## Supporting Information

# Redox Property of Enamines

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## Calculated Cartesian coordinates and energies

**Calculated Cartesian coordinates for β-ketocarbonyls derived enamines ....S2**

**Calculated Cartesian coordinates for propionic aldehyde derived enamines .....S53**

**Calculated Cartesian coordinates for phenylacetaldehyde derived enamines .....S121**

**Calculated Cartesian coordinates for butanone derived enamines.....S200**

**Calculated Cartesian coordinates for cyclohexanone derived enamines...S273**

**Calculated Cartesian coordinates for α-branched aldehyde derived enamines .....S325**

**Calculated Cartesian coordinates for α-branched ketone derived enamines .....S411**

**Calculated Cartesian coordinates for other pyrrolidine derived enamines .....S500**

## Calculated Cartesian coordinates for β-ketocarbonyls derived enamines

**1A$_1$**

Imaginary frequency: None

Electronic energies: -966.190148

Free energies: -965.738542

Corrected Free energies: -965.733446

| | | | |
|---|---|---|---|
| C | 2.278447 | 2.393352 | -0.107043 |
| C | 3.812503 | 2.358378 | -0.130076 |
| H | 4.178235 | 1.777690 | -0.982843 |
| H | 4.202658 | 3.374983 | -0.223737 |
| H | 4.229546 | 1.929100 | 0.782660 |
| C | 1.793544 | 3.215504 | -1.307302 |
| H | 2.133613 | 2.767217 | -2.246169 |
| H | 0.704068 | 3.273182 | -1.331736 |
| H | 2.192556 | 4.231741 | -1.252423 |
| C | 1.805343 | 3.063251 | 1.189128 |
| H | 0.715854 | 3.155721 | 1.225528 |
| H | 2.137177 | 2.515489 | 2.074851 |
| H | 2.217772 | 4.073720 | 1.252086 |
| C | 1.727994 | 0.952471 | -0.241257 |
| H | 2.095117 | 0.567076 | -1.196651 |
| C | 2.155687 | -0.020587 | 0.871939 |
| H | 1.657605 | 0.281002 | 1.798396 |
| H | 3.237046 | 0.040382 | 1.053562 |
| N | 0.271606 | 0.956632 | -0.303284 |
| N | 1.748341 | -1.380534 | 0.528880 |
| C | 1.139071 | -2.107864 | 1.641375 |
| H | 0.330435 | -1.478305 | 2.024397 |
| H | 0.661841 | -3.007947 | 1.244665 |
| C | 2.822171 | -2.095321 | -0.156096 |
| H | 3.148671 | -1.465046 | -0.990893 |
| H | 3.705051 | -2.221711 | 0.493196 |
| C | 2.386468 | -3.449429 | -0.699285 |
| H | 2.198483 | -4.166861 | 0.102152 |
| H | 1.471660 | -3.348728 | -1.288833 |
| H | 3.167036 | -3.863811 | -1.339403 |
| C | 2.091352 | -2.485556 | 2.778583 |
| H | 2.594995 | -1.601245 | 3.178294 |
| H | 1.541344 | -2.959612 | 3.594086 |
| H | 2.856519 | -3.187730 | 2.438738 |
| H | -0.216860 | 1.343009 | 0.498743 |

| | | | |
|---|---|---|---|
| C | -0.467313 | 0.085253 | -1.010135 |
| C | -1.805307 | -0.177374 | -0.835287 |
| C | -2.579416 | 0.427392 | 0.211139 |
| O | -2.151439 | 1.185622 | 1.076317 |
| C | 0.057153 | -0.652400 | -2.219442 |
| H | 1.036311 | -1.097738 | -2.046042 |
| H | 0.149681 | 0.061142 | -3.047482 |
| C | -2.330065 | -1.095876 | -1.913885 |
| H | -3.007783 | -1.860106 | -1.528542 |
| H | -2.877585 | -0.539279 | -2.684348 |
| C | -1.033820 | -1.703146 | -2.484971 |
| H | -0.790358 | -2.608272 | -1.922244 |
| H | -1.110685 | -1.970977 | -3.538868 |
| C | -4.721456 | 0.627738 | 1.196080 |
| H | -4.660115 | 1.717275 | 1.155566 |
| H | -4.352786 | 0.306305 | 2.172745 |
| C | -6.127324 | 0.134678 | 0.938096 |
| H | -6.805963 | 0.531991 | 1.694401 |
| H | -6.472984 | 0.461555 | -0.043800 |
| H | -6.164564 | -0.955071 | 0.976640 |
| O | -3.882739 | 0.072926 | 0.173029 |

**1A$_1$** radical cation

Imaginary frequency: None

Electronic energies: -965.991824

Free energies: -965.540959

Corrected Free energies: -965.535872

| | | | |
|---|---|---|---|
| C | 1.811816 | 2.595343 | -0.261946 |
| C | 3.283032 | 2.859062 | -0.606316 |
| H | 3.537008 | 2.442300 | -1.584757 |
| H | 3.456905 | 3.936743 | -0.643270 |
| H | 3.964154 | 2.440357 | 0.136385 |
| C | 0.930459 | 3.273104 | -1.319447 |
| H | 1.086735 | 2.824684 | -2.305087 |
| H | -0.131672 | 3.196062 | -1.073041 |
| H | 1.180785 | 4.334188 | -1.383827 |
| C | 1.497447 | 3.173612 | 1.122900 |
| H | 0.466183 | 2.981216 | 1.435793 |
| H | 2.168893 | 2.777578 | 1.887763 |
| H | 1.625264 | 4.258061 | 1.096701 |
| C | 1.568429 | 1.068430 | -0.314800 |
| H | 1.916484 | 0.705161 | -1.284271 |
| C | 2.227924 | 0.242653 | 0.809925 |

| | | | |
|---|---|---|---|
| H | 1.731149 | 0.485899 | 1.752908 |
| H | 3.277162 | 0.550616 | 0.908421 |
| N | 0.136593 | 0.774044 | -0.243610 |
| N | 2.086327 | -1.179829 | 0.540439 |
| C | 1.797634 | -1.971276 | 1.740702 |
| H | 0.927278 | -1.514871 | 2.219850 |
| H | 1.483646 | -2.968042 | 1.423136 |
| C | 3.208427 | -1.679082 | -0.258877 |
| H | 3.282626 | -1.047139 | -1.150911 |
| H | 4.163794 | -1.561425 | 0.276057 |
| C | 3.035461 | -3.129414 | -0.688293 |
| H | 3.126814 | -3.814603 | 0.156380 |
| H | 2.056591 | -3.286744 | -1.148734 |
| H | 3.804702 | -3.393641 | -1.415230 |
| C | 2.947268 | -2.080558 | 2.743416 |
| H | 3.291259 | -1.091655 | 3.057841 |
| H | 2.620082 | -2.622483 | 3.632685 |
| H | 3.798459 | -2.618038 | 2.318897 |
| H | -0.419445 | 1.236264 | 0.482535 |
| C | -0.488300 | -0.136657 | -0.927566 |
| C | -1.868661 | -0.461685 | -0.730010 |
| C | -2.724557 | 0.229700 | 0.251573 |
| O | -2.309952 | 1.100678 | 0.989345 |
| C | 0.061507 | -0.957675 | -2.057199 |
| H | 1.083354 | -1.281544 | -1.876110 |
| H | 0.044920 | -0.329427 | -2.956189 |
| C | -2.282741 | -1.527230 | -1.676729 |
| H | -2.954370 | -2.252377 | -1.214573 |
| H | -2.842432 | -1.060961 | -2.500846 |
| C | -0.946121 | -2.115825 | -2.167313 |
| H | -0.640954 | -2.922046 | -1.497696 |
| H | -1.009661 | -2.511741 | -3.177999 |
| O | -3.967061 | -0.208407 | 0.226267 |
| C | -4.887198 | 0.415972 | 1.157208 |
| H | -4.490756 | 0.281305 | 2.164441 |
| H | -4.918227 | 1.483619 | 0.935015 |
| C | -6.227764 | -0.250989 | 0.971478 |
| H | -6.156591 | -1.319073 | 1.179316 |
| H | -6.949020 | 0.189531 | 1.660848 |
| H | -6.589827 | -0.110366 | -0.047357 |

**1A$_5$**

Imaginary frequency: None

Electronic energies: -1138.031772

Free energies: -1137.518373

Corrected Free energies: -1137.512128

| | | | |
|---|---|---|---|
| C | 3.721430 | -0.670176 | -1.606209 |
| C | 4.825872 | 0.333219 | -1.961698 |
| H | 5.349072 | 0.676296 | -1.063459 |
| H | 5.559605 | -0.140738 | -2.618885 |
| H | 4.430657 | 1.207356 | -2.483680 |
| C | 4.372868 | -1.952638 | -1.075989 |
| H | 4.993780 | -1.737318 | -0.200843 |
| H | 3.614858 | -2.683127 | -0.786622 |
| H | 5.010659 | -2.399799 | -1.843216 |
| C | 2.916593 | -1.002024 | -2.869652 |
| H | 2.163792 | -1.771997 | -2.680233 |
| H | 2.417393 | -0.120914 | -3.280037 |
| H | 3.589784 | -1.388797 | -3.639422 |
| C | 2.825347 | -0.079276 | -0.490365 |
| H | 3.451552 | 0.015437 | 0.401692 |
| C | 2.233000 | 1.311188 | -0.790889 |
| H | 1.643483 | 1.259272 | -1.713781 |
| H | 3.038312 | 2.028744 | -0.972387 |
| N | 1.736490 | -0.993601 | -0.168579 |
| N | 1.403260 | 1.760111 | 0.326275 |
| C | -0.023599 | 1.820105 | 0.009850 |
| H | -0.290173 | 0.870981 | -0.465287 |
| H | -0.585459 | 1.850004 | 0.949137 |
| C | 1.943014 | 2.945125 | 0.985923 |
| H | 2.989680 | 2.728861 | 1.222857 |
| H | 1.948143 | 3.824808 | 0.319780 |
| C | 1.209777 | 3.286288 | 2.275871 |
| H | 0.188320 | 3.623551 | 2.087310 |
| H | 1.167535 | 2.410887 | 2.928805 |
| H | 1.732219 | 4.087190 | 2.802163 |
| C | -0.444476 | 2.990792 | -0.883055 |
| H | 0.144579 | 3.014458 | -1.803990 |
| H | -1.496982 | 2.897070 | -1.159095 |
| H | -0.313661 | 3.949573 | -0.374991 |
| H | 1.063826 | -1.172978 | -0.910282 |
| C | 1.182575 | -1.104295 | 1.056713 |
| C | -0.078384 | -1.569154 | 1.332923 |
| C | -1.048605 | -1.849311 | 0.296037 |
| O | -0.816485 | -1.716843 | -0.917796 |
| N | -2.292514 | -2.255490 | 0.708423 |
| H | -2.496139 | -2.211483 | 1.695068 |

| | | | |
|---|---|---|---|
| C | -3.411072 | -2.197908 | -0.205890 |
| H | -4.217080 | -2.814172 | 0.197685 |
| H | -3.099478 | -2.643557 | -1.152041 |
| C | -3.931795 | -0.793372 | -0.473568 |
| C | -4.972856 | -0.622386 | -1.388617 |
| C | -3.409993 | 0.327665 | 0.166670 |
| C | -5.481541 | 0.642105 | -1.658748 |
| H | -5.385973 | -1.490218 | -1.893900 |
| C | -3.919872 | 1.597074 | -0.100106 |
| H | -2.597850 | 0.215832 | 0.876973 |
| C | -4.955567 | 1.759443 | -1.013198 |
| H | -6.287744 | 0.757660 | -2.373801 |
| H | -3.503965 | 2.459073 | 0.409608 |
| H | -5.351404 | 2.746420 | -1.220933 |
| C | 1.946740 | -0.830273 | 2.330348 |
| H | 2.475110 | 0.122348 | 2.293206 |
| H | 2.687962 | -1.624860 | 2.478917 |
| C | -0.291380 | -1.705125 | 2.825191 |
| H | -1.263739 | -1.334562 | 3.165862 |
| H | -0.213508 | -2.748766 | 3.154001 |
| C | 0.850316 | -0.847649 | 3.407460 |
| H | 0.483100 | 0.171311 | 3.549986 |
| H | 1.210604 | -1.212727 | 4.369344 |

**1A$_5$** radical cation

Imaginary frequency: None

Electronic energies: -1137.836484

Free energies: -1137.324526

Corrected Free energies: -1137.317573

| | | | |
|---|---|---|---|
| C | 3.105127 | 2.629703 | -0.043256 |
| C | 4.610000 | 2.906426 | -0.142724 |
| H | 5.022667 | 2.505823 | -1.072964 |
| H | 4.780484 | 3.985279 | -0.135625 |
| H | 5.163556 | 2.479481 | 0.695338 |
| C | 2.386066 | 3.389616 | -1.165738 |
| H | 2.728872 | 3.051025 | -2.147746 |
| H | 1.302863 | 3.252980 | -1.114481 |
| H | 2.593611 | 4.458564 | -1.082594 |
| C | 2.583989 | 3.109487 | 1.317339 |
| H | 1.508874 | 2.942031 | 1.438742 |
| H | 3.105437 | 2.627677 | 2.147047 |
| H | 2.748811 | 4.185917 | 1.404098 |
| C | 2.868183 | 1.115419 | -0.250733 |

| | | | |
|---|---|---|---|
| H | 3.272111 | 0.838122 | -1.227572 |
| C | 3.464648 | 0.179033 | 0.826964 |
| H | 2.978569 | 0.397478 | 1.781105 |
| H | 4.529772 | 0.409235 | 0.945257 |
| N | 1.439076 | 0.819288 | -0.269245 |
| N | 3.241769 | -1.211821 | 0.463525 |
| C | 2.691773 | -2.025007 | 1.551208 |
| H | 1.813463 | -1.495439 | 1.932088 |
| H | 2.321354 | -2.959946 | 1.123784 |
| C | 4.409234 | -1.785884 | -0.207871 |
| H | 4.666605 | -1.119465 | -1.038670 |
| H | 5.287414 | -1.799088 | 0.456601 |
| C | 4.158429 | -3.185209 | -0.752134 |
| H | 4.044586 | -3.917892 | 0.048977 |
| H | 3.255241 | -3.209361 | -1.367094 |
| H | 5.002507 | -3.496401 | -1.369286 |
| C | 3.660246 | -2.320895 | 2.697285 |
| H | 4.066375 | -1.396597 | 3.117087 |
| H | 3.146102 | -2.857710 | 3.496775 |
| H | 4.497013 | -2.938708 | 2.363243 |
| H | 0.845816 | 1.193720 | 0.483043 |
| C | 0.855932 | -0.075133 | -1.012526 |
| C | -0.503589 | -0.477862 | -0.818647 |
| C | -1.362838 | 0.104310 | 0.240954 |
| O | -0.911230 | 0.930360 | 1.037690 |
| N | -2.634519 | -0.318279 | 0.262472 |
| H | -2.939846 | -1.031036 | -0.384973 |
| C | -3.595478 | 0.171240 | 1.245992 |
| H | -3.306540 | 1.195105 | 1.492024 |
| C | 1.434450 | -0.789579 | -2.199489 |
| H | 2.476330 | -1.065872 | -2.060262 |
| H | 1.362005 | -0.109255 | -3.056816 |
| C | -0.870161 | -1.501042 | -1.838817 |
| H | -1.486559 | -2.307198 | -1.435634 |
| H | -1.451220 | -1.015183 | -2.635944 |
| C | 0.492349 | -1.992345 | -2.364669 |
| H | 0.841969 | -2.811987 | -1.733829 |
| H | 0.441036 | -2.343061 | -3.392701 |
| C | -4.997470 | 0.122692 | 0.690395 |
| C | -5.306464 | 0.805183 | -0.488345 |
| C | -5.996021 | -0.593836 | 1.345008 |
| C | -6.596425 | 0.770951 | -1.002565 |
| H | -4.529913 | 1.363576 | -1.001338 |
| C | -7.291017 | -0.625154 | 0.833366 |

| | | | |
|---|---|---|---|
| H | -5.760254 | -1.130517 | 2.257548 |
| C | -7.592365 | 0.055272 | -0.340819 |
| H | -6.827591 | 1.304950 | -1.916476 |
| H | -8.061380 | -1.184585 | 1.350550 |
| H | -8.598863 | 0.029086 | -0.740737 |
| H | -3.527304 | -0.422268 | 2.161603 |

**1C$_2$**

Imaginary frequency: None

Electronic energies: -928.081373

Free energies: -927.641571

Corrected Free energies: -927.635114

| | | | |
|---|---|---|---|
| C | -1.027875 | 2.468326 | 0.334144 |
| C | -2.319886 | 3.147618 | 0.806898 |
| H | -2.642886 | 2.745365 | 1.772056 |
| H | -2.149369 | 4.220260 | 0.930321 |
| H | -3.136975 | 3.025178 | 0.093802 |
| C | 0.092529 | 2.811854 | 1.324463 |
| H | -0.119978 | 2.393088 | 2.313576 |
| H | 1.054793 | 2.419668 | 0.987762 |
| H | 0.182898 | 3.896319 | 1.426729 |
| C | -0.651729 | 2.994764 | -1.056116 |
| H | 0.273241 | 2.541890 | -1.426864 |
| H | -1.443973 | 2.810830 | -1.785954 |
| H | -0.487060 | 4.074490 | -1.008732 |
| C | -1.228469 | 0.927276 | 0.325743 |
| H | -1.583753 | 0.662041 | 1.322809 |
| C | -2.244101 | 0.421824 | -0.709503 |
| H | -1.764085 | 0.450685 | -1.691972 |
| H | -3.115959 | 1.090472 | -0.757157 |
| N | 0.046560 | 0.255087 | 0.105462 |
| N | -2.641782 | -0.954759 | -0.421144 |
| C | -2.909945 | -1.732927 | -1.632631 |
| H | -2.017651 | -1.662494 | -2.260279 |
| H | -3.002351 | -2.784665 | -1.351158 |
| C | -3.732405 | -0.986106 | 0.553479 |
| H | -3.406746 | -0.418397 | 1.431006 |
| H | -4.628326 | -0.468132 | 0.171513 |
| C | -4.102587 | -2.396967 | 0.992337 |
| H | -4.594942 | -2.955672 | 0.193669 |
| H | -3.210652 | -2.949943 | 1.297258 |
| H | -4.789412 | -2.354571 | 1.839214 |
| C | -4.140583 | -1.306330 | -2.437604 |

| | | | |
|---|---|---|---|
| H | -4.083395 | -0.251790 | -2.719725 |
| H | -4.211052 | -1.896142 | -3.353755 |
| H | -5.062820 | -1.457451 | -1.871643 |
| H | 0.643446 | 0.637791 | -0.621271 |
| C | 0.672592 | -0.598176 | 0.938563 |
| C | 2.013647 | -0.930954 | 0.817899 |
| C | -0.169166 | -1.206624 | 2.028963 |
| H | -1.151520 | -1.458589 | 1.627175 |
| H | 0.291426 | -2.104030 | 2.431133 |
| H | -0.300204 | -0.495959 | 2.850822 |
| C | 2.653378 | -1.932494 | 1.757816 |
| H | 2.522597 | -1.651654 | 2.806203 |
| H | 2.240116 | -2.938291 | 1.633902 |
| H | 3.721299 | -1.995105 | 1.568380 |
| C | 2.816238 | -0.286932 | -0.198317 |
| O | 2.428906 | 0.539283 | -1.025389 |
| O | 4.116060 | -0.661477 | -0.188328 |
| C | 4.963257 | -0.043626 | -1.165688 |
| H | 4.559913 | -0.235783 | -2.161976 |
| H | 4.963855 | 1.036914 | -1.006629 |
| C | 6.344838 | -0.634944 | -0.995878 |
| H | 6.321367 | -1.714233 | -1.153940 |
| H | 7.030037 | -0.193297 | -1.721116 |
| H | 6.726538 | -0.437022 | 0.006929 |

**1C$_2$** radical cation

Imaginary frequency: None

Electronic energies: -927.884846

Free energies: -927.441555

Corrected Free energies: -927.436945

| | | | |
|---|---|---|---|
| C | -1.538168 | 2.593054 | 0.051009 |
| C | -3.004620 | 3.036101 | 0.131717 |
| H | -3.450069 | 2.747518 | 1.087849 |
| H | -3.057923 | 4.124003 | 0.049553 |
| H | -3.608896 | 2.615296 | -0.673594 |
| C | -0.746262 | 3.313824 | 1.150612 |
| H | -1.098455 | 3.018846 | 2.143246 |
| H | 0.323791 | 3.098584 | 1.089104 |
| H | -0.874350 | 4.393700 | 1.050379 |
| C | -0.966815 | 2.962882 | -1.323804 |
| H | 0.075457 | 2.651169 | -1.448145 |
| H | -1.553804 | 2.529591 | -2.136301 |
| H | -0.988965 | 4.048758 | -1.440244 |

| | | | |
|---|---|---|---|
| C | -1.474788 | 1.068027 | 0.312291 |
| H | -1.978804 | 0.874513 | 1.259393 |
| C | -2.079552 | 0.177189 | -0.793863 |
| H | -1.456993 | 0.271582 | -1.687207 |
| H | -3.076794 | 0.557576 | -1.050308 |
| N | -0.077996 | 0.651542 | 0.442758 |
| N | -2.105673 | -1.212093 | -0.367788 |
| C | -1.761095 | -2.152654 | -1.438583 |
| H | -0.799419 | -1.829985 | -1.846921 |
| H | -1.588822 | -3.132375 | -0.987529 |
| C | -3.351073 | -1.524887 | 0.336816 |
| H | -3.470444 | -0.786702 | 1.137418 |
| H | -4.224843 | -1.398151 | -0.321955 |
| C | -3.359476 | -2.921459 | 0.942141 |
| H | -3.417688 | -3.694687 | 0.173758 |
| H | -2.456325 | -3.092229 | 1.532550 |
| H | -4.226100 | -3.036165 | 1.594763 |
| C | -2.791060 | -2.270519 | -2.563121 |
| H | -2.990929 | -1.297258 | -3.019394 |
| H | -2.419627 | -2.938315 | -3.342614 |
| H | -3.737107 | -2.676740 | -2.198083 |
| H | 0.579675 | 1.068686 | -0.228186 |
| C | 0.439956 | -0.273232 | 1.204100 |
| C | 1.843598 | -0.592721 | 1.058221 |
| C | -0.347338 | -0.982096 | 2.257319 |
| H | -1.410390 | -0.790752 | 2.180889 |
| H | -0.183026 | -2.056529 | 2.168877 |
| H | 0.013064 | -0.665055 | 3.239979 |
| C | 2.473195 | -1.629452 | 1.915119 |
| H | 2.032273 | -1.659745 | 2.909688 |
| H | 2.326387 | -2.617668 | 1.457864 |
| H | 3.544598 | -1.465306 | 1.993497 |
| C | 2.663745 | 0.057762 | -0.003754 |
| O | 2.268219 | 0.952486 | -0.727569 |
| O | 3.877476 | -0.447472 | -0.074726 |
| C | 4.755448 | 0.120457 | -1.079704 |
| H | 4.278414 | -0.002815 | -2.052863 |
| H | 4.856750 | 1.186846 | -0.873883 |
| C | 6.070227 | -0.613340 | -0.984493 |
| H | 5.930980 | -1.677626 | -1.176604 |
| H | 6.760880 | -0.213385 | -1.727779 |
| H | 6.512094 | -0.485034 | 0.004240 |

**1C$_2$** α-iminio radicals

Imaginary frequency: None

Electronic energies: -927.893642

Free energies: -927.448932

Corrected Free energies: -927.444363

| | | | |
|---|---|---|---|
| C | 2.774422 | 1.550543 | 0.732004 |
| C | 4.242914 | 1.113330 | 0.678933 |
| H | 4.589380 | 1.016898 | -0.354382 |
| H | 4.865554 | 1.861440 | 1.175188 |
| H | 4.406210 | 0.160571 | 1.188856 |
| C | 2.644804 | 2.944739 | 0.109060 |
| H | 2.957402 | 2.943539 | -0.938992 |
| H | 1.616749 | 3.310633 | 0.167772 |
| H | 3.279684 | 3.649786 | 0.650654 |
| C | 2.299972 | 1.618963 | 2.187954 |
| H | 1.246174 | 1.897406 | 2.243943 |
| H | 2.435800 | 0.674349 | 2.719058 |
| H | 2.884286 | 2.375054 | 2.718168 |
| C | 1.921400 | 0.557794 | -0.112577 |
| H | 2.273290 | 0.645105 | -1.147343 |
| C | 2.119697 | -0.899075 | 0.354848 |
| H | 2.143071 | -0.950708 | 1.442885 |
| H | 3.037795 | -1.326271 | -0.046160 |
| N | 0.502994 | 0.804906 | 0.027234 |
| N | 0.972612 | -1.761465 | -0.077997 |
| C | 0.870601 | -3.026392 | 0.726756 |
| H | 0.846512 | -2.711945 | 1.770223 |
| H | -0.098232 | -3.465813 | 0.492223 |
| C | 0.978184 | -1.980601 | -1.563238 |
| H | 0.936466 | -0.988605 | -2.013894 |
| H | 1.938333 | -2.429428 | -1.819944 |
| C | -0.193952 | -2.821037 | -2.036690 |
| H | -0.102192 | -3.864486 | -1.733985 |
| H | -1.135714 | -2.419749 | -1.657873 |
| H | -0.220791 | -2.790481 | -3.125793 |
| C | 2.004269 | -4.000724 | 0.469170 |
| H | 2.977942 | -3.560806 | 0.689029 |
| H | 1.870725 | -4.859019 | 1.127701 |
| H | 2.004063 | -4.366879 | -0.558428 |
| C | -0.215171 | 1.405381 | -0.851765 |
| C | -1.656237 | 1.412176 | -0.610979 |
| C | 0.266839 | 2.108640 | -2.100068 |
| H | 1.240778 | 1.748360 | -2.424303 |
| H | -0.447532 | 1.973517 | -2.912669 |

| | | | |
|---|---|---|---|
| H | 0.360412 | 3.181139 | -1.910710 |
| C | -2.540406 | 2.490939 | -1.135194 |
| H | -1.968260 | 3.354566 | -1.468291 |
| H | -3.142138 | 2.128016 | -1.977159 |
| H | -3.243611 | 2.804430 | -0.361928 |
| C | -2.269962 | 0.260912 | 0.079142 |
| O | -1.743954 | -0.822073 | 0.271051 |
| O | -3.529505 | 0.508747 | 0.430540 |
| C | -4.250157 | -0.573865 | 1.056087 |
| H | -4.259110 | -1.423514 | 0.371312 |
| H | -3.714071 | -0.867310 | 1.960100 |
| C | -5.640850 | -0.067995 | 1.356684 |
| H | -6.150448 | 0.225082 | 0.438011 |
| H | -6.219414 | -0.857307 | 1.838389 |
| H | -5.600316 | 0.791152 | 2.027363 |
| H | 0.111405 | -1.218572 | 0.132843 |

**2C$_2$**

Imaginary frequency: None

Electronic energies: -560.503145

Free energies: -560.255343

Corrected Free energies: -560.253747

| | | | |
|---|---|---|---|
| N | 0.351707 | 0.030711 | -0.250524 |
| H | 0.712961 | -0.899864 | -0.044104 |
| C | 1.284803 | 0.987961 | -0.287721 |
| C | 2.631860 | 0.711144 | -0.111812 |
| C | 0.840722 | 2.399796 | -0.551362 |
| H | 0.102958 | 2.724811 | 0.185334 |
| H | 1.693893 | 3.072965 | -0.514352 |
| H | 0.378046 | 2.475301 | -1.538471 |
| C | 3.138196 | -0.600340 | 0.153743 |
| O | 2.427791 | -1.616174 | 0.233365 |
| C | 4.632348 | -0.755927 | 0.355371 |
| H | 5.173250 | 0.184988 | 0.264553 |
| H | 4.810442 | -1.181011 | 1.345640 |
| H | 5.016326 | -1.466869 | -0.379371 |
| H | 3.327900 | 1.535238 | -0.170475 |
| C | -1.093334 | 0.220105 | -0.282772 |
| C | -1.746560 | -0.982328 | -0.965877 |
| C | -1.660317 | 0.414557 | 1.129338 |
| H | -1.314178 | 1.111022 | -0.878167 |
| C | -3.269734 | -0.837360 | -0.995460 |
| H | -1.476465 | -1.889154 | -0.409748 |

| | | | |
|---|---|---|---|
| H | -1.343902 | -1.087809 | -1.976387 |
| C | -3.182787 | 0.563429 | 1.096976 |
| H | -1.385681 | -0.461269 | 1.729412 |
| H | -1.193525 | 1.285665 | 1.597707 |
| C | -3.835455 | -0.639057 | 0.412424 |
| H | -3.715161 | -1.716716 | -1.466515 |
| H | -3.536301 | 0.026579 | -1.615720 |
| H | -3.566518 | 0.680555 | 2.113222 |
| H | -3.445553 | 1.476976 | 0.550178 |
| H | -4.919683 | -0.509420 | 0.369506 |
| H | -3.641548 | -1.539461 | 1.007416 |

**2C$_2$** radical cation

Imaginary frequency: None

Electronic energies: -560.292033

Free energies: -560.046477

Corrected Free energies: -560.044516

| | | | |
|---|---|---|---|
| N | -0.345253 | 0.113845 | -0.131416 |
| H | -0.702637 | -0.835134 | 0.036916 |
| C | -1.251107 | 1.047929 | -0.223262 |
| C | -2.635474 | 0.692073 | -0.108447 |
| C | -0.867028 | 2.473718 | -0.453397 |
| H | -0.424559 | 2.581236 | -1.446888 |
| H | -1.741503 | 3.115273 | -0.388859 |
| H | -0.131713 | 2.797334 | 0.284702 |
| C | -3.144683 | -0.677876 | 0.138264 |
| O | -2.377064 | -1.618442 | 0.246340 |
| C | -4.631006 | -0.825312 | 0.246868 |
| H | -5.002540 | -0.206376 | 1.067348 |
| H | -5.104416 | -0.470152 | -0.671575 |
| H | -4.882119 | -1.868512 | 0.420950 |
| H | -3.358561 | 1.490624 | -0.210888 |
| C | 1.108075 | 0.282270 | -0.209179 |
| C | 1.693727 | 0.282907 | 1.211005 |
| C | 1.694193 | -0.846268 | -1.060885 |
| H | 1.307799 | 1.241915 | -0.689137 |
| C | 3.218026 | 0.401855 | 1.142952 |
| H | 1.413964 | -0.653555 | 1.706045 |
| H | 1.261509 | 1.104498 | 1.787029 |
| C | 3.218959 | -0.723685 | -1.112378 |
| H | 1.418320 | -1.808593 | -0.613726 |
| H | 1.264850 | -0.808395 | -2.064262 |
| C | 3.822397 | -0.716733 | 0.292724 |

| | | | |
|---|---|---|---|
| H | 3.624147 | 0.377493 | 2.156118 |
| H | 3.484984 | 1.373456 | 0.712337 |
| H | 3.625067 | -1.548428 | -1.701230 |
| H | 3.488907 | 0.203202 | -1.630520 |
| H | 4.906614 | -0.598761 | 0.234473 |
| H | 3.628692 | -1.681764 | 0.774764 |

**$3A_1$**

Imaginary frequency: None

Electronic energies: -635.730201

Free energies: -635.482808

Corrected Free energies: -635.480367

| | | | |
|---|---|---|---|
| C | 3.080843 | -0.641767 | -0.131393 |
| H | 3.476239 | 0.215186 | -0.682668 |
| N | 1.622876 | -0.564817 | -0.191553 |
| H | 1.092266 | -1.419032 | -0.058206 |
| C | 0.907678 | 0.569129 | -0.159006 |
| C | -0.457447 | 0.687406 | -0.071205 |
| C | 1.545029 | 1.932175 | -0.308182 |
| H | 1.833273 | 2.067999 | -1.357214 |
| H | 2.447719 | 2.047673 | 0.294150 |
| C | -0.891218 | 2.131008 | -0.179187 |
| C | -1.324350 | -0.454423 | 0.012996 |
| O | -0.963943 | -1.624349 | 0.077766 |
| O | -2.633216 | -0.119217 | 0.019778 |
| C | -3.565807 | -1.204278 | 0.123516 |
| H | -3.392401 | -1.904707 | -0.695983 |
| H | -3.390373 | -1.734900 | 1.062139 |
| C | 3.578240 | -0.585838 | 1.313503 |
| H | 4.669576 | -0.614803 | 1.345872 |
| H | 3.239767 | 0.327052 | 1.808027 |
| H | 3.191279 | -1.442281 | 1.872038 |
| C | 3.531331 | -1.920036 | -0.828524 |
| H | 4.619571 | -1.995217 | -0.815619 |
| H | 3.125011 | -2.794872 | -0.312407 |
| H | 3.189158 | -1.938021 | -1.864289 |
| C | -4.954366 | -0.608422 | 0.068438 |
| H | -5.701731 | -1.398362 | 0.157350 |
| H | -5.099982 | 0.100340 | 0.885020 |
| H | -5.110153 | -0.087976 | -0.877733 |
| C | 0.417987 | 2.893102 | 0.106445 |
| H | -1.270492 | 2.360023 | -1.182480 |
| H | -1.680692 | 2.391754 | 0.528319 |

| | | | |
|---|---|---|---|
| H | 0.477361 | 3.851238 | -0.409679 |
| H | 0.494227 | 3.082805 | 1.179482 |

**3A$_1$** radical cation

Imaginary frequency: None

Electronic energies: -635.529701

Free energies: -635.281986

Corrected Free energies: -635.279751

| | | | |
|---|---|---|---|
| C | 3.089483 | -0.644021 | -0.126405 |
| H | 3.474326 | 0.266641 | -0.586184 |
| N | 1.624078 | -0.500606 | -0.065563 |
| H | 1.062214 | -1.350530 | 0.046416 |
| C | 0.964308 | 0.617103 | -0.114787 |
| C | -0.462357 | 0.708682 | -0.059929 |
| C | 1.552706 | 1.990104 | -0.264966 |
| H | 1.831732 | 2.120278 | -1.316964 |
| H | 2.449690 | 2.127077 | 0.338481 |
| C | -0.888698 | 2.124734 | -0.179530 |
| C | -1.343471 | -0.470048 | 0.042913 |
| O | -0.919455 | -1.601667 | 0.145702 |
| O | -2.618657 | -0.138156 | 0.011122 |
| C | -3.570483 | -1.227678 | 0.109915 |
| H | -3.367330 | -1.929508 | -0.700073 |
| H | -3.402973 | -1.734787 | 1.061254 |
| C | 3.633521 | -0.786549 | 1.293824 |
| H | 4.719060 | -0.881910 | 1.249119 |
| H | 3.382285 | 0.083837 | 1.901645 |
| H | 3.224549 | -1.680659 | 1.768442 |
| C | 3.417861 | -1.844594 | -1.004396 |
| H | 4.500890 | -1.946361 | -1.076583 |
| H | 3.016519 | -2.761544 | -0.566234 |
| H | 3.010004 | -1.720848 | -2.007860 |
| C | -4.949052 | -0.621521 | 0.015785 |
| H | -5.697355 | -1.410311 | 0.100700 |
| H | -5.108212 | 0.096726 | 0.820690 |
| H | -5.082156 | -0.117184 | -0.941820 |
| C | 0.392335 | 2.922610 | 0.130040 |
| H | -1.232335 | 2.296121 | -1.210141 |
| H | -1.733076 | 2.356014 | 0.471755 |
| H | 0.431230 | 3.869348 | -0.402989 |
| H | 0.440373 | 3.127503 | 1.199904 |

**3A$_2$**

Imaginary frequency: None

Electronic energies: -675.036042

Free energies: -674.759597

Corrected Free energies: -674.757186

| | | | |
|---|---|---|---|
| C | 2.963698 | -1.003426 | -0.029435 |
| H | 3.550361 | -0.165365 | -0.407664 |
| N | 1.551506 | -0.751983 | -0.315242 |
| H | 0.937749 | -1.555689 | -0.222928 |
| C | 0.924257 | 0.445250 | -0.196283 |
| C | -0.444079 | 0.576179 | -0.077376 |
| C | 1.819055 | 1.665912 | -0.250817 |
| H | 2.552570 | 1.516808 | -1.046446 |
| H | 2.385847 | 1.722185 | 0.686096 |
| C | -1.287792 | -0.605486 | -0.079963 |
| O | -0.926212 | -1.774863 | -0.154446 |
| C | 3.203951 | -1.139142 | 1.476020 |
| H | 4.263461 | -1.304816 | 1.683681 |
| H | 2.883095 | -0.240839 | 2.007584 |
| H | 2.637836 | -1.989401 | 1.866225 |
| C | 3.389243 | -2.264617 | -0.773305 |
| H | 4.443159 | -2.477399 | -0.587105 |
| H | 2.804779 | -3.123567 | -0.429960 |
| H | 3.237021 | -2.149642 | -1.847473 |
| C | -3.509445 | -1.415161 | 0.012146 |
| H | -3.382462 | -1.982550 | -0.912354 |
| H | -3.261960 | -2.073315 | 0.847473 |
| C | -4.906858 | -0.851312 | 0.136794 |
| H | -5.130449 | -0.190109 | -0.701745 |
| H | -5.634676 | -1.664168 | 0.141194 |
| H | -5.011404 | -0.287460 | 1.065002 |
| O | -2.601475 | -0.304569 | 0.007083 |
| C | 1.065298 | 2.971600 | -0.481282 |
| H | 0.737189 | 3.024893 | -1.525003 |
| H | 1.741469 | 3.811735 | -0.310350 |
| C | -1.125795 | 1.925755 | 0.056331 |
| H | -1.634891 | 2.188475 | -0.879805 |
| H | -1.910261 | 1.849971 | 0.811875 |
| C | -0.152829 | 3.038413 | 0.428548 |
| H | 0.167831 | 2.916764 | 1.469498 |
| H | -0.647535 | 4.009058 | 0.349536 |

**3A$_2$** radical cation

Imaginary frequency: None
Electronic energies: -674.836556
Free energies: -674.561397
Corrected Free energies: -674.558651

| | | | |
|---|---|---|---|
| C | 2.970477 | -1.026735 | -0.103426 |
| H | 3.485253 | -0.193550 | -0.577452 |
| N | 1.533459 | -0.710737 | -0.071107 |
| H | 0.891755 | -1.503549 | 0.051083 |
| C | 0.973488 | 0.470617 | -0.117935 |
| C | -0.453419 | 0.588062 | 0.020354 |
| C | 1.828593 | 1.697467 | -0.290398 |
| H | 2.532415 | 1.514151 | -1.104364 |
| H | 2.423728 | 1.807193 | 0.623977 |
| C | -1.318835 | -0.628991 | 0.028918 |
| O | -0.903193 | -1.769383 | 0.051789 |
| C | 3.465750 | -1.188440 | 1.334376 |
| H | 4.531846 | -1.417534 | 1.316694 |
| H | 3.314096 | -0.274341 | 1.909797 |
| H | 2.940640 | -2.008990 | 1.827279 |
| C | 3.162526 | -2.290589 | -0.931866 |
| H | 4.226454 | -2.521863 | -0.985967 |
| H | 2.652334 | -3.137184 | -0.465858 |
| H | 2.781223 | -2.158361 | -1.944656 |
| C | -3.534782 | -1.423064 | 0.019176 |
| H | -3.321927 | -2.051677 | -0.846455 |
| H | -3.356891 | -2.004739 | 0.924762 |
| C | -4.921971 | -0.831593 | -0.023656 |
| H | -5.061589 | -0.244135 | -0.931635 |
| H | -5.656825 | -1.637438 | -0.014867 |
| H | -5.095961 | -0.193620 | 0.843418 |
| O | -2.598122 | -0.315677 | 0.009387 |
| C | 1.028807 | 2.971071 | -0.555611 |
| H | 0.660115 | 2.966712 | -1.585590 |
| H | 1.696056 | 3.826701 | -0.452905 |
| C | -1.114007 | 1.917484 | 0.142391 |
| H | -1.663030 | 2.092490 | -0.795271 |
| H | -1.886638 | 1.846974 | 0.912476 |
| C | -0.146253 | 3.064796 | 0.406994 |
| H | 0.214498 | 3.016479 | 1.438943 |
| H | -0.673491 | 4.011405 | 0.289036 |

**3A$_3$**

Imaginary frequency: None

Electronic energies: -714.334258

Free energies: -714.028828

Corrected Free energies: -714.026509

| | | | |
|---|---|---|---|
| C | 2.937071 | -1.203873 | -0.198869 |
| H | 3.386036 | -0.328909 | -0.674586 |
| N | 1.508050 | -0.955298 | -0.012254 |
| H | 0.880179 | -1.743289 | -0.139896 |
| C | 3.635001 | -1.478171 | 1.133887 |
| H | 4.702997 | -1.646578 | 0.978280 |
| H | 3.512669 | -0.644079 | 1.827494 |
| H | 3.205888 | -2.371062 | 1.595665 |
| C | 3.087335 | -2.386947 | -1.149765 |
| H | 4.143078 | -2.592184 | -1.331627 |
| H | 2.637415 | -3.283528 | -0.713585 |
| H | 2.600216 | -2.182581 | -2.104522 |
| C | 0.428204 | 3.388627 | -0.453696 |
| C | 1.615657 | 2.438733 | -0.627940 |
| C | 1.770887 | 1.419092 | 0.518258 |
| C | -0.947449 | 2.722059 | -0.397976 |
| C | -1.090868 | 1.687594 | 0.731628 |
| C | -0.474339 | 0.338369 | 0.422792 |
| H | 0.577544 | 3.951214 | 0.476269 |
| H | 1.536450 | 1.901613 | -1.579385 |
| H | 1.497385 | 1.894292 | 1.464522 |
| H | -1.166742 | 2.231529 | -1.352791 |
| H | -2.148208 | 1.536879 | 0.938450 |
| H | 0.442331 | 4.121584 | -1.265775 |
| H | 2.529553 | 3.036228 | -0.678978 |
| H | 2.814500 | 1.130038 | 0.612926 |
| H | -1.698602 | 3.506814 | -0.263442 |
| H | -0.661602 | 2.107381 | 1.649614 |
| C | 0.901499 | 0.199923 | 0.318091 |
| C | -1.328933 | -0.788503 | 0.124840 |
| O | -0.966360 | -1.934176 | -0.136964 |
| C | -3.547063 | -1.574766 | -0.133537 |
| H | -3.317827 | -1.987808 | -1.118100 |
| H | -3.393526 | -2.364119 | 0.605525 |
| C | -4.951738 | -1.017700 | -0.073235 |
| H | -5.085294 | -0.232193 | -0.818653 |
| H | -5.674676 | -1.810524 | -0.271463 |
| H | -5.156575 | -0.600885 | 0.914178 |
| O | -2.650032 | -0.491995 | 0.143063 |

**3A$_3$** radical cation

Imaginary frequency: None

Electronic energies: -714.136308

Free energies: -713.831174

Corrected Free energies: -713.828648

| | | | |
|---|---|---|---|
| C | -2.945479 | -1.201380 | 0.225556 |
| H | -3.384787 | -0.330496 | 0.712194 |
| N | -1.518298 | -0.905030 | -0.009412 |
| H | -0.865493 | -1.693377 | 0.078341 |
| C | -3.636709 | -1.472758 | -1.109681 |
| H | -4.688905 | -1.692786 | -0.925318 |
| H | -3.572652 | -0.613764 | -1.779102 |
| H | -3.179946 | -2.334419 | -1.600149 |
| C | -3.020024 | -2.394913 | 1.168190 |
| H | -4.065567 | -2.612274 | 1.386230 |
| H | -2.576602 | -3.279409 | 0.704199 |
| H | -2.504940 | -2.187727 | 2.106831 |
| C | -0.345578 | 3.380564 | 0.463838 |
| C | -1.562912 | 2.480974 | 0.673466 |
| C | -1.809696 | 1.473371 | -0.474886 |
| C | 0.996420 | 2.658125 | 0.375052 |
| C | 1.082303 | 1.651022 | -0.804376 |
| C | 0.460188 | 0.343552 | -0.461340 |
| H | -0.493337 | 3.960684 | -0.453758 |
| H | -1.482251 | 1.940744 | 1.622179 |
| H | -1.568627 | 1.937790 | -1.434605 |
| H | 1.218636 | 2.138974 | 1.312359 |
| H | 2.123680 | 1.485831 | -1.064888 |
| H | -0.300866 | 4.098756 | 1.286377 |
| H | -2.453552 | 3.107517 | 0.744207 |
| H | -2.861665 | 1.205238 | -0.515327 |
| H | 1.787079 | 3.395860 | 0.226089 |
| H | 0.585429 | 2.084891 | -1.677296 |
| C | -0.973778 | 0.239928 | -0.320547 |
| C | 1.331102 | -0.829796 | -0.156546 |
| O | 0.914562 | -1.952151 | 0.051094 |
| C | 3.535917 | -1.591128 | 0.155396 |
| H | 3.280558 | -2.002005 | 1.133136 |
| H | 3.393193 | -2.367818 | -0.596936 |
| C | 4.924758 | -1.002958 | 0.120077 |
| H | 5.032556 | -0.222304 | 0.873751 |
| H | 5.653712 | -1.787735 | 0.325504 |
| H | 5.137333 | -0.580526 | -0.862624 |
| O | 2.609941 | -0.513357 | -0.133682 |

**3A$_4$**

Imaginary frequency: None

Electronic energies: -768.268788

Free energies: -767.987633

Corrected Free energies: -767.984073

| | | | |
|---|---|---|---|
| C | 3.886677 | -1.152112 | -0.011176 |
| H | 4.575093 | -0.372254 | -0.344078 |
| N | 2.528672 | -0.691528 | -0.290917 |
| H | 1.786325 | -1.385116 | -0.296964 |
| C | 2.102788 | 0.576287 | -0.155458 |
| C | 0.801371 | 1.013748 | -0.129397 |
| C | 3.059916 | 1.735412 | 0.001590 |
| H | 3.909447 | 1.671770 | -0.680252 |
| H | 3.458867 | 1.736456 | 1.022243 |
| C | 0.737726 | 2.514473 | 0.064449 |
| C | -0.318912 | 0.097953 | -0.151107 |
| O | -0.195039 | -1.123683 | -0.303668 |
| C | 4.092630 | -1.393073 | 1.485257 |
| H | 5.118714 | -1.709457 | 1.685872 |
| H | 3.891847 | -0.485215 | 2.057778 |
| H | 3.413952 | -2.176483 | 1.833193 |
| C | 4.150536 | -2.416049 | -0.821167 |
| H | 5.166602 | -2.773436 | -0.647430 |
| H | 3.457218 | -3.207490 | -0.521522 |
| H | 4.020610 | -2.226876 | -1.887642 |
| C | 2.174042 | 2.962393 | -0.270209 |
| H | 0.015270 | 3.009981 | -0.591667 |
| H | 0.471706 | 2.776087 | 1.096688 |
| H | 2.230307 | 3.210230 | -1.332092 |
| H | 2.486964 | 3.838612 | 0.297030 |
| C | -2.825551 | 0.089431 | 0.032565 |
| C | -3.930768 | 0.947185 | 0.131542 |
| C | -3.043214 | -1.292264 | -0.039433 |
| C | -5.220816 | 0.440040 | 0.156991 |
| H | -3.768576 | 2.018676 | 0.186147 |
| C | -4.345348 | -1.783981 | -0.014745 |
| H | -2.201713 | -1.961523 | -0.114003 |
| C | -5.440088 | -0.933398 | 0.083119 |
| H | -6.057906 | 1.123988 | 0.233394 |
| H | -4.498084 | -2.855679 | -0.071701 |
| H | -6.447153 | -1.330831 | 0.101962 |
| N | -1.556869 | 0.686134 | 0.019169 |

| | | | |
|---|---|---|---|
| H | -1.557734 | 1.689511 | 0.127698 |

**3A$_4$** radical cation

Imaginary frequency: None

Electronic energies: -768.071283

Free energies: -767.789841

Corrected Free energies: -767.786484

| | | | |
|---|---|---|---|
| C | 3.857788 | -1.190743 | 0.156382 |
| H | 4.509226 | -0.357548 | 0.418914 |
| N | 2.492858 | -0.651748 | 0.049938 |
| H | 1.711731 | -1.314376 | -0.031481 |
| C | 2.153738 | 0.602713 | 0.046869 |
| C | 0.798553 | 1.062532 | -0.015340 |
| C | 3.090663 | 1.772520 | 0.141245 |
| H | 3.982005 | 1.640421 | -0.471425 |
| H | 3.409286 | 1.866507 | 1.185383 |
| C | 0.774675 | 2.552269 | 0.045109 |
| C | -0.350128 | 0.128264 | -0.063237 |
| O | -0.165712 | -1.081783 | -0.163541 |
| C | 3.877171 | -2.230199 | 1.271575 |
| H | 4.889195 | -2.622871 | 1.373729 |
| H | 3.573291 | -1.790849 | 2.222003 |
| H | 3.209275 | -3.061395 | 1.033616 |
| C | 4.266164 | -1.771887 | -1.194881 |
| H | 5.278507 | -2.170270 | -1.118402 |
| H | 3.594694 | -2.585036 | -1.478812 |
| H | 4.246403 | -1.008240 | -1.973146 |
| C | 2.220348 | 2.963202 | -0.295162 |
| H | 0.040360 | 2.995091 | -0.631621 |
| H | 0.506091 | 2.860895 | 1.065678 |
| H | 2.310393 | 3.103714 | -1.372618 |
| H | 2.512247 | 3.887276 | 0.197687 |
| C | -2.835796 | 0.101595 | 0.001275 |
| C | -3.935446 | 0.927629 | 0.257068 |
| C | -3.029454 | -1.256898 | -0.262775 |
| C | -5.217931 | 0.401903 | 0.249898 |
| H | -3.779251 | 1.981276 | 0.461708 |
| C | -4.324185 | -1.767075 | -0.265056 |
| H | -2.187312 | -1.898898 | -0.463388 |
| C | -5.419761 | -0.951193 | -0.011062 |
| H | -6.060370 | 1.052374 | 0.450560 |
| H | -4.470244 | -2.820517 | -0.471355 |
| H | -6.421412 | -1.362261 | -0.016133 |

| | | | |
|---|---|---|---|
| N | -1.565163 | 0.718648 | 0.011430 |
| H | -1.580683 | 1.722871 | 0.126395 |

**3A$_5$**

Imaginary frequency: None

Electronic energies: -730.162703

Free energies: -729.889823

Corrected Free energies: -729.885547

| | | | |
|---|---|---|---|
| C | 4.167736 | 0.898821 | -0.040739 |
| H | 4.676833 | 0.739984 | 0.911965 |
| N | 2.816595 | 0.356798 | 0.069802 |
| H | 2.126638 | 0.678004 | -0.604229 |
| C | 2.460278 | -0.756230 | 0.745091 |
| C | 1.229595 | -1.348985 | 0.618195 |
| C | 3.462543 | -1.333159 | 1.708132 |
| H | 3.712690 | -0.602283 | 2.480907 |
| H | 3.055380 | -2.221281 | 2.185901 |
| H | 4.388824 | -1.604544 | 1.197299 |
| C | 0.203919 | -0.872711 | -0.291763 |
| O | 0.325949 | 0.119825 | -1.026573 |
| C | -2.091443 | -1.218932 | -1.112419 |
| H | -1.708764 | -0.685299 | -1.984988 |
| H | -2.593008 | -2.119920 | -1.472578 |
| C | 4.954522 | 0.202744 | -1.153504 |
| H | 5.970248 | 0.600028 | -1.213023 |
| H | 5.012902 | -0.873794 | -0.980610 |
| H | 4.461019 | 0.368299 | -2.114972 |
| C | 4.070345 | 2.400292 | -0.289350 |
| H | 5.067305 | 2.836539 | -0.369121 |
| H | 3.539896 | 2.595008 | -1.226101 |
| H | 3.533554 | 2.893658 | 0.522235 |
| H | 1.018259 | -2.220395 | 1.222572 |
| C | -3.099951 | -0.334655 | -0.398734 |
| C | -2.785186 | 0.345766 | 0.774621 |
| C | -4.372653 | -0.175089 | -0.950901 |
| C | -3.724499 | 1.174451 | 1.384577 |
| H | -1.803449 | 0.222206 | 1.218341 |
| C | -5.311091 | 0.651946 | -0.345517 |
| H | -4.628826 | -0.707067 | -1.862015 |
| C | -4.988814 | 1.331279 | 0.827190 |
| H | -3.466180 | 1.698141 | 2.297681 |
| H | -6.295527 | 0.763881 | -0.785156 |
| H | -5.719281 | 1.975125 | 1.302347 |

| | | | |
|---|---|---|---|
| N | -0.952024 | -1.604209 | -0.314249 |
| H | -1.059907 | -2.356248 | 0.347979 |

**3A$_5$** radical cation

Imaginary frequency: None

Electronic energies: -729.958317

Free energies: -729.687206

Corrected Free energies: -729.682652

| | | | |
|---|---|---|---|
| C | 4.047525 | 0.888690 | 0.170908 |
| H | 4.565354 | 0.536119 | 1.062332 |
| N | 2.767507 | 0.171401 | 0.090960 |
| H | 2.019543 | 0.573326 | -0.497964 |
| C | 2.463838 | -0.960955 | 0.668013 |
| C | 1.169135 | -1.518804 | 0.449980 |
| C | 3.445444 | -1.668691 | 1.545635 |
| H | 3.641793 | -1.071973 | 2.439629 |
| H | 3.052116 | -2.634775 | 1.850085 |
| H | 4.389809 | -1.818130 | 1.020079 |
| C | 0.143105 | -0.888978 | -0.416810 |
| O | 0.332448 | 0.192388 | -0.977870 |
| C | -2.104461 | -1.117873 | -1.356269 |
| H | -1.682260 | -0.564843 | -2.195329 |
| H | -2.627100 | -1.993088 | -1.740906 |
| C | 4.871628 | 0.562398 | -1.075833 |
| H | 5.820080 | 1.097887 | -1.020325 |
| H | 5.076607 | -0.506510 | -1.147343 |
| H | 4.341565 | 0.882911 | -1.974935 |
| C | 3.752776 | 2.378056 | 0.300260 |
| H | 4.695157 | 2.919909 | 0.381708 |
| H | 3.222844 | 2.742458 | -0.582939 |
| H | 3.152806 | 2.584523 | 1.186807 |
| H | 0.939792 | -2.452288 | 0.946074 |
| C | -3.044680 | -0.240745 | -0.558236 |
| C | -2.784609 | 1.123350 | -0.415869 |
| C | -4.164270 | -0.791941 | 0.063234 |
| C | -3.634260 | 1.922934 | 0.341268 |
| H | -1.911703 | 1.549978 | -0.897182 |
| C | -5.015484 | 0.007821 | 0.819707 |
| H | -4.374100 | -1.850399 | -0.051268 |
| C | -4.750322 | 1.366519 | 0.960655 |
| H | -3.428108 | 2.981638 | 0.445287 |
| H | -5.885906 | -0.429061 | 1.294486 |
| H | -5.412529 | 1.990897 | 1.548650 |

| | | | |
|---|---|---|---|
| N | -0.985299 | -1.599271 | -0.548333 |
| H | -1.102990 | -2.453265 | -0.022238 |

**$3B_1$**

Imaginary frequency: None

Electronic energies: -558.322941

Free energies: -558.109877

Corrected Free energies: -558.107648

| | | | |
|---|---|---|---|
| C | 2.974869 | -0.321794 | -0.084456 |
| H | 3.466288 | 0.531097 | -0.555994 |
| N | 1.530567 | -0.128470 | -0.194313 |
| H | 0.941833 | -0.951824 | -0.109365 |
| C | 0.878496 | 1.046918 | -0.174464 |
| C | -0.493026 | 1.145425 | -0.123049 |
| C | 1.702119 | 2.303468 | -0.244495 |
| H | 2.270381 | 2.334721 | -1.177054 |
| H | 1.055646 | 3.176746 | -0.201094 |
| H | 2.415975 | 2.352850 | 0.580368 |
| C | -1.354741 | -0.003030 | -0.053451 |
| O | -1.007453 | -1.178707 | -0.036885 |
| O | -2.661782 | 0.338176 | -0.002196 |
| C | -3.597207 | -0.745837 | 0.076583 |
| H | -3.482868 | -1.382620 | -0.803671 |
| H | -3.371275 | -1.348715 | 0.958719 |
| C | 3.408875 | -0.406698 | 1.379799 |
| H | 4.491666 | -0.531420 | 1.450741 |
| H | 3.127188 | 0.494404 | 1.927992 |
| H | 2.929311 | -1.263717 | 1.859927 |
| C | 3.356643 | -1.584205 | -0.850255 |
| H | 4.435262 | -1.741515 | -0.805206 |
| H | 2.868459 | -2.457967 | -0.408749 |
| H | 3.055278 | -1.509086 | -1.896029 |
| C | -4.980220 | -0.139258 | 0.152147 |
| H | -5.729218 | -0.929470 | 0.223240 |
| H | -5.068206 | 0.502089 | 1.030452 |
| H | -5.187742 | 0.456658 | -0.737922 |
| H | -0.952921 | 2.121372 | -0.133667 |

**$3B_1$** radical cation

Imaginary frequency: -8.1193

Electronic energies: -558.110942

Free energies: -557.898641

Corrected Free energies: -557.896653

| | | | |
|---|---|---|---|
| C | 2.967442 | -0.343018 | -0.110068 |
| H | 3.446668 | 0.521316 | -0.568661 |
| N | 1.518855 | -0.081363 | -0.092477 |
| H | 0.894965 | -0.894353 | -0.014450 |
| C | 0.936542 | 1.086147 | -0.133606 |
| C | -0.489809 | 1.159529 | -0.091938 |
| C | 1.737768 | 2.343031 | -0.233819 |
| H | 2.220089 | 2.393616 | -1.213315 |
| H | 1.093336 | 3.209871 | -0.117569 |
| H | 2.513775 | 2.367773 | 0.532192 |
| C | -1.370692 | -0.025685 | -0.003946 |
| O | -0.968598 | -1.168264 | 0.056399 |
| O | -2.638941 | 0.327484 | 0.001282 |
| C | -3.605924 | -0.750355 | 0.089243 |
| H | -3.439565 | -1.422476 | -0.753780 |
| H | -3.415060 | -1.297141 | 1.013880 |
| C | 3.453797 | -0.509766 | 1.330205 |
| H | 4.528881 | -0.691528 | 1.317536 |
| H | 3.256730 | 0.384612 | 1.922544 |
| H | 2.960571 | -1.362163 | 1.800958 |
| C | 3.217371 | -1.583238 | -0.958422 |
| H | 4.290532 | -1.768092 | -1.005481 |
| H | 2.738843 | -2.457924 | -0.511476 |
| H | 2.840919 | -1.448712 | -1.972636 |
| C | -4.976282 | -0.120116 | 0.064250 |
| H | -5.132760 | 0.423107 | -0.868082 |
| H | -5.733552 | -0.900934 | 0.143404 |
| H | -5.097620 | 0.567652 | 0.901575 |
| H | -0.959697 | 2.131982 | -0.132132 |

**3B$_2$**

Imaginary frequency: None

Electronic energies: -635.496265

Free energies: -635.263297

Corrected Free energies: -635.261163

| | | | |
|---|---|---|---|
| C | -0.611558 | -0.228107 | -0.061672 |
| O | -0.108571 | -1.359676 | -0.173464 |
| C | 0.153360 | 0.973346 | 0.050610 |
| C | 1.540691 | 0.997836 | 0.008164 |
| H | -0.349800 | 1.914664 | 0.206177 |
| C | 2.262466 | 2.311296 | 0.127795 |
| H | 2.787057 | 2.540476 | -0.803058 |

| | | | |
|---|---|---|---|
| H | 1.554395 | 3.110622 | 0.332422 |
| H | 3.004405 | 2.281886 | 0.928014 |
| N | 2.271364 | -0.106965 | -0.158885 |
| H | 1.731575 | -0.969435 | -0.206574 |
| C | 3.730266 | -0.202660 | -0.146655 |
| H | 4.133246 | 0.740729 | -0.519165 |
| C | 4.247270 | -0.448424 | 1.271422 |
| H | 3.854007 | -1.394500 | 1.652282 |
| H | 5.337976 | -0.500641 | 1.273415 |
| H | 3.937243 | 0.349381 | 1.948935 |
| C | 4.150405 | -1.320580 | -1.094601 |
| H | 5.237770 | -1.405468 | -1.117405 |
| H | 3.742280 | -2.276992 | -0.755210 |
| H | 3.790785 | -1.127930 | -2.106326 |
| C | -2.115064 | -0.128770 | -0.019338 |
| C | -2.808633 | 1.040809 | -0.339441 |
| C | -2.837695 | -1.272719 | 0.328132 |
| C | -4.198964 | 1.066409 | -0.302570 |
| H | -2.270730 | 1.930380 | -0.643366 |
| C | -4.225457 | -1.244862 | 0.376948 |
| H | -2.290027 | -2.178586 | 0.557563 |
| C | -4.909696 | -0.073304 | 0.061621 |
| H | -4.727619 | 1.975893 | -0.561912 |
| H | -4.775367 | -2.135528 | 0.657359 |
| H | -5.992524 | -0.050399 | 0.094264 |

**3B$_2$** radical cation

Imaginary frequency: None

Electronic energies: -635.281989

Free energies: -635.051183

Corrected Free energies: -635.048703

| | | | |
|---|---|---|---|
| C | 0.643339 | -0.260591 | 0.002789 |
| O | 0.092057 | -1.343748 | 0.147286 |
| C | -0.161104 | 0.955657 | -0.241089 |
| C | -1.596979 | 0.995750 | -0.263351 |
| H | 0.341077 | 1.887550 | -0.453534 |
| C | -2.292016 | 2.294722 | -0.515470 |
| H | -3.057891 | 2.473875 | 0.239856 |
| H | -1.579472 | 3.114656 | -0.501759 |
| H | -2.775607 | 2.266595 | -1.495446 |
| N | -2.274710 | -0.100533 | -0.075069 |
| H | -1.714272 | -0.946338 | 0.089423 |
| C | -3.740147 | -0.241956 | -0.054860 |

| | | | |
|---|---|---|---|
| H | -4.155213 | 0.605222 | -0.599824 |
| C | -4.215643 | -0.215990 | 1.398305 |
| H | -5.300448 | -0.326007 | 1.413668 |
| H | -3.772570 | -1.043104 | 1.956149 |
| H | -3.952062 | 0.722552 | 1.887010 |
| C | -4.102942 | -1.540549 | -0.764020 |
| H | -3.691697 | -2.400026 | -0.229128 |
| H | -5.188290 | -1.639551 | -0.785608 |
| H | -3.731524 | -1.545637 | -1.788944 |
| C | 2.121813 | -0.138601 | 0.023520 |
| C | 2.775744 | 1.079209 | 0.233828 |
| C | 2.868465 | -1.309208 | -0.150321 |
| C | 4.164074 | 1.121823 | 0.266116 |
| H | 2.222229 | 1.994404 | 0.401769 |
| C | 4.252935 | -1.258539 | -0.132779 |
| H | 2.347822 | -2.245758 | -0.306527 |
| C | 4.901441 | -0.042064 | 0.075741 |
| H | 4.668161 | 2.064043 | 0.439682 |
| H | 4.828498 | -2.163538 | -0.281396 |
| H | 5.983899 | -0.003198 | 0.091336 |

**3B$_3$**

Imaginary frequency: None

Electronic energies: -443.786489

Free energies: -443.603963

Corrected Free energies: -443.602434

| | | | |
|---|---|---|---|
| C | 2.119326 | -0.134605 | -0.132447 |
| H | 2.466246 | 0.752731 | -0.665089 |
| N | 0.658106 | -0.127963 | -0.145627 |
| H | 0.169390 | -1.013923 | -0.022605 |
| C | -0.139431 | 0.944929 | -0.162596 |
| C | -1.518750 | 0.839484 | -0.069068 |
| C | 0.496990 | 2.298882 | -0.311652 |
| H | 0.993499 | 2.380321 | -1.281806 |
| H | -0.259518 | 3.076923 | -0.241702 |
| H | 1.249874 | 2.468802 | 0.460622 |
| C | -2.205615 | -0.408364 | 0.064387 |
| O | -1.638296 | -1.512245 | 0.112338 |
| C | 2.650194 | -0.102321 | 1.301486 |
| H | 3.742124 | -0.092015 | 1.302935 |
| H | 2.294100 | 0.781771 | 1.833725 |
| H | 2.310663 | -0.989072 | 1.842953 |
| C | 2.605399 | -1.372271 | -0.878825 |

| | | | |
|---|---|---|---|
| H | 3.695826 | -1.397942 | -0.897205 |
| H | 2.252568 | -2.278391 | -0.377905 |
| H | 2.236055 | -1.376443 | -1.905275 |
| C | -3.719176 | -0.378761 | 0.140844 |
| H | -4.119187 | 0.629891 | 0.235143 |
| H | -4.124600 | -0.838009 | -0.764195 |
| H | -4.042947 | -0.983638 | 0.989607 |
| H | -2.098103 | 1.750857 | -0.101292 |

**3B$_3$** radical cation

Imaginary frequency: None

Electronic energies: -443.575158

Free energies: -443.392633

Corrected Free energies: -443.391521

| | | | |
|---|---|---|---|
| C | 2.132950 | -0.130299 | -0.118080 |
| H | 2.475933 | 0.800777 | -0.567254 |
| N | 0.662456 | -0.084119 | -0.082356 |
| H | 0.165023 | -0.978205 | 0.016543 |
| C | -0.089588 | 0.978943 | -0.133305 |
| C | -1.515605 | 0.832432 | -0.067560 |
| C | 0.511095 | 2.341118 | -0.264908 |
| H | 0.982927 | 2.442629 | -1.245493 |
| H | -0.256315 | 3.103868 | -0.165616 |
| H | 1.273692 | 2.499476 | 0.498717 |
| C | -2.233372 | -0.458187 | 0.058228 |
| O | -1.619550 | -1.509468 | 0.117026 |
| C | 2.654661 | -0.245493 | 1.314851 |
| H | 3.744171 | -0.283355 | 1.288592 |
| H | 2.348659 | 0.609011 | 1.919776 |
| H | 2.284579 | -1.160808 | 1.780440 |
| C | 2.550317 | -1.309247 | -0.988436 |
| H | 3.638643 | -1.345054 | -1.037103 |
| H | 2.195143 | -2.249001 | -0.558779 |
| H | 2.157671 | -1.208668 | -2.000450 |
| C | -3.728035 | -0.384004 | 0.109428 |
| H | -4.036119 | 0.243607 | 0.949246 |
| H | -4.103962 | 0.083765 | -0.803910 |
| H | -4.140539 | -1.384041 | 0.215707 |
| H | -2.104839 | 1.738998 | -0.111445 |

**3C$_1$**

Imaginary frequency: None

Electronic energies: -1017.913785
Free energies: -1017.711148
Corrected Free energies: -1017.708989

| | | | |
|---|---|---|---|
| C | 3.182096 | -0.482207 | -0.117477 |
| H | 3.612181 | 0.391514 | -0.609064 |
| N | 1.723909 | -0.359116 | -0.154586 |
| H | 1.184494 | -1.217732 | -0.100346 |
| C | 1.013086 | 0.778021 | -0.111385 |
| C | -0.371299 | 0.764166 | -0.059507 |
| C | 1.792064 | 2.063559 | -0.156184 |
| H | 2.232855 | 2.187463 | -1.148804 |
| H | 1.163561 | 2.921582 | 0.052399 |
| H | 2.605042 | 2.040474 | 0.569599 |
| C | -1.142540 | -0.460290 | -0.013465 |
| O | -0.650830 | -1.582532 | -0.016087 |
| O | -2.467689 | -0.278014 | 0.035790 |
| C | -3.266752 | -1.472669 | 0.085995 |
| H | -3.049245 | -2.079026 | -0.795252 |
| H | -2.986656 | -2.047941 | 0.970408 |
| C | 3.688145 | -0.559311 | 1.323488 |
| H | 4.777173 | -0.638189 | 1.339628 |
| H | 3.396248 | 0.322829 | 1.896525 |
| H | 3.268940 | -1.440832 | 1.815025 |
| C | 3.574965 | -1.724555 | -0.910150 |
| H | 4.659670 | -1.839764 | -0.913866 |
| H | 3.140748 | -2.618908 | -0.454115 |
| H | 3.224775 | -1.654243 | -1.940848 |
| C | -4.713209 | -1.037161 | 0.129822 |
| H | -4.965397 | -0.454497 | -0.757305 |
| H | -5.360939 | -1.914367 | 0.164475 |
| H | -4.904731 | -0.428805 | 1.014885 |
| Cl | -1.273957 | 2.273606 | -0.070923 |

**3C$_1$** radical cation
Imaginary frequency: None
Electronic energies: -1017.703819
Free energies: -1017.501302
Corrected Free energies: -1017.499036

| | | | |
|---|---|---|---|
| C | 3.172521 | -0.567101 | -0.189877 |
| H | 3.582690 | 0.165691 | -0.884612 |
| N | 1.710633 | -0.348474 | -0.131833 |
| H | 1.123136 | -1.187340 | -0.050286 |
| C | 1.074749 | 0.788557 | -0.139924 |

| | | | |
|---|---|---|---|
| C | -0.367603 | 0.774909 | -0.063993 |
| C | 1.788963 | 2.095574 | -0.221991 |
| H | 1.453001 | 2.637511 | -1.107996 |
| H | 1.531492 | 2.698808 | 0.650751 |
| H | 2.865386 | 1.973235 | -0.262038 |
| C | -1.171011 | -0.483269 | 0.003642 |
| O | -0.650230 | -1.577466 | 0.028359 |
| O | -2.460129 | -0.263237 | 0.032314 |
| C | -3.311668 | -1.440299 | 0.100000 |
| H | -3.097056 | -2.056432 | -0.773857 |
| H | -3.040325 | -1.997148 | 0.997421 |
| C | 3.766878 | -0.375127 | 1.204283 |
| H | 4.845004 | -0.530030 | 1.150303 |
| H | 3.577635 | 0.627998 | 1.588352 |
| H | 3.342816 | -1.103452 | 1.897858 |
| C | 3.409129 | -1.967954 | -0.736062 |
| H | 4.482042 | -2.138565 | -0.821298 |
| H | 2.996332 | -2.720084 | -0.059246 |
| H | 2.959787 | -2.088123 | -1.722410 |
| C | -4.737730 | -0.951138 | 0.129314 |
| H | -4.967722 | -0.380993 | -0.771096 |
| H | -5.409248 | -1.808969 | 0.178451 |
| H | -4.911367 | -0.322926 | 1.003390 |
| Cl | -1.186502 | 2.244168 | -0.064035 |

**3C$_2$**

Imaginary frequency: None

Electronic energies: -597.621464

Free energies: -597.381567

Corrected Free energies: -597.379368

| | | | |
|---|---|---|---|
| C | 3.049567 | -0.451211 | -0.101948 |
| H | 3.535643 | 0.401592 | -0.579387 |
| N | 1.603640 | -0.260061 | -0.179988 |
| H | 1.020072 | -1.090272 | -0.145070 |
| C | 0.938517 | 0.911352 | -0.130801 |
| C | -0.443601 | 1.008927 | -0.110637 |
| C | 1.786923 | 2.156944 | -0.131751 |
| H | 2.232545 | 2.306729 | -1.119494 |
| H | 1.203458 | 3.036715 | 0.118994 |
| H | 2.601510 | 2.072017 | 0.587827 |
| C | -1.136366 | 2.356410 | -0.127951 |
| H | -0.745075 | 3.004166 | -0.915292 |
| H | -2.198953 | 2.225759 | -0.315166 |

| | | | |
|---|---|---|---|
| H | -1.035784 | 2.892552 | 0.821474 |
| C | -1.238774 | -0.198803 | -0.053948 |
| O | -0.819329 | -1.353891 | -0.066393 |
| O | -2.570087 | 0.029865 | 0.028696 |
| C | -3.408810 | -1.130823 | 0.093020 |
| H | -3.238596 | -1.744645 | -0.794167 |
| H | -3.132702 | -1.723311 | 0.967812 |
| C | 3.519254 | -0.555655 | 1.350682 |
| H | 4.603701 | -0.679133 | 1.394568 |
| H | 3.248924 | 0.334664 | 1.921815 |
| H | 3.052155 | -1.421191 | 1.827756 |
| C | 3.410946 | -1.708599 | -0.886926 |
| H | 4.489629 | -1.870642 | -0.865272 |
| H | 2.928061 | -2.584449 | -0.443658 |
| H | 3.088521 | -1.622959 | -1.925625 |
| C | -4.838776 | -0.645606 | 0.173841 |
| H | -5.517381 | -1.498395 | 0.226511 |
| H | -4.985235 | -0.030406 | 1.063022 |
| H | -5.093923 | -0.053776 | -0.706638 |

**3C**$_2$ radical cation

Imaginary frequency: None

Electronic energies: -597.423160

Free energies: -597.183581

Corrected Free energies: -597.181318

| | | | |
|---|---|---|---|
| C | 3.056638 | -0.469907 | -0.115359 |
| H | 3.538869 | 0.378570 | -0.600042 |
| N | 1.603907 | -0.213261 | -0.122215 |
| H | 0.985531 | -1.033502 | -0.146285 |
| C | 1.001093 | 0.943703 | -0.091238 |
| C | -0.439685 | 1.007770 | -0.147343 |
| C | 1.787496 | 2.213953 | -0.027360 |
| H | 1.906280 | 2.614929 | -1.038532 |
| H | 1.256994 | 2.953839 | 0.568529 |
| H | 2.771570 | 2.059855 | 0.405225 |
| C | -1.128121 | 2.320408 | -0.236354 |
| H | -0.557295 | 3.033985 | -0.829537 |
| H | -2.121855 | 2.203158 | -0.659647 |
| H | -1.246362 | 2.744439 | 0.769966 |
| C | -1.254505 | -0.239225 | -0.069040 |
| O | -0.789769 | -1.361365 | -0.080262 |
| O | -2.543345 | 0.016502 | 0.019913 |
| C | -3.424119 | -1.132200 | 0.110059 |

| | | | |
|---|---|---|---|
| H | -3.276965 | -1.739285 | -0.784297 |
| H | -3.127097 | -1.717619 | 0.981107 |
| C | 3.537647 | -0.604902 | 1.328752 |
| H | 4.611934 | -0.792407 | 1.327951 |
| H | 3.341766 | 0.301266 | 1.903646 |
| H | 3.036930 | -1.444007 | 1.815535 |
| C | 3.314056 | -1.729039 | -0.933036 |
| H | 4.388106 | -1.909008 | -0.977742 |
| H | 2.841898 | -2.597012 | -0.466312 |
| H | 2.936375 | -1.620775 | -1.950159 |
| C | -4.832212 | -0.602463 | 0.224098 |
| H | -5.093135 | -0.009389 | -0.652989 |
| H | -5.527367 | -1.439576 | 0.296647 |
| H | -4.938329 | 0.015681 | 1.116158 |

**3C$_3$**

Imaginary frequency: None

Electronic energies: -522.387413

Free energies: -522.150808

Corrected Free energies: -522.149203

| | | | |
|---|---|---|---|
| C | 2.668714 | -0.359116 | -0.135381 |
| H | 3.116694 | 0.488587 | -0.657943 |
| N | 1.215020 | -0.217619 | -0.182456 |
| H | 0.651174 | -1.066149 | -0.191205 |
| C | 0.498244 | 0.915691 | -0.123127 |
| C | -0.895207 | 0.922645 | -0.129732 |
| C | 1.257488 | 2.217767 | -0.067016 |
| H | 1.387828 | 2.618929 | -1.076737 |
| H | 0.708961 | 2.954460 | 0.515720 |
| H | 2.242300 | 2.099557 | 0.378176 |
| C | -1.637329 | 2.244694 | -0.147491 |
| H | -1.116069 | 2.987829 | -0.752419 |
| H | -2.627756 | 2.135044 | -0.587336 |
| H | -1.774235 | 2.673638 | 0.852422 |
| C | -1.633592 | -0.315489 | -0.074737 |
| O | -1.106698 | -1.440935 | -0.106655 |
| C | 3.175408 | -0.398737 | 1.307534 |
| H | 4.263420 | -0.492603 | 1.328582 |
| H | 2.894389 | 0.503610 | 1.854033 |
| H | 2.742074 | -1.258561 | 1.824880 |
| C | 3.045174 | -1.633053 | -0.885303 |
| H | 4.128121 | -1.764305 | -0.885833 |
| H | 2.597613 | -2.505199 | -0.400001 |

| | | | |
|---|---|---|---|
| H | 2.695449 | -1.592632 | -1.917984 |
| C | -3.153493 | -0.246047 | 0.051804 |
| H | -3.410556 | 0.466695 | 0.841478 |
| H | -3.554482 | 0.180649 | -0.874506 |
| C | -3.786156 | -1.603738 | 0.321421 |
| H | -4.870841 | -1.511303 | 0.398378 |
| H | -3.552505 | -2.305336 | -0.479679 |
| H | -3.408633 | -2.029791 | 1.252580 |

**3C$_3$** radical cation

Imaginary frequency: None

Electronic energies: -522.190059

Free energies: -521.953340

Corrected Free energies: -521.951754

| | | | |
|---|---|---|---|
| C | 2.679662 | -0.371802 | -0.124375 |
| H | 3.132217 | 0.516507 | -0.564127 |
| N | 1.217084 | -0.179604 | -0.149722 |
| H | 0.633672 | -1.023145 | -0.216228 |
| C | 0.561049 | 0.943716 | -0.080625 |
| C | -0.888199 | 0.939651 | -0.151298 |
| C | 1.289599 | 2.243678 | 0.048701 |
| H | 1.409880 | 2.689173 | -0.943660 |
| H | 0.718086 | 2.936811 | 0.662419 |
| H | 2.271783 | 2.114113 | 0.493536 |
| C | -1.602550 | 2.242381 | -0.231269 |
| H | -1.040581 | 2.974071 | -0.810687 |
| H | -2.588868 | 2.131779 | -0.674400 |
| H | -1.738597 | 2.656803 | 0.777102 |
| C | -1.668143 | -0.331925 | -0.083789 |
| O | -1.107419 | -1.414742 | -0.135506 |
| C | 3.139103 | -0.546496 | 1.322525 |
| H | 4.220628 | -0.685925 | 1.336201 |
| H | 2.891356 | 0.324313 | 1.931140 |
| H | 2.668119 | -1.427566 | 1.762730 |
| C | 3.007721 | -1.584555 | -0.985545 |
| H | 4.089163 | -1.718138 | -1.012426 |
| H | 2.562946 | -2.489213 | -0.563772 |
| H | 2.647664 | -1.451600 | -2.006089 |
| C | -3.166538 | -0.242515 | 0.063913 |
| H | -3.396018 | 0.478794 | 0.854638 |
| H | -3.566933 | 0.187996 | -0.860774 |
| C | -3.800343 | -1.597133 | 0.342811 |
| H | -4.879945 | -1.487554 | 0.443527 |

| | | | |
|---|---|---|---|
| H | -3.595532 | -2.295359 | -0.468624 |
| H | -3.407440 | -2.026696 | 1.265305 |

**3D$_1$**

Imaginary frequency: None

Electronic energies: -481.889972

Free energies: -481.697218

Corrected Free energies: -481.695911

| | | | |
|---|---|---|---|
| C | 2.477551 | 0.163986 | -0.070205 |
| H | 2.330542 | 1.157718 | -0.495238 |
| N | 1.263464 | -0.617384 | -0.317427 |
| H | 1.393165 | -1.619570 | -0.245248 |
| C | -0.013529 | -0.190603 | -0.185787 |
| C | -1.051934 | -1.083494 | -0.109814 |
| C | -0.263997 | 1.297278 | -0.157802 |
| H | 0.427472 | 1.796173 | -0.838382 |
| H | -0.042605 | 1.670188 | 0.849456 |
| C | 2.756858 | 0.294251 | 1.427752 |
| H | 3.652534 | 0.895537 | 1.597811 |
| H | 1.920132 | 0.767735 | 1.944938 |
| H | 2.916681 | -0.695193 | 1.864600 |
| C | 3.636863 | -0.506768 | -0.797662 |
| H | 4.555803 | 0.060777 | -0.645583 |
| H | 3.795361 | -1.516294 | -0.406690 |
| H | 3.436921 | -0.574795 | -1.867763 |
| C | -1.701789 | 1.637384 | -0.543628 |
| H | -1.837894 | 1.438866 | -1.610673 |
| H | -1.879737 | 2.702294 | -0.384704 |
| C | -2.420126 | -0.686913 | 0.108700 |
| C | -2.694196 | 0.800298 | 0.253345 |
| H | -2.615461 | 1.042344 | 1.320449 |
| H | -3.726027 | 0.985569 | -0.048506 |
| H | -0.852180 | -2.149950 | -0.144339 |
| O | -3.334144 | -1.499029 | 0.222809 |

**3D$_2$** radical cation

Imaginary frequency: None

Electronic energies: -442.368969

Free energies: -442.205029

Corrected Free energies: -442.204108

| | | | |
|---|---|---|---|
| C | 2.214777 | 0.196041 | -0.116614 |
| H | 1.892563 | 1.115478 | -0.604668 |

| | | | |
|---|---|---|---|
| N | 1.002786 | -0.618880 | 0.088933 |
| H | 1.161024 | -1.591496 | 0.353530 |
| C | -0.227847 | -0.207460 | -0.001662 |
| C | -1.351759 | -1.040055 | 0.236788 |
| C | -0.645960 | 1.193186 | -0.366188 |
| H | -0.284847 | 1.427248 | -1.370026 |
| H | -0.191917 | 1.908320 | 0.322203 |
| C | -2.578563 | -0.242548 | 0.060179 |
| C | 2.828175 | 0.511501 | 1.246601 |
| H | 3.721163 | 1.118466 | 1.093603 |
| H | 2.130511 | 1.065093 | 1.875639 |
| H | 3.117381 | -0.408845 | 1.757634 |
| C | 3.165239 | -0.571749 | -1.027091 |
| H | 4.049998 | 0.039541 | -1.205862 |
| H | 3.483041 | -1.503835 | -0.553775 |
| H | 2.695582 | -0.796834 | -1.984580 |
| C | -2.181176 | 1.183390 | -0.284917 |
| H | -2.557290 | 1.847549 | 0.494194 |
| H | -2.654069 | 1.470072 | -1.224067 |
| H | -1.326319 | -2.087497 | 0.504572 |
| O | -3.699205 | -0.675617 | 0.179562 |

**4C$_2$**

Imaginary frequency: None

Electronic energies: -750.023659

Free energies: -749.761807

Corrected Free energies: -749.758268

| | | | |
|---|---|---|---|
| C | 0.677965 | 2.376610 | -0.721527 |
| H | 1.617826 | 1.896498 | -1.006179 |
| H | 0.925544 | 3.249179 | -0.111067 |
| H | 0.181282 | 2.711649 | -1.625550 |
| C | -0.172097 | 1.414225 | 0.062738 |
| C | -1.450195 | 1.093815 | -0.344878 |
| C | -2.097184 | 1.769700 | -1.536398 |
| H | -1.707757 | 1.399600 | -2.490322 |
| H | -3.169152 | 1.589323 | -1.531540 |
| H | -1.949859 | 2.850544 | -1.514013 |
| C | -2.172130 | 0.039532 | 0.345924 |
| O | -1.792490 | -0.580442 | 1.335672 |
| O | -3.360621 | -0.256781 | -0.219769 |
| C | -4.116613 | -1.307310 | 0.399751 |
| H | -4.312497 | -1.039746 | 1.440151 |
| H | -3.522226 | -2.223187 | 0.394569 |

| | | | |
|---|---|---|---|
| C | -5.395502 | -1.463176 | -0.391385 |
| H | -5.972393 | -0.537251 | -0.375200 |
| H | -5.175313 | -1.719885 | -1.428743 |
| H | -6.004030 | -2.258518 | 0.041535 |
| N | 0.403208 | 0.916424 | 1.187227 |
| H | -0.150307 | 0.223291 | 1.676527 |
| C | 1.829125 | 0.939568 | 1.445115 |
| H | 2.219602 | 1.954208 | 1.342533 |
| H | 1.966054 | 0.661238 | 2.492439 |
| C | 2.636468 | -0.004885 | 0.568628 |
| C | 3.989658 | 0.247417 | 0.341812 |
| C | 2.054034 | -1.138693 | 0.004039 |
| C | 4.751941 | -0.623269 | -0.429557 |
| H | 4.447132 | 1.134209 | 0.769311 |
| C | 2.815207 | -2.010146 | -0.770015 |
| H | 1.000532 | -1.338817 | 0.170462 |
| C | 4.165680 | -1.755938 | -0.988091 |
| H | 5.801370 | -0.414182 | -0.601328 |
| H | 2.351377 | -2.887952 | -1.204435 |
| H | 4.757113 | -2.432085 | -1.593902 |

**4C**$_2$ radical cation

Imaginary frequency: None

Electronic energies: -749.820809

Free energies: -749.559561

Corrected Free energies: -749.556034

| | | | |
|---|---|---|---|
| C | 0.680943 | 2.239944 | -0.489525 |
| H | 1.740716 | 2.008049 | -0.427413 |
| H | 0.498037 | 3.196912 | 0.009769 |
| H | 0.405673 | 2.348005 | -1.536847 |
| C | -0.153796 | 1.187351 | 0.162197 |
| C | -1.538548 | 1.040601 | -0.212298 |
| C | -2.165783 | 1.993830 | -1.160781 |
| H | -2.000850 | 1.647088 | -2.190286 |
| H | -3.240462 | 2.036294 | -1.003534 |
| H | -1.740060 | 2.992207 | -1.073559 |
| C | -2.339554 | -0.107677 | 0.304220 |
| O | -1.939781 | -0.897035 | 1.136522 |
| O | -3.530843 | -0.169307 | -0.251049 |
| C | -4.391359 | -1.252667 | 0.186069 |
| H | -4.533494 | -1.153941 | 1.263134 |
| H | -3.876026 | -2.193186 | -0.012956 |
| C | -5.684305 | -1.128584 | -0.581024 |

| | | | |
|---|---|---|---|
| H | -6.163681 | -0.170861 | -0.375863 |
| H | -5.505044 | -1.214194 | -1.653171 |
| H | -6.360778 | -1.928070 | -0.276843 |
| N | 0.355928 | 0.421074 | 1.090034 |
| H | -0.279426 | -0.276014 | 1.492060 |
| C | 1.735920 | 0.470958 | 1.585963 |
| H | 1.992658 | 1.508176 | 1.803758 |
| H | 1.734900 | -0.077679 | 2.527379 |
| C | 2.725060 | -0.137083 | 0.611496 |
| C | 3.958536 | 0.479593 | 0.413093 |
| C | 2.429544 | -1.322018 | -0.061873 |
| C | 4.893150 | -0.086195 | -0.448774 |
| H | 4.188412 | 1.405117 | 0.930554 |
| C | 3.362218 | -1.882812 | -0.926652 |
| H | 1.471478 | -1.809436 | 0.085434 |
| C | 4.595624 | -1.266734 | -1.120702 |
| H | 5.849398 | 0.400034 | -0.599106 |
| H | 3.125795 | -2.802149 | -1.448358 |
| H | 5.320343 | -1.704178 | -1.796627 |

**5A$_1$**

Imaginary frequency: None

Electronic energies: -748.828841

Free energies: -748.585168

Corrected Free energies: -748.582574

| | | | |
|---|---|---|---|
| N | 0.875113 | -0.361220 | -0.069128 |
| H | 0.365384 | -1.237945 | -0.004266 |
| C | 0.081817 | 0.735929 | 0.003513 |
| C | -1.285330 | 0.716114 | 0.038056 |
| C | 0.589110 | 2.157739 | 0.066553 |
| H | 0.854019 | 2.492948 | -0.941771 |
| H | 1.477346 | 2.258606 | 0.692674 |
| C | -1.851876 | 2.113317 | 0.127127 |
| C | -2.050711 | -0.504501 | -0.040968 |
| O | -1.581430 | -1.634858 | -0.080736 |
| O | -3.378007 | -0.288847 | -0.063385 |
| C | -4.209247 | -1.458805 | -0.136656 |
| H | -3.953426 | -2.017971 | -1.038879 |
| H | -3.999101 | -2.095361 | 0.725221 |
| C | -5.645347 | -0.988119 | -0.153146 |
| H | -6.315311 | -1.847402 | -0.208182 |
| H | -5.875531 | -0.426731 | 0.753522 |
| H | -5.829642 | -0.348389 | -1.017449 |

| | | | |
|---|---|---|---|
| C | -0.632107 | 2.929436 | 0.594792 |
| H | -2.214161 | 2.459454 | -0.848032 |
| H | -2.687522 | 2.184471 | 0.825216 |
| H | -0.648561 | 3.963188 | 0.250309 |
| H | -0.603023 | 2.934446 | 1.686609 |
| C | 2.279202 | -0.438614 | -0.062588 |
| C | 3.094384 | 0.491154 | -0.713018 |
| C | 2.868900 | -1.532042 | 0.581238 |
| C | 4.476882 | 0.342739 | -0.681915 |
| H | 2.655797 | 1.310454 | -1.265074 |
| C | 4.248616 | -1.681716 | 0.588624 |
| H | 2.234890 | -2.256584 | 1.080015 |
| C | 5.062901 | -0.739345 | -0.033859 |
| H | 5.096726 | 1.073012 | -1.188349 |
| H | 4.688968 | -2.535049 | 1.090482 |
| H | 6.139694 | -0.852684 | -0.021701 |

**5A$_1$** radical cation

Imaginary frequency: None

Electronic energies: -748.622473

Free energies: -748.379065

Corrected Free energies: -748.376606

| | | | |
|---|---|---|---|
| N | 0.877721 | -0.278541 | -0.020607 |
| H | 0.340579 | -1.153326 | 0.028332 |
| C | 0.127856 | 0.805929 | -0.002728 |
| C | -1.285118 | 0.741458 | 0.024380 |
| C | 0.573327 | 2.239210 | 0.034547 |
| H | 0.817497 | 2.557444 | -0.984716 |
| H | 1.460181 | 2.379159 | 0.654397 |
| C | -1.864160 | 2.106673 | 0.099233 |
| C | -2.044615 | -0.524661 | -0.032108 |
| O | -1.510257 | -1.614937 | -0.037297 |
| O | -3.344394 | -0.322793 | -0.067493 |
| C | -4.179056 | -1.508822 | -0.118724 |
| H | -3.900612 | -2.078335 | -1.006404 |
| H | -3.960492 | -2.110939 | 0.764248 |
| C | -5.612915 | -1.041833 | -0.158925 |
| H | -6.273089 | -1.909165 | -0.195040 |
| H | -5.853087 | -0.459657 | 0.731279 |
| H | -5.793806 | -0.430355 | -1.043494 |
| C | -0.676071 | 2.976754 | 0.550009 |
| H | -2.216632 | 2.392410 | -0.902275 |
| H | -2.731040 | 2.148179 | 0.760117 |

| | | | |
|---|---|---|---|
| H | -0.734268 | 3.993157 | 0.168234 |
| H | -0.650180 | 3.016619 | 1.639503 |
| C | 2.278970 | -0.408455 | -0.045235 |
| C | 3.120841 | 0.570660 | -0.580370 |
| C | 2.800392 | -1.601991 | 0.466873 |
| C | 4.491001 | 0.355962 | -0.567403 |
| H | 2.721852 | 1.464106 | -1.036266 |
| C | 4.170771 | -1.797378 | 0.477189 |
| H | 2.129822 | -2.355023 | 0.864009 |
| C | 5.018813 | -0.817062 | -0.034495 |
| H | 5.148635 | 1.106464 | -0.986555 |
| H | 4.577430 | -2.714903 | 0.882484 |
| H | 6.090163 | -0.972880 | -0.028745 |

**5A$_2$**

Imaginary frequency: None

Electronic energies: -788.133104

Free energies: -787.861914

Corrected Free energies: -787.858829

| | | | |
|---|---|---|---|
| N | -0.870424 | -0.540246 | 0.069505 |
| H | -0.353825 | -1.406749 | -0.044066 |
| C | -0.112164 | 0.590825 | 0.023858 |
| C | 1.262478 | 0.556674 | -0.025357 |
| C | 1.958982 | -0.718626 | 0.037496 |
| O | 1.451857 | -1.834510 | 0.059165 |
| O | 3.298368 | -0.576876 | 0.076090 |
| C | 4.065482 | -1.789191 | 0.127068 |
| H | 3.782678 | -2.351511 | 1.019278 |
| H | 3.822449 | -2.398557 | -0.745670 |
| C | -2.290229 | -0.614038 | 0.044888 |
| C | -3.051810 | -0.215264 | 1.144182 |
| C | -2.923643 | -1.159118 | -1.071413 |
| C | -4.436393 | -0.334058 | 1.111286 |
| H | -2.551812 | 0.171601 | 2.024561 |
| C | -4.307933 | -1.295078 | -1.092145 |
| H | -2.322786 | -1.471431 | -1.917827 |
| C | -5.068145 | -0.874858 | -0.005435 |
| H | -5.021222 | -0.019524 | 1.967456 |
| H | -4.791259 | -1.723384 | -1.962008 |
| H | -6.146518 | -0.975181 | -0.024357 |
| C | -0.868339 | 1.899453 | -0.018442 |
| H | -1.365956 | 1.951980 | -0.995183 |
| H | -1.667189 | 1.880064 | 0.723041 |

| | | | |
|---|---|---|---|
| C | 2.100694 | 1.815250 | -0.150590 |
| H | 2.565596 | 2.058029 | 0.813200 |
| H | 2.923903 | 1.625137 | -0.841789 |
| C | 0.013297 | 3.125859 | 0.194297 |
| H | -0.552966 | 4.022641 | -0.065097 |
| H | 0.279410 | 3.204919 | 1.253868 |
| C | 1.285506 | 3.008903 | -0.633389 |
| H | 1.881944 | 3.921334 | -0.564864 |
| H | 1.018707 | 2.869766 | -1.687211 |
| C | 5.524608 | -1.394575 | 0.149348 |
| H | 6.149031 | -2.288650 | 0.183491 |
| H | 5.782015 | -0.826397 | -0.745810 |
| H | 5.744642 | -0.784223 | 1.026507 |

**5A$_2$** radical cation

Imaginary frequency: None

Electronic energies: -787.926635

Free energies: -787.656032

Corrected Free energies: -787.652808

| | | | |
|---|---|---|---|
| N | -0.862192 | -0.508719 | -0.064658 |
| H | -0.318847 | -1.375520 | -0.163740 |
| C | -0.171984 | 0.607052 | -0.029133 |
| C | 1.261632 | 0.555561 | -0.102953 |
| C | 1.977040 | -0.755521 | -0.047510 |
| O | 1.428826 | -1.836921 | -0.104548 |
| O | 3.277452 | -0.594293 | 0.066047 |
| C | 4.077349 | -1.803681 | 0.125830 |
| H | 3.738460 | -2.389479 | 0.981320 |
| H | 3.890062 | -2.374194 | -0.784773 |
| C | -2.295279 | -0.611488 | -0.010004 |
| C | -2.955135 | -0.398692 | 1.195256 |
| C | -2.977422 | -0.973323 | -1.165220 |
| C | -4.336921 | -0.537721 | 1.234679 |
| H | -2.392705 | -0.142869 | 2.085328 |
| C | -4.360365 | -1.106688 | -1.110924 |
| H | -2.432627 | -1.141473 | -2.085995 |
| C | -5.038002 | -0.888276 | 0.084196 |
| H | -4.862602 | -0.376893 | 2.167256 |
| H | -4.905546 | -1.382442 | -2.004718 |
| H | -6.114905 | -0.995986 | 0.120833 |
| C | -0.890944 | 1.925396 | 0.035034 |
| H | -1.367131 | 2.057252 | -0.945506 |
| H | -1.700586 | 1.854116 | 0.760721 |

| | | | |
|---|---|---|---|
| C | 2.076742 | 1.796051 | -0.208488 |
| H | 2.592469 | 1.918963 | 0.756544 |
| H | 2.876785 | 1.622493 | -0.933170 |
| C | 0.027755 | 3.104837 | 0.342593 |
| H | -0.527020 | 4.028734 | 0.179927 |
| H | 0.320941 | 3.080199 | 1.396359 |
| C | 1.267645 | 3.045629 | -0.538374 |
| H | 1.895248 | 3.924340 | -0.389936 |
| H | 0.972003 | 3.027711 | -1.591699 |
| C | 5.518158 | -1.375088 | 0.254052 |
| H | 6.154403 | -2.259966 | 0.294342 |
| H | 5.817043 | -0.771150 | -0.603300 |
| H | 5.668065 | -0.797390 | 1.166613 |

**5B$_4$**

Imaginary frequency: None

Electronic energies: -854.614991

Free energies: -854.463076

Corrected Free energies: -854.460261

| | | | |
|---|---|---|---|
| C | -2.002428 | -0.253356 | 0.079461 |
| O | -1.521683 | -1.351796 | 0.373502 |
| C | -1.318028 | 0.935897 | -0.246426 |
| C | 0.072366 | 1.009503 | -0.266316 |
| H | -1.880383 | 1.819386 | -0.503748 |
| C | -3.540694 | -0.214952 | 0.068327 |
| F | -4.020608 | -1.108767 | -0.804987 |
| F | -4.023069 | -0.539705 | 1.273849 |
| F | -4.051032 | 0.977701 | -0.258349 |
| C | 0.734817 | 2.302555 | -0.637729 |
| H | 1.661721 | 2.131320 | -1.185033 |
| H | 0.053760 | 2.893471 | -1.246521 |
| H | 0.971479 | 2.879188 | 0.259077 |
| N | 0.816619 | -0.063552 | 0.021886 |
| H | 0.281949 | -0.916474 | 0.192325 |
| C | 2.232672 | -0.169268 | 0.047115 |
| C | 2.817467 | -1.262914 | -0.590889 |
| C | 3.026242 | 0.746891 | 0.734703 |
| C | 4.196252 | -1.427046 | -0.556462 |
| H | 2.187119 | -1.971671 | -1.115204 |
| C | 4.406954 | 0.583138 | 0.750571 |
| H | 2.567569 | 1.566684 | 1.272188 |
| C | 4.995767 | -0.500438 | 0.106510 |
| H | 4.646158 | -2.277497 | -1.053927 |

| | | | |
|---|---|---|---|
| H | 5.020721 | 1.298582 | 1.283944 |
| H | 6.071095 | -0.626874 | 0.127864 |

**5B$_4$** radical cation

Imaginary frequency: None

Electronic energies: -854.383901

Free energies: -854.232550

Corrected Free energies: -854.229904

| | | | |
|---|---|---|---|
| C | 1.958088 | -0.334202 | -0.029426 |
| O | 1.398217 | -1.406352 | -0.080048 |
| C | 1.318923 | 0.976671 | 0.030070 |
| C | -0.038118 | 1.196888 | 0.040277 |
| H | 1.967616 | 1.841192 | 0.076474 |
| C | 3.499606 | -0.297939 | -0.014203 |
| F | 3.928530 | 0.288477 | 1.106354 |
| F | 4.009033 | -1.515230 | -0.080359 |
| F | 3.951830 | 0.416379 | -1.047494 |
| C | -0.576428 | 2.585855 | 0.115787 |
| H | -1.267506 | 2.687733 | 0.954284 |
| H | 0.247748 | 3.279962 | 0.257014 |
| H | -1.091956 | 2.850977 | -0.809473 |
| N | -0.853929 | 0.098985 | 0.000967 |
| H | -0.323533 | -0.781210 | -0.009728 |
| C | -2.206455 | -0.072574 | -0.007362 |
| C | -2.630585 | -1.429414 | 0.092833 |
| C | -3.176243 | 0.958991 | -0.120653 |
| C | -3.966921 | -1.739607 | 0.096567 |
| H | -1.882556 | -2.209621 | 0.176917 |
| C | -4.509510 | 0.622306 | -0.119925 |
| H | -2.896879 | 1.992480 | -0.227789 |
| C | -4.915454 | -0.714854 | -0.008427 |
| H | -4.283609 | -2.770437 | 0.178941 |
| H | -5.252549 | 1.403007 | -0.213893 |
| H | -5.970974 | -0.955520 | -0.008871 |

**5D$_2$**

Imaginary frequency: None

Electronic energies: -555.682517

Free energies: -555.523537

Corrected Free energies: -555.521822

| | | | |
|---|---|---|---|
| N | 0.064240 | -0.976387 | -0.491475 |
| H | 0.025026 | -1.960830 | -0.719650 |

| | | | |
|---|---|---|---|
| C | -1.121146 | -0.378681 | -0.230167 |
| C | -2.346680 | -0.947569 | -0.413678 |
| C | -1.217280 | 1.013901 | 0.351414 |
| H | -0.860714 | 1.754409 | -0.364677 |
| H | -0.589045 | 1.097186 | 1.241458 |
| C | -3.384571 | -0.058116 | 0.054818 |
| C | -2.713484 | 1.187518 | 0.634236 |
| H | -2.927816 | 1.226850 | 1.704133 |
| H | -3.137087 | 2.083367 | 0.179096 |
| H | -2.531610 | -1.930610 | -0.825053 |
| O | -4.591421 | -0.235721 | 0.034086 |
| C | 1.358836 | -0.452914 | -0.248061 |
| C | 2.280409 | -1.240926 | 0.442947 |
| C | 1.739294 | 0.801377 | -0.725205 |
| C | 3.567598 | -0.769897 | 0.668382 |
| H | 1.977606 | -2.216855 | 0.805007 |
| C | 3.022050 | 1.275370 | -0.473666 |
| H | 1.048111 | 1.388962 | -1.314924 |
| C | 3.939996 | 0.494856 | 0.221680 |
| H | 4.276622 | -1.389243 | 1.204242 |
| H | 3.309591 | 2.252169 | -0.843423 |
| H | 4.940864 | 0.865562 | 0.405240 |

**5D$_2$** radical cation

Imaginary frequency: None

Electronic energies: -555.462388

Free energies: -555.303615

Corrected Free energies: -555.302315

| | | | |
|---|---|---|---|
| N | 0.103885 | -0.876054 | 0.035358 |
| H | 0.068940 | -1.894531 | 0.041914 |
| C | -1.116696 | -0.291258 | 0.023126 |
| C | -2.254550 | -1.057103 | 0.036751 |
| C | -1.409665 | 1.186349 | -0.015757 |
| C | -3.435857 | -0.173317 | -0.005248 |
| C | -2.942997 | 1.261775 | -0.078791 |
| H | -2.306643 | -2.137315 | 0.069870 |
| O | -4.584592 | -0.542230 | 0.010737 |
| C | 1.382823 | -0.370250 | 0.022593 |
| C | 2.419200 | -1.332890 | -0.031512 |
| C | 1.697997 | 1.006159 | 0.062042 |
| C | 3.734220 | -0.928505 | -0.056159 |
| H | 2.168060 | -2.387008 | -0.058712 |
| C | 3.022833 | 1.388412 | 0.038380 |

| | | | |
|---|---|---|---|
| H | 0.933397 | 1.761838 | 0.121186 |
| C | 4.042726 | 0.434374 | -0.022727 |
| H | 4.523919 | -1.666415 | -0.102134 |
| H | 3.269136 | 2.441535 | 0.070103 |
| H | 5.076846 | 0.754273 | -0.041392 |
| H | -1.020068 | 1.669895 | 0.882200 |
| H | -0.938654 | 1.647092 | -0.886025 |
| H | -3.370448 | 1.833651 | 0.744776 |
| H | -3.295145 | 1.704721 | -1.011385 |

**6C$_2$**

Imaginary frequency: None

Electronic energies: -1890.142395

Free energies: -1889.665824

Corrected Free energies: -1889.658213

| | | | |
|---|---|---|---|
| S | 2.174344 | -0.759500 | 0.675198 |
| F | 2.648907 | -2.583281 | -1.145295 |
| F | 4.418329 | -1.866405 | -0.134560 |
| F | 3.074376 | -3.222519 | 0.872845 |
| O | 0.825941 | -1.346170 | 0.781923 |
| O | 2.334795 | 0.243106 | -0.373223 |
| O | 2.794799 | -0.451835 | 1.959406 |
| C | 3.140078 | -2.192640 | 0.032982 |
| O | -0.084024 | 2.331008 | -1.308510 |
| O | 1.620783 | 3.360791 | -0.305039 |
| N | -1.554629 | 0.732302 | 0.187985 |
| N | -1.433891 | -1.937528 | -0.564298 |
| C | -2.788187 | -0.029471 | 0.253417 |
| C | -2.685555 | -1.149705 | -0.791337 |
| C | -1.639788 | -3.111244 | 0.352414 |
| C | -2.337714 | -4.286208 | -0.307912 |
| C | -0.708409 | -2.310381 | -1.825519 |
| C | -0.094218 | -1.088027 | -2.487140 |
| C | -4.053672 | 0.856481 | 0.062368 |
| C | -5.308353 | -0.026164 | 0.055890 |
| C | -3.981925 | 1.665028 | -1.238349 |
| C | -4.134346 | 1.826224 | 1.246562 |
| C | -0.800779 | 1.188330 | 1.233940 |
| C | -1.058263 | 0.543263 | 2.568261 |
| C | 0.191558 | 2.122755 | 1.069829 |
| C | 1.051226 | 2.607142 | 2.217234 |
| C | 0.524039 | 2.585093 | -0.273024 |
| C | 2.069894 | 3.770654 | -1.603817 |

| | | | |
|---|---|---|---|
| C | 3.294705 | 4.633434 | -1.401614 |
| H | -2.870444 | -0.488396 | 1.242028 |
| H | -3.530392 | -1.833011 | -0.743608 |
| H | -2.641255 | -0.729389 | -1.795097 |
| H | -2.211758 | -2.739723 | 1.204421 |
| H | -0.644605 | -3.382284 | 0.704976 |
| H | -2.510841 | -5.047239 | 0.453236 |
| H | -3.306270 | -4.012118 | -0.729048 |
| H | -1.725441 | -4.732683 | -1.091277 |
| H | -1.414416 | -2.826039 | -2.477083 |
| H | 0.072174 | -3.009333 | -1.521791 |
| H | 0.548294 | -1.424406 | -3.301695 |
| H | 0.516869 | -0.523507 | -1.779412 |
| H | -0.844921 | -0.420682 | -2.912897 |
| H | -6.199746 | 0.603061 | 0.110855 |
| H | -5.386138 | -0.622800 | -0.856041 |
| H | -5.320180 | -0.702640 | 0.916151 |
| H | -4.878747 | 2.282771 | -1.328517 |
| H | -3.118018 | 2.334920 | -1.247261 |
| H | -3.937503 | 1.025923 | -2.123900 |
| H | -4.997954 | 2.485153 | 1.129344 |
| H | -4.250415 | 1.284400 | 2.189800 |
| H | -3.239547 | 2.451396 | 1.309455 |
| H | -2.013911 | 0.864208 | 2.990281 |
| H | -1.078023 | -0.541886 | 2.448273 |
| H | -0.268536 | 0.774722 | 3.275314 |
| H | 1.442664 | 3.597860 | 1.994651 |
| H | 0.481325 | 2.686582 | 3.142459 |
| H | 1.905442 | 1.945027 | 2.394399 |
| H | 1.267942 | 4.315541 | -2.105531 |
| H | 2.293942 | 2.878421 | -2.192621 |
| H | 3.676470 | 4.967326 | -2.367663 |
| H | 3.049169 | 5.512756 | -0.803829 |
| H | 4.079870 | 4.072381 | -0.892681 |
| H | -0.761022 | -1.322890 | -0.067689 |
| H | -1.348556 | 1.192442 | -0.695465 |

**6C$_2$** radical cation

Imaginary frequency: None

Electronic energies: -1889.940495

Free energies: -1889.462564

Corrected Free energies: -1889.455474

| | | | |
|---|---|---|---|
| S | 1.774791 | -1.046636 | 0.962225 |

| | | | |
|---|---|---|---|
| F | 2.079765 | -2.901834 | -0.843172 |
| F | 3.885426 | -2.426784 | 0.245316 |
| F | 2.333320 | -3.594806 | 1.186783 |
| O | 0.341978 | -1.418157 | 0.966619 |
| O | 2.110945 | -0.046168 | -0.052465 |
| O | 2.327614 | -0.813920 | 2.288905 |
| C | 2.575274 | -2.591880 | 0.354041 |
| O | 0.309525 | 2.267030 | -1.443189 |
| O | 2.258423 | 2.931598 | -0.582948 |
| N | -1.345479 | 1.107398 | 0.232575 |
| N | -1.569572 | -1.637498 | -0.924355 |
| C | -2.587569 | 0.326295 | 0.253701 |
| C | -2.584696 | -0.541041 | -1.006569 |
| C | -2.102180 | -2.864707 | -0.225603 |
| C | -3.068212 | -3.676032 | -1.067575 |
| C | -0.948927 | -1.959177 | -2.256471 |
| C | 0.012529 | -0.869468 | -2.695377 |
| C | -3.836940 | 1.254757 | 0.347636 |
| C | -5.087535 | 0.375888 | 0.485958 |
| C | -3.951957 | 2.150889 | -0.890311 |
| C | -3.715490 | 2.127073 | 1.601976 |
| C | -0.521017 | 1.388667 | 1.212562 |
| C | -0.746683 | 0.930466 | 2.614608 |
| C | 0.655655 | 2.173127 | 0.926951 |
| C | 1.569773 | 2.585193 | 2.019528 |
| C | 1.039892 | 2.455189 | -0.487949 |
| C | 2.761329 | 3.148807 | -1.924963 |
| C | 4.179685 | 3.645078 | -1.790366 |
| H | -2.576963 | -0.312763 | 1.137272 |
| H | -3.557778 | -1.001040 | -1.157807 |
| H | -2.362360 | 0.063416 | -1.885438 |
| H | -2.571264 | -2.516619 | 0.695638 |
| H | -1.221745 | -3.446634 | 0.048633 |
| H | -3.432501 | -4.499908 | -0.453879 |
| H | -3.935487 | -3.096322 | -1.387240 |
| H | -2.583663 | -4.103419 | -1.945068 |
| H | -1.760832 | -2.107589 | -2.968871 |
| H | -0.424482 | -2.905814 | -2.122833 |
| H | 0.512601 | -1.199808 | -3.606120 |
| H | 0.775979 | -0.684413 | -1.936005 |
| H | -0.490584 | 0.071591 | -2.921769 |
| H | -5.942737 | 1.011340 | 0.724240 |
| H | -5.330769 | -0.159018 | -0.433659 |
| H | -4.974384 | -0.352040 | 1.294459 |

| | | | |
|---|---|---|---|
| H | -4.810226 | 2.815518 | -0.772830 |
| H | -3.066742 | 2.780521 | -1.020806 |
| H | -4.109154 | 1.573785 | -1.804661 |
| H | -4.607124 | 2.750808 | 1.688277 |
| H | -3.646966 | 1.517879 | 2.507256 |
| H | -2.853812 | 2.797037 | 1.556188 |
| H | -1.070342 | 1.782980 | 3.218888 |
| H | -1.492254 | 0.146213 | 2.686861 |
| H | 0.191375 | 0.557085 | 3.027870 |
| H | 2.158328 | 3.448642 | 1.720241 |
| H | 1.029900 | 2.805361 | 2.939481 |
| H | 2.267514 | 1.760923 | 2.227418 |
| H | 2.109902 | 3.870948 | -2.418685 |
| H | 2.700846 | 2.198934 | -2.458773 |
| H | 4.599140 | 3.813970 | -2.782832 |
| H | 4.208035 | 4.583876 | -1.236296 |
| H | 4.795061 | 2.908223 | -1.273373 |
| H | -0.785739 | -1.331304 | -0.310258 |
| H | -1.064147 | 1.507520 | -0.675043 |

**1'$C_2$**

Imaginary frequency: None

Electronic energies: -849.483071

Free energies: -849.093508

Corrected Free energies: -849.088869

| | | | |
|---|---|---|---|
| C | 1.559602 | -2.248915 | 0.065248 |
| C | 1.006236 | -2.596926 | -1.322587 |
| H | 0.010981 | -2.171537 | -1.480797 |
| H | 1.665565 | -2.252509 | -2.122789 |
| H | 0.913306 | -3.682490 | -1.414986 |
| C | 2.912429 | -2.944360 | 0.260884 |
| H | 3.601528 | -2.733080 | -0.559462 |
| H | 3.384140 | -2.630281 | 1.197045 |
| H | 2.768783 | -4.027065 | 0.300909 |
| C | 0.581655 | -2.758461 | 1.131872 |
| H | -0.402290 | -2.294751 | 1.021930 |
| H | 0.457612 | -3.840830 | 1.042189 |
| H | 0.954514 | -2.543201 | 2.138196 |
| C | 1.731908 | -0.716996 | 0.260902 |
| H | 2.074777 | -0.568362 | 1.286650 |
| C | 2.766371 | -0.055323 | -0.650442 |
| H | 2.478660 | -0.185219 | -1.706888 |
| H | 3.737513 | -0.537762 | -0.513682 |

| | | | |
|---|---|---|---|
| N | 0.450575 | -0.031665 | 0.099547 |
| N | 2.909252 | 1.350299 | -0.288139 |
| C | 3.880581 | 2.048698 | -1.127050 |
| H | 4.858147 | 1.581861 | -0.969953 |
| H | 3.646780 | 1.941644 | -2.198449 |
| C | 3.947014 | 3.522585 | -0.757163 |
| H | 4.690427 | 4.043659 | -1.362581 |
| H | 2.979900 | 4.005564 | -0.920729 |
| H | 4.211251 | 3.637582 | 0.295717 |
| H | -0.079165 | -0.270911 | -0.733043 |
| C | -0.302209 | 0.506546 | 1.088819 |
| C | -1.663800 | 0.718808 | 0.980291 |
| C | 0.429380 | 0.909245 | 2.342841 |
| H | -0.105513 | 1.693365 | 2.871836 |
| H | 0.531292 | 0.054810 | 3.019115 |
| H | 1.427044 | 1.271679 | 2.094233 |
| C | -2.438551 | 1.372739 | 2.105775 |
| H | -3.505604 | 1.318360 | 1.909009 |
| H | -2.255950 | 0.880314 | 3.063873 |
| H | -2.180799 | 2.429849 | 2.225033 |
| C | -2.364047 | 0.278324 | -0.211135 |
| O | -1.861008 | -0.246272 | -1.202879 |
| O | -3.697308 | 0.485637 | -0.166416 |
| C | -4.446449 | 0.053728 | -1.311001 |
| H | -4.060451 | 0.556249 | -2.200186 |
| H | -4.305243 | -1.020934 | -1.444480 |
| C | -5.895388 | 0.401014 | -1.053552 |
| H | -6.260004 | -0.110151 | -0.161292 |
| H | -6.012485 | 1.476662 | -0.912809 |
| H | -6.506552 | 0.094049 | -1.903684 |
| H | 2.001180 | 1.793834 | -0.407638 |

**1'$C_2$** radical cation

Imaginary frequency: None

Electronic energies: -849.282571

Free energies: -848.894543

Corrected Free energies: -848.889717

| | | | |
|---|---|---|---|
| C | 2.128230 | -2.109998 | -0.082782 |
| C | 1.430501 | -2.563193 | -1.372455 |
| H | 0.339818 | -2.541296 | -1.288779 |
| H | 1.726398 | -1.964645 | -2.236499 |
| H | 1.707484 | -3.599496 | -1.578843 |
| C | 3.639042 | -2.334705 | -0.215746 |

| | | | |
|---|---|---|---|
| H | 4.037242 | -1.885802 | -1.127898 |
| H | 4.177918 | -1.921044 | 0.641543 |
| H | 3.841714 | -3.406986 | -0.256751 |
| C | 1.600147 | -2.936250 | 1.096363 |
| H | 0.525851 | -2.793064 | 1.240693 |
| H | 1.772435 | -3.998818 | 0.911565 |
| H | 2.112181 | -2.664295 | 2.023525 |
| C | 1.885467 | -0.608257 | 0.227559 |
| H | 2.289564 | -0.402155 | 1.218781 |
| C | 2.523747 | 0.385159 | -0.754997 |
| H | 2.255309 | 0.135372 | -1.790853 |
| H | 3.605915 | 0.274571 | -0.661723 |
| N | 0.440435 | -0.358480 | 0.275192 |
| N | 2.180949 | 1.754533 | -0.391604 |
| C | 3.082564 | 2.737258 | -1.000149 |
| H | 4.081268 | 2.571990 | -0.585785 |
| H | 3.157871 | 2.599627 | -2.089138 |
| C | 2.617286 | 4.150029 | -0.686767 |
| H | 3.306664 | 4.884322 | -1.105996 |
| H | 1.627637 | 4.335227 | -1.112507 |
| H | 2.560372 | 4.301730 | 0.392761 |
| H | -0.117026 | -0.714566 | -0.511261 |
| C | -0.237958 | 0.260189 | 1.206562 |
| C | -1.675883 | 0.335535 | 1.104705 |
| C | 0.471758 | 0.862885 | 2.377486 |
| H | -0.149457 | 1.603525 | 2.871304 |
| H | 0.718479 | 0.078934 | 3.100307 |
| H | 1.387312 | 1.341191 | 2.034144 |
| C | -2.476838 | 0.907363 | 2.217558 |
| H | -3.519865 | 0.619473 | 2.129902 |
| H | -2.088994 | 0.588999 | 3.186101 |
| H | -2.427136 | 2.003791 | 2.187111 |
| C | -2.370370 | -0.134154 | -0.130292 |
| O | -1.820326 | -0.716967 | -1.044891 |
| O | -3.653301 | 0.158978 | -0.121688 |
| C | -4.418057 | -0.247795 | -1.285252 |
| H | -3.966383 | 0.215428 | -2.163416 |
| H | -4.334690 | -1.331213 | -1.380441 |
| C | -5.839392 | 0.205237 | -1.060366 |
| H | -6.256496 | -0.262890 | -0.168239 |
| H | -5.883446 | 1.288878 | -0.946799 |
| H | -6.448116 | -0.079180 | -1.919443 |
| H | 1.238050 | 1.958097 | -0.714408 |

**6'$C_2$**

Imaginary frequency: None

Electronic energies: -1811.542202

Free energies: -1811.118250

Corrected Free energies: -1811.111462

| | | | |
|---|---|---|---|
| C | -0.227560 | 3.714142 | 0.325608 |
| C | -0.271801 | 4.303729 | -1.087455 |
| H | -1.144359 | 3.939755 | -1.635637 |
| H | -0.331917 | 5.393482 | -1.034385 |
| H | 0.629996 | 4.043401 | -1.649874 |
| C | -1.462629 | 4.188158 | 1.099001 |
| H | -1.496568 | 3.791344 | 2.116732 |
| H | -1.447108 | 5.278075 | 1.175193 |
| H | -2.382587 | 3.903800 | 0.582966 |
| C | 1.047713 | 4.196079 | 1.028642 |
| H | 1.939775 | 3.766801 | 0.562110 |
| H | 1.118319 | 5.284052 | 0.958443 |
| H | 1.053783 | 3.934117 | 2.089681 |
| C | -0.195100 | 2.170297 | 0.207398 |
| H | 0.618018 | 1.903879 | -0.473287 |
| C | 0.117743 | 1.483207 | 1.546121 |
| H | -0.529550 | 1.829708 | 2.353836 |
| H | 1.159756 | 1.641112 | 1.815523 |
| N | -1.440559 | 1.624019 | -0.334699 |
| N | -0.086216 | 0.010630 | 1.428923 |
| C | 0.548311 | -0.782971 | 2.521955 |
| H | 1.620560 | -0.600078 | 2.447544 |
| H | 0.183008 | -0.384827 | 3.468877 |
| C | 0.211881 | -2.252564 | 2.350368 |
| H | 0.707956 | -2.831601 | 3.129220 |
| H | -0.864347 | -2.419305 | 2.430460 |
| H | 0.557756 | -2.613381 | 1.380117 |
| H | -2.160746 | 1.489745 | 0.365191 |
| C | -1.480424 | 0.699433 | -1.347638 |
| C | -2.344999 | -0.367687 | -1.370954 |
| C | -0.577916 | 0.945484 | -2.526703 |
| H | 0.182499 | 0.163833 | -2.591711 |
| H | -1.166107 | 0.918001 | -3.445954 |
| H | -0.090089 | 1.915224 | -2.467004 |
| C | -2.470338 | -1.212429 | -2.618401 |
| H | -1.487679 | -1.520591 | -2.982385 |
| H | -3.047643 | -2.110620 | -2.417076 |
| H | -2.967103 | -0.670621 | -3.429328 |

| | | | |
|---|---|---|---|
| C | -3.107339 | -0.725605 | -0.182719 |
| O | -2.950925 | -0.256116 | 0.948598 |
| O | -4.016173 | -1.680773 | -0.392240 |
| C | -4.751692 | -2.140354 | 0.757282 |
| H | -4.045593 | -2.547777 | 1.483285 |
| H | -5.256880 | -1.288205 | 1.214381 |
| C | -5.728469 | -3.185216 | 0.270282 |
| H | -5.200167 | -4.020120 | -0.192209 |
| H | -6.309145 | -3.565086 | 1.112024 |
| H | -6.416156 | -2.756866 | -0.460230 |
| H | -1.100605 | -0.185703 | 1.390565 |
| S | 2.643920 | -0.472243 | -0.691605 |
| F | 3.594770 | -2.914192 | -0.803932 |
| F | 4.923763 | -1.485731 | 0.119637 |
| F | 3.192825 | -2.202262 | 1.194766 |
| O | 3.240286 | -0.188600 | -1.988016 |
| O | 2.758410 | 0.577322 | 0.324137 |
| O | 1.289984 | -1.063192 | -0.744120 |
| C | 3.654390 | -1.854316 | -0.006842 |
| H | 0.312134 | -0.333993 | 0.532260 |

**6'$C_2$** radical cation

Imaginary frequency: None

Electronic energies: -1811.330757

Free energies: -1810.910499

Corrected Free energies: -1810.902143

| | | | |
|---|---|---|---|
| C | -0.266672 | 3.649043 | 0.208282 |
| C | -0.413717 | 4.047557 | -1.264430 |
| H | -1.275534 | 3.563649 | -1.732537 |
| H | -0.567596 | 5.126176 | -1.334201 |
| H | 0.485139 | 3.799830 | -1.835274 |
| C | -1.536067 | 4.049419 | 0.967105 |
| H | -1.491635 | 3.796884 | 2.028594 |
| H | -1.661811 | 5.131874 | 0.897635 |
| H | -2.428726 | 3.589919 | 0.534841 |
| C | 0.953885 | 4.360678 | 0.804243 |
| H | 1.880022 | 4.021492 | 0.331231 |
| H | 0.860661 | 5.435003 | 0.634418 |
| H | 1.034512 | 4.203644 | 1.882178 |
| C | -0.010864 | 2.120433 | 0.276123 |
| H | 0.826126 | 1.880425 | -0.376660 |
| C | 0.351828 | 1.624070 | 1.687355 |
| H | -0.269090 | 2.072378 | 2.462333 |

| | | | |
|---|---|---|---|
| H | 1.396898 | 1.863190 | 1.874313 |
| N | -1.173201 | 1.346762 | -0.175467 |
| N | 0.216203 | 0.139381 | 1.810607 |
| C | 1.078506 | -0.462596 | 2.879637 |
| H | 2.106351 | -0.281587 | 2.564251 |
| H | 0.882254 | 0.082393 | 3.802597 |
| C | 0.772677 | -1.942168 | 3.008913 |
| H | 1.456032 | -2.386487 | 3.732153 |
| H | -0.248612 | -2.104266 | 3.357783 |
| H | 0.908673 | -2.451276 | 2.053317 |
| H | -1.905663 | 1.208713 | 0.523953 |
| C | -1.334647 | 0.661738 | -1.280585 |
| C | -2.433775 | -0.272459 | -1.358747 |
| C | -0.442166 | 0.824700 | -2.462513 |
| H | -0.155397 | -0.154065 | -2.845747 |
| H | -1.002310 | 1.353704 | -3.240120 |
| H | 0.454136 | 1.395764 | -2.244506 |
| C | -2.821360 | -0.895772 | -2.645541 |
| H | -2.321743 | -1.870152 | -2.739274 |
| H | -3.892572 | -1.091055 | -2.660099 |
| H | -2.543386 | -0.287258 | -3.502200 |
| C | -3.089271 | -0.748576 | -0.102629 |
| O | -2.802548 | -0.350482 | 1.013524 |
| O | -4.000176 | -1.660787 | -0.338164 |
| C | -4.690301 | -2.205627 | 0.819225 |
| H | -3.939777 | -2.634842 | 1.483933 |
| H | -5.181937 | -1.378804 | 1.332863 |
| C | -5.667423 | -3.234137 | 0.307461 |
| H | -5.144571 | -4.031826 | -0.220998 |
| H | -6.203277 | -3.669940 | 1.151395 |
| H | -6.392577 | -2.775945 | -0.365666 |
| H | -0.762506 | -0.116666 | 1.984395 |
| S | 2.428425 | -0.492380 | -0.771903 |
| F | 3.200222 | -2.982483 | -1.049073 |
| F | 4.752273 | -1.630246 | -0.400517 |
| F | 3.219272 | -2.257820 | 0.985660 |
| O | 2.768475 | -0.240013 | -2.161592 |
| O | 2.791255 | 0.545994 | 0.197003 |
| O | 1.044808 | -0.983186 | -0.552441 |
| C | 3.467092 | -1.935064 | -0.282094 |
| H | 0.475346 | -0.320495 | 0.907471 |

## Calculated Cartesian coordinates for propionic aldehyde derived enamines

**1E-*E***

Imaginary frequency: None

Electronic energies: -621.589624

Free energies: -621.239132

Corrected Free energies: -621.235742

| | | | |
|---|---|---|---|
| C | -2.560173 | -0.343111 | 0.091322 |
| C | -2.802036 | -1.686020 | 0.795633 |
| H | -2.407325 | -1.666685 | 1.816264 |
| H | -3.875882 | -1.882141 | 0.854991 |
| H | -2.345444 | -2.524827 | 0.267780 |
| C | -3.404068 | 0.721575 | 0.802223 |
| H | -3.098856 | 0.818505 | 1.849009 |
| H | -3.293782 | 1.695934 | 0.326102 |
| H | -4.460017 | 0.438111 | 0.781606 |
| C | -3.007059 | -0.449461 | -1.372085 |
| H | -2.883248 | 0.499780 | -1.901433 |
| H | -2.450861 | -1.221469 | -1.910405 |
| H | -4.067763 | -0.711336 | -1.418708 |
| C | -1.062282 | 0.041916 | 0.195691 |
| H | -0.819145 | 0.059637 | 1.264597 |
| C | -0.105531 | -0.945698 | -0.499088 |
| H | -0.120151 | -0.727908 | -1.572022 |
| H | -0.448844 | -1.984322 | -0.383851 |
| N | -0.836289 | 1.403957 | -0.285420 |
| N | 1.259690 | -0.782168 | -0.005572 |
| C | 2.273902 | -0.962099 | -1.043038 |
| H | 2.019989 | -0.277286 | -1.857357 |
| H | 3.235111 | -0.621492 | -0.649354 |
| C | 1.481013 | -1.588851 | 1.192082 |
| H | 0.672507 | -1.361704 | 1.893065 |
| H | 1.400843 | -2.667646 | 0.973062 |
| C | 2.814214 | -1.298112 | 1.868530 |
| H | 3.659158 | -1.654322 | 1.275695 |
| H | 2.932323 | -0.222743 | 2.022814 |
| H | 2.858139 | -1.795382 | 2.839019 |
| C | 2.418002 | -2.384308 | -1.592745 |
| H | 1.463022 | -2.758265 | -1.971603 |
| H | 3.136067 | -2.399522 | -2.415189 |
| H | 2.774317 | -3.076777 | -0.826252 |
| H | -0.976979 | 1.498973 | -1.285030 |

| | | | |
|---|---|---|---|
| C | 0.267467 | 2.112524 | 0.175236 |
| C | 0.942295 | 3.058426 | -0.487633 |
| C | 2.055278 | 3.860242 | 0.125742 |
| H | 1.824355 | 4.930129 | 0.151394 |
| H | 2.989708 | 3.752082 | -0.433667 |
| H | 0.676087 | 3.273030 | -1.520862 |
| H | 0.533353 | 1.875447 | 1.203359 |
| H | 2.243379 | 3.537531 | 1.152704 |

**1E-*Z***

Imaginary frequency: None

Electronic energies: -621.590171

Free energies: -621.240357

Corrected Free energies: -621.236540

| | | | |
|---|---|---|---|
| C | 2.224277 | -1.105388 | 0.025787 |
| C | 2.041256 | -2.599660 | -0.276282 |
| H | 1.645028 | -2.748492 | -1.285737 |
| H | 3.007141 | -3.108346 | -0.216362 |
| H | 1.369668 | -3.089962 | 0.430409 |
| C | 3.341161 | -0.570898 | -0.878299 |
| H | 3.070364 | -0.683699 | -1.932879 |
| H | 3.529931 | 0.485732 | -0.687673 |
| H | 4.265018 | -1.128951 | -0.703451 |
| C | 2.633747 | -0.930396 | 1.493426 |
| H | 2.802820 | 0.121532 | 1.741952 |
| H | 1.878605 | -1.330439 | 2.175174 |
| H | 3.569027 | -1.463695 | 1.684602 |
| C | 0.911665 | -0.342701 | -0.287481 |
| H | 0.677891 | -0.543681 | -1.339636 |
| C | -0.293707 | -0.779753 | 0.565916 |
| H | -0.184199 | -0.327128 | 1.556544 |
| H | -0.303649 | -1.869167 | 0.715369 |
| N | 1.104734 | 1.101674 | -0.188927 |
| N | -1.542950 | -0.315923 | -0.030306 |
| C | -2.526177 | 0.133003 | 0.953856 |
| H | -2.032972 | 0.886928 | 1.574356 |
| H | -3.330338 | 0.652736 | 0.426396 |
| C | -2.054633 | -1.287605 | -0.993097 |
| H | -1.238927 | -1.519696 | -1.684291 |
| H | -2.321655 | -2.240732 | -0.504610 |
| C | -3.242491 | -0.767251 | -1.791697 |
| H | -4.139010 | -0.674615 | -1.175218 |
| H | -3.012631 | 0.214076 | -2.213902 |

| | | | |
|---|---|---|---|
| H | -3.472583 | -1.452267 | -2.609486 |
| C | -3.120049 | -0.961874 | 1.844879 |
| H | -2.334577 | -1.508469 | 2.373889 |
| H | -3.786730 | -0.522996 | 2.590061 |
| H | -3.699954 | -1.680376 | 1.260891 |
| H | 1.275782 | 1.420008 | 0.757650 |
| C | 0.311385 | 1.961621 | -0.932113 |
| C | 0.035590 | 3.233027 | -0.610819 |
| C | 0.497135 | 3.872124 | 0.672711 |
| H | 0.049368 | 4.856913 | 0.808042 |
| H | 1.585656 | 4.000915 | 0.704255 |
| H | -0.532507 | 3.824779 | -1.317043 |
| H | -0.048296 | 1.534305 | -1.862905 |
| H | 0.224280 | 3.269041 | 1.547512 |

**1E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -621.408289

Free energies: -621.057200

Corrected Free energies: -621.054179

| | | | |
|---|---|---|---|
| C | -2.643726 | -0.223254 | 0.100321 |
| C | -3.065563 | -1.472911 | 0.884352 |
| H | -2.751618 | -1.406206 | 1.929804 |
| H | -4.153981 | -1.560794 | 0.864322 |
| H | -2.653968 | -2.388137 | 0.455826 |
| C | -3.385821 | 0.989911 | 0.676732 |
| H | -3.121506 | 1.145660 | 1.726422 |
| H | -3.155650 | 1.906361 | 0.127742 |
| H | -4.463972 | 0.826343 | 0.617622 |
| C | -3.015100 | -0.402509 | -1.376848 |
| H | -2.739629 | 0.460208 | -1.991257 |
| H | -2.554364 | -1.293668 | -1.807578 |
| H | -4.098276 | -0.516443 | -1.461256 |
| C | -1.127036 | -0.009560 | 0.296472 |
| H | -0.929509 | 0.061243 | 1.370503 |
| C | -0.203618 | -1.110489 | -0.297863 |
| H | -0.342191 | -1.132137 | -1.380964 |
| H | -0.532291 | -2.079160 | 0.098152 |
| N | -0.678541 | 1.251716 | -0.280348 |
| N | 1.182588 | -0.829603 | 0.010323 |
| C | 2.100363 | -1.037786 | -1.111851 |
| H | 1.686199 | -0.497797 | -1.967753 |
| H | 3.048976 | -0.551543 | -0.873412 |

| | | | |
|---|---|---|---|
| C | 1.605735 | -1.423312 | 1.279929 |
| H | 0.872782 | -1.129942 | 2.037931 |
| H | 1.578506 | -2.522867 | 1.233376 |
| C | 2.986795 | -0.955202 | 1.716847 |
| H | 3.774034 | -1.364082 | 1.080768 |
| H | 3.050952 | 0.135391 | 1.683545 |
| H | 3.182053 | -1.282657 | 2.738824 |
| C | 2.341153 | -2.501165 | -1.484217 |
| H | 1.398624 | -3.011666 | -1.699135 |
| H | 2.971396 | -2.563594 | -2.373317 |
| H | 2.844771 | -3.039311 | -0.677892 |
| H | -1.059773 | 1.522545 | -1.184047 |
| C | 0.404391 | 1.865052 | 0.154000 |
| C | 1.025697 | 2.902921 | -0.542164 |
| C | 2.237731 | 3.584973 | -0.042272 |
| H | 2.044591 | 4.657389 | 0.063278 |
| H | 3.044442 | 3.490304 | -0.776210 |
| H | 0.603906 | 3.215849 | -1.492078 |
| H | 0.789313 | 1.540460 | 1.113024 |
| H | 2.571849 | 3.183453 | 0.913304 |

**1E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -621.406735

Free energies: -621.056537

Corrected Free energies: -621.053198

| | | | |
|---|---|---|---|
| C | 2.449862 | -0.744342 | -0.022644 |
| C | 2.618248 | -2.237986 | -0.329217 |
| H | 2.311082 | -2.467180 | -1.353660 |
| H | 3.670189 | -2.511858 | -0.223027 |
| H | 2.043180 | -2.864843 | 0.354609 |
| C | 3.420668 | 0.053135 | -0.903514 |
| H | 3.211521 | -0.114921 | -1.963502 |
| H | 3.356207 | 1.126426 | -0.708147 |
| H | 4.446817 | -0.263398 | -0.704066 |
| C | 2.774225 | -0.493267 | 1.455729 |
| H | 2.700027 | 0.562176 | 1.735200 |
| H | 2.132981 | -1.074666 | 2.120896 |
| H | 3.806524 | -0.794175 | 1.648079 |
| C | 1.008643 | -0.326694 | -0.384883 |
| H | 0.856481 | -0.512191 | -1.452907 |
| C | -0.129020 | -1.052342 | 0.396459 |
| H | 0.013339 | -0.874227 | 1.464441 |

| | | | |
|---|---|---|---|
| H | -0.020022 | -2.128534 | 0.220510 |
| N | 0.791880 | 1.098255 | -0.183472 |
| N | -1.425139 | -0.561556 | -0.016353 |
| C | -2.327497 | -0.234018 | 1.089192 |
| H | -1.771221 | 0.410870 | 1.775877 |
| H | -3.145991 | 0.372273 | 0.694913 |
| C | -2.012281 | -1.344448 | -1.104127 |
| H | -1.245870 | -1.447607 | -1.878622 |
| H | -2.257627 | -2.365361 | -0.773465 |
| C | -3.243945 | -0.683588 | -1.707042 |
| H | -4.093767 | -0.705063 | -1.022478 |
| H | -3.034782 | 0.358395 | -1.961994 |
| H | -3.536973 | -1.210612 | -2.615966 |
| C | -2.883039 | -1.443215 | 1.841766 |
| H | -2.074187 | -2.074389 | 2.219100 |
| H | -3.482943 | -1.115537 | 2.692752 |
| H | -3.520136 | -2.054113 | 1.198287 |
| H | 1.177679 | 1.516124 | 0.659382 |
| C | -0.150754 | 1.749121 | -0.831642 |
| C | -0.609097 | 3.017234 | -0.447745 |
| H | -0.545194 | 1.272283 | -1.719112 |
| C | -0.120154 | 3.737703 | 0.754256 |
| H | -0.371611 | 3.180642 | 1.664687 |
| H | 0.969148 | 3.850620 | 0.734439 |
| H | -0.566113 | 4.726018 | 0.826522 |
| H | -1.371076 | 3.462199 | -1.073493 |

**2E-*E***

Imaginary frequency: None

Electronic energies: -407.849942

Free energies: -407.638506

Corrected Free energies: -407.636974

| | | | |
|---|---|---|---|
| N | 0.911285 | -0.915767 | 0.171779 |
| C | 2.061872 | -0.269052 | -0.280245 |
| C | 3.207681 | -0.115379 | 0.389041 |
| C | 4.445712 | 0.487351 | -0.210518 |
| H | 5.273532 | -0.228027 | -0.235944 |
| H | 4.790698 | 1.351011 | 0.365587 |
| H | 3.265614 | -0.461977 | 1.419014 |
| H | 0.930731 | -1.093270 | 1.171162 |
| C | -0.377331 | -0.370765 | -0.257490 |
| C | -1.492599 | -1.347847 | 0.107397 |
| C | -0.667965 | 1.021106 | 0.317083 |

| | | | |
|---|---|---|---|
| H | -0.334533 | -0.290220 | -1.352001 |
| C | -2.860451 | -0.829960 | -0.342584 |
| H | -1.495367 | -1.481087 | 1.197463 |
| H | -1.277197 | -2.322659 | -0.337407 |
| C | -2.032406 | 1.542328 | -0.139664 |
| H | -0.648941 | 0.949571 | 1.412763 |
| H | 0.130353 | 1.710197 | 0.025251 |
| C | -3.145220 | 0.560055 | 0.231681 |
| H | -3.642108 | -1.533172 | -0.044496 |
| H | -2.880865 | -0.776395 | -1.437681 |
| H | -2.225780 | 2.524523 | 0.299223 |
| H | -2.020222 | 1.676897 | -1.228026 |
| H | -4.110834 | 0.926780 | -0.126211 |
| H | -3.212886 | 0.490784 | 1.324156 |
| H | 1.982964 | 0.081679 | -1.308817 |
| H | 4.260093 | 0.818710 | -1.234707 |

**2E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -407.664197

Free energies: -407.451271

Corrected Free energies: -407.450217

| | | | |
|---|---|---|---|
| N | 0.966260 | -0.212062 | 0.410238 |
| C | 2.091541 | -0.003160 | -0.235778 |
| C | 3.343405 | -0.096036 | 0.372609 |
| C | 4.607742 | 0.138472 | -0.353176 |
| H | 5.241338 | -0.751924 | -0.287096 |
| H | 5.165400 | 0.946304 | 0.131375 |
| H | 3.384340 | -0.349870 | 1.427308 |
| H | 1.012886 | -0.453387 | 1.399473 |
| C | -0.373658 | -0.079031 | -0.167930 |
| C | -1.211959 | -1.309519 | 0.184714 |
| C | -1.025959 | 1.213767 | 0.337632 |
| H | -0.237638 | -0.020257 | -1.251442 |
| C | -2.624611 | -1.162766 | -0.385965 |
| H | -1.265092 | -1.399439 | 1.276399 |
| H | -0.725846 | -2.207918 | -0.201302 |
| C | -2.438366 | 1.345063 | -0.236449 |
| H | -1.071926 | 1.181021 | 1.431939 |
| H | -0.406197 | 2.067844 | 0.055324 |
| C | -3.291349 | 0.122566 | 0.107034 |
| H | -3.217437 | -2.036028 | -0.106618 |
| H | -2.570721 | -1.148646 | -1.480296 |

| | | | |
|---|---|---|---|
| H | -2.898562 | 2.257162 | 0.148817 |
| H | -2.376119 | 1.451896 | -1.325255 |
| H | -4.286005 | 0.222938 | -0.332835 |
| H | -3.423021 | 0.067655 | 1.193814 |
| H | 2.006045 | 0.252556 | -1.287333 |
| H | 4.444018 | 0.388394 | -1.400084 |

**2E-*Z***

Imaginary frequency: None

Electronic energies: -407.850347

Free energies: -407.637791

Corrected Free energies: -407.636626

| | | | |
|---|---|---|---|
| N | 1.086965 | -0.644268 | -0.214763 |
| C | 2.068379 | 0.100327 | -0.861166 |
| C | 3.302362 | 0.350455 | -0.407432 |
| H | 1.289331 | -0.824167 | 0.762887 |
| C | -0.308824 | -0.265286 | -0.431561 |
| C | -1.231818 | -1.362774 | 0.093912 |
| C | -0.665059 | 1.087889 | 0.195033 |
| H | -0.447853 | -0.189824 | -1.518251 |
| C | -2.703840 | -1.010066 | -0.132433 |
| H | -1.048857 | -1.487378 | 1.169538 |
| H | -0.977152 | -2.309150 | -0.389798 |
| C | -2.134929 | 1.443873 | -0.037087 |
| H | -0.466264 | 1.027180 | 1.273204 |
| H | -0.006797 | 1.861616 | -0.211696 |
| C | -3.054581 | 0.341756 | 0.493392 |
| H | -3.343003 | -1.796903 | 0.275655 |
| H | -2.900014 | -0.967650 | -1.210446 |
| H | -2.369766 | 2.399938 | 0.437613 |
| H | -2.309252 | 1.571043 | -1.112371 |
| H | -4.100331 | 0.590418 | 0.294564 |
| H | -2.941909 | 0.273496 | 1.582154 |
| H | 1.768247 | 0.446407 | -1.847099 |
| H | 3.984468 | 0.871662 | -1.067905 |
| C | 3.803103 | -0.081566 | 0.944402 |
| H | 4.088203 | -1.139472 | 0.962345 |
| H | 4.679979 | 0.495678 | 1.239789 |
| H | 3.043451 | 0.059332 | 1.720796 |

**2E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -407.662655

Free energies: -407.450790

Corrected Free energies: -407.449259

| | | | |
|---|---|---|---|
| N | -1.106386 | 0.012915 | -0.020628 |
| C | -2.095473 | -0.004264 | -0.880471 |
| C | -3.444070 | -0.007695 | -0.496651 |
| H | -1.324738 | 0.024774 | 0.974775 |
| C | 0.318921 | 0.005699 | -0.365877 |
| C | 0.986120 | 1.270973 | 0.180511 |
| C | 0.972247 | -1.263205 | 0.189698 |
| H | 0.371230 | 0.001204 | -1.457763 |
| C | 2.483795 | 1.253730 | -0.137117 |
| H | 0.841045 | 1.304981 | 1.266423 |
| H | 0.504568 | 2.152027 | -0.248712 |
| C | 2.469896 | -1.264626 | -0.127896 |
| H | 0.825879 | -1.288002 | 1.275717 |
| H | 0.480988 | -2.141701 | -0.233813 |
| C | 3.152215 | -0.007178 | 0.412669 |
| H | 2.948569 | 2.149573 | 0.279314 |
| H | 2.621965 | 1.295761 | -1.223256 |
| H | 2.924979 | -2.162528 | 0.294796 |
| H | 2.607336 | -1.315955 | -1.213739 |
| H | 4.213095 | -0.013971 | 0.153015 |
| H | 3.087829 | -0.002821 | 1.506796 |
| H | -1.824915 | -0.018561 | -1.930275 |
| H | -4.168922 | -0.036226 | -1.299254 |
| C | -3.898916 | 0.007575 | 0.914520 |
| H | -3.441565 | 0.831548 | 1.471482 |
| H | -4.979208 | 0.106655 | 0.974481 |
| H | -3.611842 | -0.923228 | 1.418089 |

**3E-*E***

Imaginary frequency: None

Electronic energies: -291.132197

Free energies: -290.983881

Corrected Free energies: -290.982997

| | | | |
|---|---|---|---|
| C | -1.465032 | 0.031052 | 0.341392 |
| H | -1.247080 | 0.083478 | 1.418057 |
| N | -0.281781 | -0.439689 | -0.393488 |
| C | 0.951827 | 0.130995 | -0.075409 |
| C | 2.136601 | -0.485606 | -0.100168 |
| C | 3.441633 | 0.208898 | 0.163159 |
| H | 4.101932 | 0.173478 | -0.708891 |

| | | | |
|---|---|---|---|
| H | 3.984051 | -0.257618 | 0.990755 |
| H | 2.172014 | -1.546466 | -0.341406 |
| H | -0.232997 | -1.451869 | -0.417800 |
| C | -2.591367 | -0.970747 | 0.123330 |
| H | -3.498041 | -0.644833 | 0.635182 |
| H | -2.806890 | -1.059871 | -0.944889 |
| H | -2.319004 | -1.957746 | 0.505394 |
| C | -1.875186 | 1.417984 | -0.145098 |
| H | -2.125300 | 1.375223 | -1.208247 |
| H | -2.749722 | 1.766974 | 0.408345 |
| H | -1.079253 | 2.152344 | -0.009020 |
| H | 0.902698 | 1.190271 | 0.167707 |
| H | 3.279205 | 1.259001 | 0.415993 |

**3E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -290.947568

Free energies: -290.798768

Corrected Free energies: -290.798121

| | | | |
|---|---|---|---|
| C | -1.514930 | 0.000044 | -0.350068 |
| H | -1.289234 | 0.000155 | -1.417494 |
| N | -0.212795 | -0.000077 | 0.335531 |
| C | 0.957552 | -0.000006 | -0.259811 |
| C | 2.164371 | -0.000093 | 0.441810 |
| C | 3.481865 | 0.000054 | -0.224281 |
| H | 4.056424 | -0.875183 | 0.095952 |
| H | 4.056356 | 0.875231 | 0.096243 |
| H | 2.128061 | -0.000266 | 1.526716 |
| H | -0.237602 | -0.000196 | 1.354440 |
| C | -2.273442 | 1.269155 | 0.026094 |
| H | -3.225325 | 1.282298 | -0.505789 |
| H | -2.479621 | 1.290546 | 1.098830 |
| H | -1.706408 | 2.159559 | -0.246027 |
| C | -2.273528 | -1.269105 | 0.025802 |
| H | -2.479721 | -1.290718 | 1.098530 |
| H | -3.225404 | -1.282071 | -0.506099 |
| H | -1.706542 | -2.159480 | -0.246507 |
| H | 0.948879 | 0.000122 | -1.345206 |
| H | 3.398375 | 0.000239 | -1.309585 |

**3E-*Z***

Imaginary frequency: None

Electronic energies: -291.132525
Free energies: -290.984284
Corrected Free energies: -290.983331

| | | | |
|---|---|---|---|
| C | -1.399796 | 0.016403 | -0.337371 |
| H | -1.393922 | -0.190079 | -1.417347 |
| N | -0.025157 | 0.168186 | 0.154358 |
| C | 0.924528 | -0.776651 | -0.223362 |
| C | 2.249093 | -0.591482 | -0.190954 |
| H | 0.310093 | 1.120968 | 0.081357 |
| C | -2.143107 | 1.323698 | -0.097815 |
| H | -3.176319 | 1.243485 | -0.438604 |
| H | -2.145674 | 1.559460 | 0.969882 |
| H | -1.669044 | 2.149536 | -0.634152 |
| C | -2.093370 | -1.139701 | 0.377710 |
| H | -2.143821 | -0.932495 | 1.449694 |
| H | -3.108324 | -1.265741 | -0.005416 |
| H | -1.562098 | -2.082576 | 0.235349 |
| H | 0.513159 | -1.734256 | -0.528249 |
| C | 2.882370 | 0.703949 | 0.241516 |
| H | 2.751025 | 1.496159 | -0.505200 |
| H | 2.442907 | 1.069986 | 1.175717 |
| H | 3.953726 | 0.586607 | 0.404030 |
| H | 2.886089 | -1.415652 | -0.485905 |

**3E-*Z*** radical cation
Imaginary frequency: None
Electronic energies: -290.946017
Free energies: -290.798542
Corrected Free energies: -290.797069

| | | | |
|---|---|---|---|
| C | -1.461112 | 0.001721 | 0.309085 |
| H | -1.534315 | 0.007796 | 1.397542 |
| N | -0.020417 | -0.001369 | 0.003065 |
| C | 0.942487 | 0.003551 | 0.890829 |
| C | 2.303275 | 0.002211 | 0.549793 |
| H | 0.226457 | -0.003417 | -0.985846 |
| C | -2.088399 | -1.269414 | -0.253702 |
| H | -3.151060 | -1.277684 | -0.008923 |
| H | -1.987424 | -1.298145 | -1.341111 |
| H | -1.622363 | -2.158129 | 0.171840 |
| C | -2.085152 | 1.268250 | -0.267649 |
| H | -1.981398 | 1.285985 | -1.355102 |
| H | -3.148350 | 1.280689 | -0.025519 |
| H | -1.618574 | 2.160344 | 0.150210 |

| | | | |
|---|---|---|---|
| H | 0.641375 | 0.011124 | 1.932402 |
| H | 3.001020 | 0.028824 | 1.376035 |
| C | 2.807590 | -0.009735 | -0.844157 |
| H | 3.881004 | -0.177342 | -0.866651 |
| H | 2.319988 | -0.783937 | -1.444131 |
| H | 2.604417 | 0.953971 | -1.327399 |

**4E-*Z***

Imaginary frequency: None

Electronic energies: -443.534480

Free energies: -443.364602

Corrected Free energies: -443.362611

| | | | |
|---|---|---|---|
| C | -2.983564 | -0.418724 | 0.816108 |
| C | -2.077641 | 0.561505 | 0.731572 |
| N | -1.567737 | 1.111356 | -0.440530 |
| C | -0.217266 | 1.640166 | -0.409901 |
| H | -0.162935 | 2.391750 | 0.384069 |
| H | -1.791814 | 0.598303 | -1.283148 |
| H | -1.698385 | 1.038373 | 1.631621 |
| C | 0.896855 | 0.625851 | -0.197721 |
| C | 2.175016 | 1.079134 | 0.136223 |
| C | 0.689196 | -0.743144 | -0.351320 |
| C | 3.225673 | 0.185732 | 0.305817 |
| H | 2.345711 | 2.143753 | 0.265344 |
| C | 1.740265 | -1.641902 | -0.180281 |
| H | -0.299052 | -1.115895 | -0.595830 |
| C | 3.010511 | -1.181715 | 0.146884 |
| H | 4.211115 | 0.554078 | 0.566212 |
| H | 1.562532 | -2.704236 | -0.301339 |
| H | 3.826151 | -1.882015 | 0.281554 |
| H | -0.040360 | 2.170928 | -1.349040 |
| C | -3.548654 | -1.148350 | -0.371860 |
| H | -4.364845 | -0.595560 | -0.849658 |
| H | -2.788764 | -1.324073 | -1.141483 |
| H | -3.943701 | -2.122063 | -0.079977 |
| H | -3.343838 | -0.684145 | 1.802266 |

**4E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -443.342988

Free energies: -443.172759

Corrected Free energies: -443.170981

| | | | |
|---|---|---|---|
| C | 3.546309 | 0.506367 | 0.149816 |
| C | 2.453109 | -0.100619 | 0.784844 |
| N | 1.445735 | -0.627212 | 0.131699 |
| C | 0.275228 | -1.255784 | 0.753792 |
| H | 0.427372 | -1.225498 | 1.832539 |
| H | 1.442526 | -0.589798 | -0.885696 |
| H | 2.410931 | -0.155551 | 1.866768 |
| C | -0.986100 | -0.532802 | 0.343703 |
| C | -1.899981 | -1.135607 | -0.516522 |
| C | -1.231567 | 0.754591 | 0.823564 |
| C | -3.057332 | -0.458095 | -0.891016 |
| H | -1.711317 | -2.136274 | -0.889586 |
| C | -2.384547 | 1.430957 | 0.447431 |
| H | -0.522532 | 1.224500 | 1.497587 |
| C | -3.299041 | 0.823968 | -0.410890 |
| H | -3.767719 | -0.932873 | -1.556756 |
| H | -2.572756 | 2.428248 | 0.825842 |
| H | -4.199773 | 1.350948 | -0.701646 |
| H | 0.250862 | -2.297906 | 0.431470 |
| C | 3.689066 | 0.619906 | -1.320948 |
| H | 3.821668 | -0.373343 | -1.766538 |
| H | 2.798384 | 1.063115 | -1.777233 |
| H | 4.551522 | 1.226816 | -1.582428 |
| H | 4.319821 | 0.890801 | 0.801140 |

**4E-*E***

Imaginary frequency: None

Electronic energies: -443.533955

Free energies: -443.363222

Corrected Free energies: -443.361641

| | | | |
|---|---|---|---|
| C | 3.018758 | -0.443601 | 0.205849 |
| C | 2.138155 | 0.478655 | -0.189755 |
| N | 1.407435 | 1.336068 | 0.633313 |
| C | 0.094274 | 1.750198 | 0.175738 |
| H | 0.209257 | 2.213326 | -0.809490 |
| H | 1.439490 | 1.087766 | 1.614196 |
| H | 1.969246 | 0.654488 | -1.251316 |
| C | -0.967528 | 0.664782 | 0.083662 |
| C | -2.146117 | 0.925302 | -0.619108 |
| C | -0.817153 | -0.572469 | 0.706912 |
| C | -3.156639 | -0.025411 | -0.692659 |
| H | -2.270420 | 1.884799 | -1.112353 |
| C | -1.828045 | -1.528985 | 0.633153 |

| | | | |
|---|---|---|---|
| H | 0.096548 | -0.799037 | 1.244169 |
| C | -3.000093 | -1.259158 | -0.064007 |
| H | -4.064709 | 0.193276 | -1.242469 |
| H | -1.695707 | -2.488168 | 1.120442 |
| H | -3.784550 | -2.004255 | -0.123137 |
| H | -0.262977 | 2.537693 | 0.844907 |
| C | 3.852489 | -1.256337 | -0.742142 |
| H | 3.693425 | -2.328805 | -0.596696 |
| H | 3.607585 | -1.017193 | -1.779417 |
| H | 4.921638 | -1.071815 | -0.599656 |
| H | 3.160532 | -0.612398 | 1.271760 |

**4E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -443.344479

Free energies: -443.174712

Corrected Free energies: -443.172922

| | | | |
|---|---|---|---|
| C | -3.383523 | -0.120872 | -0.626755 |
| C | -2.368308 | 0.229251 | 0.264577 |
| N | -1.269219 | 0.840893 | -0.116756 |
| C | -0.158905 | 1.205052 | 0.767605 |
| H | -0.461854 | 0.961471 | 1.785639 |
| H | -1.150167 | 1.056790 | -1.104567 |
| H | -2.455938 | 0.003756 | 1.322914 |
| C | 1.097035 | 0.467246 | 0.364882 |
| C | 2.151616 | 1.146137 | -0.239537 |
| C | 1.195684 | -0.906364 | 0.591428 |
| C | 3.303856 | 0.457846 | -0.609499 |
| H | 2.075258 | 2.213453 | -0.415844 |
| C | 2.344836 | -1.592673 | 0.221147 |
| H | 0.374769 | -1.436572 | 1.064168 |
| C | 3.400633 | -0.909932 | -0.379605 |
| H | 4.123328 | 0.990631 | -1.076385 |
| H | 2.420008 | -2.657611 | 0.403929 |
| H | 4.297691 | -1.445837 | -0.665446 |
| H | -0.017715 | 2.284284 | 0.692021 |
| C | -4.619689 | -0.810755 | -0.209033 |
| H | -4.711332 | -1.756918 | -0.752465 |
| H | -4.647468 | -1.004586 | 0.861630 |
| H | -5.489915 | -0.210851 | -0.493824 |
| H | -3.251551 | 0.126113 | -1.675739 |

**5E-*E***

Imaginary frequency: None

Electronic energies: -404.237928

Free energies: -404.096459

Corrected Free energies: -404.094389

| | | | |
|---|---|---|---|
| N | -0.747444 | -0.734182 | -0.044614 |
| C | -1.885193 | 0.054279 | 0.060546 |
| C | -3.135064 | -0.387625 | -0.098476 |
| C | -4.345499 | 0.480863 | 0.075492 |
| H | -4.988846 | 0.114617 | 0.880979 |
| H | -4.954851 | 0.501681 | -0.832643 |
| H | -3.297320 | -1.431814 | -0.356597 |
| H | -0.889688 | -1.729449 | -0.135476 |
| C | 0.567958 | -0.299913 | -0.026456 |
| C | 1.591275 | -1.260708 | 0.033512 |
| C | 0.925468 | 1.055804 | -0.071616 |
| C | 2.922668 | -0.877163 | 0.056985 |
| H | 1.326584 | -2.312434 | 0.066203 |
| C | 2.266082 | 1.424353 | -0.036965 |
| H | 0.169741 | 1.825835 | -0.150814 |
| C | 3.276051 | 0.470829 | 0.027703 |
| H | 3.691190 | -1.640188 | 0.104486 |
| H | 2.518083 | 2.478273 | -0.071292 |
| H | 4.316418 | 0.769678 | 0.050174 |
| H | -1.701724 | 1.091387 | 0.318386 |
| H | -4.059957 | 1.507374 | 0.314552 |

**5E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -404.043133

Free energies: -403.900428

Corrected Free energies: -403.899258

| | | | |
|---|---|---|---|
| N | -0.764521 | -0.641017 | -0.053886 |
| C | -1.853363 | 0.135561 | 0.015706 |
| C | -3.119790 | -0.397463 | -0.026659 |
| C | -4.345865 | 0.423745 | 0.054265 |
| H | -4.944105 | 0.106506 | 0.914399 |
| H | -4.965268 | 0.246998 | -0.830573 |
| H | -3.227621 | -1.474301 | -0.122195 |
| H | -0.923854 | -1.644638 | -0.123449 |
| C | 0.574466 | -0.251470 | -0.030364 |
| C | 1.536100 | -1.270549 | 0.011561 |
| C | 0.959227 | 1.096148 | -0.049027 |

| | | | |
|---|---|---|---|
| C | 2.879556 | -0.940006 | 0.045622 |
| H | 1.222089 | -2.308101 | 0.023836 |
| C | 2.306909 | 1.407207 | -0.014157 |
| H | 0.229906 | 1.892487 | -0.102738 |
| C | 3.268707 | 0.397552 | 0.034885 |
| H | 3.622733 | -1.725879 | 0.081918 |
| H | 2.611406 | 2.445788 | -0.030101 |
| H | 4.320030 | 0.654999 | 0.060875 |
| H | -1.701504 | 1.201995 | 0.116113 |
| H | -4.127847 | 1.486917 | 0.138128 |

**5E-*Z***

Imaginary frequency: None

Electronic energies: -404.238295

Free energies: -404.094860

Corrected Free energies: -404.093629

| | | | |
|---|---|---|---|
| N | -0.928442 | 0.300369 | -0.109897 |
| C | -1.850523 | -0.715752 | -0.329462 |
| C | -3.170566 | -0.594730 | -0.157210 |
| H | -1.273857 | 1.247891 | -0.090704 |
| C | 0.448273 | 0.142790 | -0.040640 |
| C | 1.269616 | 1.277778 | -0.130330 |
| C | 1.050914 | -1.111433 | 0.130604 |
| C | 2.648995 | 1.157268 | -0.063536 |
| H | 0.812391 | 2.253309 | -0.259153 |
| C | 2.436633 | -1.217447 | 0.181010 |
| H | 0.444802 | -2.000409 | 0.246807 |
| C | 3.248338 | -0.092413 | 0.084778 |
| H | 3.261240 | 2.049054 | -0.133579 |
| H | 2.882344 | -2.197028 | 0.311992 |
| H | 4.326055 | -0.184658 | 0.131120 |
| H | -1.427351 | -1.642691 | -0.698475 |
| C | -3.853009 | 0.640090 | 0.358344 |
| H | -4.152896 | 1.312695 | -0.452439 |
| H | -4.757274 | 0.380870 | 0.911082 |
| H | -3.204101 | 1.205595 | 1.032720 |
| H | -3.784279 | -1.444127 | -0.431435 |

**5E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -404.040948

Free energies: -403.898507

Corrected Free energies: -403.896767

| | | | |
|---|---|---|---|
| N | 0.934716 | 0.156782 | -0.008796 |
| C | 1.830040 | -0.832904 | -0.014922 |
| C | 3.189949 | -0.590911 | -0.006600 |
| H | 1.298456 | 1.107891 | -0.000100 |
| C | -0.459704 | 0.065187 | -0.004766 |
| C | -1.173455 | 1.270623 | -0.006488 |
| C | -1.129283 | -1.164887 | 0.003091 |
| C | -2.557356 | 1.244404 | -0.001256 |
| H | -0.638100 | 2.213117 | -0.012528 |
| C | -2.513018 | -1.171750 | 0.008057 |
| H | -0.591668 | -2.102658 | 0.006877 |
| C | -3.230189 | 0.025111 | 0.005955 |
| H | -3.110577 | 2.174413 | -0.002639 |
| H | -3.037896 | -2.118193 | 0.014709 |
| H | -4.312499 | 0.004607 | 0.010561 |
| H | 1.454146 | -1.845687 | -0.022211 |
| C | 3.814883 | 0.756056 | 0.011452 |
| H | 3.337902 | 1.444923 | -0.690677 |
| H | 3.728214 | 1.192947 | 1.013796 |
| H | 4.872179 | 0.692096 | -0.233042 |
| H | 3.825634 | -1.466499 | 0.009685 |

**6E-*E***

Imaginary frequency: None

Electronic energies: -1583.652712

Free energies: -1583.268813

Corrected Free energies: -1583.262517

| | | | |
|---|---|---|---|
| S | -2.032898 | 0.720258 | -0.079905 |
| F | -3.478359 | -1.360793 | -0.787139 |
| F | -4.557829 | 0.128571 | 0.342166 |
| F | -4.061917 | 0.492190 | -1.726965 |
| O | -1.140657 | 0.428365 | -1.205594 |
| O | -1.685838 | -0.024971 | 1.142797 |
| O | -2.378739 | 2.122157 | 0.118262 |
| C | -3.629618 | -0.050358 | -0.592951 |
| N | 1.689590 | 0.825438 | 0.695173 |
| H | 2.291318 | 0.861117 | 1.510678 |
| N | 0.499431 | -1.736610 | 0.603822 |
| H | 0.065679 | -0.802026 | 0.700789 |
| C | 2.123764 | -0.121273 | -0.325130 |
| H | 1.415362 | -0.012313 | -1.156118 |
| C | 1.946055 | -1.513466 | 0.287303 |

| | | | |
|---|---|---|---|
| H | 2.275101 | -2.311678 | -0.373571 |
| H | 2.510723 | -1.586437 | 1.216641 |
| C | -0.233947 | -2.426145 | -0.513862 |
| H | -1.292257 | -2.268946 | -0.310236 |
| H | 0.013755 | -1.878351 | -1.422754 |
| C | 0.086869 | -3.904823 | -0.632750 |
| H | -0.255380 | -4.468926 | 0.234923 |
| H | 1.151387 | -4.094037 | -0.777837 |
| H | -0.437114 | -4.291128 | -1.507310 |
| C | 0.263403 | -2.399446 | 1.929890 |
| H | -0.786591 | -2.694182 | 1.935604 |
| H | 0.882926 | -3.296139 | 1.962626 |
| C | 0.553308 | -1.455332 | 3.082511 |
| H | 0.293239 | -1.957047 | 4.014801 |
| H | -0.050787 | -0.551645 | 2.990840 |
| H | 1.606107 | -1.176651 | 3.138230 |
| C | 3.552850 | 0.091319 | -0.899041 |
| C | 3.767498 | -0.850651 | -2.091821 |
| H | 3.803216 | -1.901114 | -1.794817 |
| H | 4.719094 | -0.619695 | -2.576820 |
| H | 2.973629 | -0.728500 | -2.834796 |
| C | 4.626879 | -0.170240 | 0.162786 |
| H | 4.481972 | 0.458393 | 1.046322 |
| H | 5.612564 | 0.064900 | -0.246396 |
| H | 4.645011 | -1.216171 | 0.480137 |
| C | 3.678563 | 1.536314 | -1.394718 |
| H | 2.891679 | 1.774320 | -2.117255 |
| H | 4.644535 | 1.671797 | -1.887611 |
| H | 3.610650 | 2.250773 | -0.572558 |
| C | 1.154015 | 2.065371 | 0.331887 |
| C | 1.182724 | 3.174340 | 1.072530 |
| H | 0.632144 | 2.046678 | -0.621086 |
| C | 0.492403 | 4.445747 | 0.672061 |
| H | 0.017633 | 4.336008 | -0.305067 |
| H | 1.193698 | 5.283628 | 0.617835 |
| H | 1.714810 | 3.163921 | 2.021736 |
| H | -0.284661 | 4.725264 | 1.390129 |

**6E-*Z***

Imaginary frequency: None

Electronic energies: -1583.653028

Free energies: -1583.269485

Corrected Free energies: -1583.263264

| | | | |
|---|---|---|---|
| S | -2.060374 | 0.888308 | -0.201013 |
| F | -3.618039 | -1.193563 | -0.594359 |
| F | -4.603371 | 0.490607 | 0.327916 |
| F | -4.126740 | 0.537972 | -1.777003 |
| O | -1.200213 | 0.371739 | -1.270203 |
| O | -1.734075 | 0.329514 | 1.122149 |
| O | -2.326000 | 2.321062 | -0.227818 |
| C | -3.702036 | 0.137021 | -0.582847 |
| N | 1.757429 | 0.861487 | 0.419001 |
| H | 2.434296 | 0.949649 | 1.168244 |
| N | 0.345501 | -1.577030 | 0.817629 |
| H | -0.026481 | -0.614885 | 0.758505 |
| C | 1.997038 | -0.264906 | -0.473429 |
| H | 1.214868 | -0.212038 | -1.241275 |
| C | 1.773062 | -1.526508 | 0.363870 |
| H | 1.983918 | -2.439877 | -0.187108 |
| H | 2.409899 | -1.510107 | 1.248746 |
| C | -0.513766 | -2.410739 | -0.093230 |
| H | -1.541371 | -2.136539 | 0.141205 |
| H | -0.299310 | -2.069746 | -1.106239 |
| C | -0.295141 | -3.903944 | 0.067869 |
| H | -0.619520 | -4.259317 | 1.046018 |
| H | 0.745100 | -4.195570 | -0.085136 |
| H | -0.894315 | -4.414363 | -0.686421 |
| C | 0.174769 | -1.953312 | 2.261133 |
| H | -0.888210 | -2.157148 | 2.394395 |
| H | 0.734711 | -2.873682 | 2.430054 |
| C | 0.616637 | -0.831859 | 3.183464 |
| H | 0.407715 | -1.126776 | 4.212100 |
| H | 0.061375 | 0.080791 | 2.961972 |
| H | 1.684883 | -0.626690 | 3.106379 |
| C | 3.369790 | -0.273979 | -1.202367 |
| C | 3.366803 | -1.372427 | -2.274219 |
| H | 3.311964 | -2.375808 | -1.846238 |
| H | 4.288931 | -1.319970 | -2.858274 |
| H | 2.525744 | -1.245204 | -2.962178 |
| C | 4.522649 | -0.513347 | -0.221418 |
| H | 4.524101 | 0.224230 | 0.587187 |
| H | 5.477103 | -0.423316 | -0.745745 |
| H | 4.484014 | -1.512516 | 0.220526 |
| C | 3.571370 | 1.078760 | -1.894515 |
| H | 2.733943 | 1.309661 | -2.560004 |
| H | 4.484420 | 1.051613 | -2.494374 |
| H | 3.662420 | 1.891140 | -1.170514 |

| | | | |
|---|---|---|---|
| C | 1.269881 | 2.074607 | -0.065450 |
| C | 1.455013 | 3.257184 | 0.528627 |
| H | 0.665479 | 1.977063 | -0.960695 |
| C | 2.290549 | 3.432798 | 1.768130 |
| H | 3.277959 | 2.967681 | 1.656531 |
| H | 1.821125 | 2.980240 | 2.648926 |
| H | 0.963778 | 4.120293 | 0.097922 |
| H | 2.452870 | 4.487295 | 1.989581 |

**6E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1583.458135

Free energies: -1583.073102

Corrected Free energies: -1583.067284

| | | | |
|---|---|---|---|
| S | -1.975089 | 0.545309 | -0.041535 |
| F | -3.225802 | -1.542763 | -0.999339 |
| F | -4.431273 | -0.301242 | 0.292522 |
| F | -3.975824 | 0.351341 | -1.713668 |
| O | -1.033892 | 0.422914 | -1.160645 |
| O | -1.577736 | -0.281375 | 1.117870 |
| O | -2.393522 | 1.900581 | 0.288353 |
| C | -3.501256 | -0.288734 | -0.653141 |
| N | 1.542065 | 1.167412 | 0.670791 |
| H | 1.836153 | 1.121345 | 1.644587 |
| N | 0.670130 | -1.792059 | 0.588849 |
| H | -0.023889 | -1.048871 | 0.808768 |
| C | 2.058390 | 0.147032 | -0.251355 |
| H | 1.366454 | 0.142856 | -1.098042 |
| C | 2.038159 | -1.200295 | 0.471099 |
| H | 2.657325 | -1.925353 | -0.050243 |
| H | 2.442538 | -1.094618 | 1.477747 |
| C | 0.179646 | -2.407983 | -0.700130 |
| H | -0.885994 | -2.581139 | -0.544050 |
| H | 0.273752 | -1.644138 | -1.469994 |
| C | 0.896106 | -3.689084 | -1.082634 |
| H | 0.755754 | -4.477837 | -0.343816 |
| H | 1.964137 | -3.540719 | -1.248034 |
| H | 0.468624 | -4.036164 | -2.023710 |
| C | 0.574142 | -2.758788 | 1.741623 |
| H | -0.331144 | -3.340750 | 1.568811 |
| H | 1.434839 | -3.425396 | 1.680400 |
| C | 0.494539 | -2.038873 | 3.075701 |
| H | 0.338226 | -2.783213 | 3.856525 |

| | | | |
|---|---|---|---|
| H | -0.348561 | -1.346585 | 3.088000 |
| H | 1.408453 | -1.496756 | 3.320438 |
| C | 3.476437 | 0.516894 | -0.789108 |
| C | 3.841069 | -0.480531 | -1.898103 |
| H | 4.028217 | -1.486189 | -1.517961 |
| H | 4.759115 | -0.147514 | -2.386005 |
| H | 3.055775 | -0.533351 | -2.657488 |
| C | 4.524120 | 0.475909 | 0.327701 |
| H | 4.281928 | 1.167453 | 1.139598 |
| H | 5.492502 | 0.776843 | -0.077474 |
| H | 4.643014 | -0.526193 | 0.746724 |
| C | 3.430040 | 1.921405 | -1.401047 |
| H | 2.655450 | 1.996677 | -2.169961 |
| H | 4.390200 | 2.135426 | -1.873944 |
| H | 3.258860 | 2.695551 | -0.649929 |
| C | 0.797125 | 2.190844 | 0.301412 |
| C | 0.348267 | 3.160940 | 1.200755 |
| H | 0.516889 | 2.235670 | -0.745375 |
| C | -0.496952 | 4.296694 | 0.791684 |
| H | -0.682636 | 4.306878 | -0.280326 |
| H | -0.029730 | 5.236202 | 1.102234 |
| H | 0.623808 | 3.061753 | 2.246350 |
| H | -1.455713 | 4.230141 | 1.316243 |

**6E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1583.458192

Free energies: -1583.072720

Corrected Free energies: -1583.067363

| | | | |
|---|---|---|---|
| S | 2.158219 | 0.983427 | 0.130040 |
| F | 2.810105 | -1.538355 | 0.147166 |
| F | 3.915906 | -0.359277 | -1.284835 |
| F | 4.392712 | -0.224151 | 0.815688 |
| O | 1.675839 | 0.819111 | 1.500902 |
| O | 1.147094 | 0.583380 | -0.880518 |
| O | 2.866359 | 2.215092 | -0.173881 |
| C | 3.409900 | -0.357593 | -0.059973 |
| N | -1.505141 | 1.063477 | 0.003379 |
| H | -1.144675 | 1.195149 | -0.940752 |
| N | -0.351947 | -1.622286 | 0.020520 |
| H | 0.239933 | -0.818110 | -0.273659 |
| C | -2.369387 | -0.095449 | 0.239557 |
| H | -2.417600 | -0.234644 | 1.322430 |

| | | | |
|---|---|---|---|
| C | -1.749716 | -1.322574 | -0.425687 |
| H | -2.354123 | -2.200874 | -0.210030 |
| H | -1.710611 | -1.191513 | -1.506897 |
| C | -0.196883 | -1.753922 | 1.514627 |
| H | 0.860107 | -1.960027 | 1.678634 |
| H | -0.390569 | -0.772351 | 1.945936 |
| C | -1.075633 | -2.833804 | 2.114787 |
| H | -0.879828 | -3.811395 | 1.672549 |
| H | -2.139213 | -2.609166 | 2.020086 |
| H | -0.848285 | -2.898531 | 3.178641 |
| C | 0.186392 | -2.829904 | -0.714070 |
| H | 1.029765 | -3.190974 | -0.128059 |
| H | -0.594069 | -3.590391 | -0.703912 |
| C | 0.625262 | -2.484591 | -2.126083 |
| H | 1.058977 | -3.378506 | -2.574263 |
| H | 1.384086 | -1.700987 | -2.118909 |
| H | -0.205434 | -2.168268 | -2.757217 |
| C | -3.826107 | 0.191020 | -0.248070 |
| C | -4.690412 | -1.043139 | 0.043494 |
| H | -4.443241 | -1.885329 | -0.605608 |
| H | -5.737581 | -0.792465 | -0.135888 |
| H | -4.597295 | -1.361341 | 1.085848 |
| C | -3.873790 | 0.518924 | -1.744186 |
| H | -3.270411 | 1.395966 | -1.993170 |
| H | -4.904868 | 0.748778 | -2.020960 |
| H | -3.551410 | -0.319183 | -2.365527 |
| C | -4.370654 | 1.379075 | 0.553083 |
| H | -4.324872 | 1.188974 | 1.629152 |
| H | -5.416153 | 1.543215 | 0.285954 |
| H | -3.830725 | 2.303625 | 0.336378 |
| C | -1.169249 | 1.948306 | 0.914274 |
| C | -0.438773 | 3.112536 | 0.634923 |
| H | -1.499181 | 1.753721 | 1.929500 |
| C | -0.035223 | 3.590283 | -0.703648 |
| H | 1.003475 | 3.925352 | -0.673468 |
| H | -0.138617 | 2.851123 | -1.495848 |
| H | -0.646894 | 4.465959 | -0.953327 |
| H | -0.199778 | 3.729414 | 1.492100 |

**7E-*E***

Imaginary frequency: None

Electronic energies: -541.788499

Free energies: -541.507009

Corrected Free energies: -541.505255

| | | | |
|---|---|---|---|
| N | 1.180656 | 0.005456 | -0.630399 |
| C | 2.437968 | -0.373583 | -0.162876 |
| C | 3.536668 | 0.386920 | -0.149281 |
| C | 4.886460 | -0.108681 | 0.283831 |
| H | 5.287900 | 0.486909 | 1.109177 |
| H | 5.617323 | -0.055802 | -0.529142 |
| H | 3.464709 | 1.418718 | -0.488104 |
| H | 1.071913 | 1.011785 | -0.722545 |
| C | 0.008937 | -0.551532 | 0.040539 |
| C | -1.215032 | 0.301384 | -0.326752 |
| C | -0.239396 | -2.006246 | -0.367319 |
| H | 0.135328 | -0.527440 | 1.135609 |
| C | -2.462365 | -0.242047 | 0.384674 |
| H | -1.358902 | 0.180517 | -1.408944 |
| C | -1.489922 | -2.565496 | 0.312504 |
| H | -0.355143 | -2.040027 | -1.456817 |
| H | 0.631875 | -2.617486 | -0.116952 |
| C | -2.713277 | -1.702315 | -0.000564 |
| H | -3.331445 | 0.371341 | 0.131598 |
| H | -2.322811 | -0.174854 | 1.469737 |
| H | -1.658895 | -3.597121 | -0.005770 |
| H | -1.332844 | -2.587916 | 1.397325 |
| H | -3.594308 | -2.083735 | 0.521533 |
| H | -2.927565 | -1.758550 | -1.074354 |
| N | -0.937823 | 1.730227 | -0.128452 |
| C | -1.883225 | 2.587029 | -0.827998 |
| H | -2.896712 | 2.558231 | -0.397377 |
| H | -1.532773 | 3.620668 | -0.784683 |
| H | -1.944928 | 2.289965 | -1.876771 |
| C | -0.813136 | 2.133267 | 1.266007 |
| H | -0.466731 | 3.168244 | 1.304135 |
| H | -1.763093 | 2.074693 | 1.819213 |
| H | -0.074064 | 1.514790 | 1.777967 |
| H | 2.497806 | -1.406890 | 0.174851 |
| H | 4.831450 | -1.148020 | 0.615673 |

**7E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -541.605342

Free energies: -541.323398

Corrected Free energies: -541.321976

| | | | |
|---|---|---|---|
| N | 1.204012 | 0.187483 | 0.231339 |

| | | | |
|---|---|---|---|
| C | 2.410830 | -0.315697 | 0.130111 |
| C | 3.531052 | 0.485065 | -0.099960 |
| C | 4.901514 | -0.054908 | -0.210534 |
| H | 5.540286 | 0.401111 | 0.552818 |
| H | 5.332663 | 0.226784 | -1.176443 |
| H | 3.381497 | 1.555920 | -0.198604 |
| H | 1.041012 | 1.199105 | 0.138449 |
| C | -0.055208 | -0.523432 | 0.454544 |
| C | -1.128073 | 0.276225 | -0.312939 |
| C | -0.024314 | -1.986872 | 0.027437 |
| H | -0.262594 | -0.463185 | 1.530870 |
| C | -2.503237 | -0.360525 | -0.092850 |
| H | -0.874982 | 0.183225 | -1.376401 |
| C | -1.412924 | -2.609289 | 0.207599 |
| H | 0.279417 | -2.044131 | -1.024264 |
| H | 0.704398 | -2.546030 | 0.618486 |
| C | -2.487625 | -1.822671 | -0.544034 |
| H | -3.258888 | 0.207331 | -0.641928 |
| H | -2.766344 | -0.312704 | 0.969526 |
| H | -1.385400 | -3.645404 | -0.134582 |
| H | -1.659954 | -2.630672 | 1.274755 |
| H | -3.467420 | -2.275772 | -0.379574 |
| H | -2.288085 | -1.869615 | -1.620468 |
| N | -0.997819 | 1.700233 | 0.014618 |
| C | -1.484922 | 2.562130 | -1.058240 |
| H | -2.568260 | 2.462205 | -1.221025 |
| H | -1.275061 | 3.602075 | -0.802756 |
| H | -0.966570 | 2.324564 | -1.988276 |
| C | -1.603523 | 2.078816 | 1.289601 |
| H | -1.300885 | 3.098253 | 1.533319 |
| H | -2.701488 | 2.043472 | 1.260420 |
| H | -1.257538 | 1.424796 | 2.091617 |
| H | 2.518485 | -1.390438 | 0.231953 |
| H | 4.930935 | -1.137953 | -0.104007 |

**7E-*Z***

Imaginary frequency: None

Electronic energies: -541.789258

Free energies: -541.507991

Corrected Free energies: -541.505856

| | | | |
|---|---|---|---|
| N | 1.214813 | -0.585807 | -0.415558 |
| C | 2.237295 | -1.338806 | 0.148961 |
| C | 3.523470 | -0.973177 | 0.215052 |

| | | | |
|---|---|---|---|
| H | 1.438385 | 0.397270 | -0.539718 |
| C | -0.132414 | -0.725367 | 0.128683 |
| C | -0.971519 | 0.477150 | -0.329450 |
| C | -0.802116 | -2.023003 | -0.331194 |
| H | -0.107952 | -0.735082 | 1.230510 |
| C | -2.384106 | 0.378843 | 0.265120 |
| H | -1.056768 | 0.395334 | -1.421657 |
| C | -2.220612 | -2.137434 | 0.228397 |
| H | -0.827117 | -2.025377 | -1.426928 |
| H | -0.201901 | -2.882760 | -0.021085 |
| C | -3.062882 | -0.923366 | -0.168464 |
| H | -2.981408 | 1.239526 | -0.047982 |
| H | -2.324910 | 0.405627 | 1.359100 |
| H | -2.689186 | -3.059193 | -0.124759 |
| H | -2.173829 | -2.201421 | 1.321902 |
| H | -4.061218 | -0.991928 | 0.270891 |
| H | -3.192286 | -0.915836 | -1.257123 |
| N | -0.257579 | 1.737935 | -0.089493 |
| C | -0.829857 | 2.855138 | -0.825261 |
| H | -1.811385 | 3.172564 | -0.439508 |
| H | -0.154891 | 3.711649 | -0.762783 |
| H | -0.943502 | 2.584406 | -1.876808 |
| C | -0.085927 | 2.077717 | 1.316438 |
| H | 0.549905 | 2.962778 | 1.388313 |
| H | -1.035185 | 2.301312 | 1.827123 |
| H | 0.412929 | 1.265015 | 1.847806 |
| H | 1.928894 | -2.312706 | 0.518432 |
| H | 4.233241 | -1.683304 | 0.621492 |
| C | 4.029755 | 0.358534 | -0.270697 |
| H | 5.026552 | 0.566741 | 0.118914 |
| H | 4.088727 | 0.404728 | -1.364025 |
| H | 3.375740 | 1.178377 | 0.047749 |

**7E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -541.604351

Free energies: -541.321484

Corrected Free energies: -541.320127

| | | | |
|---|---|---|---|
| N | 1.245232 | -0.469230 | 0.227992 |
| C | 2.192019 | -1.362446 | 0.105309 |
| C | 3.530222 | -1.005483 | -0.118206 |
| H | 1.443523 | 0.538753 | 0.158647 |
| C | -0.185724 | -0.692583 | 0.443152 |

| | | | |
|---|---|---|---|
| C | -0.901108 | 0.453882 | -0.300252 |
| C | -0.674982 | -2.060184 | -0.018274 |
| H | -0.359200 | -0.588536 | 1.521752 |
| C | -2.412855 | 0.344577 | -0.083053 |
| H | -0.697235 | 0.298964 | -1.367025 |
| C | -2.193588 | -2.152996 | 0.163218 |
| H | -0.414718 | -2.193163 | -1.074690 |
| H | -0.189043 | -2.856112 | 0.550223 |
| C | -2.918783 | -1.018358 | -0.561913 |
| H | -2.917403 | 1.154267 | -0.616621 |
| H | -2.642679 | 0.461850 | 0.981597 |
| H | -2.538206 | -3.122671 | -0.200443 |
| H | -2.429998 | -2.109340 | 1.232094 |
| H | -3.995175 | -1.096173 | -0.396100 |
| H | -2.751486 | -1.110440 | -1.640813 |
| N | -0.267462 | 1.729251 | 0.053719 |
| C | -0.420606 | 2.735384 | -0.993098 |
| H | -1.467296 | 3.043180 | -1.132880 |
| H | 0.159267 | 3.619872 | -0.724523 |
| H | -0.039275 | 2.346869 | -1.938591 |
| C | -0.685272 | 2.266960 | 1.346848 |
| H | -0.038861 | 3.107478 | 1.603262 |
| H | -1.724724 | 2.622824 | 1.337898 |
| H | -0.583140 | 1.513627 | 2.129783 |
| H | 1.913275 | -2.406626 | 0.181221 |
| H | 4.241075 | -1.817211 | -0.195063 |
| C | 3.986677 | 0.400182 | -0.244162 |
| H | 3.441609 | 0.918791 | -1.040492 |
| H | 3.799667 | 0.951154 | 0.684896 |
| H | 5.049635 | 0.448887 | -0.463520 |

**8E-*E***

Imaginary frequency: None

Electronic energies: -847.793664

Free energies: -847.453268

Corrected Free energies: -847.448717

| | | | |
|---|---|---|---|
| N | 2.004492 | -0.728078 | 0.451356 |
| C | 3.193697 | -0.377444 | -0.189041 |
| C | 4.284158 | -1.141318 | -0.292186 |
| C | 5.572459 | -0.672484 | -0.903991 |
| H | 5.879287 | -1.315449 | -1.734126 |
| H | 6.391171 | -0.680286 | -0.177923 |
| H | 4.254460 | -2.154561 | 0.103747 |

| | | | |
|---|---|---|---|
| H | 1.922717 | -1.714318 | 0.677151 |
| C | 0.761208 | -0.235681 | -0.127385 |
| C | -0.402372 | -0.957611 | 0.590039 |
| H | 0.712982 | -0.448096 | -1.205325 |
| H | -0.346303 | -0.638097 | 1.636620 |
| N | -0.173894 | -2.410639 | 0.622260 |
| C | -1.047400 | -3.076274 | 1.578632 |
| H | -2.106098 | -3.051484 | 1.275988 |
| H | -0.743246 | -4.120535 | 1.673588 |
| H | -0.956251 | -2.599865 | 2.557026 |
| C | -0.225966 | -3.080981 | -0.670508 |
| H | 0.112524 | -4.110817 | -0.539880 |
| H | -1.237428 | -3.106491 | -1.102594 |
| H | 0.446872 | -2.597972 | -1.382196 |
| C | 0.624705 | 1.266467 | 0.048362 |
| C | 0.936699 | 1.863770 | 1.270632 |
| C | 0.150403 | 2.063563 | -0.991510 |
| C | 0.767250 | 3.231897 | 1.450821 |
| H | 1.326636 | 1.247136 | 2.072859 |
| C | -0.020560 | 3.434023 | -0.814291 |
| H | -0.088051 | 1.607874 | -1.947047 |
| C | 0.285922 | 4.021096 | 0.408757 |
| H | 1.013052 | 3.684940 | 2.404260 |
| H | -0.387973 | 4.042018 | -1.632632 |
| H | 0.155934 | 5.087715 | 0.549256 |
| C | -1.764802 | -0.539257 | 0.059876 |
| C | -2.756994 | -0.143971 | 0.957941 |
| C | -2.072744 | -0.557391 | -1.304264 |
| C | -4.023303 | 0.225234 | 0.513347 |
| H | -2.531750 | -0.120230 | 2.019695 |
| C | -3.337363 | -0.191045 | -1.753456 |
| H | -1.321277 | -0.849505 | -2.029067 |
| C | -4.316840 | 0.201831 | -0.845766 |
| H | -4.777318 | 0.534450 | 1.227704 |
| H | -3.556019 | -0.208076 | -2.814751 |
| H | -5.300179 | 0.491510 | -1.196552 |
| H | 3.199262 | 0.638541 | -0.581432 |
| H | 5.473853 | 0.346073 | -1.285732 |

**8E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -847.605721

Free energies: -847.262877

Corrected Free energies: -847.259307

| | | | |
|---|---|---|---|
| N | 1.857668 | -1.013385 | -0.135782 |
| C | 3.078433 | -0.578935 | -0.348128 |
| C | 4.205189 | -1.356680 | -0.079361 |
| C | 5.583178 | -0.884659 | -0.320276 |
| H | 6.089570 | -1.566104 | -1.011527 |
| H | 6.153059 | -0.919993 | 0.613754 |
| H | 4.056438 | -2.353497 | 0.323444 |
| H | 1.669508 | -1.963910 | 0.211941 |
| C | 0.618623 | -0.282307 | -0.427018 |
| C | -0.485015 | -0.964391 | 0.416339 |
| H | 0.417180 | -0.418800 | -1.493998 |
| H | -0.260059 | -0.722806 | 1.460221 |
| N | -0.344233 | -2.424203 | 0.318477 |
| C | -1.021093 | -3.107568 | 1.417678 |
| H | -2.113270 | -2.989042 | 1.370642 |
| H | -0.786617 | -4.171760 | 1.370399 |
| H | -0.665295 | -2.715531 | 2.371919 |
| C | -0.742927 | -2.998361 | -0.964990 |
| H | -0.468504 | -4.054012 | -0.969262 |
| H | -1.823180 | -2.918140 | -1.145858 |
| H | -0.213737 | -2.514274 | -1.788596 |
| C | 0.733108 | 1.195093 | -0.131953 |
| C | 1.139537 | 1.633599 | 1.130425 |
| C | 0.395765 | 2.128374 | -1.108181 |
| C | 1.204091 | 2.992669 | 1.409034 |
| H | 1.414517 | 0.914837 | 1.896025 |
| C | 0.454335 | 3.490230 | -0.825879 |
| H | 0.082324 | 1.790491 | -2.089956 |
| C | 0.857963 | 3.923079 | 0.431935 |
| H | 1.522853 | 3.326244 | 2.388964 |
| H | 0.187352 | 4.209793 | -1.590131 |
| H | 0.905722 | 4.982705 | 0.651770 |
| C | -1.862240 | -0.404943 | 0.108021 |
| C | -2.704874 | -0.063240 | 1.166347 |
| C | -2.328533 | -0.245525 | -1.199724 |
| C | -3.987539 | 0.421394 | 0.929722 |
| H | -2.349696 | -0.173059 | 2.185949 |
| C | -3.609394 | 0.239995 | -1.439390 |
| H | -1.699815 | -0.500079 | -2.045951 |
| C | -4.442468 | 0.573776 | -0.375413 |
| H | -4.626705 | 0.683673 | 1.764246 |
| H | -3.956264 | 0.358851 | -2.458771 |
| H | -5.439322 | 0.954001 | -0.563692 |

| | | | |
|---|---|---|---|
| H | 3.182296 | 0.427684 | -0.742565 |
| H | 5.610774 | 0.126247 | -0.722965 |

**8E-*Z***

Imaginary frequency: None

Electronic energies: -847.794341

Free energies: -847.453221

Corrected Free energies: -847.448743

| | | | |
|---|---|---|---|
| N | 2.183956 | -0.024884 | 0.199322 |
| C | 3.182267 | 0.615777 | -0.528165 |
| C | 4.428825 | 0.162987 | -0.702388 |
| H | 2.379853 | -0.985681 | 0.460095 |
| C | 0.809344 | 0.112269 | -0.261403 |
| C | -0.051408 | -0.889514 | 0.541367 |
| H | 0.728795 | -0.114824 | -1.333687 |
| H | -0.012545 | -0.545834 | 1.581194 |
| N | 0.575420 | -2.220121 | 0.556640 |
| C | -0.018553 | -3.089024 | 1.563182 |
| H | -1.057171 | -3.366682 | 1.324650 |
| H | 0.571970 | -4.004202 | 1.638064 |
| H | -0.008864 | -2.590058 | 2.534479 |
| C | 0.639646 | -2.896336 | -0.732551 |
| H | 1.257124 | -3.790417 | -0.624044 |
| H | -0.347109 | -3.207010 | -1.106615 |
| H | 1.112069 | -2.254629 | -1.479578 |
| C | 0.288883 | 1.524193 | -0.057384 |
| C | 0.534429 | 2.202421 | 1.137625 |
| C | -0.473037 | 2.147205 | -1.043866 |
| C | 0.017348 | 3.476403 | 1.344611 |
| H | 1.145275 | 1.727723 | 1.897631 |
| C | -0.992011 | 3.422940 | -0.839702 |
| H | -0.662721 | 1.629179 | -1.978312 |
| C | -0.749749 | 4.089598 | 0.356724 |
| H | 0.215043 | 3.993370 | 2.276449 |
| H | -1.581092 | 3.896323 | -1.616408 |
| H | -1.151196 | 5.083314 | 0.516940 |
| C | -1.510971 | -0.875328 | 0.113850 |
| C | -2.505919 | -0.754292 | 1.085233 |
| C | -1.900343 | -0.999233 | -1.223503 |
| C | -3.853769 | -0.751785 | 0.737890 |
| H | -2.218768 | -0.652463 | 2.127197 |
| C | -3.246191 | -0.998073 | -1.575561 |
| H | -1.153744 | -1.087387 | -2.004738 |

| | | | |
|---|---|---|---|
| C | -4.227390 | -0.873632 | -0.595956 |
| H | -4.609369 | -0.649684 | 1.508056 |
| H | -3.528560 | -1.090295 | -2.617725 |
| H | -5.275287 | -0.868769 | -0.872019 |
| H | 2.885268 | 1.581432 | -0.929145 |
| C | 4.916371 | -1.164603 | -0.188243 |
| H | 5.189639 | -1.123548 | 0.871937 |
| H | 4.151998 | -1.942119 | -0.293409 |
| H | 5.797880 | -1.497077 | -0.737675 |
| H | 5.129251 | 0.802533 | -1.225632 |

**8E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -847.604725

Free energies: -847.261622

Corrected Free energies: -847.258075

| | | | |
|---|---|---|---|
| N | 2.069742 | -0.475015 | -0.293118 |
| C | 3.165077 | 0.217193 | -0.489988 |
| C | 4.449694 | -0.298451 | -0.283011 |
| H | 2.081730 | -1.460523 | 0.002121 |
| C | 0.695047 | -0.010367 | -0.519588 |
| C | -0.200002 | -0.931081 | 0.344949 |
| H | 0.483871 | -0.166859 | -1.581588 |
| H | 0.028406 | -0.679726 | 1.385665 |
| N | 0.234811 | -2.326128 | 0.177576 |
| C | -0.195046 | -3.166900 | 1.292266 |
| H | -1.287984 | -3.280848 | 1.328696 |
| H | 0.251543 | -4.155911 | 1.181601 |
| H | 0.146333 | -2.735545 | 2.234708 |
| C | -0.138405 | -2.937448 | -1.096964 |
| H | 0.354883 | -3.907281 | -1.171349 |
| H | -1.222262 | -3.088955 | -1.188908 |
| H | 0.200221 | -2.326786 | -1.936357 |
| C | 0.512778 | 1.452118 | -0.188932 |
| C | 0.834407 | 1.932723 | 1.082348 |
| C | -0.006850 | 2.323569 | -1.142580 |
| C | 0.633556 | 3.271211 | 1.393680 |
| H | 1.250779 | 1.264096 | 1.829124 |
| C | -0.213438 | 3.663912 | -0.827699 |
| H | -0.253071 | 1.954285 | -2.132282 |
| C | 0.106068 | 4.138058 | 0.439074 |
| H | 0.887046 | 3.637942 | 2.380752 |
| H | -0.620544 | 4.335482 | -1.573649 |

| | | | |
|---|---|---|---|
| H | -0.052767 | 5.181397 | 0.683313 |
| C | -1.678792 | -0.667290 | 0.129266 |
| C | -2.517908 | -0.594635 | 1.241940 |
| C | -2.238230 | -0.528999 | -1.143920 |
| C | -3.886292 | -0.391841 | 1.091989 |
| H | -2.093631 | -0.692296 | 2.236181 |
| C | -3.605100 | -0.323945 | -1.296719 |
| H | -1.614643 | -0.579463 | -2.029933 |
| C | -4.432590 | -0.255943 | -0.179557 |
| H | -4.522110 | -0.337100 | 1.967494 |
| H | -4.023834 | -0.215751 | -2.290096 |
| H | -5.496943 | -0.094450 | -0.301234 |
| H | 3.041839 | 1.241299 | -0.825987 |
| C | 4.776901 | -1.661117 | 0.186993 |
| H | 3.912698 | -2.261155 | 0.466019 |
| H | 5.328665 | -2.186689 | -0.599720 |
| H | 5.452925 | -1.595864 | 1.043922 |
| H | 5.269722 | 0.374105 | -0.501004 |

**9E-*E***

Imaginary frequency: None

Electronic energies: -329.227183

Free energies: -329.069912

Corrected Free energies: -329.069312

| | | | |
|---|---|---|---|
| C | -2.436362 | 0.478158 | 0.445238 |
| C | -2.243953 | -0.934641 | -0.116035 |
| C | -0.728901 | -1.117008 | -0.036867 |
| C | -1.249776 | 1.246164 | -0.145227 |
| H | -3.395883 | 0.922551 | 0.181337 |
| H | -2.354768 | 0.453791 | 1.535113 |
| H | -2.567379 | -0.970989 | -1.159726 |
| H | -2.786615 | -1.698614 | 0.440164 |
| H | -0.417278 | -1.460483 | 0.962390 |
| H | -0.345260 | -1.836436 | -0.766877 |
| H | -0.908046 | 2.051311 | 0.510010 |
| H | -1.511823 | 1.684742 | -1.115299 |
| N | -0.216361 | 0.217939 | -0.302194 |
| C | 1.119211 | 0.500115 | -0.155760 |
| C | 2.110203 | -0.384813 | 0.042114 |
| H | 1.355711 | 1.559752 | -0.233354 |
| C | 3.554175 | 0.018123 | 0.151163 |
| H | 4.164107 | -0.431625 | -0.638987 |
| H | 3.662763 | 1.102881 | 0.076366 |

| | | | |
|---|---|---|---|
| H | 3.991939 | -0.295424 | 1.104057 |
| H | 1.879477 | -1.443615 | 0.112406 |

**9E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -329.047063

Free energies: -328.888869

Corrected Free energies: -328.888517

| | | | |
|---|---|---|---|
| C | -2.486195 | 0.467456 | 0.330906 |
| C | -2.220559 | -0.945786 | -0.196198 |
| C | -0.722097 | -1.134029 | 0.038319 |
| C | -1.261896 | 1.238961 | -0.148611 |
| H | -3.408800 | 0.899477 | -0.051282 |
| H | -2.522321 | 0.467987 | 1.422095 |
| H | -2.438087 | -0.997250 | -1.264631 |
| H | -2.801836 | -1.710656 | 0.314384 |
| H | -0.506963 | -1.505381 | 1.043900 |
| H | -0.236639 | -1.777761 | -0.694672 |
| H | -0.998556 | 2.109076 | 0.450508 |
| H | -1.358431 | 1.536281 | -1.196861 |
| N | -0.180636 | 0.236371 | -0.063906 |
| C | 1.097828 | 0.553162 | -0.060917 |
| C | 2.127716 | -0.377243 | 0.040487 |
| H | 1.327981 | 1.611083 | -0.137532 |
| C | 3.553770 | 0.011588 | 0.044617 |
| H | 4.073563 | -0.486701 | -0.779912 |
| H | 3.690418 | 1.088418 | -0.040201 |
| H | 4.029464 | -0.343934 | 0.964126 |
| H | 1.883261 | -1.429890 | 0.125801 |

**9E-*Z***

Imaginary frequency: None

Electronic energies: -329.222341

Free energies: -329.064629

Corrected Free energies: -329.063849

| | | | |
|---|---|---|---|
| C | -2.369193 | 0.227498 | 0.311991 |
| C | -1.849369 | -1.179624 | 0.013770 |
| C | -0.331779 | -1.015419 | 0.126519 |
| C | -1.353133 | 1.101580 | -0.421648 |
| H | -3.392485 | 0.393223 | -0.025218 |
| H | -2.319034 | 0.422825 | 1.386825 |
| H | -2.118845 | -1.466699 | -1.006377 |

| | | | |
|---|---|---|---|
| H | -2.230905 | -1.939494 | 0.695689 |
| H | 0.005017 | -1.139088 | 1.164520 |
| H | 0.201369 | -1.743087 | -0.486830 |
| H | -1.256959 | 2.100884 | 0.008999 |
| H | -1.635405 | 1.217163 | -1.474054 |
| N | -0.082947 | 0.370454 | -0.307640 |
| C | 1.031970 | 1.044937 | 0.170198 |
| C | 2.273729 | 0.554922 | 0.293630 |
| H | 0.842976 | 2.076357 | 0.462568 |
| H | 3.010809 | 1.211322 | 0.741619 |
| C | 2.741636 | -0.786275 | -0.206562 |
| H | 2.551809 | -1.602647 | 0.497925 |
| H | 2.242835 | -1.043423 | -1.144664 |
| H | 3.816283 | -0.766232 | -0.394914 |

**9E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -329.041849

Free energies: -328.883030

Corrected Free energies: -328.882638

| | | | |
|---|---|---|---|
| C | -2.425350 | 0.096007 | 0.320064 |
| C | -1.815257 | -1.166153 | -0.294160 |
| C | -0.329206 | -1.017868 | 0.023691 |
| C | -1.407105 | 1.169208 | -0.043491 |
| H | -3.411850 | 0.330177 | -0.074571 |
| H | -2.494872 | -0.003241 | 1.405187 |
| H | -1.964534 | -1.172135 | -1.375669 |
| H | -2.220181 | -2.087245 | 0.119990 |
| H | -0.105450 | -1.361643 | 1.037377 |
| H | 0.330622 | -1.513205 | -0.684999 |
| H | -1.359055 | 2.010318 | 0.646238 |
| H | -1.558361 | 1.542539 | -1.059934 |
| N | -0.114175 | 0.443157 | -0.021876 |
| C | 1.032113 | 1.088880 | -0.080952 |
| C | 2.324680 | 0.561404 | -0.048853 |
| H | 0.936051 | 2.166407 | -0.163015 |
| C | 2.765175 | -0.845456 | 0.126937 |
| H | 2.149768 | -1.401440 | 0.832177 |
| H | 2.728286 | -1.371301 | -0.835576 |
| H | 3.799686 | -0.865527 | 0.464565 |
| H | 3.098812 | 1.308061 | -0.178057 |

**10E-*E***

Imaginary frequency: None

Electronic energies: -368.538594

Free energies: -368.351862

Corrected Free energies: -368.351486

| | | | |
|---|---|---|---|
| C | -3.881947 | -0.015801 | 0.065183 |
| C | -2.432047 | 0.378012 | 0.092944 |
| C | -1.446501 | -0.473411 | -0.215759 |
| H | -4.443480 | 0.563818 | -0.673919 |
| H | -4.360127 | 0.157825 | 1.033578 |
| C | 0.358042 | 1.109786 | 0.108192 |
| C | 0.756457 | -1.297021 | 0.226530 |
| C | 1.819621 | 1.350858 | -0.259698 |
| H | 0.214774 | 1.237082 | 1.196276 |
| H | -0.271229 | 1.848643 | -0.391853 |
| C | 2.216779 | -1.111952 | -0.165176 |
| H | 0.675128 | -1.330526 | 1.326693 |
| H | 0.371661 | -2.243345 | -0.160200 |
| C | 2.720011 | 0.252616 | 0.302372 |
| H | 2.122573 | 2.333088 | 0.110697 |
| H | 1.907311 | 1.368636 | -1.350995 |
| H | 2.810656 | -1.919060 | 0.270533 |
| H | 2.304271 | -1.183687 | -1.254326 |
| H | 3.756345 | 0.410012 | -0.005035 |
| H | 2.696620 | 0.288988 | 1.398131 |
| H | -2.208432 | 1.404772 | 0.362785 |
| N | -0.077681 | -0.216601 | -0.307117 |
| H | -1.697951 | -1.505168 | -0.457681 |
| H | -3.996846 | -1.073385 | -0.182387 |

**10E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -368.354724

Free energies: -368.168573

Corrected Free energies: -368.167840

| | | | |
|---|---|---|---|
| C | -3.727082 | -0.023434 | -0.419213 |
| C | -2.361364 | 0.386854 | -0.025916 |
| C | -1.329602 | -0.537085 | 0.121930 |
| H | -4.011985 | 0.487919 | -1.344282 |
| H | -4.442598 | 0.303367 | 0.342016 |
| C | 0.458859 | 1.069871 | 0.725485 |
| C | 0.929374 | -1.337709 | 0.505626 |
| C | 1.510270 | 1.398050 | -0.338018 |

| | | | |
|---|---|---|---|
| H | 0.916872 | 1.032583 | 1.717548 |
| H | -0.343106 | 1.799940 | 0.746438 |
| C | 1.997651 | -1.059096 | -0.554249 |
| H | 1.368049 | -1.327090 | 1.507346 |
| H | 0.432894 | -2.292539 | 0.345722 |
| C | 2.603499 | 0.330839 | -0.363129 |
| H | 1.925148 | 2.381138 | -0.110417 |
| H | 1.016323 | 1.462645 | -1.312074 |
| H | 2.760412 | -1.835452 | -0.475530 |
| H | 1.539198 | -1.141223 | -1.543993 |
| H | 3.313871 | 0.541277 | -1.164102 |
| H | 3.159749 | 0.359062 | 0.579717 |
| H | -2.183920 | 1.440960 | 0.141361 |
| N | -0.083092 | -0.271067 | 0.467908 |
| H | -1.543400 | -1.585580 | -0.059848 |
| H | -3.815503 | -1.099276 | -0.560354 |

**10E-*Z***

Imaginary frequency: None

Electronic energies: -368.531773

Free energies: -368.345184

Corrected Free energies: -368.344378

| | | | |
|---|---|---|---|
| C | -2.625325 | -0.529823 | -0.121049 |
| C | -1.393539 | -1.041692 | -0.275613 |
| C | 0.024342 | 0.949396 | 0.062003 |
| C | 0.915078 | -1.305973 | 0.357007 |
| C | 1.396656 | 1.451565 | -0.381914 |
| H | -0.099930 | 1.135069 | 1.142204 |
| H | -0.754219 | 1.497661 | -0.466706 |
| C | 2.303827 | -0.857236 | -0.083059 |
| H | 0.849825 | -1.264984 | 1.457636 |
| H | 0.734885 | -2.340312 | 0.056781 |
| C | 2.514493 | 0.620399 | 0.244671 |
| H | 1.494786 | 2.505549 | -0.110531 |
| H | 1.458394 | 1.382904 | -1.473056 |
| H | 3.055889 | -1.478353 | 0.409660 |
| H | 2.399618 | -1.011535 | -1.162780 |
| H | 3.491212 | 0.959677 | -0.107696 |
| H | 2.498056 | 0.754057 | 1.333130 |
| N | -0.125975 | -0.468772 | -0.239918 |
| H | -1.338024 | -2.100600 | -0.518996 |
| C | -3.096477 | 0.853597 | 0.258108 |
| H | -2.440578 | 1.347630 | 0.972963 |

| | | | |
|---|---|---|---|
| H | -3.198416 | 1.511859 | -0.611546 |
| H | -4.084188 | 0.783560 | 0.717568 |
| H | -3.419809 | -1.242176 | -0.320117 |

**10E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -368.348634

Free energies: -368.161943

Corrected Free energies: -368.160979

| | | | |
|---|---|---|---|
| C | -2.486592 | -0.549853 | -0.247974 |
| C | -1.240019 | -1.145401 | -0.016167 |
| C | 0.069671 | 0.781200 | 0.866779 |
| C | 1.143229 | -1.362261 | 0.354976 |
| C | 0.982327 | 1.524955 | -0.111570 |
| H | 0.554101 | 0.703979 | 1.844189 |
| H | -0.891634 | 1.259174 | 1.007196 |
| C | 2.087621 | -0.679321 | -0.638758 |
| H | 1.568160 | -1.351632 | 1.361951 |
| H | 0.921645 | -2.388417 | 0.069947 |
| C | 2.313065 | 0.784877 | -0.260071 |
| H | 1.136179 | 2.535772 | 0.269075 |
| H | 0.480909 | 1.606565 | -1.080854 |
| H | 3.028500 | -1.231742 | -0.646282 |
| H | 1.651863 | -0.750590 | -1.639576 |
| H | 2.930436 | 1.274316 | -1.014820 |
| H | 2.858748 | 0.833663 | 0.687879 |
| N | -0.115744 | -0.600331 | 0.402561 |
| H | -1.170062 | -2.208343 | -0.221271 |
| C | -2.872654 | 0.883655 | -0.295728 |
| H | -3.102755 | 1.253901 | 0.711053 |
| H | -2.093235 | 1.517533 | -0.718842 |
| H | -3.778353 | 0.992554 | -0.889746 |
| H | -3.264190 | -1.271513 | -0.466751 |

**11E-*E***

Imaginary frequency: None

Electronic energies: -517.799002

Free energies: -517.630977

Corrected Free energies: -517.629393

| | | | |
|---|---|---|---|
| C | 1.885059 | 1.217867 | 0.020148 |
| C | 0.947258 | 2.423032 | -0.067144 |
| C | -0.409792 | 1.857688 | 0.365913 |

| | | | |
|---|---|---|---|
| C | 0.984084 | 0.067083 | -0.462735 |
| H | 2.786837 | 1.311969 | -0.582204 |
| H | 2.172600 | 1.036850 | 1.059842 |
| H | 0.889125 | 2.766953 | -1.102356 |
| H | 1.272531 | 3.256990 | 0.553583 |
| H | -0.594039 | 1.999331 | 1.437395 |
| H | -1.238675 | 2.322302 | -0.179108 |
| H | 1.016359 | -0.003758 | -1.559502 |
| N | -0.318461 | 0.439002 | 0.040686 |
| C | -1.438489 | -0.327081 | -0.195768 |
| C | -2.710192 | 0.016544 | 0.054321 |
| H | -1.219647 | -1.311399 | -0.603568 |
| C | -3.868714 | -0.901224 | -0.216905 |
| H | -4.581356 | -0.458684 | -0.919627 |
| H | -3.524838 | -1.846712 | -0.642911 |
| H | -4.426063 | -1.130495 | 0.696624 |
| H | -2.931317 | 0.985645 | 0.491215 |
| C | 1.473209 | -1.254910 | 0.093424 |
| O | 0.957878 | -1.892398 | 0.970615 |
| O | 2.607568 | -1.625506 | -0.516461 |
| H | 2.909607 | -2.452753 | -0.114948 |

**11E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -517.611502

Free energies: -517.443177

Corrected Free energies: -517.441835

| | | | |
|---|---|---|---|
| C | 1.941449 | 1.164806 | 0.019347 |
| C | 1.033996 | 2.393922 | -0.020109 |
| C | -0.316982 | 1.843398 | 0.424963 |
| C | 1.032133 | 0.045962 | -0.514557 |
| H | 2.839802 | 1.260927 | -0.585274 |
| H | 2.233861 | 0.940937 | 1.047972 |
| H | 0.959012 | 2.780541 | -1.037801 |
| H | 1.377544 | 3.191543 | 0.634942 |
| H | -0.387918 | 1.760009 | 1.513125 |
| H | -1.168470 | 2.403719 | 0.044483 |
| H | 1.089043 | -0.022693 | -1.605220 |
| N | -0.322487 | 0.477974 | -0.139436 |
| C | -1.387179 | -0.279397 | -0.309504 |
| C | -2.673437 | 0.089108 | 0.082462 |
| H | -1.223955 | -1.244688 | -0.775000 |
| C | -3.847452 | -0.778716 | -0.140636 |

| | | | |
|---|---|---|---|
| H | -4.597155 | -0.238146 | -0.727312 |
| H | -3.588990 | -1.705945 | -0.648640 |
| H | -4.321509 | -1.008658 | 0.819152 |
| H | -2.825632 | 1.039327 | 0.580688 |
| C | 1.373535 | -1.315294 | 0.073381 |
| O | 0.641291 | -1.990055 | 0.739336 |
| O | 2.620838 | -1.633800 | -0.253390 |
| H | 2.838371 | -2.494586 | 0.135286 |

**11E-*Z***

Imaginary frequency: None

Electronic energies: -517.795596

Free energies: -517.627089

Corrected Free energies: -517.625530

| | | | |
|---|---|---|---|
| C | 1.403998 | 1.565721 | 0.124339 |
| C | 0.144821 | 2.414148 | -0.050114 |
| C | -0.971997 | 1.436970 | 0.321572 |
| C | 0.952977 | 0.207632 | -0.441803 |
| H | 2.279648 | 1.951771 | -0.394164 |
| H | 1.643619 | 1.460736 | 1.186612 |
| H | 0.044594 | 2.713508 | -1.096464 |
| H | 0.145419 | 3.309815 | 0.570692 |
| H | -1.158277 | 1.455203 | 1.400169 |
| H | -1.912085 | 1.649841 | -0.191662 |
| H | 1.119143 | 0.183863 | -1.529063 |
| N | -0.454737 | 0.128842 | -0.109165 |
| C | -1.243047 | -0.777128 | -0.808267 |
| C | -2.528003 | -1.074002 | -0.578824 |
| H | -0.720856 | -1.280653 | -1.620707 |
| C | 1.756653 | -0.930157 | 0.154651 |
| O | 1.350108 | -1.770451 | 0.909256 |
| O | 3.029423 | -0.874495 | -0.266007 |
| H | 3.515651 | -1.602267 | 0.147267 |
| C | -3.359905 | -0.581883 | 0.573814 |
| H | -2.730639 | -0.254453 | 1.403132 |
| H | -4.014091 | 0.252382 | 0.300649 |
| H | -4.004203 | -1.383988 | 0.940940 |
| H | -2.994000 | -1.765892 | -1.271451 |

**11E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -517.606581

Free energies: -517.437080

Corrected Free energies: -517.435868

| | | | |
|---|---|---|---|
| C | 1.423875 | 1.583880 | 0.089163 |
| C | 0.147854 | 2.414382 | -0.036204 |
| C | -0.947147 | 1.414675 | 0.319487 |
| C | 1.010101 | 0.230013 | -0.506985 |
| H | 2.274509 | 2.002707 | -0.442770 |
| H | 1.695045 | 1.458750 | 1.140082 |
| H | 0.015090 | 2.759876 | -1.063009 |
| H | 0.135922 | 3.274554 | 0.629681 |
| H | -1.032354 | 1.286249 | 1.402129 |
| H | -1.919189 | 1.651592 | -0.104710 |
| H | 1.182118 | 0.206673 | -1.587250 |
| N | -0.441763 | 0.152607 | -0.260869 |
| C | -1.136947 | -0.909926 | -0.610573 |
| C | -2.494404 | -1.159563 | -0.380395 |
| H | -0.573349 | -1.673185 | -1.134443 |
| C | 1.743104 | -0.946690 | 0.120469 |
| O | 1.225298 | -1.864945 | 0.689108 |
| O | 3.050999 | -0.795009 | -0.054835 |
| H | 3.511339 | -1.546595 | 0.348356 |
| C | -3.467578 | -0.389260 | 0.430806 |
| H | -3.012565 | 0.129644 | 1.271699 |
| H | -3.968467 | 0.356369 | -0.200323 |
| H | -4.241685 | -1.060853 | 0.799754 |
| H | -2.857591 | -2.059460 | -0.861915 |

**12E-*E***

Imaginary frequency: None

Electronic energies: -905.782033

Free energies: -905.442842

Corrected Free energies: -905.439720

| | | | |
|---|---|---|---|
| C | 0.205888 | -1.222932 | -0.408489 |
| C | -0.274305 | -2.681827 | -0.277871 |
| C | 0.674118 | -3.308297 | 0.752442 |
| C | 1.997693 | -2.611064 | 0.459220 |
| H | -0.155137 | -3.183338 | -1.241186 |
| H | -1.326642 | -2.758487 | 0.001687 |
| H | 0.747844 | -4.390590 | 0.648746 |
| H | 0.351399 | -3.082355 | 1.769306 |
| H | 2.551297 | -3.130326 | -0.338401 |
| H | 2.652147 | -2.553365 | 1.333576 |
| C | -0.623310 | -0.231190 | 0.465572 |

| | | | |
|---|---|---|---|
| O | -0.584809 | -0.647004 | 1.825223 |
| C | -2.082301 | -0.125170 | 0.009559 |
| C | -3.004021 | 0.427903 | 0.904084 |
| C | -2.530832 | -0.515111 | -1.253250 |
| C | -4.337166 | 0.586120 | 0.548661 |
| H | -2.662717 | 0.736969 | 1.885282 |
| C | -3.867754 | -0.353864 | -1.612146 |
| H | -1.850835 | -0.954078 | -1.973037 |
| C | -4.774588 | 0.196188 | -0.714777 |
| H | -5.035422 | 1.016737 | 1.256882 |
| H | -4.196905 | -0.664710 | -2.596552 |
| H | -5.813752 | 0.319459 | -0.995192 |
| C | 0.039980 | 1.139317 | 0.400122 |
| C | -0.100811 | 1.932670 | -0.740006 |
| C | 0.875841 | 1.572265 | 1.427152 |
| C | 0.596553 | 3.129409 | -0.859762 |
| H | -0.754292 | 1.611466 | -1.544598 |
| C | 1.569299 | 2.774047 | 1.310233 |
| H | 0.990166 | 0.957122 | 2.309585 |
| C | 1.437951 | 3.553213 | 0.165852 |
| H | 0.480814 | 3.732251 | -1.752860 |
| H | 2.219147 | 3.097750 | 2.115047 |
| H | 1.981455 | 4.486146 | 0.074579 |
| N | 1.607206 | -1.280072 | 0.013999 |
| H | 0.150813 | -0.879008 | -1.445225 |
| C | 2.557358 | -0.470025 | -0.580818 |
| C | 3.884881 | -0.660884 | -0.578278 |
| C | 4.842012 | 0.304687 | -1.219316 |
| H | 5.443539 | -0.177004 | -1.996369 |
| H | 5.543588 | 0.723928 | -0.491192 |
| H | 4.309619 | -1.526966 | -0.080142 |
| H | 2.147640 | 0.411172 | -1.068474 |
| H | 4.304972 | 1.136984 | -1.680832 |
| H | -1.169622 | -1.405952 | 1.920497 |

**12E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -905.598618

Free energies: -905.259547

Corrected Free energies: -905.256409

| | | | |
|---|---|---|---|
| C | 0.041734 | -1.261151 | -0.631882 |
| C | -0.498085 | -2.691509 | -0.508505 |
| C | 0.386796 | -3.376799 | 0.548683 |

| | | | |
|---|---|---|---|
| C | 1.726543 | -2.634357 | 0.502252 |
| H | -0.394025 | -3.189827 | -1.473351 |
| H | -1.553329 | -2.705397 | -0.237742 |
| H | 0.521623 | -4.433509 | 0.327526 |
| H | -0.048388 | -3.292705 | 1.541579 |
| H | 2.510116 | -3.211750 | 0.009495 |
| H | 2.076578 | -2.323794 | 1.488660 |
| C | -0.607558 | -0.243149 | 0.370162 |
| O | -0.468221 | -0.763069 | 1.683084 |
| C | -2.081547 | -0.000180 | 0.048513 |
| C | -2.845758 | 0.644263 | 1.026250 |
| C | -2.686301 | -0.355219 | -1.156137 |
| C | -4.188819 | 0.918196 | 0.807960 |
| H | -2.376515 | 0.933160 | 1.960236 |
| C | -4.034364 | -0.077817 | -1.374901 |
| H | -2.129867 | -0.857446 | -1.938383 |
| C | -4.788322 | 0.556099 | -0.395925 |
| H | -4.766439 | 1.418095 | 1.576114 |
| H | -4.491412 | -0.364290 | -2.314250 |
| H | -5.836507 | 0.768077 | -0.568494 |
| C | 0.174750 | 1.065091 | 0.313554 |
| C | 0.030062 | 1.927088 | -0.775250 |
| C | 1.132342 | 1.347988 | 1.286216 |
| C | 0.851441 | 3.041892 | -0.900831 |
| H | -0.721112 | 1.725349 | -1.532138 |
| C | 1.951367 | 2.466937 | 1.160750 |
| H | 1.244658 | 0.680279 | 2.130514 |
| C | 1.819551 | 3.311310 | 0.064240 |
| H | 0.734312 | 3.702160 | -1.751619 |
| H | 2.697098 | 2.672060 | 1.919688 |
| H | 2.461567 | 4.177987 | -0.036577 |
| N | 1.468649 | -1.431269 | -0.311413 |
| H | -0.025739 | -0.859000 | -1.643085 |
| C | 2.399706 | -0.588817 | -0.713952 |
| C | 3.742642 | -0.675999 | -0.352330 |
| C | 4.739257 | 0.321148 | -0.796224 |
| H | 5.555199 | -0.177952 | -1.328457 |
| H | 5.192254 | 0.799277 | 0.078684 |
| H | 4.071260 | -1.483808 | 0.291238 |
| H | 2.071369 | 0.223136 | -1.355298 |
| H | 4.301508 | 1.086560 | -1.435656 |
| H | -1.221602 | -1.333305 | 1.870663 |

**12E-*Z***

Imaginary frequency: None

Electronic energies: -905.777827

Free energies: -905.438272

Corrected Free energies: -905.435127

| | | | |
|---|---|---|---|
| C | 0.245077 | -1.205624 | -0.516706 |
| C | -0.104258 | -2.687960 | -0.286825 |
| C | 1.031005 | -3.209079 | 0.600171 |
| C | 2.239922 | -2.430136 | 0.097404 |
| H | -0.093937 | -3.211714 | -1.245757 |
| H | -1.093940 | -2.830860 | 0.151091 |
| H | 1.172023 | -4.286541 | 0.515965 |
| H | 0.846042 | -2.964864 | 1.647227 |
| H | 2.685797 | -2.913786 | -0.783625 |
| H | 3.015300 | -2.340908 | 0.858480 |
| C | -0.543019 | -0.238336 | 0.415591 |
| O | -0.348517 | -0.617520 | 1.773976 |
| C | -2.045455 | -0.216449 | 0.113748 |
| C | -2.880970 | 0.407544 | 1.046188 |
| C | -2.618587 | -0.757667 | -1.037002 |
| C | -4.250590 | 0.489124 | 0.835958 |
| H | -2.441270 | 0.831785 | 1.941908 |
| C | -3.994064 | -0.675129 | -1.250378 |
| H | -2.009310 | -1.256146 | -1.780902 |
| C | -4.813408 | -0.052809 | -0.317690 |
| H | -4.880194 | 0.978056 | 1.570023 |
| H | -4.420792 | -1.102884 | -2.149858 |
| H | -5.881898 | 0.009793 | -0.485533 |
| C | 0.033774 | 1.162852 | 0.254465 |
| C | -0.242228 | 1.899647 | -0.898517 |
| C | 0.901617 | 1.694059 | 1.205773 |
| C | 0.349380 | 3.140754 | -1.104079 |
| H | -0.924494 | 1.500874 | -1.642957 |
| C | 1.488433 | 2.940919 | 1.004316 |
| H | 1.123344 | 1.122740 | 2.097339 |
| C | 1.219841 | 3.665302 | -0.152065 |
| H | 0.126811 | 3.700067 | -2.005246 |
| H | 2.163737 | 3.342710 | 1.751062 |
| H | 1.680435 | 4.633567 | -0.309350 |
| N | 1.687113 | -1.119785 | -0.273184 |
| H | 0.036431 | -0.905315 | -1.549604 |
| C | 2.435548 | -0.295161 | -1.116108 |
| C | 3.721487 | 0.036346 | -0.952476 |
| H | 1.892750 | 0.092916 | -1.977037 |

| | | | |
|---|---|---|---|
| H | -0.889070 | -1.395882 | 1.943531 |
| C | 4.555195 | -0.291751 | 0.254896 |
| H | 3.933950 | -0.314309 | 1.154621 |
| H | 5.056024 | -1.262868 | 0.177232 |
| H | 5.331805 | 0.461672 | 0.397805 |
| H | 4.176621 | 0.631881 | -1.735923 |

**12E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -905.592967

Free energies: -905.254311

Corrected Free energies: -905.250740

| | | | |
|---|---|---|---|
| C | 0.179364 | -1.152252 | -0.721848 |
| C | -0.165715 | -2.639720 | -0.606271 |
| C | 0.868495 | -3.235089 | 0.371095 |
| C | 2.044601 | -2.246579 | 0.402671 |
| H | -0.068789 | -3.099593 | -1.590094 |
| H | -1.190448 | -2.790874 | -0.268530 |
| H | 1.199205 | -4.216381 | 0.036915 |
| H | 0.453608 | -3.346408 | 1.370709 |
| H | 2.969205 | -2.666209 | 0.010203 |
| H | 2.213750 | -1.856989 | 1.407244 |
| C | -0.531847 | -0.239546 | 0.335094 |
| O | -0.227261 | -0.737216 | 1.628281 |
| C | -2.044308 | -0.201880 | 0.118994 |
| C | -2.830624 | 0.259811 | 1.178276 |
| C | -2.664846 | -0.557220 | -1.078092 |
| C | -4.209532 | 0.355949 | 1.045964 |
| H | -2.352382 | 0.550299 | 2.106928 |
| C | -4.047706 | -0.455800 | -1.211184 |
| H | -2.090952 | -0.920180 | -1.922310 |
| C | -4.822865 | -0.001505 | -0.151791 |
| H | -4.805045 | 0.714209 | 1.876965 |
| H | -4.515148 | -0.737026 | -2.147008 |
| H | -5.898314 | 0.074261 | -0.257710 |
| C | 0.056269 | 1.164635 | 0.232689 |
| C | -0.298315 | 1.990102 | -0.836388 |
| C | 1.029821 | 1.594659 | 1.133103 |
| C | 0.322973 | 3.220952 | -1.011086 |
| H | -1.063774 | 1.672824 | -1.536952 |
| C | 1.648756 | 2.830503 | 0.958017 |
| H | 1.307780 | 0.958960 | 1.964390 |
| C | 1.302424 | 3.642897 | -0.115723 |

| | | | |
|---|---|---|---|
| H | 0.039538 | 3.851383 | -1.845202 |
| H | 2.405775 | 3.154578 | 1.662308 |
| H | 1.786986 | 4.602150 | -0.252259 |
| N | 1.630899 | -1.132814 | -0.470523 |
| H | 0.009388 | -0.746675 | -1.718650 |
| C | 2.412444 | -0.221705 | -1.014943 |
| C | 3.770493 | 0.007984 | -0.769045 |
| H | 1.923719 | 0.430851 | -1.731036 |
| H | -0.863716 | -1.424205 | 1.854356 |
| C | 4.652625 | -0.593561 | 0.261284 |
| H | 4.130413 | -0.813762 | 1.190777 |
| H | 5.084999 | -1.530638 | -0.112014 |
| H | 5.482383 | 0.080412 | 0.468298 |
| H | 4.208566 | 0.750645 | -1.424825 |

**13E-*E***

Imaginary frequency: None

Electronic energies: -1314.451926

Free energies: -1314.018628

Corrected Free energies: -1314.014771

| | | | |
|---|---|---|---|
| Si | 0.704963 | 2.380515 | -0.803078 |
| O | 0.087889 | 0.817579 | -0.798264 |
| N | -1.978650 | 0.005176 | 0.976774 |
| C | -0.571122 | -0.124618 | 1.320478 |
| C | -0.554391 | -1.321104 | 2.289334 |
| C | -1.806448 | -2.142433 | 1.938493 |
| C | -2.804435 | -1.102017 | 1.427310 |
| C | 0.331153 | -0.299697 | 0.051696 |
| C | -0.470350 | 3.282739 | -1.941040 |
| C | 0.725808 | 3.182134 | 0.894965 |
| C | 2.447056 | 2.469781 | -1.482253 |
| C | 1.826514 | -0.349566 | 0.383365 |
| C | 2.351545 | -0.026943 | 1.634100 |
| C | 3.730879 | 0.001613 | 1.841115 |
| C | 4.602540 | -0.300797 | 0.803228 |
| C | 4.089180 | -0.632240 | -0.449144 |
| C | 2.717215 | -0.650899 | -0.653072 |
| C | -0.125200 | -1.548660 | -0.697158 |
| C | -1.245288 | -1.470864 | -1.527532 |
| C | -1.761090 | -2.614333 | -2.128576 |
| C | -1.161781 | -3.852463 | -1.912299 |
| C | -0.037707 | -3.936733 | -1.097509 |
| C | 0.476724 | -2.792265 | -0.495147 |

| | | | |
|---|---|---|---|
| C | -2.558213 | 1.197418 | 0.622015 |
| C | -3.867349 | 1.423818 | 0.420968 |
| H | -0.238066 | 0.793383 | 1.815070 |
| H | -0.629272 | -0.944039 | 3.311995 |
| H | 0.361465 | -1.909085 | 2.217252 |
| H | -1.586294 | -2.866792 | 1.153928 |
| H | -2.193007 | -2.684091 | 2.801596 |
| H | -3.420623 | -1.489201 | 0.607616 |
| H | -3.485767 | -0.756185 | 2.218363 |
| H | -0.413254 | 2.874504 | -2.953232 |
| H | -0.220520 | 4.345793 | -1.990671 |
| H | -1.504084 | 3.189710 | -1.598589 |
| H | -0.260205 | 3.279884 | 1.353908 |
| H | 1.134295 | 4.191207 | 0.777895 |
| H | 1.378997 | 2.646320 | 1.588442 |
| H | 3.184812 | 2.121336 | -0.755495 |
| H | 2.674666 | 3.511734 | -1.728148 |
| H | 2.555990 | 1.874752 | -2.392166 |
| H | 1.699887 | 0.206432 | 2.467492 |
| H | 4.118156 | 0.257456 | 2.820202 |
| H | 5.673362 | -0.281479 | 0.967056 |
| H | 4.759128 | -0.868450 | -1.267489 |
| H | 2.322077 | -0.894324 | -1.633552 |
| H | -1.711393 | -0.506439 | -1.687491 |
| H | -2.633868 | -2.539396 | -2.767136 |
| H | -1.564246 | -4.743180 | -2.380210 |
| H | 0.441796 | -4.893980 | -0.929057 |
| H | 1.349988 | -2.875003 | 0.141710 |
| H | -1.855612 | 2.014894 | 0.502582 |
| H | -4.579493 | 0.610351 | 0.519403 |
| C | -4.406751 | 2.777014 | 0.049527 |
| H | -4.917870 | 2.761095 | -0.918325 |
| H | -5.132254 | 3.141366 | 0.783587 |
| H | -3.601781 | 3.514043 | -0.011916 |

**13E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1314.267090

Free energies: -1313.833597

Corrected Free energies: -1313.829925

| | | | |
|---|---|---|---|
| Si | -1.013686 | -2.331732 | -0.732546 |
| O | -0.128453 | -0.886558 | -0.699870 |
| N | 1.931801 | -0.217968 | 1.138147 |

| | | | |
|---|---|---|---|
| C | 0.510605 | 0.066345 | 1.411370 |
| C | 0.577120 | 1.264211 | 2.367947 |
| C | 1.903428 | 1.980411 | 2.061812 |
| C | 2.828115 | 0.895732 | 1.508642 |
| C | -0.275703 | 0.292245 | 0.070147 |
| C | -0.006378 | -3.376523 | -1.903922 |
| C | -1.091942 | -3.117557 | 0.969009 |
| C | -2.756084 | -2.131049 | -1.370961 |
| C | -1.761634 | 0.553477 | 0.339379 |
| C | -2.388119 | 0.256036 | 1.548953 |
| C | -3.766675 | 0.408653 | 1.689562 |
| C | -4.532846 | 0.865982 | 0.625486 |
| C | -3.915437 | 1.169700 | -0.585709 |
| C | -2.544820 | 1.009734 | -0.725942 |
| C | 0.374802 | 1.440339 | -0.705141 |
| C | 1.430707 | 1.170548 | -1.576607 |
| C | 2.097466 | 2.208695 | -2.221406 |
| C | 1.710535 | 3.527625 | -2.009935 |
| C | 0.644997 | 3.802892 | -1.158072 |
| C | -0.018863 | 2.766446 | -0.510989 |
| C | 2.363257 | -1.380363 | 0.687400 |
| C | 3.699692 | -1.655307 | 0.406502 |
| H | 0.094086 | -0.825157 | 1.883385 |
| H | 0.574998 | 0.892223 | 3.393596 |
| H | -0.280950 | 1.924496 | 2.250708 |
| H | 1.764303 | 2.765025 | 1.321392 |
| H | 2.328071 | 2.428955 | 2.957705 |
| H | 3.384501 | 1.215238 | 0.625720 |
| H | 3.527963 | 0.519000 | 2.257304 |
| H | 0.058479 | -2.897839 | -2.883961 |
| H | -0.473442 | -4.355912 | -2.035131 |
| H | 1.010928 | -3.537120 | -1.539371 |
| H | -0.114993 | -3.302978 | 1.422559 |
| H | -1.586961 | -4.088040 | 0.864756 |
| H | -1.690461 | -2.522899 | 1.663824 |
| H | -3.415594 | -1.670695 | -0.631621 |
| H | -3.146942 | -3.126570 | -1.603522 |
| H | -2.789177 | -1.532890 | -2.284160 |
| H | -1.823403 | -0.091674 | 2.405909 |
| H | -4.235244 | 0.173565 | 2.637436 |
| H | -5.603498 | 0.987552 | 0.738114 |
| H | -4.504033 | 1.521914 | -1.424282 |
| H | -2.073364 | 1.229647 | -1.677259 |
| H | 1.719280 | 0.142122 | -1.757809 |

| | | | |
|---|---|---|---|
| H | 2.916185 | 1.983297 | -2.894382 |
| H | 2.227692 | 4.335351 | -2.513970 |
| H | 0.326431 | 4.825742 | -0.996892 |
| H | -0.849185 | 2.996394 | 0.147209 |
| H | 1.615456 | -2.148156 | 0.540795 |
| H | 4.442754 | -0.876969 | 0.535199 |
| C | 4.152176 | -2.978644 | -0.071241 |
| H | 4.618070 | -2.874676 | -1.056842 |
| H | 4.929745 | -3.364713 | 0.594965 |
| H | 3.338523 | -3.699500 | -0.131522 |

**13E-*Z***

Imaginary frequency: None

Electronic energies: -1314.447514

Free energies: -1314.014680

Corrected Free energies: -1314.010655

| | | | |
|---|---|---|---|
| Si | -1.342076 | -2.217023 | -0.732367 |
| O | -0.312436 | -0.890689 | -0.736819 |
| N | 1.839310 | -0.588747 | 1.063205 |
| C | 0.505854 | -0.081756 | 1.371177 |
| C | 0.752941 | 1.095365 | 2.332552 |
| C | 2.215388 | 1.491768 | 2.098465 |
| C | 2.890488 | 0.171309 | 1.745952 |
| C | -0.265174 | 0.287442 | 0.060667 |
| C | -0.386821 | -3.494179 | -1.704518 |
| C | -1.746476 | -2.871491 | 0.980593 |
| C | -2.968953 | -1.843835 | -1.583203 |
| C | -1.696452 | 0.770912 | 0.316717 |
| C | -2.340973 | 0.656142 | 1.547985 |
| C | -3.677329 | 1.029562 | 1.689470 |
| C | -4.384339 | 1.529821 | 0.603888 |
| C | -3.748974 | 1.654606 | -0.630135 |
| C | -2.421854 | 1.274300 | -0.768309 |
| C | 0.551335 | 1.326181 | -0.703262 |
| C | 1.598252 | 0.900406 | -1.523238 |
| C | 2.434912 | 1.825074 | -2.139749 |
| C | 2.236607 | 3.189859 | -1.946571 |
| C | 1.188211 | 3.622579 | -1.141534 |
| C | 0.350382 | 2.696098 | -0.526498 |
| C | 2.010524 | -1.941151 | 0.806445 |
| C | 3.100947 | -2.525688 | 0.290583 |
| H | -0.079349 | -0.872354 | 1.856547 |
| H | 0.619090 | 0.748814 | 3.360225 |

| | | | |
|---|---|---|---|
| H | 0.062568 | 1.923341 | 2.169116 |
| H | 2.293334 | 2.181940 | 1.256509 |
| H | 2.665663 | 1.961742 | 2.972832 |
| H | 3.761672 | 0.324167 | 1.108090 |
| H | 3.219868 | -0.368205 | 2.645522 |
| H | -0.204173 | -3.146889 | -2.724657 |
| H | -0.943678 | -4.433235 | -1.760943 |
| H | 0.580502 | -3.692389 | -1.235766 |
| H | -0.878225 | -3.239572 | 1.530198 |
| H | -2.434995 | -3.713452 | 0.853673 |
| H | -2.255670 | -2.125325 | 1.595129 |
| H | -3.632632 | -1.254355 | -0.946125 |
| H | -3.471198 | -2.786556 | -1.820863 |
| H | -2.817384 | -1.295548 | -2.516301 |
| H | -1.816385 | 0.275399 | 2.416228 |
| H | -4.159671 | 0.930026 | 2.654757 |
| H | -5.421264 | 1.823116 | 0.716403 |
| H | -4.290827 | 2.041700 | -1.485085 |
| H | -1.934326 | 1.361154 | -1.733580 |
| H | 1.748525 | -0.162389 | -1.666096 |
| H | 3.245048 | 1.479205 | -2.771806 |
| H | 2.889777 | 3.909992 | -2.425343 |
| H | 1.017795 | 4.682299 | -0.991483 |
| H | -0.463903 | 3.048613 | 0.096599 |
| H | 1.157405 | -2.563877 | 1.067454 |
| H | 3.087639 | -3.608504 | 0.231309 |
| C | 4.303404 | -1.809543 | -0.261347 |
| H | 5.062057 | -1.596741 | 0.500042 |
| H | 4.782768 | -2.413419 | -1.033874 |
| H | 4.011930 | -0.856316 | -0.710235 |

**13E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1314.262456

Free energies: -1313.828740

Corrected Free energies: -1313.824956

| | | | |
|---|---|---|---|
| Si | 1.663558 | 2.146960 | -0.609643 |
| O | 0.424274 | 0.996178 | -0.592977 |
| N | -1.753738 | 0.615761 | 1.212991 |
| C | -0.403853 | 0.076913 | 1.453307 |
| C | -0.634292 | -1.103082 | 2.406374 |
| C | -2.143019 | -1.432067 | 2.369525 |
| C | -2.799094 | -0.397503 | 1.446867 |

| | | | |
|---|---|---|---|
| C | 0.263098 | -0.243287 | 0.061955 |
| C | 0.935667 | 3.480265 | -1.690887 |
| C | 1.992058 | 2.806909 | 1.114115 |
| C | 3.252674 | 1.493461 | -1.340215 |
| C | 1.619515 | -0.928948 | 0.237896 |
| C | 2.373911 | -0.807462 | 1.405068 |
| C | 3.662790 | -1.330660 | 1.473369 |
| C | 4.211315 | -1.983066 | 0.375671 |
| C | 3.463586 | -2.114011 | -0.791274 |
| C | 2.179486 | -1.589338 | -0.858701 |
| C | -0.714555 | -1.078653 | -0.766982 |
| C | -1.532376 | -0.451439 | -1.707731 |
| C | -2.522634 | -1.169262 | -2.372691 |
| C | -2.705904 | -2.522431 | -2.106437 |
| C | -1.875325 | -3.160234 | -1.189974 |
| C | -0.881548 | -2.444863 | -0.528976 |
| C | -1.938034 | 1.868341 | 0.843858 |
| C | -3.118651 | 2.456368 | 0.380872 |
| H | 0.187107 | 0.871269 | 1.911260 |
| H | -0.335029 | -0.808157 | 3.411447 |
| H | -0.024966 | -1.959849 | 2.127692 |
| H | -2.324013 | -2.435237 | 1.987937 |
| H | -2.570928 | -1.368909 | 3.368253 |
| H | -3.087221 | -0.837285 | 0.488962 |
| H | -3.662755 | 0.089765 | 1.894310 |
| H | 0.756253 | 3.100520 | -2.699681 |
| H | 1.620848 | 4.328494 | -1.764603 |
| H | -0.013751 | 3.846750 | -1.292034 |
| H | 1.099435 | 3.218911 | 1.592366 |
| H | 2.716894 | 3.622742 | 1.031449 |
| H | 2.426615 | 2.055144 | 1.777428 |
| H | 3.770294 | 0.809552 | -0.663328 |
| H | 3.915005 | 2.341405 | -1.539945 |
| H | 3.075185 | 0.974119 | -2.284757 |
| H | 1.974252 | -0.310890 | 2.281426 |
| H | 4.232732 | -1.228901 | 2.388874 |
| H | 5.213533 | -2.390655 | 0.430341 |
| H | 3.883155 | -2.619619 | -1.652647 |
| H | 1.608520 | -1.682053 | -1.775786 |
| H | -1.390588 | 0.602085 | -1.912293 |
| H | -3.151528 | -0.667707 | -3.098765 |
| H | -3.480722 | -3.079207 | -2.619507 |
| H | -1.995528 | -4.218321 | -0.990857 |
| H | -0.229880 | -2.962942 | 0.165660 |

| | | | |
|---|---|---|---|
| H | -1.056474 | 2.494694 | 0.900484 |
| H | -3.052095 | 3.530293 | 0.253414 |
| C | -4.397920 | 1.805310 | 0.005291 |
| H | -5.065657 | 1.753850 | 0.874695 |
| H | -4.904000 | 2.410176 | -0.746141 |
| H | -4.263895 | 0.795205 | -0.379573 |

**14E-*E***

Imaginary frequency: None

Electronic energies: -2662.631154

Free energies: -2662.201175

Corrected Free energies: -2662.190914

| | | | |
|---|---|---|---|
| Si | 0.800953 | -2.707735 | 1.642637 |
| O | -0.215268 | -1.549247 | 0.951092 |
| N | -1.753273 | -2.040072 | -1.392475 |
| C | -0.410677 | -1.496826 | -1.457411 |
| C | -0.426624 | -0.665921 | -2.754305 |
| C | -1.903673 | -0.306959 | -2.989327 |
| C | -2.684001 | -1.455183 | -2.345419 |
| C | -0.054960 | -0.686440 | -0.160779 |
| C | -0.364905 | -3.662530 | 2.739939 |
| C | 1.610580 | -3.813441 | 0.362090 |
| C | 2.167595 | -1.930021 | 2.659265 |
| C | 1.376201 | -0.146449 | -0.156575 |
| C | 2.346863 | -0.543220 | -1.067233 |
| C | 3.666867 | -0.117559 | -0.919082 |
| C | 4.041292 | 0.714645 | 0.120556 |
| C | 3.063454 | 1.119782 | 1.024629 |
| C | 1.752204 | 0.696794 | 0.893767 |
| C | -1.082522 | 0.428557 | -0.008332 |
| C | -2.338224 | 0.100270 | 0.494742 |
| C | -3.357975 | 1.045044 | 0.497385 |
| C | -3.147507 | 2.331816 | 0.026242 |
| C | -1.882517 | 2.661533 | -0.445874 |
| C | -0.856950 | 1.724932 | -0.469038 |
| C | -2.070575 | -3.202694 | -0.729167 |
| C | -3.285327 | -3.769314 | -0.659700 |
| H | 0.311563 | -2.318225 | -1.515883 |
| H | -0.059431 | -1.290872 | -3.570904 |
| H | 0.209854 | 0.219311 | -2.704679 |
| H | -2.157530 | 0.638463 | -2.509196 |
| H | -2.130588 | -0.209615 | -4.050286 |

| | | | |
|---|---|---|---|
| H | -3.590800 | -1.101689 | -1.841513 |
| H | -2.986781 | -2.217166 | -3.076543 |
| H | -0.772614 | -3.011342 | 3.517075 |
| H | 0.155622 | -4.489497 | 3.229426 |
| H | -1.202542 | -4.073048 | 2.170807 |
| H | 0.904846 | -4.370781 | -0.256945 |
| H | 2.225213 | -4.543718 | 0.898054 |
| H | 2.280074 | -3.251464 | -0.295055 |
| H | 2.993124 | -1.579135 | 2.034862 |
| H | 2.565572 | -2.688488 | 3.340139 |
| H | 1.810091 | -1.091472 | 3.261795 |
| H | 2.102815 | -1.195622 | -1.897601 |
| H | 5.069277 | 1.032887 | 0.235342 |
| H | 1.013187 | 1.001341 | 1.627503 |
| H | 0.109995 | 2.010046 | -0.866947 |
| H | -1.230811 | -3.677941 | -0.232909 |
| H | -4.133150 | -3.287648 | -1.137365 |
| C | -3.538135 | -5.062319 | 0.063435 |
| H | -4.257156 | -4.936952 | 0.878769 |
| H | -3.947263 | -5.825420 | -0.605561 |
| H | -2.613382 | -5.458783 | 0.490220 |
| C | 4.676114 | -0.606623 | -1.916677 |
| C | 3.433205 | 2.039663 | 2.151764 |
| F | 4.372270 | -0.208308 | -3.160991 |
| F | 4.720309 | -1.948502 | -1.946464 |
| F | 5.911136 | -0.173197 | -1.649304 |
| F | 3.271970 | 3.328121 | 1.813656 |
| F | 4.712417 | 1.891159 | 2.517512 |
| F | 2.677646 | 1.826003 | 3.237074 |
| H | -3.948016 | 3.060863 | 0.024391 |
| H | -2.518076 | -0.903925 | 0.861325 |
| C | -1.629826 | 4.066495 | -0.907139 |
| C | -4.702321 | 0.622399 | 1.011632 |
| F | -2.671469 | 4.557716 | -1.593440 |
| F | -1.425658 | 4.898986 | 0.126892 |
| F | -0.552875 | 4.155796 | -1.696713 |
| F | -4.639948 | 0.223170 | 2.290739 |
| F | -5.189852 | -0.417924 | 0.313762 |
| F | -5.608980 | 1.602987 | 0.944725 |

**14E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -2662.440699

Free energies: -2662.008010

Corrected Free energies: -2661.998441

| | | | |
|---|---|---|---|
| Si | 0.953332 | -2.721609 | 1.555359 |
| O | -0.148813 | -1.650088 | 0.817945 |
| N | -1.629137 | -2.012310 | -1.603261 |
| C | -0.259587 | -1.469743 | -1.578316 |
| C | -0.192857 | -0.628503 | -2.860715 |
| C | -1.641362 | -0.229268 | -3.196310 |
| C | -2.526135 | -1.281499 | -2.522989 |
| C | -0.010385 | -0.713123 | -0.222577 |
| C | -0.149539 | -3.656143 | 2.727125 |
| C | 1.720496 | -3.850675 | 0.272636 |
| C | 2.316245 | -1.842455 | 2.481540 |
| C | 1.388868 | -0.095538 | -0.170646 |
| C | 2.432548 | -0.506241 | -0.992244 |
| C | 3.720429 | -0.017959 | -0.785779 |
| C | 3.992502 | 0.887884 | 0.226133 |
| C | 2.943528 | 1.301435 | 1.038590 |
| C | 1.658824 | 0.818428 | 0.849366 |
| C | -1.104162 | 0.338829 | -0.037533 |
| C | -2.278685 | -0.017482 | 0.619411 |
| C | -3.343694 | 0.872079 | 0.678549 |
| C | -3.254553 | 2.139834 | 0.121814 |
| C | -2.064794 | 2.503068 | -0.493537 |
| C | -0.996828 | 1.617408 | -0.579050 |
| C | -2.001019 | -3.069212 | -0.905205 |
| C | -3.309657 | -3.547568 | -0.863665 |
| H | 0.425497 | -2.319349 | -1.599800 |
| H | 0.222228 | -1.247450 | -3.656617 |
| H | 0.455462 | 0.239715 | -2.748828 |
| H | -1.878733 | 0.762467 | -2.819371 |
| H | -1.805061 | -0.222404 | -4.271592 |
| H | -3.348154 | -0.846658 | -1.949908 |
| H | -2.931820 | -2.003891 | -3.232918 |
| H | -0.580554 | -2.976607 | 3.466110 |
| H | 0.426763 | -4.416148 | 3.260499 |
| H | -0.969939 | -4.158667 | 2.209695 |
| H | 0.988814 | -4.391727 | -0.332419 |
| H | 2.316424 | -4.600571 | 0.801793 |
| H | 2.401620 | -3.318460 | -0.396905 |
| H | 3.092323 | -1.456728 | 1.815804 |
| H | 2.785777 | -2.570069 | 3.150682 |
| H | 1.940719 | -1.019285 | 3.093317 |
| H | 2.274410 | -1.211376 | -1.800534 |

| | | | |
|---|---|---|---|
| H | 4.995827 | 1.262123 | 0.380928 |
| H | 0.862414 | 1.142067 | 1.511580 |
| H | -0.084920 | 1.931552 | -1.077405 |
| H | -1.228123 | -3.570176 | -0.336376 |
| H | -4.084375 | -3.031253 | -1.418292 |
| C | -3.692184 | -4.732104 | -0.069597 |
| H | -4.418344 | -4.436913 | 0.695911 |
| H | -4.203248 | -5.457271 | -0.709999 |
| H | -2.837238 | -5.207101 | 0.408434 |
| C | 4.810300 | -0.509115 | -1.695369 |
| C | 3.193371 | 2.229558 | 2.192762 |
| F | 4.599580 | -0.131171 | -2.964262 |
| F | 4.867895 | -1.850114 | -1.700138 |
| F | 6.014058 | -0.056525 | -1.337618 |
| F | 2.252994 | 3.179402 | 2.273814 |
| F | 4.378766 | 2.839249 | 2.106190 |
| F | 3.173300 | 1.566776 | 3.360572 |
| H | -4.087985 | 2.828026 | 0.169787 |
| H | -2.357037 | -0.995157 | 1.081062 |
| C | -1.909462 | 3.854439 | -1.129283 |
| C | -4.612840 | 0.395997 | 1.323804 |
| F | -2.978067 | 4.632101 | -0.940045 |
| F | -0.843573 | 4.507704 | -0.647565 |
| F | -1.724442 | 3.745342 | -2.455332 |
| F | -4.410783 | 0.003587 | 2.588594 |
| F | -5.112175 | -0.667752 | 0.669225 |
| F | -5.562125 | 1.334371 | 1.339466 |

**14E-*Z***

Imaginary frequency: None

Electronic energies: -2662.628068

Free energies: -2662.196762

Corrected Free energies: -2662.186564

| | | | |
|---|---|---|---|
| Si | 0.888816 | -2.796937 | 1.596362 |
| O | -0.152334 | -1.635595 | 0.949180 |
| N | -1.719194 | -2.068938 | -1.345356 |
| C | -0.382478 | -1.499303 | -1.446005 |
| C | -0.419492 | -0.635102 | -2.720048 |
| C | -1.908167 | -0.359623 | -2.969089 |
| C | -2.609871 | -1.595909 | -2.413227 |
| C | -0.019932 | -0.730031 | -0.129275 |
| C | -0.263391 | -3.907965 | 2.550646 |
| C | 1.832851 | -3.761906 | 0.293991 |

| | | | |
|---|---|---|---|
| C | 2.144620 | -2.012273 | 2.744815 |
| C | 1.399073 | -0.159335 | -0.126531 |
| C | 2.357264 | -0.477124 | -1.079552 |
| C | 3.666665 | -0.016039 | -0.941300 |
| C | 4.040879 | 0.774190 | 0.130376 |
| C | 3.074653 | 1.099978 | 1.078343 |
| C | 1.774707 | 0.641146 | 0.957301 |
| C | -1.063569 | 0.361703 | 0.064251 |
| C | -2.299527 | 0.005299 | 0.609307 |
| C | -3.336758 | 0.924070 | 0.635370 |
| C | -3.173230 | 2.214259 | 0.137656 |
| C | -1.936124 | 2.568215 | -0.371492 |
| C | -0.883605 | 1.654680 | -0.409267 |
| C | -1.866981 | -3.353907 | -0.832766 |
| C | -3.013743 | -3.944756 | -0.474317 |
| H | 0.353425 | -2.307801 | -1.535213 |
| H | -0.002420 | -1.211941 | -3.548484 |
| H | 0.162230 | 0.284320 | -2.634077 |
| H | -2.233623 | 0.532121 | -2.430257 |
| H | -2.127126 | -0.209444 | -4.025762 |
| H | -3.602894 | -1.350720 | -2.032075 |
| H | -2.723279 | -2.377500 | -3.175930 |
| H | -0.775713 | -3.348250 | 3.337112 |
| H | 0.290374 | -4.724391 | 3.021356 |
| H | -1.020681 | -4.336822 | 1.890082 |
| H | 1.196752 | -4.365952 | -0.355390 |
| H | 2.503083 | -4.447625 | 0.822705 |
| H | 2.459427 | -3.119420 | -0.329903 |
| H | 2.986393 | -1.576626 | 2.201211 |
| H | 2.541182 | -2.785379 | 3.409693 |
| H | 1.695594 | -1.233041 | 3.365784 |
| H | 2.112543 | -1.095907 | -1.935438 |
| H | 5.060843 | 1.120499 | 0.235930 |
| H | 1.044179 | 0.882310 | 1.722263 |
| H | 0.069145 | 1.962882 | -0.827289 |
| H | -0.938496 | -3.912352 | -0.737193 |
| H | -2.944031 | -4.982002 | -0.165434 |
| C | -4.366356 | -3.290736 | -0.415790 |
| H | -4.908625 | -3.348725 | -1.365712 |
| H | -4.987269 | -3.772087 | 0.341574 |
| H | -4.280057 | -2.234538 | -0.153955 |
| C | 4.665272 | -0.424104 | -1.984370 |
| C | 3.448646 | 1.975160 | 2.239144 |
| F | 4.316899 | 0.019255 | -3.201658 |

| | | | |
|---|---|---|---|
| F | 4.752483 | -1.760943 | -2.077198 |
| F | 5.892122 | 0.037803 | -1.727035 |
| F | 3.311371 | 3.276833 | 1.942741 |
| F | 4.723326 | 1.794645 | 2.607993 |
| F | 2.683004 | 1.737416 | 3.311644 |
| H | -3.989307 | 2.925292 | 0.158539 |
| H | -2.430320 | -0.994175 | 1.003418 |
| C | -1.708165 | 3.931361 | -0.952349 |
| C | -4.685614 | 0.501382 | 1.135607 |
| F | -2.746633 | 4.750945 | -0.759508 |
| F | -0.626139 | 4.524220 | -0.425647 |
| F | -1.497256 | 3.865398 | -2.278333 |
| F | -4.609161 | -0.507644 | 2.012004 |
| F | -5.468385 | 0.074820 | 0.125652 |
| F | -5.343573 | 1.504110 | 1.730332 |

**14E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -2662.435915

Free energies: -2662.003389

Corrected Free energies: -2661.993533

| | | | |
|---|---|---|---|
| Si | 1.101834 | -2.717233 | 1.605201 |
| O | -0.044053 | -1.715237 | 0.843145 |
| N | -1.531089 | -2.125064 | -1.551360 |
| C | -0.168901 | -1.561610 | -1.543313 |
| C | -0.096169 | -0.762096 | -2.849745 |
| C | -1.548695 | -0.466361 | -3.278649 |
| C | -2.452577 | -1.339427 | -2.397263 |
| C | 0.046555 | -0.776922 | -0.198364 |
| C | 0.026580 | -3.720116 | 2.745814 |
| C | 1.970096 | -3.807713 | 0.354512 |
| C | 2.376478 | -1.737491 | 2.554329 |
| C | 1.409989 | -0.083071 | -0.155617 |
| C | 2.479815 | -0.471794 | -0.953302 |
| C | 3.738800 | 0.092412 | -0.760251 |
| C | 3.954266 | 1.049636 | 0.216592 |
| C | 2.878397 | 1.440322 | 1.006515 |
| C | 1.621896 | 0.885351 | 0.828385 |
| C | -1.096545 | 0.221398 | -0.017084 |
| C | -2.178152 | -0.108002 | 0.794939 |
| C | -3.272821 | 0.745519 | 0.875820 |
| C | -3.313553 | 1.935006 | 0.162623 |
| C | -2.219289 | 2.266867 | -0.624574 |

| | | | |
|---|---|---|---|
| C | -1.114502 | 1.428856 | -0.711072 |
| C | -1.816712 | -3.232599 | -0.893079 |
| C | -3.070221 | -3.822938 | -0.700275 |
| H | 0.530637 | -2.399030 | -1.532781 |
| H | 0.401529 | -1.374760 | -3.601017 |
| H | 0.489010 | 0.149069 | -2.737547 |
| H | -1.799978 | 0.583968 | -3.144193 |
| H | -1.694022 | -0.709250 | -4.328807 |
| H | -3.097331 | -0.735626 | -1.754590 |
| H | -3.068197 | -2.031142 | -2.969170 |
| H | -0.473265 | -3.071614 | 3.469076 |
| H | 0.630857 | -4.443568 | 3.298486 |
| H | -0.740302 | -4.270650 | 2.195323 |
| H | 1.289598 | -4.420103 | -0.242672 |
| H | 2.614156 | -4.496644 | 0.910009 |
| H | 2.617878 | -3.244533 | -0.322114 |
| H | 3.134682 | -1.298061 | 1.901379 |
| H | 2.885673 | -2.419495 | 3.241976 |
| H | 1.922678 | -0.940060 | 3.147329 |
| H | 2.363552 | -1.215809 | -1.733502 |
| H | 4.935524 | 1.483169 | 0.360736 |
| H | 0.803480 | 1.195800 | 1.469010 |
| H | -0.266556 | 1.732204 | -1.316645 |
| H | -0.962560 | -3.730549 | -0.451951 |
| H | -3.019546 | -4.788282 | -0.210457 |
| C | -4.418826 | -3.316986 | -1.049864 |
| H | -4.691179 | -3.659817 | -2.056726 |
| H | -5.151449 | -3.740078 | -0.363449 |
| H | -4.496667 | -2.232897 | -1.029488 |
| C | 4.857782 | -0.362364 | -1.653072 |
| C | 3.090338 | 2.415074 | 2.129481 |
| F | 4.660063 | 0.021125 | -2.922597 |
| F | 4.952018 | -1.700944 | -1.667784 |
| F | 6.041896 | 0.120440 | -1.270158 |
| F | 2.021194 | 3.196676 | 2.318747 |
| F | 4.141972 | 3.211221 | 1.912533 |
| F | 3.314934 | 1.775452 | 3.288793 |
| H | -4.170224 | 2.592755 | 0.225804 |
| H | -2.157880 | -1.032865 | 1.359500 |
| C | -2.216788 | 3.526561 | -1.442160 |
| C | -4.432217 | 0.326034 | 1.733560 |
| F | -3.238712 | 4.331167 | -1.140937 |
| F | -1.086821 | 4.224746 | -1.272370 |
| F | -2.302391 | 3.249612 | -2.755104 |

| | | | |
|---|---|---|---|
| F | -4.038514 | 0.006218 | 2.973216 |
| F | -5.038573 | -0.763751 | 1.231674 |
| F | -5.359941 | 1.280837 | 1.838285 |

**15E-*E***

Imaginary frequency: None

Electronic energies: -655.140350

Free energies: -654.854195

Corrected Free energies: -654.852622

| | | | |
|---|---|---|---|
| C | 1.193348 | -1.616710 | 0.262374 |
| C | -0.317033 | -1.502533 | 0.426831 |
| C | 0.580827 | 0.453255 | -0.660832 |
| H | -0.549490 | -1.314086 | 1.486561 |
| H | 0.621904 | 0.753251 | -1.716952 |
| N | -0.611059 | -0.363227 | -0.422228 |
| C | -1.884924 | 0.152862 | -0.578914 |
| C | -2.978845 | -0.174345 | 0.119202 |
| H | -1.961123 | 0.868702 | -1.395395 |
| C | -4.340805 | 0.371538 | -0.200143 |
| H | -4.788398 | 0.858086 | 0.671053 |
| H | -4.285914 | 1.106478 | -1.006609 |
| H | -5.031742 | -0.417019 | -0.513708 |
| H | -2.900480 | -0.871914 | 0.947948 |
| N | 1.634360 | -0.519890 | -0.389040 |
| O | 1.879396 | -2.564358 | 0.600997 |
| C | 2.978680 | -0.482028 | -0.940005 |
| H | 3.725305 | -0.276138 | -0.170766 |
| H | 3.202677 | -1.451525 | -1.388147 |
| H | 3.033673 | 0.290904 | -1.703995 |
| C | -0.974316 | -2.802740 | -0.026330 |
| H | -2.054799 | -2.776765 | 0.102273 |
| H | -0.749858 | -2.979344 | -1.080313 |
| H | -0.566648 | -3.624734 | 0.563242 |
| C | 0.701406 | 1.734552 | 0.220684 |
| C | 0.450002 | 1.390312 | 1.690335 |
| H | 1.143930 | 0.622707 | 2.045478 |
| H | 0.594049 | 2.280323 | 2.308430 |
| H | -0.573739 | 1.036893 | 1.840037 |
| C | 2.107121 | 2.328406 | 0.063873 |
| H | 2.348404 | 2.515739 | -0.987124 |
| H | 2.156874 | 3.283585 | 0.591495 |
| H | 2.871456 | 1.676427 | 0.488606 |
| C | -0.309569 | 2.795029 | -0.238231 |

| | | | |
|---|---|---|---|
| H | -0.093742 | 3.739210 | 0.267969 |
| H | -0.239746 | 2.970274 | -1.316400 |
| H | -1.336215 | 2.520036 | 0.004144 |

**15E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -654.945740

Free energies: -654.659071

Corrected Free energies: -654.657517

| | | | |
|---|---|---|---|
| C | -0.963949 | 1.739482 | 0.236688 |
| C | 0.493998 | 1.414276 | 0.570353 |
| C | -0.604125 | -0.420306 | -0.615914 |
| H | 0.593497 | 1.222937 | 1.643420 |
| H | -0.517895 | -0.718835 | -1.665966 |
| N | 0.688443 | 0.158933 | -0.177401 |
| C | 1.837158 | -0.406348 | -0.500309 |
| C | 3.071668 | -0.094874 | 0.065285 |
| H | 1.778402 | -1.196589 | -1.242288 |
| C | 4.327902 | -0.719057 | -0.393862 |
| H | 4.820459 | -1.216117 | 0.447555 |
| H | 4.169332 | -1.432364 | -1.200442 |
| H | 5.017917 | 0.061977 | -0.730983 |
| H | 3.116650 | 0.593871 | 0.899485 |
| N | -1.486755 | 0.718946 | -0.475707 |
| O | -1.516004 | 2.779990 | 0.512720 |
| C | -2.770431 | 0.864470 | -1.149988 |
| H | -3.601694 | 0.712228 | -0.460745 |
| H | -2.829921 | 1.874160 | -1.555852 |
| H | -2.834692 | 0.140836 | -1.960473 |
| C | 1.376863 | 2.574493 | 0.118827 |
| H | 2.395316 | 2.506798 | 0.491184 |
| H | 1.389233 | 2.638535 | -0.970374 |
| H | 0.928027 | 3.484141 | 0.517516 |
| C | -1.000828 | -1.652341 | 0.252774 |
| C | -1.040107 | -1.278618 | 1.735940 |
| H | -1.716967 | -0.441006 | 1.922919 |
| H | -1.403034 | -2.132579 | 2.311490 |
| H | -0.046675 | -1.028327 | 2.118303 |
| C | -2.390314 | -2.119143 | -0.202746 |
| H | -2.420213 | -2.303123 | -1.280226 |
| H | -2.628265 | -3.056537 | 0.303164 |
| H | -3.167055 | -1.399918 | 0.056745 |
| C | -0.008034 | -2.798428 | 0.029022 |

| | | | |
|---|---|---|---|
| H | -0.390486 | -3.695061 | 0.520031 |
| H | 0.112198 | -3.027315 | -1.033933 |
| H | 0.973275 | -2.594420 | 0.463040 |

**15E-*Z***

Imaginary frequency: None

Electronic energies: -655.140141

Free energies: -654.853304

Corrected Free energies: -654.851595

| | | | |
|---|---|---|---|
| C | -0.238797 | 1.888811 | 0.306129 |
| C | 1.078121 | 1.131475 | 0.349211 |
| C | -0.681752 | -0.231082 | -0.607353 |
| H | 1.384207 | 1.021957 | 1.396896 |
| H | -0.796825 | -0.426151 | -1.685695 |
| N | 0.732776 | -0.155775 | -0.254431 |
| C | 1.653079 | -0.869791 | -1.029724 |
| C | 2.849995 | -1.262428 | -0.585308 |
| H | 1.332400 | -1.105922 | -2.044017 |
| N | -1.157704 | 1.112023 | -0.300884 |
| O | -0.412271 | 3.029338 | 0.700258 |
| C | -2.469414 | 1.628321 | -0.639520 |
| H | -3.190432 | 1.477353 | 0.167695 |
| H | -2.373122 | 2.698608 | -0.820664 |
| H | -2.832614 | 1.136072 | -1.541585 |
| C | 2.127664 | 1.946136 | -0.404262 |
| H | 3.098985 | 1.453924 | -0.397310 |
| H | 1.817993 | 2.090552 | -1.442359 |
| H | 2.218557 | 2.920916 | 0.076445 |
| C | -1.424908 | -1.354321 | 0.170635 |
| C | -1.435637 | -1.029896 | 1.664672 |
| H | -2.004195 | -0.119498 | 1.873218 |
| H | -1.894893 | -1.849916 | 2.222682 |
| H | -0.415452 | -0.895250 | 2.036033 |
| C | -2.858635 | -1.520117 | -0.349759 |
| H | -2.873596 | -1.631805 | -1.438467 |
| H | -3.299308 | -2.421918 | 0.082551 |
| H | -3.502266 | -0.683063 | -0.079533 |
| C | -0.677878 | -2.673005 | -0.063239 |
| H | -1.229396 | -3.492465 | 0.404162 |
| H | -0.588524 | -2.893293 | -1.132287 |
| H | 0.325535 | -2.641978 | 0.364128 |
| H | 3.516585 | -1.747168 | -1.289519 |
| C | 3.300636 | -1.096204 | 0.836931 |

| | | | |
|---|---|---|---|
| H | 3.826891 | -0.150477 | 1.011318 |
| H | 2.436104 | -1.117114 | 1.506769 |
| H | 3.981191 | -1.899198 | 1.124198 |

**15E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -654.941477

Free energies: -654.653333

Corrected Free energies: -654.652042

| | | | |
|---|---|---|---|
| C | -0.330533 | 1.848871 | 0.295822 |
| C | 0.992232 | 1.086310 | 0.388283 |
| C | -0.767369 | -0.258556 | -0.644572 |
| H | 1.185048 | 0.828627 | 1.433264 |
| H | -0.925068 | -0.488025 | -1.703712 |
| N | 0.690101 | -0.127586 | -0.394289 |
| C | 1.541738 | -0.961388 | -0.963597 |
| C | 2.878753 | -1.193466 | -0.627873 |
| H | 1.120302 | -1.564244 | -1.762151 |
| N | -1.237354 | 1.075258 | -0.336285 |
| O | -0.490821 | 2.987358 | 0.672044 |
| C | -2.492856 | 1.640870 | -0.814698 |
| H | -3.230753 | 1.707239 | -0.014756 |
| H | -2.293977 | 2.642462 | -1.195816 |
| H | -2.882759 | 1.017069 | -1.616524 |
| C | 2.098758 | 1.948571 | -0.208359 |
| H | 3.086840 | 1.512059 | -0.094773 |
| H | 1.900534 | 2.128605 | -1.266210 |
| H | 2.078220 | 2.902208 | 0.318694 |
| C | -1.386768 | -1.383967 | 0.237190 |
| C | -1.067353 | -1.150089 | 1.715253 |
| H | -1.402353 | -0.165048 | 2.050971 |
| H | -1.587044 | -1.898488 | 2.316687 |
| H | 0.001829 | -1.253352 | 1.920012 |
| C | -2.906801 | -1.366763 | 0.027201 |
| H | -3.169884 | -1.438059 | -1.031841 |
| H | -3.342541 | -2.227347 | 0.538138 |
| H | -3.362820 | -0.469737 | 0.446458 |
| C | -0.849133 | -2.749455 | -0.204159 |
| H | -1.392664 | -3.530824 | 0.330195 |
| H | -0.996488 | -2.914240 | -1.275640 |
| H | 0.208673 | -2.882116 | 0.033085 |
| C | 3.602583 | -0.841438 | 0.612059 |
| H | 3.971373 | -1.773448 | 1.052892 |

| | | | |
|---|---|---|---|
| H | 4.495050 | -0.253741 | 0.372865 |
| H | 3.004819 | -0.318319 | 1.352448 |
| H | 3.411486 | -1.810843 | -1.341920 |

**16E-*Z***

Imaginary frequency: None

Electronic energies: -886.150853

Free energies: -885.788390

Corrected Free energies: -885.784937

| | | | |
|---|---|---|---|
| C | 0.539171 | 1.518599 | -0.616110 |
| C | -0.125248 | 0.160221 | -0.442804 |
| C | 2.277240 | -0.055529 | -0.467677 |
| H | -0.782567 | -0.005000 | -1.302400 |
| H | 2.887507 | -0.339733 | -1.335748 |
| N | 0.997532 | -0.776563 | -0.508354 |
| C | 0.932759 | -1.855239 | -1.403509 |
| C | -0.110661 | -2.654054 | -1.649089 |
| H | 1.863310 | -2.038467 | -1.934347 |
| N | 1.873113 | 1.337890 | -0.618267 |
| O | -0.037820 | 2.588990 | -0.719054 |
| C | 2.777485 | 2.441859 | -0.883551 |
| H | 3.664599 | 2.070731 | -1.395970 |
| H | 2.258736 | 3.155891 | -1.522678 |
| H | 3.077356 | 2.951289 | 0.034827 |
| C | -0.964546 | 0.127016 | 0.861831 |
| H | -0.746553 | -0.804547 | 1.385266 |
| H | -0.635036 | 0.937401 | 1.521234 |
| C | 3.101811 | -0.365709 | 0.807010 |
| C | 2.361008 | 0.104286 | 2.057456 |
| H | 1.410918 | -0.422190 | 2.168639 |
| H | 2.964409 | -0.098817 | 2.945763 |
| H | 2.162304 | 1.179517 | 2.021817 |
| C | 3.308673 | -1.884040 | 0.861355 |
| H | 3.826121 | -2.242857 | -0.034500 |
| H | 3.921611 | -2.141643 | 1.728349 |
| H | 2.355476 | -2.409415 | 0.942790 |
| C | 4.479090 | 0.306750 | 0.731548 |
| H | 5.113694 | -0.077462 | 1.533792 |
| H | 4.977000 | 0.091483 | -0.219034 |
| H | 4.419260 | 1.388528 | 0.854223 |
| C | -2.454910 | 0.246204 | 0.639256 |
| C | -2.979175 | 1.212310 | -0.223657 |
| C | -3.336847 | -0.612338 | 1.297565 |

| | | | |
|---|---|---|---|
| C | -4.352442 | 1.309260 | -0.427183 |
| H | -2.301247 | 1.892407 | -0.729457 |
| C | -4.710431 | -0.515738 | 1.096889 |
| H | -2.943245 | -1.368990 | 1.969039 |
| C | -5.222977 | 0.445469 | 0.230879 |
| H | -4.743468 | 2.062258 | -1.101801 |
| H | -5.379079 | -1.194526 | 1.613492 |
| H | -6.291853 | 0.519705 | 0.069436 |
| C | -1.441983 | -2.654062 | -0.949702 |
| H | -1.332340 | -2.405637 | 0.107370 |
| H | -2.156951 | -1.943932 | -1.377630 |
| H | -1.897229 | -3.643714 | -1.011812 |
| H | 0.047214 | -3.405066 | -2.414926 |

**16E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -885.950563

Free energies: -885.586573

Corrected Free energies: -885.583727

| | | | |
|---|---|---|---|
| C | 0.553293 | 1.556575 | -0.569201 |
| C | -0.120693 | 0.188228 | -0.524650 |
| C | 2.324563 | 0.001916 | -0.523188 |
| H | -0.747220 | 0.111572 | -1.415969 |
| H | 2.964032 | -0.253050 | -1.374491 |
| N | 1.028765 | -0.712520 | -0.697226 |
| C | 1.009664 | -1.953448 | -1.148561 |
| C | -0.081968 | -2.792939 | -1.398380 |
| H | 1.989657 | -2.368752 | -1.352100 |
| N | 1.890331 | 1.381551 | -0.618180 |
| O | -0.032716 | 2.616571 | -0.585503 |
| C | 2.773591 | 2.504987 | -0.905882 |
| H | 3.690517 | 2.131674 | -1.358328 |
| H | 2.262322 | 3.164951 | -1.605884 |
| H | 3.013547 | 3.066326 | -0.002418 |
| C | -0.953349 | -0.051515 | 0.756674 |
| H | -0.784957 | -1.075433 | 1.098337 |
| H | -0.582000 | 0.607092 | 1.546093 |
| C | 3.059594 | -0.367816 | 0.797371 |
| C | 2.208909 | -0.026355 | 2.020135 |
| H | 1.330600 | -0.671835 | 2.091495 |
| H | 2.800919 | -0.185267 | 2.923801 |
| H | 1.889017 | 1.019040 | 2.012285 |
| C | 3.403779 | -1.861809 | 0.810615 |

| | | | |
|---|---|---|---|
| H | 3.973013 | -2.155774 | -0.076238 |
| H | 4.025478 | -2.068300 | 1.683750 |
| H | 2.517291 | -2.494360 | 0.894641 |
| C | 4.373674 | 0.427154 | 0.838233 |
| H | 4.977667 | 0.063415 | 1.671392 |
| H | 4.953328 | 0.293785 | -0.079477 |
| H | 4.204109 | 1.491693 | 0.997892 |
| C | -2.439759 | 0.171101 | 0.573152 |
| C | -2.936792 | 1.215973 | -0.207102 |
| C | -3.340090 | -0.679609 | 1.217317 |
| C | -4.310069 | 1.399063 | -0.344732 |
| H | -2.249262 | 1.897757 | -0.696032 |
| C | -4.711356 | -0.492408 | 1.084783 |
| H | -2.965195 | -1.497409 | 1.824405 |
| C | -5.200581 | 0.547294 | 0.299685 |
| H | -4.682025 | 2.213089 | -0.955462 |
| H | -5.396650 | -1.163026 | 1.589327 |
| H | -6.268763 | 0.691662 | 0.190764 |
| C | -1.535633 | -2.601697 | -1.201910 |
| H | -1.808874 | -3.006758 | -0.216939 |
| H | -1.884552 | -1.574398 | -1.243466 |
| H | -2.077169 | -3.194230 | -1.939149 |
| H | 0.222555 | -3.767423 | -1.762520 |

**16E-*E***

Imaginary frequency: None

Electronic energies: -886.158003

Free energies: -885.794303

Corrected Free energies: -885.791481

| | | | |
|---|---|---|---|
| C | -1.422058 | 1.876637 | 0.530747 |
| C | -0.089412 | 1.152442 | 0.478794 |
| C | -1.923155 | -0.422448 | 0.473230 |
| H | 0.467000 | 1.414859 | 1.388051 |
| H | -2.258695 | -0.961470 | 1.370593 |
| N | -0.458709 | -0.256510 | 0.507978 |
| C | 0.242139 | -1.130483 | 1.348196 |
| C | 1.478454 | -0.988957 | 1.833860 |
| H | -0.317766 | -2.030235 | 1.589315 |
| C | 2.125758 | -2.027400 | 2.705255 |
| H | 1.445606 | -2.859307 | 2.900363 |
| H | 3.027922 | -2.431264 | 2.235307 |
| H | 2.430604 | -1.608167 | 3.668437 |
| H | 2.077840 | -0.122686 | 1.573494 |

| | | | |
|---|---|---|---|
| N | -2.403257 | 0.952602 | 0.545029 |
| O | -1.570952 | 3.085643 | 0.560064 |
| C | -3.787636 | 1.339176 | 0.743194 |
| H | -3.797226 | 2.268026 | 1.312788 |
| H | -4.303188 | 1.507428 | -0.205056 |
| H | -4.307707 | 0.561994 | 1.302842 |
| C | 0.713806 | 1.616275 | -0.749792 |
| H | 0.128160 | 1.417294 | -1.650195 |
| H | 0.828138 | 2.699833 | -0.661903 |
| C | -2.413258 | -1.216545 | -0.767300 |
| C | -3.920498 | -1.489950 | -0.666636 |
| H | -4.185478 | -1.906198 | 0.310228 |
| H | -4.519084 | -0.594881 | -0.836362 |
| H | -4.205658 | -2.220508 | -1.427599 |
| C | -2.105973 | -0.455834 | -2.055433 |
| H | -2.563978 | 0.537262 | -2.054912 |
| H | -1.028286 | -0.343823 | -2.188668 |
| H | -2.495192 | -1.007381 | -2.914880 |
| C | -1.686973 | -2.567453 | -0.785882 |
| H | -0.605988 | -2.437370 | -0.870426 |
| H | -1.900074 | -3.144797 | 0.119587 |
| H | -2.029690 | -3.153249 | -1.642152 |
| C | 2.060646 | 0.951799 | -0.834032 |
| C | 3.179087 | 1.547690 | -0.249367 |
| C | 2.198510 | -0.307344 | -1.420504 |
| C | 4.405569 | 0.890861 | -0.228699 |
| H | 3.082735 | 2.529602 | 0.203766 |
| C | 3.422525 | -0.966730 | -1.403167 |
| H | 1.334883 | -0.779024 | -1.877650 |
| C | 4.528427 | -0.372412 | -0.800421 |
| H | 5.264422 | 1.364662 | 0.232317 |
| H | 3.514694 | -1.946883 | -1.856870 |
| H | 5.481628 | -0.887452 | -0.784239 |

**16E-*E*** radical cation

Imaginary frequency: None

Electronic energies: -885.961292

Free energies: -885.597315

Corrected Free energies: -885.594675

| | | | |
|---|---|---|---|
| C | -1.502973 | 1.905093 | 0.413559 |
| C | -0.144881 | 1.218377 | 0.443810 |
| C | -1.984368 | -0.404614 | 0.557319 |
| H | 0.417030 | 1.603530 | 1.298519 |

| | | | |
|---|---|---|---|
| H | -2.335919 | -0.885177 | 1.477247 |
| N | -0.517727 | -0.175394 | 0.713032 |
| C | 0.248324 | -1.071329 | 1.316833 |
| C | 1.578362 | -0.880602 | 1.683238 |
| H | -0.229015 | -2.015765 | 1.553729 |
| C | 2.390257 | -1.954625 | 2.288686 |
| H | 1.829354 | -2.875823 | 2.435042 |
| H | 3.253729 | -2.152037 | 1.642279 |
| H | 2.798432 | -1.612315 | 3.244486 |
| H | 2.044537 | 0.086359 | 1.541714 |
| N | -2.468217 | 0.962922 | 0.497539 |
| O | -1.662973 | 3.101942 | 0.335100 |
| C | -3.859323 | 1.348981 | 0.694142 |
| H | -3.869050 | 2.287983 | 1.246053 |
| H | -4.372628 | 1.494166 | -0.257280 |
| H | -4.369651 | 0.580368 | 1.272394 |
| C | 0.636520 | 1.499934 | -0.858582 |
| H | 0.057986 | 1.157987 | -1.716239 |
| H | 0.687423 | 2.590241 | -0.912403 |
| C | -2.373809 | -1.305397 | -0.649114 |
| C | -3.893782 | -1.526641 | -0.599022 |
| H | -4.218475 | -1.872464 | 0.386049 |
| H | -4.450834 | -0.627454 | -0.859406 |
| H | -4.157952 | -2.296088 | -1.326836 |
| C | -1.993279 | -0.664623 | -1.982218 |
| H | -2.375211 | 0.355786 | -2.067516 |
| H | -0.911935 | -0.655477 | -2.127960 |
| H | -2.421986 | -1.251321 | -2.797245 |
| C | -1.693621 | -2.673895 | -0.522176 |
| H | -0.609213 | -2.614523 | -0.639072 |
| H | -1.927148 | -3.156441 | 0.431760 |
| H | -2.065378 | -3.322576 | -1.317343 |
| C | 2.018175 | 0.906029 | -0.852579 |
| C | 3.074834 | 1.599928 | -0.257994 |
| C | 2.248547 | -0.375942 | -1.355932 |
| C | 4.328715 | 1.010407 | -0.139990 |
| H | 2.908670 | 2.601303 | 0.126112 |
| C | 3.504274 | -0.966660 | -1.241860 |
| H | 1.444499 | -0.918475 | -1.842285 |
| C | 4.543413 | -0.278425 | -0.623752 |
| H | 5.138855 | 1.555861 | 0.328879 |
| H | 3.667575 | -1.963221 | -1.634222 |
| H | 5.519383 | -0.738644 | -0.527465 |

**17E-*E***

Imaginary frequency: None

Electronic energies: -807.556792

Free energies: -807.249203

Corrected Free energies: -807.246530

| | | | |
|---|---|---|---|
| C | 0.197356 | 1.603068 | 1.224521 |
| C | -0.695495 | 0.377942 | 1.325388 |
| C | -0.704801 | 1.269452 | -0.939009 |
| H | -1.508840 | 0.588383 | 2.034756 |
| N | -1.180803 | 0.224885 | -0.022401 |
| C | -2.242950 | -0.592916 | -0.340214 |
| C | -2.946614 | -1.364142 | 0.500730 |
| H | -2.488270 | -0.606435 | -1.399708 |
| C | -4.068036 | -2.253313 | 0.043511 |
| H | -3.859456 | -3.307385 | 0.250800 |
| H | -5.005047 | -2.009706 | 0.552929 |
| H | -4.235147 | -2.151114 | -1.031123 |
| H | -2.713616 | -1.365637 | 1.560994 |
| N | 0.166111 | 2.040734 | -0.048063 |
| O | 0.851669 | 2.071458 | 2.141386 |
| C | 0.987306 | 3.136308 | -0.518965 |
| H | 1.465252 | 3.582517 | 0.350751 |
| H | 1.756859 | 2.777791 | -1.206905 |
| H | 0.379404 | 3.890713 | -1.021028 |
| C | 0.128738 | -0.822649 | 1.847150 |
| H | 0.585282 | -0.507404 | 2.788507 |
| H | -0.539537 | -1.658140 | 2.058753 |
| C | 0.097050 | 0.670994 | -2.094958 |
| C | 1.177050 | -1.238556 | 0.849140 |
| C | 2.406627 | -0.578773 | 0.782776 |
| C | 0.902673 | -2.242499 | -0.081004 |
| C | 3.339937 | -0.914844 | -0.193854 |
| H | 2.624005 | 0.209127 | 1.497042 |
| C | 1.835541 | -2.585734 | -1.054216 |
| H | -0.058171 | -2.746830 | -0.043155 |
| C | 3.056805 | -1.919754 | -1.114938 |
| H | 4.290017 | -0.394554 | -0.232987 |
| H | 1.608804 | -3.369128 | -1.768255 |
| H | 3.784160 | -2.183621 | -1.873668 |
| H | 0.959934 | 0.128410 | -1.703802 |
| H | -0.531830 | -0.022966 | -2.656820 |
| H | 0.432464 | 1.451135 | -2.781983 |
| C | -1.848484 | 2.149858 | -1.449028 |

| | | | |
|---|---|---|---|
| H | -2.407901 | 2.555519 | -0.604112 |
| H | -1.460596 | 2.972445 | -2.052550 |
| H | -2.524486 | 1.569213 | -2.078448 |

**17E-*Z***

Imaginary frequency: None

Electronic energies: -807.552274

Free energies: -807.243153

Corrected Free energies: -807.241002

| | | | |
|---|---|---|---|
| C | -0.606805 | 1.318570 | 1.295054 |
| C | -1.005561 | -0.136259 | 1.127317 |
| C | -0.990919 | 1.016856 | -1.020340 |
| H | -1.881036 | -0.314603 | 1.760374 |
| N | -1.308279 | -0.219264 | -0.289376 |
| C | -1.517287 | -1.413169 | -0.965350 |
| C | -2.199688 | -2.471137 | -0.507172 |
| H | -1.061404 | -1.470498 | -1.950552 |
| N | -0.627547 | 1.906356 | 0.085478 |
| O | -0.297664 | 1.841610 | 2.353797 |
| C | -0.200555 | 3.274929 | -0.118149 |
| H | -0.187248 | 3.763597 | 0.854115 |
| H | 0.802997 | 3.313681 | -0.549996 |
| H | -0.895946 | 3.798733 | -0.775035 |
| C | 0.126575 | -1.064957 | 1.617961 |
| H | 0.307399 | -0.806940 | 2.664875 |
| H | -0.227161 | -2.097288 | 1.583207 |
| C | 1.390137 | -0.932721 | 0.806730 |
| C | 1.686231 | -1.862834 | -0.190592 |
| C | 2.261037 | 0.144420 | 0.997933 |
| C | 2.814295 | -1.716182 | -0.992022 |
| H | 1.014290 | -2.700534 | -0.345545 |
| C | 3.388380 | 0.295828 | 0.196426 |
| H | 2.047005 | 0.870420 | 1.775971 |
| C | 3.666002 | -0.631865 | -0.804867 |
| H | 3.026293 | -2.447449 | -1.763535 |
| H | 4.053219 | 1.136868 | 0.356001 |
| H | 4.543776 | -0.513569 | -1.429125 |
| C | -2.239245 | 1.524390 | -1.744225 |
| H | -2.565728 | 0.771377 | -2.465126 |
| H | -3.039716 | 1.690880 | -1.021722 |
| H | -2.039558 | 2.449300 | -2.288959 |
| C | 0.182571 | 0.889511 | -1.997192 |
| H | 1.077880 | 0.539790 | -1.481827 |

| | | | |
|---|---|---|---|
| H | -0.059222 | 0.203328 | -2.810063 |
| H | 0.385862 | 1.863032 | -2.449224 |
| C | -3.004513 | -2.512441 | 0.762109 |
| H | -3.748867 | -3.307875 | 0.711602 |
| H | -2.397208 | -2.697127 | 1.656353 |
| H | -3.533441 | -1.568359 | 0.915462 |
| H | -2.194015 | -3.356931 | -1.132053 |

**17E-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -807.356234

Free energies: -807.046207

Corrected Free energies: -807.044369

| | | | |
|---|---|---|---|
| C | -0.665174 | 1.322524 | 1.335608 |
| C | -1.037708 | -0.139894 | 1.140645 |
| C | -1.019420 | 1.089591 | -0.998678 |
| H | -1.958466 | -0.341228 | 1.690323 |
| N | -1.277758 | -0.220488 | -0.303781 |
| C | -1.633019 | -1.276172 | -1.007850 |
| C | -2.051740 | -2.539614 | -0.574823 |
| H | -1.608551 | -1.130209 | -2.082240 |
| N | -0.654533 | 1.928834 | 0.134463 |
| O | -0.384996 | 1.809236 | 2.410189 |
| C | -0.215328 | 3.303423 | -0.035659 |
| H | -0.163605 | 3.749549 | 0.954954 |
| H | 0.773367 | 3.337447 | -0.497921 |
| H | -0.926652 | 3.860362 | -0.645151 |
| C | 0.117156 | -1.041050 | 1.631894 |
| H | 0.297950 | -0.733338 | 2.664324 |
| H | -0.202485 | -2.081980 | 1.649969 |
| C | 1.360292 | -0.889625 | 0.791414 |
| C | 1.645148 | -1.822471 | -0.206994 |
| C | 2.214519 | 0.203957 | 0.959610 |
| C | 2.747450 | -1.657199 | -1.039894 |
| H | 1.003769 | -2.690035 | -0.329624 |
| C | 3.317215 | 0.370206 | 0.128056 |
| H | 2.012197 | 0.926416 | 1.744036 |
| C | 3.581767 | -0.555965 | -0.878233 |
| H | 2.954130 | -2.389369 | -1.811203 |
| H | 3.972608 | 1.221477 | 0.268249 |
| H | 4.439685 | -0.424029 | -1.526335 |
| C | -2.314953 | 1.569075 | -1.649915 |
| H | -2.615139 | 0.896362 | -2.454111 |

| | | | |
|---|---|---|---|
| H | -3.110423 | 1.628744 | -0.906672 |
| H | -2.155212 | 2.555521 | -2.086182 |
| C | 0.126866 | 0.976017 | -1.999970 |
| H | 1.042193 | 0.646146 | -1.507979 |
| H | -0.124352 | 0.289096 | -2.808577 |
| H | 0.292162 | 1.957698 | -2.446812 |
| C | -2.428780 | -3.045544 | 0.762447 |
| H | -3.406354 | -3.527910 | 0.672876 |
| H | -1.733274 | -3.840519 | 1.057173 |
| H | -2.477447 | -2.299558 | 1.547682 |
| H | -2.165831 | -3.246515 | -1.389005 |

**17E-*E*** radical cation

Imaginary frequency: -33.4822

Electronic energies: -807.362681

Free energies: -807.052718

Corrected Free energies: -807.051015

| | | | |
|---|---|---|---|
| C | 0.374211 | 1.648705 | 1.218866 |
| C | -0.680632 | 0.559616 | 1.359597 |
| C | -0.500921 | 1.357814 | -0.969597 |
| H | -1.468333 | 0.892427 | 2.039856 |
| N | -1.210183 | 0.457744 | -0.003112 |
| C | -2.223009 | -0.296326 | -0.381310 |
| C | -3.009908 | -1.055310 | 0.483332 |
| H | -2.453257 | -0.296074 | -1.442094 |
| C | -4.110513 | -1.914139 | 0.004093 |
| H | -3.908645 | -2.953017 | 0.287898 |
| H | -5.039605 | -1.636670 | 0.511144 |
| H | -4.248076 | -1.855475 | -1.073885 |
| H | -2.832833 | -1.002238 | 1.550956 |
| N | 0.447034 | 2.012094 | -0.076443 |
| O | 1.056777 | 2.051096 | 2.136395 |
| C | 1.457635 | 2.931396 | -0.570233 |
| H | 1.975783 | 3.333344 | 0.297540 |
| H | 2.173001 | 2.406712 | -1.206496 |
| H | 0.998936 | 3.749491 | -1.126140 |
| C | -0.018971 | -0.738765 | 1.878542 |
| H | 0.493376 | -0.448347 | 2.798342 |
| H | -0.782807 | -1.468938 | 2.144719 |
| C | 0.202337 | 0.550964 | -2.057383 |
| C | 0.946851 | -1.324619 | 0.879854 |
| C | 2.233547 | -0.796833 | 0.739028 |
| C | 0.547028 | -2.366073 | 0.041092 |

| | | | |
|---|---|---|---|
| C | 3.094335 | -1.289070 | -0.236256 |
| H | 2.558102 | 0.004591 | 1.395024 |
| C | 1.408391 | -2.861192 | -0.933899 |
| H | -0.443147 | -2.797671 | 0.154091 |
| C | 2.681531 | -2.318809 | -1.078263 |
| H | 4.088879 | -0.870997 | -0.336556 |
| H | 1.085364 | -3.670205 | -1.577876 |
| H | 3.352979 | -2.701801 | -1.837205 |
| H | 0.940633 | -0.126163 | -1.627198 |
| H | -0.523347 | -0.020144 | -2.637964 |
| H | 0.698898 | 1.242082 | -2.740246 |
| C | -1.497818 | 2.361238 | -1.547046 |
| H | -2.001139 | 2.899090 | -0.743140 |
| H | -0.963948 | 3.072840 | -2.177188 |
| H | -2.237561 | 1.857943 | -2.170357 |

## Calculated Cartesian coordinates for phenylacetaldehyde derived enamines

**1F-*E***

Imaginary frequency: None

Electronic energies: -813.306882

Free energies: -812.907712

Corrected Free energies: -812.903060

| | | | |
|---|---|---|---|
| C | 3.240398 | -1.538517 | 0.199746 |
| C | 4.337973 | -0.879396 | 1.046865 |
| H | 3.986394 | -0.699296 | 2.067303 |
| H | 5.206479 | -1.540796 | 1.102255 |
| H | 4.675372 | 0.070284 | 0.628089 |
| C | 2.929252 | -2.911629 | 0.807569 |
| H | 2.519973 | -2.803754 | 1.816750 |
| H | 2.202432 | -3.458711 | 0.205995 |
| H | 3.844137 | -3.506764 | 0.872078 |
| C | 3.752770 | -1.722715 | -1.234667 |
| H | 2.999654 | -2.177970 | -1.884759 |
| H | 4.061637 | -0.773252 | -1.679313 |
| H | 4.622252 | -2.385476 | -1.233597 |
| C | 1.965330 | -0.661207 | 0.241292 |
| H | 1.728779 | -0.499665 | 1.299396 |
| C | 2.113789 | 0.713975 | -0.436443 |
| H | 2.112483 | 0.558063 | -1.519593 |

| | | | |
|---|---|---|---|
| H | 3.077229 | 1.179737 | -0.182842 |
| N | 0.815507 | -1.366010 | -0.317712 |
| N | 0.991448 | 1.574758 | -0.080998 |
| C | 0.510919 | 2.399069 | -1.188114 |
| H | 0.297946 | 1.721103 | -2.019759 |
| H | -0.448406 | 2.836979 | -0.900149 |
| C | 1.254565 | 2.311011 | 1.152347 |
| H | 1.591185 | 1.585850 | 1.899285 |
| H | 2.083691 | 3.028615 | 1.027796 |
| C | 0.023580 | 3.031129 | 1.686668 |
| H | -0.259210 | 3.877574 | 1.057389 |
| H | -0.823758 | 2.342546 | 1.736603 |
| H | 0.219615 | 3.415458 | 2.689123 |
| C | 1.465103 | 3.502918 | -1.650864 |
| H | 2.440742 | 3.090362 | -1.921811 |
| H | 1.057988 | 4.011110 | -2.527332 |
| H | 1.617338 | 4.252568 | -0.870818 |
| H | 0.924526 | -1.662889 | -1.280167 |
| C | -0.457476 | -1.002430 | 0.030925 |
| C | -1.569289 | -1.217890 | -0.703300 |
| H | -1.460157 | -1.643603 | -1.697828 |
| H | -0.517122 | -0.536734 | 1.009473 |
| C | -2.933066 | -0.898812 | -0.283056 |
| C | -3.983023 | -1.048368 | -1.204390 |
| C | -3.268579 | -0.441719 | 1.004467 |
| C | -5.297616 | -0.751089 | -0.865483 |
| H | -3.754978 | -1.402590 | -2.204557 |
| C | -4.581534 | -0.140457 | 1.340411 |
| H | -2.498820 | -0.326133 | 1.759104 |
| C | -5.609075 | -0.291552 | 0.410427 |
| H | -6.081466 | -0.879272 | -1.603680 |
| H | -4.806231 | 0.210059 | 2.341644 |
| H | -6.632512 | -0.058564 | 0.678486 |

**1F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -813.125388

Free energies: -812.724536

Corrected Free energies: -812.720355

| | | | |
|---|---|---|---|
| C | 3.167034 | -1.633882 | 0.222870 |
| C | 4.318873 | -1.076029 | 1.069223 |
| H | 3.995764 | -0.888533 | 2.096919 |
| H | 5.131046 | -1.805792 | 1.099231 |

| | | | |
|---|---|---|---|
| H | 4.724289 | -0.149799 | 0.658572 |
| C | 2.740473 | -2.984290 | 0.813602 |
| H | 2.355677 | -2.860055 | 1.829721 |
| H | 1.966248 | -3.469015 | 0.213830 |
| H | 3.600140 | -3.656665 | 0.853763 |
| C | 3.647713 | -1.824907 | -1.220903 |
| H | 2.859329 | -2.189401 | -1.886445 |
| H | 4.048186 | -0.899023 | -1.639312 |
| H | 4.447018 | -2.569239 | -1.237758 |
| C | 1.977165 | -0.653623 | 0.310624 |
| H | 1.747940 | -0.493443 | 1.368696 |
| C | 2.185289 | 0.725148 | -0.362825 |
| H | 2.280832 | 0.573203 | -1.440689 |
| H | 3.131640 | 1.150617 | -0.006252 |
| N | 0.768040 | -1.221001 | -0.282459 |
| N | 1.053437 | 1.592249 | -0.091926 |
| C | 0.616775 | 2.368035 | -1.256178 |
| H | 0.458121 | 1.656075 | -2.070843 |
| H | -0.361254 | 2.799578 | -1.032300 |
| C | 1.247759 | 2.374346 | 1.131594 |
| H | 1.498406 | 1.671542 | 1.932358 |
| H | 2.109330 | 3.053988 | 1.036392 |
| C | 0.009720 | 3.163737 | 1.533096 |
| H | -0.183193 | 3.991242 | 0.847925 |
| H | -0.870855 | 2.517226 | 1.545950 |
| H | 0.145996 | 3.583504 | 2.530720 |
| C | 1.584131 | 3.464549 | -1.702704 |
| H | 2.574616 | 3.052054 | -1.912852 |
| H | 1.216581 | 3.942135 | -2.612779 |
| H | 1.692473 | 4.237550 | -0.938549 |
| H | 0.867691 | -1.744242 | -1.149117 |
| C | -0.437578 | -0.858741 | 0.090720 |
| C | -1.586947 | -1.206101 | -0.633127 |
| H | -1.448403 | -1.758876 | -1.557452 |
| H | -0.491259 | -0.283712 | 1.005378 |
| C | -2.920036 | -0.877043 | -0.254882 |
| C | -3.971755 | -1.262186 | -1.118568 |
| C | -3.243463 | -0.187123 | 0.938271 |
| C | -5.285359 | -0.966988 | -0.807376 |
| H | -3.732245 | -1.793966 | -2.032155 |
| C | -4.559027 | 0.102866 | 1.240383 |
| H | -2.467700 | 0.112265 | 1.630998 |
| C | -5.583415 | -0.282767 | 0.371517 |
| H | -6.081239 | -1.266989 | -1.477026 |

| | | | |
|---|---|---|---|
| H | -4.796738 | 0.630053 | 2.155549 |
| H | -6.612870 | -0.051023 | 0.616203 |

**1F-*Z***

Imaginary frequency: None

Electronic energies: -813.305915

Free energies: -812.906381

Corrected Free energies: -812.901116

| | | | |
|---|---|---|---|
| C | 1.628374 | 2.492190 | 0.053438 |
| C | 3.141097 | 2.754103 | 0.064193 |
| H | 3.599798 | 2.429699 | -0.875148 |
| H | 3.328451 | 3.824952 | 0.177515 |
| H | 3.647033 | 2.244755 | 0.886119 |
| C | 0.992029 | 3.406078 | -1.000576 |
| H | 1.376921 | 3.172924 | -1.998321 |
| H | -0.092590 | 3.291686 | -1.020580 |
| H | 1.227603 | 4.450927 | -0.780881 |
| C | 1.045168 | 2.827747 | 1.431848 |
| H | -0.036469 | 2.665318 | 1.465219 |
| H | 1.508678 | 2.233267 | 2.223311 |
| H | 1.222410 | 3.881789 | 1.661913 |
| C | 1.359277 | 1.014790 | -0.329621 |
| H | 1.837182 | 0.851158 | -1.301859 |
| C | 1.919705 | -0.013374 | 0.668975 |
| H | 1.288638 | 0.003920 | 1.563131 |
| H | 2.933712 | 0.264160 | 0.991552 |
| N | -0.066969 | 0.780318 | -0.539442 |
| N | 1.890027 | -1.355617 | 0.096799 |
| C | 1.530745 | -2.390206 | 1.065976 |
| H | 0.580434 | -2.087731 | 1.515574 |
| H | 1.328542 | -3.316715 | 0.522710 |
| C | 3.110152 | -1.634241 | -0.656440 |
| H | 3.257967 | -0.805848 | -1.355533 |
| H | 3.997257 | -1.642981 | -0.000467 |
| C | 3.038656 | -2.934407 | -1.446454 |
| H | 3.054556 | -3.810290 | -0.794690 |
| H | 2.121820 | -2.964089 | -2.040418 |
| H | 3.892921 | -3.008369 | -2.121554 |
| C | 2.562063 | -2.652933 | 2.166987 |
| H | 2.800358 | -1.733890 | 2.708923 |
| H | 2.171431 | -3.376941 | 2.885043 |
| H | 3.491155 | -3.056627 | 1.757766 |
| H | -0.627277 | 0.868419 | 0.299663 |

| | | | |
|---|---|---|---|
| C | -0.493146 | -0.180087 | -1.421156 |
| C | -1.717157 | -0.746676 | -1.510246 |
| H | 0.270408 | -0.486210 | -2.129000 |
| C | -2.884494 | -0.476314 | -0.666188 |
| C | -3.119232 | 0.765488 | -0.050402 |
| C | -3.850671 | -1.481387 | -0.482395 |
| C | -4.245888 | 0.975642 | 0.738457 |
| H | -2.441999 | 1.593095 | -0.227795 |
| C | -4.975143 | -1.269915 | 0.302468 |
| H | -3.703261 | -2.442855 | -0.963785 |
| C | -5.176298 | -0.040609 | 0.928478 |
| H | -4.401129 | 1.945834 | 1.197027 |
| H | -5.699136 | -2.066917 | 0.429127 |
| H | -6.051965 | 0.125201 | 1.544294 |
| H | -1.836284 | -1.515881 | -2.264413 |

**1F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -813.119808

Free energies: -812.717819

Corrected Free energies: -812.713928

| | | | |
|---|---|---|---|
| C | 1.730960 | 2.491946 | 0.017903 |
| C | 3.245962 | 2.735844 | 0.034640 |
| H | 3.700168 | 2.456459 | -0.920072 |
| H | 3.438117 | 3.797858 | 0.201853 |
| H | 3.744794 | 2.182111 | 0.831691 |
| C | 1.101088 | 3.416719 | -1.032845 |
| H | 1.477517 | 3.183445 | -2.032721 |
| H | 0.011322 | 3.336657 | -1.052404 |
| H | 1.352616 | 4.455356 | -0.807349 |
| C | 1.153357 | 2.808550 | 1.403680 |
| H | 0.077514 | 2.617780 | 1.472784 |
| H | 1.651268 | 2.236581 | 2.189363 |
| H | 1.301641 | 3.868695 | 1.620623 |
| C | 1.474048 | 1.026156 | -0.392647 |
| H | 1.966638 | 0.852457 | -1.354347 |
| C | 1.960915 | -0.050409 | 0.611923 |
| H | 1.407056 | 0.070271 | 1.545937 |
| H | 3.020440 | 0.135767 | 0.829408 |
| N | 0.053040 | 0.773943 | -0.616358 |
| N | 1.730669 | -1.380420 | 0.083884 |
| C | 1.280642 | -2.347144 | 1.089129 |
| H | 0.421548 | -1.903358 | 1.598979 |

| | | | |
|---|---|---|---|
| H | 0.904996 | -3.230450 | 0.568163 |
| C | 2.837931 | -1.839006 | -0.758438 |
| H | 3.021855 | -1.063600 | -1.508339 |
| H | 3.768459 | -1.931177 | -0.177144 |
| C | 2.536368 | -3.150515 | -1.470006 |
| H | 2.514855 | -3.993942 | -0.777700 |
| H | 1.569991 | -3.097779 | -1.977470 |
| H | 3.307759 | -3.351136 | -2.214770 |
| C | 2.340387 | -2.754516 | 2.113406 |
| H | 2.740532 | -1.880200 | 2.633466 |
| H | 1.905556 | -3.422852 | 2.858850 |
| H | 3.172541 | -3.279159 | 1.638354 |
| H | -0.618951 | 1.278838 | -0.046425 |
| C | -0.370372 | -0.196831 | -1.392285 |
| C | -1.700493 | -0.645902 | -1.492131 |
| H | 0.368372 | -0.622075 | -2.059908 |
| C | -2.789483 | -0.388583 | -0.598946 |
| C | -2.626856 | -0.034086 | 0.759678 |
| C | -4.100578 | -0.539459 | -1.103308 |
| C | -3.731866 | 0.203110 | 1.557189 |
| H | -1.641803 | -0.006923 | 1.209077 |
| C | -5.198609 | -0.285195 | -0.303245 |
| H | -4.235002 | -0.837911 | -2.136469 |
| C | -5.017913 | 0.093289 | 1.027228 |
| H | -3.595250 | 0.460427 | 2.599788 |
| H | -6.197266 | -0.387054 | -0.708713 |
| H | -5.878234 | 0.285712 | 1.656394 |
| H | -1.917944 | -1.229271 | -2.379150 |

**2F-*E***

Imaginary frequency: None

Electronic energies: -599.565528

Free energies: -599.305893

Corrected Free energies: -599.303107

| | | | |
|---|---|---|---|
| N | -1.010817 | -1.072844 | -0.214917 |
| C | 0.237530 | -0.504082 | -0.298139 |
| C | 1.359499 | -0.952255 | 0.296374 |
| H | 1.285979 | -1.782675 | 0.994145 |
| H | -1.101966 | -1.795631 | 0.490544 |
| C | -2.193981 | -0.224661 | -0.345772 |
| C | -3.423193 | -1.089889 | -0.614660 |
| C | -2.413665 | 0.671179 | 0.878462 |
| H | -2.023409 | 0.416669 | -1.220225 |

| | | | |
|---|---|---|---|
| C | -4.683192 | -0.234088 | -0.764255 |
| H | -3.552830 | -1.783100 | 0.226872 |
| H | -3.250493 | -1.693207 | -1.509352 |
| C | -3.670770 | 1.529799 | 0.724365 |
| H | -2.512835 | 0.025799 | 1.760981 |
| H | -1.529456 | 1.297081 | 1.033730 |
| C | -4.899350 | 0.656796 | 0.460986 |
| H | -5.551287 | -0.877386 | -0.927509 |
| H | -4.583888 | 0.398267 | -1.654636 |
| H | -3.819495 | 2.141078 | 1.617952 |
| H | -3.533923 | 2.221123 | -0.115857 |
| H | -5.786035 | 1.280767 | 0.322370 |
| H | -5.085652 | 0.024103 | 1.337210 |
| H | 0.269153 | 0.370207 | -0.945354 |
| C | 2.692231 | -0.375160 | 0.101029 |
| C | 3.022746 | 0.434770 | -0.998166 |
| C | 3.699555 | -0.633790 | 1.043130 |
| C | 4.290646 | 0.987171 | -1.125088 |
| H | 2.287167 | 0.618099 | -1.773301 |
| C | 4.971248 | -0.088974 | 0.910247 |
| H | 3.471337 | -1.265323 | 1.895659 |
| C | 5.274507 | 0.731663 | -0.172375 |
| H | 4.518355 | 1.608986 | -1.983590 |
| H | 5.727310 | -0.303600 | 1.657049 |
| H | 6.264803 | 1.157785 | -0.279098 |

**2F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -599.378867

Free energies: -599.117915

Corrected Free energies: -599.115413

| | | | |
|---|---|---|---|
| C | -2.267851 | -0.762693 | -0.618443 |
| C | -3.462527 | -0.159101 | 1.540978 |
| C | -4.065522 | 1.041518 | -0.594011 |
| C | -4.589027 | 0.490157 | 0.733867 |
| C | -3.363559 | -0.047720 | -1.412535 |
| C | -2.786851 | -1.269713 | 0.735656 |
| N | -1.134640 | 0.156625 | -0.407126 |
| C | 1.170088 | 0.666775 | -0.103937 |
| C | 2.545172 | 0.309160 | -0.024955 |
| C | 5.278451 | -0.260490 | 0.152727 |
| C | 3.014476 | -1.019155 | -0.166718 |
| C | 3.486721 | 1.339184 | 0.209918 |

| | | | |
|---|---|---|---|
| C | 4.835864 | 1.054871 | 0.296745 |
| C | 4.364080 | -1.292504 | -0.077868 |
| C | 0.118380 | -0.224553 | -0.345772 |
| H | -1.868571 | -1.597319 | -1.197270 |
| H | -2.723767 | 0.602026 | 1.819102 |
| H | -3.849534 | -0.572809 | 2.474271 |
| H | -3.384382 | 1.878563 | -0.395983 |
| H | -4.882938 | 1.457954 | -1.185945 |
| H | -5.059315 | 1.288109 | 1.312454 |
| H | -5.362012 | -0.260135 | 0.531460 |
| H | -2.944443 | 0.357661 | -2.336306 |
| H | -4.094272 | -0.810906 | -1.695009 |
| H | -1.963251 | -1.723194 | 1.292862 |
| H | -3.511142 | -2.061871 | 0.521656 |
| H | -1.344689 | 1.141645 | -0.264507 |
| H | 0.915556 | 1.713207 | 0.032966 |
| H | 6.336013 | -0.484124 | 0.220527 |
| H | 2.323894 | -1.833700 | -0.342286 |
| H | 3.132943 | 2.357760 | 0.319771 |
| H | 5.547461 | 1.850822 | 0.475269 |
| H | 4.715548 | -2.310519 | -0.186572 |
| H | 0.292006 | -1.283953 | -0.500493 |

**2F-*Z***

Imaginary frequency: None

Electronic energies: -599.563505

Free energies: -599.301829

Corrected Free energies: -599.299358

| | | | |
|---|---|---|---|
| N | 0.513119 | -0.667940 | -0.568487 |
| C | -0.216061 | -1.676544 | 0.010792 |
| C | -1.532981 | -1.705622 | 0.299680 |
| H | -1.940912 | -2.662405 | 0.604826 |
| H | 0.042213 | 0.217634 | -0.693457 |
| C | 1.947417 | -0.566387 | -0.321261 |
| C | 2.584947 | 0.357641 | -1.356853 |
| C | 2.264828 | -0.092226 | 1.102065 |
| H | 2.364539 | -1.573720 | -0.451984 |
| C | 4.092822 | 0.489295 | -1.131606 |
| H | 2.117719 | 1.347980 | -1.273529 |
| H | 2.370039 | -0.020445 | -2.359543 |
| C | 3.773172 | 0.030413 | 1.326336 |
| H | 1.789249 | 0.885986 | 1.251474 |
| H | 1.816706 | -0.784140 | 1.821963 |
| C | 4.403069 | 0.963590 | 0.290020 |

| | | | |
|---|---|---|---|
| H | 4.518696 | 1.177744 | -1.865547 |
| H | 4.566396 | -0.485895 | -1.296208 |
| H | 3.974300 | 0.389691 | 2.338600 |
| H | 4.232332 | -0.962122 | 1.242862 |
| H | 5.483880 | 1.024788 | 0.440552 |
| H | 4.001222 | 1.974754 | 0.427018 |
| H | 0.368269 | -2.578370 | 0.178963 |
| C | -2.491728 | -0.596876 | 0.169347 |
| C | -2.160173 | 0.733504 | 0.471275 |
| C | -3.810611 | -0.864789 | -0.225690 |
| C | -3.097862 | 1.753157 | 0.349097 |
| H | -1.169409 | 0.968764 | 0.845387 |
| C | -4.749381 | 0.152703 | -0.344047 |
| H | -4.093925 | -1.888683 | -0.446687 |
| C | -4.395939 | 1.470643 | -0.066022 |
| H | -2.815698 | 2.771198 | 0.592535 |
| H | -5.760527 | -0.083550 | -0.655360 |
| H | -5.126039 | 2.265350 | -0.161246 |

**2F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -599.375264

Free energies: -599.113781

Corrected Free energies: -599.111167

| | | | |
|---|---|---|---|
| N | 0.511591 | -0.574231 | 0.139822 |
| C | -0.221737 | -1.520968 | 0.670783 |
| C | -1.624826 | -1.594747 | 0.616572 |
| H | -2.038976 | -2.567822 | 0.853239 |
| H | 0.053647 | 0.141661 | -0.420611 |
| C | 1.974995 | -0.495909 | 0.212790 |
| C | 2.566489 | -0.573657 | -1.196743 |
| C | 2.378607 | 0.796021 | 0.930608 |
| H | 2.300377 | -1.359087 | 0.799672 |
| C | 4.090276 | -0.439155 | -1.136808 |
| H | 2.149327 | 0.240440 | -1.801163 |
| H | 2.273690 | -1.517076 | -1.662660 |
| C | 3.903601 | 0.920320 | 0.975398 |
| H | 1.957376 | 1.650297 | 0.387486 |
| H | 1.954499 | 0.799990 | 1.937171 |
| C | 4.504929 | 0.851835 | -0.429040 |
| H | 4.494390 | -0.470487 | -2.150564 |
| H | 4.506424 | -1.298577 | -0.599205 |
| H | 4.173654 | 1.857867 | 1.465382 |

| | | | |
|---|---|---|---|
| H | 4.313563 | 0.108927 | 1.587115 |
| H | 5.593874 | 0.917166 | -0.375102 |
| H | 4.158855 | 1.712149 | -1.013447 |
| H | 0.322907 | -2.324125 | 1.156268 |
| C | -2.543762 | -0.559967 | 0.253463 |
| C | -2.243610 | 0.818380 | 0.345564 |
| C | -3.834350 | -0.943814 | -0.174860 |
| C | -3.181866 | 1.763289 | -0.026891 |
| H | -1.305365 | 1.150707 | 0.773146 |
| C | -4.760248 | 0.007552 | -0.559098 |
| H | -4.082248 | -1.998003 | -0.218447 |
| C | -4.434606 | 1.362656 | -0.493071 |
| H | -2.947295 | 2.816469 | 0.060236 |
| H | -5.739444 | -0.299982 | -0.903208 |
| H | -5.163732 | 2.108085 | -0.786069 |

**3F-*E***

Imaginary frequency: None

Electronic energies: -482.847566

Free energies: -482.650657

Corrected Free energies: -482.648827

| | | | |
|---|---|---|---|
| C | -3.341710 | 0.118188 | 0.394982 |
| H | -3.106447 | 0.222334 | 1.462702 |
| N | -2.223602 | -0.535675 | -0.296069 |
| C | -0.935581 | -0.104846 | -0.097906 |
| C | 0.177655 | -0.841998 | -0.275699 |
| H | 0.069729 | -1.894173 | -0.527838 |
| H | -2.323811 | -1.537406 | -0.399342 |
| C | -4.572461 | -0.766841 | 0.252720 |
| H | -5.430807 | -0.303008 | 0.740138 |
| H | -4.808685 | -0.909131 | -0.805331 |
| H | -4.407399 | -1.746505 | 0.707468 |
| C | -3.595666 | 1.503246 | -0.193089 |
| H | -3.876290 | 1.411294 | -1.245269 |
| H | -4.406754 | 1.997355 | 0.345944 |
| H | -2.712801 | 2.141900 | -0.127597 |
| H | -0.860716 | 0.935568 | 0.207864 |
| C | 1.548792 | -0.347678 | -0.128156 |
| C | 1.880274 | 1.017482 | -0.098923 |
| C | 2.598943 | -1.271935 | -0.015837 |
| C | 3.195555 | 1.431430 | 0.064651 |
| H | 1.105849 | 1.765901 | -0.224050 |
| C | 3.916124 | -0.856989 | 0.139209 |

| | | | |
|---|---|---|---|
| H | 2.370325 | -2.332372 | -0.045675 |
| C | 4.224392 | 0.499269 | 0.185959 |
| H | 3.421323 | 2.491711 | 0.084040 |
| H | 4.704007 | -1.596677 | 0.225825 |
| H | 5.249786 | 0.826961 | 0.306135 |

**3F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -482.664197

Free energies: -482.466428

Corrected Free energies: -482.464722

| | | | |
|---|---|---|---|
| C | -3.375014 | 0.391075 | 0.001524 |
| H | -3.053285 | 1.433775 | 0.005660 |
| N | -2.141252 | -0.411190 | -0.002099 |
| C | -0.922447 | 0.068554 | 0.000166 |
| C | 0.210416 | -0.755868 | -0.002219 |
| H | 0.045585 | -1.829020 | -0.005140 |
| H | -2.261721 | -1.422558 | -0.007026 |
| C | -4.165206 | 0.083142 | 1.269465 |
| H | -5.070690 | 0.690884 | 1.281180 |
| H | -4.459227 | -0.969074 | 1.292828 |
| H | -3.578690 | 0.308828 | 2.160324 |
| C | -4.166055 | 0.093388 | -1.268291 |
| H | -4.462557 | -0.957925 | -1.298236 |
| H | -5.070103 | 0.703314 | -1.276073 |
| H | -3.579028 | 0.323368 | -2.157705 |
| H | -0.841256 | 1.149673 | 0.004806 |
| C | 1.557529 | -0.298851 | -0.000719 |
| C | 2.585777 | -1.270771 | -0.001848 |
| C | 1.918771 | 1.070588 | 0.001480 |
| C | 3.914248 | -0.892930 | -0.000874 |
| C | 3.249078 | 1.437477 | 0.002201 |
| H | 1.160273 | 1.842933 | 0.002450 |
| C | 4.250062 | 0.461583 | 0.001033 |
| H | 4.692193 | -1.645681 | -0.001700 |
| H | 3.517495 | 2.486337 | 0.003607 |
| H | 5.291441 | 0.759661 | 0.001582 |
| H | 2.315376 | -2.320506 | -0.003370 |

**3F-*Z***

Imaginary frequency: None

Electronic energies: -482.848849

Free energies: -482.650356

Corrected Free energies: -482.648853

| | | | |
|---|---|---|---|
| C | -3.079862 | 0.054826 | -0.068073 |
| H | -3.587814 | -0.539460 | -0.834212 |
| N | -1.657165 | 0.052625 | -0.424128 |
| C | -1.053079 | -1.153437 | -0.703203 |
| C | 0.257654 | -1.467569 | -0.669218 |
| H | 0.512317 | -2.494033 | -0.906923 |
| H | -1.105028 | 0.684846 | 0.145752 |
| C | -3.601148 | 1.484524 | -0.128992 |
| H | -4.668779 | 1.511597 | 0.095171 |
| H | -3.086206 | 2.106092 | 0.610008 |
| H | -3.437023 | 1.914803 | -1.117972 |
| C | -3.332646 | -0.576842 | 1.301166 |
| H | -2.832651 | 0.006613 | 2.079969 |
| H | -4.401426 | -0.603997 | 1.524823 |
| H | -2.946567 | -1.598102 | 1.336337 |
| H | -1.756286 | -1.925212 | -1.006614 |
| C | 1.373331 | -0.587449 | -0.303905 |
| C | 1.353283 | 0.801317 | -0.510195 |
| C | 2.537862 | -1.147747 | 0.246397 |
| C | 2.437852 | 1.595201 | -0.148986 |
| H | 0.501382 | 1.261848 | -0.996559 |
| C | 3.619087 | -0.355372 | 0.606133 |
| H | 2.582178 | -2.221501 | 0.396469 |
| C | 3.572739 | 1.024839 | 0.417485 |
| H | 2.397672 | 2.664256 | -0.323580 |
| H | 4.502405 | -0.814349 | 1.035185 |
| H | 4.415534 | 1.644483 | 0.699383 |

**3F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -482.658468

Free energies: -482.462751

Corrected Free energies: -482.459875

| | | | |
|---|---|---|---|
| C | -3.088133 | -0.041739 | -0.011685 |
| H | -3.523583 | -0.904888 | -0.517764 |
| N | -1.633659 | -0.275087 | 0.003363 |
| C | -1.035139 | -1.324473 | -0.501411 |
| C | 0.352218 | -1.554593 | -0.500340 |
| H | 0.643133 | -2.580671 | -0.693057 |
| H | -1.074022 | 0.413682 | 0.502666 |
| C | -3.378280 | 1.227763 | -0.806665 |

| | | | |
|---|---|---|---|
| H | -4.456767 | 1.385808 | -0.842424 |
| H | -2.920897 | 2.095847 | -0.326360 |
| H | -3.000538 | 1.144590 | -1.825939 |
| C | -3.594219 | 0.035623 | 1.424215 |
| H | -3.133982 | 0.876785 | 1.948291 |
| H | -4.673700 | 0.189282 | 1.413865 |
| H | -3.375128 | -0.884452 | 1.966526 |
| H | -1.687602 | -2.086587 | -0.914713 |
| C | 1.395601 | -0.612051 | -0.237778 |
| C | 1.246262 | 0.784343 | -0.403362 |
| C | 2.652413 | -1.115342 | 0.166589 |
| C | 2.298910 | 1.635998 | -0.122559 |
| H | 0.332861 | 1.195785 | -0.816358 |
| C | 3.693214 | -0.254845 | 0.460483 |
| H | 2.782730 | -2.186761 | 0.265909 |
| C | 3.517439 | 1.122548 | 0.323517 |
| H | 2.179699 | 2.702371 | -0.265931 |
| H | 4.645456 | -0.650421 | 0.790302 |
| H | 4.336232 | 1.795847 | 0.545420 |

**4F-*E***

Imaginary frequency: None

Electronic energies: -635.250625

Free energies: -635.032005

Corrected Free energies: -635.028926

| | | | |
|---|---|---|---|
| C | -1.475811 | -0.215422 | 0.083801 |
| C | -0.640932 | 0.663553 | -0.506772 |
| H | -1.070408 | -1.086709 | 0.587316 |
| N | 0.728449 | 0.643726 | -0.451563 |
| C | 1.426218 | -0.494758 | 0.118810 |
| H | 1.085500 | -0.612537 | 1.154068 |
| H | 1.176483 | -1.425331 | -0.409001 |
| C | 2.917846 | -0.269581 | 0.096393 |
| C | 3.772277 | -1.190861 | -0.504710 |
| C | 3.459317 | 0.875918 | 0.684829 |
| C | 5.148874 | -0.977442 | -0.513994 |
| H | 3.358649 | -2.079885 | -0.968648 |
| C | 4.831642 | 1.092814 | 0.673769 |
| H | 2.794868 | 1.597616 | 1.148194 |
| C | 5.680578 | 0.164366 | 0.074249 |
| H | 5.803570 | -1.701640 | -0.984231 |
| H | 5.241207 | 1.984546 | 1.133456 |
| H | 6.750785 | 0.333010 | 0.065737 |

| | | | |
|---|---|---|---|
| H | 1.205627 | 1.103156 | -1.214061 |
| H | -1.035106 | 1.501574 | -1.073776 |
| C | -2.938719 | -0.105328 | 0.067575 |
| C | -3.712633 | -1.227756 | 0.400344 |
| C | -3.619587 | 1.078944 | -0.258372 |
| C | -5.101505 | -1.179009 | 0.387944 |
| H | -3.209579 | -2.151844 | 0.665962 |
| C | -5.007426 | 1.124684 | -0.280225 |
| H | -3.062002 | 1.981845 | -0.479602 |
| C | -5.760004 | -0.002946 | 0.041614 |
| H | -5.670898 | -2.063949 | 0.648918 |
| H | -5.506289 | 2.052520 | -0.536217 |
| H | -6.842361 | 0.038492 | 0.031286 |

**4F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -635.059940

Free energies: -634.841596

Corrected Free energies: -634.838171

| | | | |
|---|---|---|---|
| C | 1.503282 | 0.233056 | 0.072870 |
| C | 0.600476 | -0.836204 | -0.002550 |
| H | 1.104359 | 1.236046 | 0.171285 |
| N | -0.702235 | -0.687926 | 0.038793 |
| C | -1.423021 | 0.589592 | 0.169891 |
| H | -1.157638 | 1.033028 | 1.132654 |
| H | -1.082784 | 1.254270 | -0.627172 |
| C | -2.905421 | 0.348187 | 0.070343 |
| C | -3.528285 | 0.346406 | -1.177104 |
| C | -3.653598 | 0.086213 | 1.217206 |
| C | -4.890284 | 0.085255 | -1.276986 |
| H | -2.946908 | 0.556093 | -2.068706 |
| C | -5.015967 | -0.175378 | 1.116822 |
| H | -3.169594 | 0.092004 | 2.187964 |
| C | -5.634021 | -0.176443 | -0.129884 |
| H | -5.370760 | 0.089474 | -2.247691 |
| H | -5.593495 | -0.375975 | 2.010961 |
| H | -6.695672 | -0.377642 | -0.207383 |
| H | -1.275037 | -1.523967 | -0.021101 |
| H | 0.944824 | -1.857906 | -0.102696 |
| C | 2.918097 | 0.101905 | 0.025590 |
| C | 3.585909 | -1.143391 | -0.083732 |
| C | 3.695863 | 1.284126 | 0.089969 |
| C | 4.963599 | -1.191382 | -0.126797 |

| | | | |
|---|---|---|---|
| H | 3.027036 | -2.068691 | -0.133067 |
| C | 5.074435 | 1.224875 | 0.044454 |
| H | 3.191821 | 2.239992 | 0.174533 |
| C | 5.712447 | -0.011899 | -0.063866 |
| H | 5.466261 | -2.146393 | -0.210853 |
| H | 5.658297 | 2.135111 | 0.091895 |
| H | 6.793870 | -0.059479 | -0.099536 |

**4F-*Z***

Imaginary frequency: None

Electronic energies: -635.248942

Free energies: -635.028772

Corrected Free energies: -635.025862

| | | | |
|---|---|---|---|
| C | 1.357214 | 0.634509 | -1.535617 |
| C | 0.205269 | 1.235302 | -1.180706 |
| H | 1.495153 | 0.438852 | -2.592509 |
| N | -0.230554 | 1.564884 | 0.086875 |
| C | -1.652046 | 1.766101 | 0.296705 |
| H | -2.005918 | 2.489055 | -0.444240 |
| H | 0.237245 | 1.084238 | 0.845180 |
| H | -0.493795 | 1.521056 | -1.962325 |
| C | 2.418220 | 0.165302 | -0.635059 |
| C | 3.187904 | -0.952237 | -0.996750 |
| C | 2.727771 | 0.807606 | 0.574002 |
| C | 4.198461 | -1.427370 | -0.172167 |
| H | 2.979184 | -1.451394 | -1.937301 |
| C | 3.739835 | 0.330056 | 1.400731 |
| H | 2.202950 | 1.714412 | 0.851912 |
| C | 4.475496 | -0.792915 | 1.037468 |
| H | 4.773468 | -2.295843 | -0.472714 |
| H | 3.960606 | 0.847034 | 2.327428 |
| H | 5.262275 | -1.164332 | 1.682800 |
| H | -1.786057 | 2.236286 | 1.273985 |
| C | -2.517757 | 0.517772 | 0.223263 |
| C | -1.974362 | -0.758098 | 0.092821 |
| C | -3.905761 | 0.654940 | 0.305496 |
| C | -2.804361 | -1.877514 | 0.043829 |
| H | -0.900086 | -0.887071 | 0.022320 |
| C | -4.733999 | -0.458933 | 0.259068 |
| H | -4.337870 | 1.645969 | 0.407826 |
| C | -4.183514 | -1.732843 | 0.126635 |
| H | -2.367386 | -2.863852 | -0.061053 |
| H | -5.808792 | -0.335178 | 0.323869 |
| H | -4.827313 | -2.603466 | 0.088379 |

**4F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -635.055219

Free energies: -634.836553

Corrected Free energies: -634.833313

| | | | |
|---|---|---|---|
| C | 1.738322 | -1.710438 | 0.129932 |
| C | 0.458452 | -1.789355 | -0.446424 |
| H | 2.056095 | -2.602740 | 0.656647 |
| N | -0.260012 | -0.768518 | -0.846511 |
| C | -1.601731 | -0.869039 | -1.434824 |
| H | -1.812826 | -1.928490 | -1.576597 |
| H | 0.078887 | 0.173430 | -0.664616 |
| H | -0.008437 | -2.763945 | -0.546089 |
| C | 2.628266 | -0.591695 | 0.127240 |
| C | 3.637141 | -0.542530 | 1.115995 |
| C | 2.575817 | 0.439534 | -0.839093 |
| C | 4.509727 | 0.527336 | 1.176622 |
| H | 3.702905 | -1.344651 | 1.841803 |
| C | 3.463155 | 1.497842 | -0.778749 |
| H | 1.889384 | 0.376301 | -1.674659 |
| C | 4.420304 | 1.553490 | 0.235051 |
| H | 5.265708 | 0.565554 | 1.950604 |
| H | 3.423052 | 2.275613 | -1.530605 |
| H | 5.109944 | 2.387455 | 0.278915 |
| H | -1.566364 | -0.385225 | -2.412094 |
| C | -2.623932 | -0.208822 | -0.540241 |
| C | -3.089753 | -0.878412 | 0.591650 |
| C | -3.089504 | 1.072699 | -0.825174 |
| C | -4.015452 | -0.270400 | 1.430162 |
| H | -2.733212 | -1.879553 | 0.811207 |
| C | -4.015597 | 1.682568 | 0.016186 |
| H | -2.731684 | 1.591867 | -1.707860 |
| C | -4.478054 | 1.011849 | 1.143143 |
| H | -4.378818 | -0.796503 | 2.304512 |
| H | -4.376343 | 2.678236 | -0.211286 |
| H | -5.201180 | 1.484521 | 1.796840 |

**5F-*E***

Imaginary frequency: None

Electronic energies: -595.952316

Free energies: -595.760096

Corrected Free energies: -595.757964

| | | | |
|---|---|---|---|
| N | 1.226124 | -0.992223 | 0.057051 |
| C | -0.000970 | -0.372974 | 0.041161 |
| C | -1.177221 | -1.020890 | -0.017315 |
| H | -1.171854 | -2.103778 | -0.111370 |
| H | 1.232278 | -1.998729 | 0.143593 |
| C | 2.470270 | -0.370141 | 0.000717 |
| C | 3.612912 | -1.134191 | 0.279026 |
| C | 2.626203 | 0.981928 | -0.329967 |
| C | 4.873152 | -0.557718 | 0.237653 |
| H | 3.500256 | -2.182346 | 0.534421 |
| C | 3.895642 | 1.548686 | -0.355405 |
| H | 1.771432 | 1.593063 | -0.587830 |
| C | 5.027431 | 0.791470 | -0.073749 |
| H | 5.741086 | -1.168158 | 0.458328 |
| H | 3.995168 | 2.596903 | -0.612322 |
| H | 6.011776 | 1.241057 | -0.101964 |
| H | 0.036971 | 0.708094 | 0.096483 |
| C | -2.494269 | -0.378530 | 0.015202 |
| C | -2.686452 | 0.970366 | 0.355067 |
| C | -3.629521 | -1.138806 | -0.301889 |
| C | -3.954889 | 1.533757 | 0.352851 |
| H | -1.841362 | 1.586108 | 0.640882 |
| C | -4.900321 | -0.575769 | -0.296903 |
| H | -3.506052 | -2.185591 | -0.559242 |
| C | -5.071662 | 0.766391 | 0.026412 |
| H | -4.074950 | 2.577663 | 0.618874 |
| H | -5.758736 | -1.188169 | -0.548325 |
| H | -6.060714 | 1.207969 | 0.031956 |

**5F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -595.758736

Free energies: -595.565804

Corrected Free energies: -595.563806

| | | | |
|---|---|---|---|
| N | 1.178919 | -0.869968 | 0.000226 |
| C | 0.010080 | -0.239438 | 0.000382 |
| C | -1.187325 | -0.938533 | 0.000278 |
| H | -1.136224 | -2.023610 | 0.000072 |
| H | 1.152068 | -1.887206 | 0.000221 |
| C | 2.467339 | -0.310118 | 0.000052 |
| C | 3.545114 | -1.200896 | -0.000067 |
| C | 2.681958 | 1.071551 | -0.000048 |

| | | | |
|---|---|---|---|
| C | 4.839836 | -0.707140 | -0.000174 |
| H | 3.362933 | -2.269658 | -0.000142 |
| C | 3.982974 | 1.548002 | -0.000140 |
| H | 1.860084 | 1.773896 | -0.000153 |
| C | 5.062987 | 0.666935 | -0.000177 |
| H | 5.674260 | -1.396375 | -0.000256 |
| H | 4.154064 | 2.616782 | -0.000206 |
| H | 6.074618 | 1.052227 | -0.000239 |
| H | 0.039030 | 0.840676 | 0.000551 |
| C | -2.486458 | -0.347130 | 0.000206 |
| C | -3.606531 | -1.208701 | -0.000126 |
| C | -2.703566 | 1.050571 | 0.000312 |
| C | -4.889923 | -0.695464 | -0.000367 |
| H | -3.446338 | -2.280579 | -0.000204 |
| C | -3.988724 | 1.553759 | 0.000046 |
| H | -1.868802 | 1.739677 | 0.000615 |
| C | -5.084357 | 0.685720 | -0.000309 |
| H | -5.741188 | -1.364018 | -0.000595 |
| H | -4.147804 | 2.624388 | 0.000110 |
| H | -6.089565 | 1.088866 | -0.000563 |

**5F-*Z***

Imaginary frequency: None

Electronic energies: -595.951343

Free energies: -595.758242

Corrected Free energies: -595.756059

| | | | |
|---|---|---|---|
| N | 0.697516 | -0.195645 | -0.091477 |
| C | 0.067013 | -1.420718 | -0.042182 |
| C | -1.259815 | -1.639507 | -0.010347 |
| H | -1.574635 | -2.673553 | -0.087499 |
| H | 0.137619 | 0.600932 | -0.362953 |
| C | 2.076716 | 0.001837 | -0.066910 |
| C | 2.596331 | 1.209366 | -0.554010 |
| C | 2.957917 | -0.955490 | 0.451113 |
| C | 3.962895 | 1.445032 | -0.534005 |
| H | 1.918323 | 1.955507 | -0.954477 |
| C | 4.326798 | -0.711172 | 0.450642 |
| H | 2.581826 | -1.877256 | 0.875849 |
| C | 4.842226 | 0.484135 | -0.039103 |
| H | 4.343216 | 2.385309 | -0.916167 |
| H | 4.994416 | -1.464212 | 0.853051 |
| H | 5.909041 | 0.667820 | -0.029790 |
| H | 0.735339 | -2.272639 | -0.082458 |

| | | | |
|---|---|---|---|
| C | -2.331441 | -0.634762 | 0.042115 |
| C | -2.198025 | 0.596457 | 0.702800 |
| C | -3.564408 | -0.924869 | -0.561324 |
| C | -3.246780 | 1.509761 | 0.728605 |
| H | -1.282230 | 0.828316 | 1.234365 |
| C | -4.610213 | -0.012321 | -0.536124 |
| H | -3.693229 | -1.880163 | -1.059295 |
| C | -4.454527 | 1.215152 | 0.104128 |
| H | -3.120955 | 2.452278 | 1.248728 |
| H | -5.550141 | -0.258911 | -1.016093 |
| H | -5.269320 | 1.928686 | 0.124686 |

**5F-Z** radical cation

Imaginary frequency: None

Electronic energies: -595.753186

Free energies: -595.559618

Corrected Free energies: -595.557644

| | | | |
|---|---|---|---|
| N | 0.693017 | -0.268795 | -0.158573 |
| C | 0.084718 | -1.446712 | -0.061490 |
| C | -1.293680 | -1.626548 | -0.088504 |
| H | -1.616911 | -2.648046 | -0.252717 |
| H | 0.118868 | 0.539374 | -0.389497 |
| C | 2.076831 | -0.030091 | -0.087234 |
| C | 2.554741 | 1.171048 | -0.619013 |
| C | 2.944881 | -0.951214 | 0.505577 |
| C | 3.913964 | 1.437472 | -0.578972 |
| H | 1.864608 | 1.877390 | -1.066180 |
| C | 4.301583 | -0.670317 | 0.533554 |
| H | 2.571602 | -1.857642 | 0.963776 |
| C | 4.790053 | 0.516949 | -0.008917 |
| H | 4.289381 | 2.364186 | -0.993655 |
| H | 4.980346 | -1.377003 | 0.993529 |
| H | 5.851462 | 0.727911 | 0.022142 |
| H | 0.726298 | -2.317334 | -0.019009 |
| C | -2.317579 | -0.628514 | 0.025119 |
| C | -2.132196 | 0.606850 | 0.685159 |
| C | -3.584569 | -0.922472 | -0.524086 |
| C | -3.162532 | 1.528353 | 0.738791 |
| H | -1.209722 | 0.815665 | 1.213990 |
| C | -4.602726 | 0.011144 | -0.479694 |
| H | -3.741242 | -1.882090 | -1.002972 |
| C | -4.391879 | 1.240639 | 0.145543 |
| H | -3.017478 | 2.467146 | 1.257727 |

| | | | |
|---|---|---|---|
| H | -5.564400 | -0.215087 | -0.922293 |
| H | -5.193587 | 1.967580 | 0.190179 |

**6F-*E***

Imaginary frequency: -15.0452

Electronic energies: -1775.368231

Free energies: -1774.932058

Corrected Free energies: -1774.925524

| | | | |
|---|---|---|---|
| S | -0.365230 | 2.040893 | -0.021456 |
| F | -2.560764 | 3.287673 | -0.749040 |
| F | -1.144894 | 4.528310 | 0.307401 |
| F | -0.773155 | 3.973282 | -1.745446 |
| O | -0.606166 | 1.083561 | -1.106621 |
| O | -1.057332 | 1.680667 | 1.227611 |
| O | 1.011981 | 2.491675 | 0.135001 |
| C | -1.264246 | 3.550976 | -0.585249 |
| N | 0.138452 | -1.691169 | 0.574618 |
| H | 0.222515 | -2.297373 | 1.383329 |
| N | -2.518800 | -0.694120 | 0.713261 |
| H | -1.625138 | -0.178620 | 0.742121 |
| C | -0.844964 | -2.131965 | -0.410133 |
| H | -0.842726 | -1.370855 | -1.200357 |
| C | -2.200997 | -2.098116 | 0.298068 |
| H | -3.009533 | -2.452238 | -0.335879 |
| H | -2.176112 | -2.719105 | 1.193537 |
| C | -3.378334 | 0.022309 | -0.292930 |
| H | -3.294914 | 1.080111 | -0.046959 |
| H | -2.905082 | -0.134321 | -1.262220 |
| C | -4.826901 | -0.429457 | -0.283682 |
| H | -5.327589 | -0.174759 | 0.650446 |
| H | -4.935406 | -1.500613 | -0.460147 |
| H | -5.344615 | 0.090358 | -1.090229 |
| C | -3.061844 | -0.578228 | 2.108453 |
| H | -3.436567 | 0.441625 | 2.199324 |
| H | -3.897465 | -1.273208 | 2.193857 |
| C | -1.985088 | -0.839693 | 3.145874 |
| H | -2.407526 | -0.661899 | 4.135124 |
| H | -1.145082 | -0.159360 | 2.997827 |
| H | -1.623771 | -1.868575 | 3.122249 |
| C | -0.561059 | -3.506114 | -1.079596 |
| C | -1.607170 | -3.764220 | -2.173498 |
| H | -2.599935 | -3.961904 | -1.764081 |
| H | -1.318496 | -4.641224 | -2.757656 |

| | | | |
|---|---|---|---|
| H | -1.677179 | -2.913180 | -2.857762 |
| C | -0.592991 | -4.645702 | -0.055388 |
| H | 0.133320 | -4.487191 | 0.746916 |
| H | -0.334160 | -5.586724 | -0.547000 |
| H | -1.582955 | -4.772009 | 0.390830 |
| C | 0.823496 | -3.459815 | -1.736374 |
| H | 0.896708 | -2.627178 | -2.442871 |
| H | 0.998592 | -4.387152 | -2.287117 |
| H | 1.617951 | -3.350663 | -0.996072 |
| C | 1.325119 | -1.087781 | 0.190639 |
| C | 2.469938 | -1.134635 | 0.890946 |
| H | 1.247825 | -0.528564 | -0.737445 |
| H | 2.513848 | -1.759916 | 1.779941 |
| C | 3.706676 | -0.440670 | 0.515686 |
| C | 3.729078 | 0.649956 | -0.367698 |
| C | 4.927055 | -0.879046 | 1.049610 |
| C | 4.929906 | 1.250692 | -0.723250 |
| H | 2.796166 | 1.054602 | -0.743173 |
| C | 6.126740 | -0.270835 | 0.699095 |
| H | 4.929446 | -1.714400 | 1.742282 |
| C | 6.136746 | 0.794504 | -0.196245 |
| H | 4.922632 | 2.094298 | -1.404241 |
| H | 7.056106 | -0.632384 | 1.124510 |
| H | 7.069751 | 1.271613 | -0.471084 |

**6F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1775.175312

Free energies: -1774.741041

Corrected Free energies: -1774.733568

| | | | |
|---|---|---|---|
| S | 0.364752 | 1.823251 | -0.120789 |
| F | -1.312255 | 3.715411 | -0.796370 |
| F | 0.416225 | 4.409337 | 0.296314 |
| F | 0.607845 | 3.834418 | -1.775565 |
| O | -0.183962 | 1.015295 | -1.216963 |
| O | -0.400331 | 1.666117 | 1.133255 |
| O | 1.811178 | 1.773197 | 0.032193 |
| C | -0.001699 | 3.557176 | -0.630342 |
| N | -0.252294 | -1.838001 | 0.511531 |
| H | -0.323121 | -2.291715 | 1.419725 |
| N | -2.646832 | 0.093140 | 0.839018 |
| H | -1.674621 | 0.441779 | 0.955940 |
| C | -1.460640 | -1.799247 | -0.322542 |

| | | | |
|---|---|---|---|
| H | -1.267255 | -1.040872 | -1.085717 |
| C | -2.633407 | -1.377018 | 0.564126 |
| H | -3.584205 | -1.628039 | 0.101817 |
| H | -2.592851 | -1.897052 | 1.521437 |
| C | -3.199590 | 0.900172 | -0.311778 |
| H | -2.937303 | 1.933468 | -0.082816 |
| H | -2.635971 | 0.610227 | -1.197509 |
| C | -4.694556 | 0.743972 | -0.513691 |
| H | -5.265876 | 1.082188 | 0.350706 |
| H | -4.983344 | -0.280505 | -0.752234 |
| H | -4.977641 | 1.365725 | -1.363333 |
| C | -3.333299 | 0.427625 | 2.138356 |
| H | -3.543202 | 1.496604 | 2.099548 |
| H | -4.279585 | -0.113529 | 2.156584 |
| C | -2.456992 | 0.102127 | 3.334946 |
| H | -2.954832 | 0.464174 | 4.234400 |
| H | -1.491925 | 0.605165 | 3.251090 |
| H | -2.294522 | -0.968930 | 3.459770 |
| C | -1.704503 | -3.157413 | -1.048401 |
| C | -2.845836 | -2.965256 | -2.057304 |
| H | -3.814379 | -2.810320 | -1.578687 |
| H | -2.931860 | -3.865175 | -2.669479 |
| H | -2.646324 | -2.122188 | -2.724507 |
| C | -2.060147 | -4.265728 | -0.052734 |
| H | -1.263648 | -4.426923 | 0.679112 |
| H | -2.199308 | -5.204932 | -0.592180 |
| H | -2.989312 | -4.055291 | 0.482585 |
| C | -0.437973 | -3.542954 | -1.820976 |
| H | -0.132461 | -2.747302 | -2.507095 |
| H | -0.639347 | -4.436402 | -2.414981 |
| H | 0.397670 | -3.773888 | -1.156801 |
| C | 0.944131 | -1.453264 | 0.112902 |
| C | 2.084875 | -1.635339 | 0.900770 |
| H | 0.987599 | -0.991722 | -0.867239 |
| H | 1.957620 | -2.127794 | 1.860542 |
| C | 3.398456 | -1.249137 | 0.528364 |
| C | 3.692585 | -0.537603 | -0.661880 |
| C | 4.464091 | -1.603235 | 1.392304 |
| C | 4.997256 | -0.213272 | -0.968688 |
| H | 2.896216 | -0.216919 | -1.319941 |
| C | 5.765974 | -1.274500 | 1.074329 |
| H | 4.241586 | -2.142667 | 2.305706 |
| C | 6.036035 | -0.581213 | -0.107604 |
| H | 5.217619 | 0.334019 | -1.876173 |

| | | | |
|---|---|---|---|
| H | 6.574753 | -1.552276 | 1.737737 |
| H | 7.057684 | -0.321593 | -0.357459 |

**6F-*Z***

Imaginary frequency: None

Electronic energies: -1775.366761

Free energies: -1774.931823

Corrected Free energies: -1774.924595

| | | | |
|---|---|---|---|
| S | 1.967989 | -1.172595 | -0.623781 |
| F | 4.322954 | -0.184977 | 0.023096 |
| F | 4.158003 | -2.322040 | 0.269077 |
| F | 4.340943 | -1.475017 | -1.707504 |
| O | 1.760688 | 0.003594 | -1.471982 |
| O | 1.567439 | -0.956780 | 0.778642 |
| O | 1.586731 | -2.459501 | -1.191464 |
| C | 3.806863 | -1.297430 | -0.502466 |
| N | -1.234039 | 0.573008 | -0.382513 |
| H | -1.899834 | 0.309389 | 0.337587 |
| N | 0.759485 | 1.731475 | 1.138513 |
| H | 0.639842 | 0.801953 | 0.698434 |
| C | -1.056806 | 2.013227 | -0.533304 |
| H | -0.318099 | 2.148113 | -1.332855 |
| C | -0.449297 | 2.533257 | 0.774380 |
| H | -0.150239 | 3.574800 | 0.695741 |
| H | -1.166986 | 2.448532 | 1.589764 |
| C | 2.028963 | 2.299622 | 0.566054 |
| H | 2.767809 | 1.504666 | 0.653291 |
| H | 1.840615 | 2.460955 | -0.494830 |
| C | 2.504788 | 3.563242 | 1.259739 |
| H | 2.782975 | 3.379581 | 2.297762 |
| H | 1.767199 | 4.366238 | 1.228650 |
| H | 3.394042 | 3.914668 | 0.735722 |
| C | 0.873325 | 1.458901 | 2.610552 |
| H | 1.879996 | 1.070891 | 2.768496 |
| H | 0.774989 | 2.414270 | 3.126575 |
| C | -0.157155 | 0.444967 | 3.074299 |
| H | -0.016721 | 0.271759 | 4.141532 |
| H | -0.014452 | -0.499903 | 2.549727 |
| H | -1.182971 | 0.788587 | 2.930160 |
| C | -2.338440 | 2.802714 | -0.934869 |
| C | -2.045125 | 4.309684 | -0.913210 |
| H | -1.929469 | 4.693500 | 0.103072 |
| H | -2.875209 | 4.850465 | -1.373401 |

| | | | |
|---|---|---|---|
| H | -1.137397 | 4.544543 | -1.478069 |
| C | -3.504968 | 2.490923 | 0.009764 |
| H | -3.793724 | 1.437485 | -0.044639 |
| H | -4.376139 | 3.081994 | -0.283037 |
| H | -3.279751 | 2.737044 | 1.050773 |
| C | -2.743716 | 2.408354 | -2.360524 |
| H | -1.933103 | 2.600589 | -3.069543 |
| H | -3.610468 | 2.998301 | -2.669125 |
| H | -3.017945 | 1.353858 | -2.424809 |
| C | -1.273109 | -0.239031 | -1.510103 |
| C | -1.835677 | -1.453913 | -1.598727 |
| H | -0.772712 | 0.188707 | -2.371447 |
| C | -2.485758 | -2.160784 | -0.480620 |
| C | -1.895728 | -2.188232 | 0.790612 |
| C | -3.694419 | -2.843720 | -0.666432 |
| C | -2.512779 | -2.845695 | 1.850193 |
| H | -0.925244 | -1.719367 | 0.925544 |
| C | -4.308380 | -3.504995 | 0.390836 |
| H | -4.155004 | -2.846164 | -1.648741 |
| C | -3.725014 | -3.501652 | 1.655829 |
| H | -2.038193 | -2.856737 | 2.825049 |
| H | -5.246899 | -4.022442 | 0.228666 |
| H | -4.206762 | -4.015080 | 2.479488 |
| H | -1.807462 | -1.947875 | -2.562638 |

**6F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1775.170670

Free energies: -1774.731810

Corrected Free energies: -1774.725994

| | | | |
|---|---|---|---|
| S | -0.734042 | 1.876289 | -0.709201 |
| F | -3.148828 | 2.622720 | -0.029664 |
| F | -1.671328 | 4.195303 | 0.061728 |
| F | -2.415671 | 3.524119 | -1.849969 |
| O | -1.328107 | 0.768856 | -1.465944 |
| O | -0.517081 | 1.524127 | 0.713184 |
| O | 0.381528 | 2.561032 | -1.343089 |
| C | -2.077459 | 3.137567 | -0.627149 |
| N | 0.839079 | -1.342934 | -0.467438 |
| H | 1.487045 | -1.463399 | 0.308641 |
| N | -1.596296 | -0.919972 | 1.366216 |
| H | -1.047479 | -0.106429 | 1.018744 |
| C | -0.382779 | -2.162184 | -0.470208 |

| | | | |
|---|---|---|---|
| H | -1.076417 | -1.646940 | -1.140029 |
| C | -0.929167 | -2.192888 | 0.957468 |
| H | -1.657987 | -2.989465 | 1.078071 |
| H | -0.121551 | -2.385334 | 1.663934 |
| C | -2.969869 | -0.750617 | 0.762923 |
| H | -3.236311 | 0.289785 | 0.951938 |
| H | -2.858301 | -0.867126 | -0.313858 |
| C | -4.012535 | -1.694987 | 1.330787 |
| H | -4.174823 | -1.537889 | 2.396983 |
| H | -3.770750 | -2.744447 | 1.157743 |
| H | -4.953134 | -1.491042 | 0.818830 |
| C | -1.621024 | -0.759022 | 2.865358 |
| H | -2.365496 | 0.009706 | 3.073224 |
| H | -1.966780 | -1.703239 | 3.287380 |
| C | -0.266829 | -0.345512 | 3.412947 |
| H | -0.363098 | -0.199816 | 4.488936 |
| H | 0.056088 | 0.597724 | 2.969093 |
| H | 0.503116 | -1.101780 | 3.254526 |
| C | -0.133635 | -3.594171 | -1.040436 |
| C | -1.494542 | -4.287933 | -1.200576 |
| H | -1.964277 | -4.527629 | -0.244972 |
| H | -1.351373 | -5.231160 | -1.730990 |
| H | -2.185284 | -3.674097 | -1.785478 |
| C | 0.773353 | -4.412541 | -0.116135 |
| H | 1.746941 | -3.934337 | 0.024015 |
| H | 0.951998 | -5.392459 | -0.563931 |
| H | 0.320988 | -4.579567 | 0.864345 |
| C | 0.512233 | -3.484606 | -2.426016 |
| H | -0.092632 | -2.872524 | -3.101523 |
| H | 0.590147 | -4.482182 | -2.861967 |
| H | 1.522708 | -3.072634 | -2.381598 |
| C | 1.232123 | -0.610197 | -1.489673 |
| C | 2.425286 | 0.127476 | -1.537676 |
| H | 0.582154 | -0.612439 | -2.356678 |
| C | 3.259596 | 0.483797 | -0.431625 |
| C | 2.754856 | 0.645543 | 0.878304 |
| C | 4.628570 | 0.730167 | -0.673217 |
| C | 3.607291 | 0.983580 | 1.913579 |
| H | 1.686795 | 0.594198 | 1.056934 |
| C | 5.474716 | 1.050169 | 0.371943 |
| H | 5.012121 | 0.639334 | -1.682732 |
| C | 4.968280 | 1.169403 | 1.667212 |
| H | 3.211220 | 1.122786 | 2.911743 |
| H | 6.527693 | 1.216257 | 0.183551 |

| | | | |
|---|---|---|---|
| H | 5.631447 | 1.430862 | 2.482628 |
| H | 2.741355 | 0.425325 | -2.530654 |

**7F-*E***

Imaginary frequency: None

Electronic energies: -733.504190

Free energies: -733.173924

Corrected Free energies: -733.170823

| | | | |
|---|---|---|---|
| N | 0.441250 | -0.184691 | -0.577050 |
| C | -0.850711 | 0.155248 | -0.272312 |
| C | -1.928158 | -0.636417 | -0.445748 |
| H | -1.769320 | -1.645419 | -0.818624 |
| H | 0.631630 | -1.176482 | -0.683069 |
| C | 1.564193 | 0.514220 | 0.035595 |
| C | 2.842555 | -0.282748 | -0.268432 |
| C | 1.711914 | 1.943062 | -0.494933 |
| H | 1.433474 | 0.571184 | 1.127673 |
| C | 4.046934 | 0.396601 | 0.397721 |
| H | 2.982340 | -0.231143 | -1.356609 |
| C | 2.921942 | 2.637684 | 0.132717 |
| H | 1.826387 | 1.893923 | -1.583836 |
| H | 0.801723 | 2.513503 | -0.290986 |
| C | 4.201193 | 1.833511 | -0.106984 |
| H | 4.956112 | -0.175838 | 0.194197 |
| H | 3.906985 | 0.409321 | 1.484495 |
| H | 3.023721 | 3.646954 | -0.273004 |
| H | 2.758657 | 2.741945 | 1.211766 |
| H | 5.050531 | 2.315617 | 0.383252 |
| H | 4.419259 | 1.815936 | -1.181171 |
| N | 2.657439 | -1.707693 | 0.033357 |
| C | 3.656430 | -2.549097 | -0.609362 |
| H | 4.664494 | -2.425355 | -0.183636 |
| H | 3.371960 | -3.597213 | -0.493808 |
| H | 3.700647 | -2.321362 | -1.675996 |
| C | 2.567651 | -2.012700 | 1.455351 |
| H | 2.288338 | -3.061511 | 1.574596 |
| H | 3.516621 | -1.852325 | 1.989150 |
| H | 1.795084 | -1.404956 | 1.929187 |
| H | -0.965028 | 1.166575 | 0.109128 |
| C | -3.318021 | -0.263595 | -0.177342 |
| C | -4.321870 | -1.232680 | -0.335243 |
| C | -3.719036 | 1.019470 | 0.234183 |
| C | -5.658805 | -0.941551 | -0.090652 |

| | | | |
|---|---|---|---|
| H | -4.040167 | -2.230757 | -0.654784 |
| C | -5.053892 | 1.308612 | 0.481458 |
| H | -2.984314 | 1.806490 | 0.359087 |
| C | -6.036218 | 0.332184 | 0.322301 |
| H | -6.407761 | -1.714245 | -0.223374 |
| H | -5.331860 | 2.307704 | 0.797745 |
| H | -7.076948 | 0.563312 | 0.514562 |

**7F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -733.321817

Free energies: -732.989662

Corrected Free energies: -732.987196

| | | | |
|---|---|---|---|
| N | -0.407217 | -0.298265 | -0.336138 |
| C | 0.823959 | 0.136235 | -0.274097 |
| C | 1.912789 | -0.731335 | -0.107221 |
| H | 1.697666 | -1.793004 | -0.037089 |
| H | -0.623351 | -1.299405 | -0.252249 |
| C | -1.631362 | 0.492617 | -0.487407 |
| C | -2.712549 | -0.243042 | 0.328922 |
| C | -1.481125 | 1.944076 | -0.046251 |
| H | -1.898375 | 0.462529 | -1.551263 |
| C | -4.051383 | 0.486480 | 0.186908 |
| H | -2.399135 | -0.176851 | 1.378365 |
| C | -2.830482 | 2.663452 | -0.141855 |
| H | -1.117811 | 1.963868 | 0.987685 |
| H | -0.749064 | 2.463018 | -0.669132 |
| C | -3.915598 | 1.937350 | 0.654305 |
| H | -4.815390 | -0.038169 | 0.766320 |
| H | -4.370614 | 0.473821 | -0.860968 |
| H | -2.713803 | 3.688425 | 0.214722 |
| H | -3.131442 | 2.722353 | -1.193626 |
| H | -4.870435 | 2.455621 | 0.544732 |
| H | -3.660291 | 1.954957 | 1.719767 |
| N | -2.693608 | -1.670046 | -0.011794 |
| C | -3.196586 | -2.505618 | 1.074162 |
| H | -4.266083 | -2.341596 | 1.273071 |
| H | -3.058371 | -3.555264 | 0.809764 |
| H | -2.635033 | -2.303356 | 1.987350 |
| C | -3.371933 | -1.997082 | -1.264138 |
| H | -3.150977 | -3.034067 | -1.521773 |
| H | -4.463105 | -1.885186 | -1.194187 |
| H | -3.010376 | -1.365297 | -2.077049 |

| | | | |
|---|---|---|---|
| H | 0.967012 | 1.206569 | -0.358665 |
| C | 3.275493 | -0.325687 | -0.023509 |
| C | 3.690325 | 1.026228 | -0.085305 |
| C | 4.261028 | -1.328335 | 0.132694 |
| C | 5.029595 | 1.348428 | 0.003871 |
| H | 2.966436 | 1.822453 | -0.201293 |
| C | 5.599422 | -0.995543 | 0.220855 |
| H | 3.950907 | -2.365841 | 0.181827 |
| C | 5.988220 | 0.342668 | 0.156098 |
| H | 5.337615 | 2.385231 | -0.043948 |
| H | 6.343929 | -1.772369 | 0.340338 |
| H | 7.036982 | 0.604393 | 0.224630 |

**7F-Z**

Imaginary frequency: None

Electronic energies: -733.504500

Free energies: -733.173271

Corrected Free energies: -733.170251

| | | | |
|---|---|---|---|
| N | -0.194236 | -0.809537 | -0.158151 |
| C | 0.574953 | -1.853937 | 0.296988 |
| C | 1.918520 | -1.921435 | 0.403993 |
| H | 0.217842 | 0.116717 | -0.086641 |
| C | -1.613562 | -0.765390 | 0.179193 |
| C | -2.153561 | 0.618068 | -0.215227 |
| C | -2.410189 | -1.850340 | -0.549342 |
| H | -1.758135 | -0.908282 | 1.262139 |
| C | -3.636508 | 0.723456 | 0.166137 |
| H | -2.077871 | 0.673815 | -1.309279 |
| C | -3.897369 | -1.757521 | -0.205278 |
| H | -2.261439 | -1.718501 | -1.627249 |
| H | -2.025046 | -2.839657 | -0.289136 |
| C | -4.451524 | -0.369119 | -0.531865 |
| H | -4.018702 | 1.712800 | -0.100026 |
| H | -3.743620 | 0.615388 | 1.251449 |
| H | -4.453355 | -2.527343 | -0.745503 |
| H | -4.033202 | -1.957285 | 0.864002 |
| H | -5.501957 | -0.300115 | -0.238581 |
| H | -4.410455 | -0.211075 | -1.615841 |
| N | -1.279931 | 1.683669 | 0.291617 |
| C | -1.452396 | 2.939352 | -0.423487 |
| H | -2.431500 | 3.410481 | -0.242512 |
| H | -0.679652 | 3.642393 | -0.104778 |
| H | -1.341581 | 2.772052 | -1.496526 |

| | | | |
|---|---|---|---|
| C | -1.362789 | 1.893914 | 1.731126 |
| H | -0.568433 | 2.578532 | 2.035261 |
| H | -2.323945 | 2.327245 | 2.047065 |
| H | -1.215289 | 0.952364 | 2.262845 |
| H | 0.003453 | -2.729137 | 0.594265 |
| H | 2.318151 | -2.837364 | 0.824105 |
| C | 2.900812 | -0.885311 | 0.071977 |
| C | 4.156519 | -0.918480 | 0.701690 |
| C | 2.672489 | 0.133604 | -0.868406 |
| C | 5.126723 | 0.036014 | 0.432953 |
| H | 4.361198 | -1.707716 | 1.417786 |
| C | 3.646684 | 1.090327 | -1.137148 |
| H | 1.744060 | 0.156853 | -1.425907 |
| C | 4.874519 | 1.054470 | -0.484566 |
| H | 6.083533 | -0.013511 | 0.940149 |
| H | 3.445933 | 1.863250 | -1.870415 |
| H | 5.629254 | 1.803135 | -0.693355 |

**7F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -733.317815

Free energies: -732.985424

Corrected Free energies: -732.982707

| | | | |
|---|---|---|---|
| N | -0.232761 | -0.949848 | 0.425577 |
| C | 0.455666 | -2.041299 | 0.226522 |
| C | 1.859692 | -2.077488 | 0.128577 |
| H | 0.233797 | -0.045903 | 0.570387 |
| C | -1.684655 | -0.775097 | 0.467887 |
| C | -1.942141 | 0.595300 | -0.196542 |
| C | -2.466456 | -1.890601 | -0.212286 |
| H | -1.968088 | -0.721198 | 1.526398 |
| C | -3.438064 | 0.916310 | -0.150059 |
| H | -1.651798 | 0.482630 | -1.248868 |
| C | -3.960778 | -1.550322 | -0.206391 |
| H | -2.109227 | -1.997784 | -1.243008 |
| H | -2.303713 | -2.842139 | 0.299204 |
| C | -4.233311 | -0.189277 | -0.849800 |
| H | -3.618630 | 1.883830 | -0.625731 |
| H | -3.767734 | 0.996475 | 0.891481 |
| H | -4.508344 | -2.337378 | -0.727901 |
| H | -4.321183 | -1.540132 | 0.828002 |
| H | -5.300878 | 0.036223 | -0.808613 |
| H | -3.952918 | -0.223782 | -1.908578 |

| | | | |
|---|---|---|---|
| N | -1.024743 | 1.588673 | 0.375174 |
| C | -0.735300 | 2.681217 | -0.548985 |
| H | -1.619409 | 3.299560 | -0.762171 |
| H | 0.031381 | 3.323547 | -0.112224 |
| H | -0.354537 | 2.282399 | -1.491336 |
| C | -1.443177 | 2.113732 | 1.673857 |
| H | -0.621846 | 2.691475 | 2.100093 |
| H | -2.322595 | 2.767960 | 1.598278 |
| H | -1.674626 | 1.299848 | 2.362863 |
| H | -0.095489 | -2.973503 | 0.167999 |
| H | 2.306854 | -3.058030 | 0.240878 |
| C | 2.743340 | -0.964709 | -0.058386 |
| C | 4.093587 | -1.121895 | 0.323988 |
| C | 2.345595 | 0.262039 | -0.638615 |
| C | 4.989138 | -0.076170 | 0.196508 |
| H | 4.416085 | -2.068630 | 0.741701 |
| C | 3.252118 | 1.297773 | -0.775636 |
| H | 1.347004 | 0.384754 | -1.040484 |
| C | 4.569720 | 1.138835 | -0.345746 |
| H | 6.016649 | -0.203937 | 0.512483 |
| H | 2.937565 | 2.227507 | -1.233262 |
| H | 5.274364 | 1.954352 | -0.452198 |

**8F-*E***

Imaginary frequency: None

Electronic energies: -1039.508936

Free energies: -1039.118640

Corrected Free energies: -1039.113085

| | | | |
|---|---|---|---|
| N | -0.654407 | -0.731932 | -0.687140 |
| C | -1.903672 | -0.332840 | -0.275907 |
| C | -3.039804 | -1.038839 | -0.423806 |
| H | -2.978244 | -2.047362 | -0.825175 |
| H | -0.546890 | -1.702590 | -0.962622 |
| C | 0.526913 | -0.219722 | -0.007821 |
| C | 1.751779 | -0.956470 | -0.594456 |
| H | 0.468035 | -0.411386 | 1.071978 |
| H | 1.814808 | -0.640598 | -1.641878 |
| N | 1.507977 | -2.406412 | -0.647067 |
| C | 2.477585 | -3.091107 | -1.491272 |
| H | 3.489855 | -3.095305 | -1.057677 |
| H | 2.160811 | -4.126479 | -1.630930 |
| H | 2.523215 | -2.608377 | -2.469650 |
| C | 1.399284 | -3.066616 | 0.647637 |

| | | | |
|---|---|---|---|
| H | 1.077878 | -4.097156 | 0.484433 |
| H | 2.350036 | -3.088970 | 1.200202 |
| H | 0.644434 | -2.577178 | 1.266649 |
| C | 0.674326 | 1.278953 | -0.199056 |
| C | 0.499827 | 1.851176 | -1.460584 |
| C | 1.013628 | 2.099260 | 0.874820 |
| C | 0.672576 | 3.218208 | -1.644225 |
| H | 0.214323 | 1.218146 | -2.293825 |
| C | 1.188580 | 3.468662 | 0.693528 |
| H | 1.143155 | 1.663714 | 1.860386 |
| C | 1.019529 | 4.031023 | -0.567209 |
| H | 0.533985 | 3.651736 | -2.627915 |
| H | 1.452160 | 4.094582 | 1.537960 |
| H | 1.152232 | 5.096803 | -0.710980 |
| C | 3.053585 | -0.552801 | 0.080312 |
| C | 4.150550 | -0.206108 | -0.710269 |
| C | 3.207273 | -0.545876 | 1.470131 |
| C | 5.370353 | 0.138085 | -0.135581 |
| H | 4.043905 | -0.201611 | -1.790572 |
| C | 4.424818 | -0.203057 | 2.049094 |
| H | 2.373933 | -0.803512 | 2.114065 |
| C | 5.510362 | 0.139838 | 1.248053 |
| H | 6.208231 | 0.407815 | -0.767694 |
| H | 4.524716 | -0.200775 | 3.128127 |
| H | 6.457331 | 0.409028 | 1.700537 |
| H | -1.920960 | 0.657137 | 0.174957 |
| C | -4.374768 | -0.565207 | -0.047329 |
| C | -4.675215 | 0.788356 | 0.177994 |
| C | -5.415258 | -1.495033 | 0.099313 |
| C | -5.948802 | 1.183478 | 0.565654 |
| H | -3.911037 | 1.543461 | 0.031430 |
| C | -6.692074 | -1.097920 | 0.478506 |
| H | -5.210241 | -2.545388 | -0.080663 |
| C | -6.966962 | 0.244718 | 0.720706 |
| H | -6.152341 | 2.234871 | 0.734610 |
| H | -7.474005 | -1.840933 | 0.587526 |
| H | -7.960786 | 0.557762 | 1.016768 |

**8F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1039.322331

Free energies: -1038.932723

Corrected Free energies: -1038.926834

| | | | |
|---|---|---|---|
| N | -0.645933 | -0.871677 | 0.018502 |
| C | -1.842388 | -0.362308 | 0.176330 |
| C | -3.004046 | -1.086537 | -0.117679 |
| H | -2.879139 | -2.098320 | -0.489944 |
| H | -0.503899 | -1.838334 | -0.300932 |
| C | 0.621265 | -0.210445 | 0.354496 |
| C | 1.722839 | -0.982519 | -0.410711 |
| H | 0.760876 | -0.320873 | 1.434086 |
| H | 1.570683 | -0.752688 | -1.470400 |
| N | 1.486347 | -2.428430 | -0.290367 |
| C | 2.178683 | -3.178967 | -1.334369 |
| H | 3.271995 | -3.131102 | -1.226026 |
| H | 1.872005 | -4.224462 | -1.281277 |
| H | 1.905155 | -2.786642 | -2.315242 |
| C | 1.776884 | -2.994301 | 1.025236 |
| H | 1.436638 | -4.030567 | 1.036613 |
| H | 2.848500 | -2.977042 | 1.265358 |
| H | 1.235332 | -2.458047 | 1.807306 |
| C | 0.616944 | 1.261289 | 0.009271 |
| C | 0.284657 | 1.683872 | -1.279913 |
| C | 0.985908 | 2.202800 | 0.966171 |
| C | 0.325903 | 3.033685 | -1.604635 |
| H | -0.014280 | 0.959611 | -2.031094 |
| C | 1.033551 | 3.554868 | 0.638142 |
| H | 1.242436 | 1.879141 | 1.969128 |
| C | 0.703906 | 3.971356 | -0.646448 |
| H | 0.064262 | 3.353943 | -2.605739 |
| H | 1.325417 | 4.279932 | 1.388052 |
| H | 0.737767 | 5.023667 | -0.901625 |
| C | 3.115330 | -0.505279 | -0.038429 |
| C | 4.037708 | -0.252015 | -1.054584 |
| C | 3.517723 | -0.337610 | 1.289282 |
| C | 5.333425 | 0.158382 | -0.756503 |
| H | 3.735161 | -0.371370 | -2.090036 |
| C | 4.811040 | 0.075051 | 1.590351 |
| H | 2.826874 | -0.527025 | 2.103220 |
| C | 5.722387 | 0.323584 | 0.568219 |
| H | 6.035403 | 0.352547 | -1.558561 |
| H | 5.106132 | 0.203181 | 2.624808 |
| H | 6.729253 | 0.646293 | 0.804402 |
| H | -1.882153 | 0.658026 | 0.542851 |
| C | -4.333271 | -0.601994 | 0.035215 |
| C | -5.397690 | -1.469629 | -0.305920 |
| C | -4.641944 | 0.695833 | 0.509955 |

| | | | |
|---|---|---|---|
| C | -6.710681 | -1.059337 | -0.179351 |
| H | -5.168786 | -2.465324 | -0.668108 |
| C | -5.957043 | 1.095744 | 0.633090 |
| H | -3.853940 | 1.386518 | 0.781102 |
| C | -6.994340 | 0.223624 | 0.289874 |
| H | -7.516780 | -1.731753 | -0.443359 |
| H | -6.185082 | 2.089614 | 0.996576 |
| H | -8.023214 | 0.546937 | 0.389348 |

**8F-*Z***

Imaginary frequency: None

Electronic energies: -1039.508381

Free energies: -1039.117069

Corrected Free energies: -1039.111444

| | | | |
|---|---|---|---|
| N | 0.962348 | 0.624690 | -0.159083 |
| C | 1.705665 | 1.552134 | -0.838807 |
| C | 3.048386 | 1.609344 | -0.957311 |
| H | 3.456508 | 2.500207 | -1.420228 |
| H | 1.412865 | -0.197981 | 0.218246 |
| C | -0.447088 | 0.424537 | -0.437650 |
| C | -0.912391 | -0.771448 | 0.426998 |
| H | -0.602811 | 0.191762 | -1.499205 |
| H | -0.876896 | -0.419339 | 1.464076 |
| N | 0.066774 | -1.868304 | 0.365198 |
| C | -0.155031 | -2.856498 | 1.412396 |
| H | -1.080958 | -3.432819 | 1.261442 |
| H | 0.685208 | -3.553298 | 1.427847 |
| H | -0.210948 | -2.359479 | 2.382972 |
| C | 0.193143 | -2.514801 | -0.934517 |
| H | 1.047784 | -3.194295 | -0.902405 |
| H | -0.696581 | -3.097980 | -1.212708 |
| H | 0.383674 | -1.773672 | -1.714374 |
| C | -1.276381 | 1.654603 | -0.108070 |
| C | -1.013827 | 2.385399 | 1.051537 |
| C | -2.329026 | 2.047343 | -0.932430 |
| C | -1.795745 | 3.485271 | 1.384801 |
| H | -0.182332 | 2.092704 | 1.683520 |
| C | -3.114984 | 3.148107 | -0.600009 |
| H | -2.537445 | 1.487315 | -1.838436 |
| C | -2.850325 | 3.868838 | 0.559806 |
| H | -1.580220 | 4.046149 | 2.286718 |
| H | -3.930130 | 3.444241 | -1.249681 |
| H | -3.458108 | 4.728108 | 0.817731 |

| | | | |
|---|---|---|---|
| C | -2.348192 | -1.176233 | 0.134805 |
| C | -3.238007 | -1.342034 | 1.197144 |
| C | -2.809097 | -1.418784 | -1.163055 |
| C | -4.553838 | -1.738036 | 0.976986 |
| H | -2.895117 | -1.152750 | 2.209628 |
| C | -4.123243 | -1.816330 | -1.387584 |
| H | -2.146844 | -1.292219 | -2.012221 |
| C | -4.999749 | -1.976841 | -0.318411 |
| H | -5.229765 | -1.856439 | 1.815588 |
| H | -4.463669 | -1.997528 | -2.400295 |
| H | -6.023818 | -2.283474 | -0.495216 |
| H | 1.111908 | 2.355368 | -1.268300 |
| C | 4.021769 | 0.632317 | -0.448769 |
| C | 3.771155 | -0.748823 | -0.401329 |
| C | 5.282042 | 1.077970 | -0.020420 |
| C | 4.725583 | -1.635618 | 0.085693 |
| H | 2.838550 | -1.145071 | -0.788442 |
| C | 6.236352 | 0.192455 | 0.463580 |
| H | 5.504456 | 2.139133 | -0.064009 |
| C | 5.960460 | -1.171300 | 0.528553 |
| H | 4.505059 | -2.696914 | 0.107805 |
| H | 7.198252 | 0.567617 | 0.794085 |
| H | 6.701752 | -1.863485 | 0.909432 |

**8F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1039.317935

Free energies: -1038.925923

Corrected Free energies: -1038.920595

| | | | |
|---|---|---|---|
| N | 0.938489 | 0.612737 | -0.348112 |
| C | 1.640780 | 1.662550 | -0.687344 |
| C | 3.038176 | 1.758765 | -0.561320 |
| H | 3.438731 | 2.762813 | -0.635006 |
| H | 1.366754 | -0.223720 | 0.069848 |
| C | -0.508452 | 0.435645 | -0.519831 |
| C | -0.887057 | -0.764942 | 0.382801 |
| H | -0.675251 | 0.189030 | -1.572095 |
| H | -0.813482 | -0.402198 | 1.413293 |
| N | 0.144375 | -1.808998 | 0.266960 |
| C | 0.110749 | -2.737901 | 1.393304 |
| H | -0.800061 | -3.353342 | 1.396906 |
| H | 0.975775 | -3.399832 | 1.331394 |
| H | 0.164867 | -2.183129 | 2.331361 |

| | | | |
|---|---|---|---|
| C | 0.143475 | -2.535772 | -1.000738 |
| H | 1.023145 | -3.181138 | -1.027934 |
| H | -0.750152 | -3.160876 | -1.129314 |
| H | 0.208965 | -1.844650 | -1.844423 |
| C | -1.298979 | 1.677930 | -0.177303 |
| C | -1.088593 | 2.338208 | 1.034998 |
| C | -2.274037 | 2.145097 | -1.054717 |
| C | -1.847105 | 3.454940 | 1.361988 |
| H | -0.326721 | 1.985731 | 1.723146 |
| C | -3.039572 | 3.259370 | -0.722268 |
| H | -2.438271 | 1.635526 | -1.998067 |
| C | -2.825967 | 3.915451 | 0.484486 |
| H | -1.676190 | 3.964315 | 2.302449 |
| H | -3.797282 | 3.615764 | -1.409353 |
| H | -3.418108 | 4.785338 | 0.741953 |
| C | -2.318151 | -1.218947 | 0.162364 |
| C | -3.116303 | -1.490455 | 1.274390 |
| C | -2.858492 | -1.405561 | -1.113049 |
| C | -4.424492 | -1.938874 | 1.121776 |
| H | -2.709631 | -1.343732 | 2.269949 |
| C | -4.167071 | -1.850788 | -1.268595 |
| H | -2.266767 | -1.205485 | -1.999700 |
| C | -4.953058 | -2.118593 | -0.151901 |
| H | -5.029678 | -2.143873 | 1.996725 |
| H | -4.572731 | -1.986959 | -2.263938 |
| H | -5.972269 | -2.464468 | -0.274891 |
| H | 1.083941 | 2.522071 | -1.048423 |
| C | 3.963132 | 0.699449 | -0.297019 |
| C | 3.699908 | -0.663163 | -0.572385 |
| C | 5.220704 | 1.047321 | 0.245382 |
| C | 4.636473 | -1.631171 | -0.261074 |
| H | 2.796081 | -0.959061 | -1.091289 |
| C | 6.145026 | 0.070887 | 0.566096 |
| H | 5.442469 | 2.091826 | 0.431294 |
| C | 5.852240 | -1.271154 | 0.322357 |
| H | 4.429688 | -2.669756 | -0.487051 |
| H | 7.096597 | 0.349631 | 1.000530 |
| H | 6.579533 | -2.035754 | 0.566319 |

**9F-*E***

Imaginary frequency: None

Electronic energies: -520.944416

Free energies: -520.739408

Corrected Free energies: -520.737254

| | | | |
|---|---|---|---|
| C | -4.296637 | 0.549646 | 0.330563 |
| C | -4.097011 | -0.906086 | -0.107705 |
| C | -2.591697 | -1.127358 | 0.073582 |
| C | -3.052550 | 1.238523 | -0.228585 |
| H | -5.221755 | 0.987066 | -0.043611 |
| H | -4.294297 | 0.615940 | 1.421462 |
| H | -4.360639 | -1.013032 | -1.162810 |
| H | -4.692262 | -1.614492 | 0.467159 |
| H | -2.347793 | -1.517868 | 1.070385 |
| H | -2.177916 | -1.821173 | -0.665622 |
| H | -2.770961 | 2.134991 | 0.327095 |
| H | -3.198690 | 1.512298 | -1.280918 |
| N | -2.028041 | 0.205378 | -0.091728 |
| C | -0.698826 | 0.447135 | -0.101453 |
| C | 0.279561 | -0.484385 | 0.016519 |
| H | -0.448794 | 1.498357 | -0.216786 |
| H | 0.003456 | -1.530197 | 0.101552 |
| C | 1.713442 | -0.198810 | 0.018093 |
| C | 2.256721 | 1.098053 | 0.064762 |
| C | 2.619775 | -1.271924 | -0.021016 |
| C | 3.629754 | 1.303181 | 0.055521 |
| H | 1.602561 | 1.960791 | 0.118619 |
| C | 3.993903 | -1.065605 | -0.024691 |
| H | 2.230336 | -2.284424 | -0.052863 |
| C | 4.512356 | 0.225362 | 0.010258 |
| H | 4.015356 | 2.315966 | 0.091975 |
| H | 4.662149 | -1.918934 | -0.055984 |
| H | 5.582786 | 0.390666 | 0.007345 |

**9F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -520.763005

Free energies: -520.556209

Corrected Free energies: -520.554523

| | | | |
|---|---|---|---|
| C | -4.282457 | 0.483739 | 0.377844 |
| C | -4.056383 | -0.906002 | -0.225075 |
| C | -2.558917 | -1.138276 | -0.025918 |
| C | -3.050323 | 1.252434 | -0.085295 |
| H | -5.202564 | 0.953354 | 0.036026 |
| H | -4.298488 | 0.428762 | 1.468205 |
| H | -4.292665 | -0.897717 | -1.290840 |
| H | -4.646818 | -1.683446 | 0.255378 |

| | | | |
|---|---|---|---|
| H | -2.338148 | -1.574333 | 0.952050 |
| H | -2.100209 | -1.748783 | -0.803438 |
| H | -2.763834 | 2.089381 | 0.549251 |
| H | -3.158132 | 1.598394 | -1.117008 |
| N | -1.988409 | 0.224590 | -0.058985 |
| C | -0.708852 | 0.511081 | -0.047646 |
| C | 0.298605 | -0.459314 | -0.002146 |
| H | -0.469739 | 1.568232 | -0.070276 |
| H | 0.003316 | -1.501680 | 0.034735 |
| C | 1.698654 | -0.186029 | 0.005108 |
| C | 2.243700 | 1.118908 | -0.041026 |
| C | 2.584423 | -1.286782 | 0.057441 |
| C | 3.612312 | 1.301664 | -0.035329 |
| H | 1.598048 | 1.986692 | -0.081153 |
| C | 3.952962 | -1.093853 | 0.062429 |
| H | 2.174855 | -2.289662 | 0.093390 |
| C | 4.471223 | 0.200273 | 0.015842 |
| H | 4.020653 | 2.303596 | -0.071592 |
| H | 4.619612 | -1.945856 | 0.101581 |
| H | 5.543288 | 0.353872 | 0.019214 |

**9F-*Z***

Imaginary frequency: None

Electronic energies: -520.937745

Free energies: -520.730984

Corrected Free energies: -520.729381

| | | | |
|---|---|---|---|
| C | 3.721080 | -0.420479 | -0.518848 |
| C | 2.672749 | -1.527470 | -0.651991 |
| C | 1.341927 | -0.798992 | -0.415450 |
| C | 3.150455 | 0.413108 | 0.624833 |
| H | 4.722873 | -0.797214 | -0.312471 |
| H | 3.752295 | 0.181511 | -1.431175 |
| H | 2.828687 | -2.279170 | 0.126127 |
| H | 2.692986 | -2.031131 | -1.618050 |
| H | 0.891667 | -0.446823 | -1.351787 |
| H | 0.612791 | -1.445280 | 0.076041 |
| H | 3.497886 | 1.447352 | 0.628939 |
| H | 3.403727 | -0.034463 | 1.592007 |
| N | 1.699227 | 0.367847 | 0.403891 |
| C | 0.993002 | 1.539276 | 0.323977 |
| C | -0.321678 | 1.729542 | 0.074119 |
| H | 1.607439 | 2.427213 | 0.455776 |
| H | -0.621069 | 2.759847 | -0.085890 |

| | | | |
|---|---|---|---|
| C | -1.408735 | 0.740743 | 0.050375 |
| C | -1.446526 | -0.347101 | 0.935796 |
| C | -2.501449 | 0.921070 | -0.810590 |
| C | -2.517090 | -1.234587 | 0.935319 |
| H | -0.634039 | -0.477684 | 1.642707 |
| C | -3.570300 | 0.034031 | -0.813439 |
| H | -2.501111 | 1.768303 | -1.488587 |
| C | -3.582003 | -1.053780 | 0.056914 |
| H | -2.524257 | -2.065432 | 1.631750 |
| H | -4.397553 | 0.191749 | -1.496003 |
| H | -4.415487 | -1.745871 | 0.057298 |

**9F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -520.751226

Free energies: -520.543817

Corrected Free energies: -520.542396

| | | | |
|---|---|---|---|
| C | -3.760117 | -0.389862 | 0.477839 |
| C | -2.719746 | -1.495975 | 0.685522 |
| C | -1.366637 | -0.810971 | 0.439482 |
| C | -3.147508 | 0.424156 | -0.652442 |
| H | -4.743121 | -0.776038 | 0.215679 |
| H | -3.849428 | 0.232335 | 1.370536 |
| H | -2.868015 | -2.288010 | -0.049818 |
| H | -2.762749 | -1.938164 | 1.678751 |
| H | -0.854843 | -0.514515 | 1.357195 |
| H | -0.695641 | -1.431192 | -0.149031 |
| H | -3.509126 | 1.445877 | -0.742479 |
| H | -3.251030 | -0.086455 | -1.613687 |
| N | -1.713346 | 0.430662 | -0.297476 |
| C | -0.986405 | 1.516216 | -0.387522 |
| C | 0.367106 | 1.682894 | -0.031761 |
| H | -1.524628 | 2.402105 | -0.711577 |
| H | 0.625143 | 2.697416 | 0.253961 |
| C | 1.425850 | 0.721043 | -0.042656 |
| C | 1.425807 | -0.393867 | -0.908642 |
| C | 2.555637 | 0.950504 | 0.772462 |
| C | 2.494849 | -1.270798 | -0.915020 |
| H | 0.609837 | -0.529128 | -1.609180 |
| C | 3.609852 | 0.056039 | 0.776548 |
| H | 2.575261 | 1.824675 | 1.412933 |
| C | 3.580166 | -1.058249 | -0.062786 |
| H | 2.495008 | -2.115818 | -1.591798 |

| | | | |
|---|---|---|---|
| H | 4.461384 | 0.227044 | 1.422793 |
| H | 4.412250 | -1.751545 | -0.068094 |

**10F-*E***

Imaginary frequency: None

Electronic energies: -560.253752

Free energies: -560.018168

Corrected Free energies: -560.016542

| | | | |
|---|---|---|---|
| C | 0.641606 | -0.533086 | -0.064073 |
| C | -0.322786 | 0.409675 | -0.038227 |
| C | -2.194360 | -1.136399 | -0.148288 |
| C | -2.503050 | 1.180448 | 0.624470 |
| C | -3.644601 | -1.177569 | -0.621969 |
| H | -2.108119 | -1.585038 | 0.855721 |
| H | -1.573288 | -1.724393 | -0.825758 |
| C | -3.944849 | 1.181388 | 0.133361 |
| H | -2.482775 | 0.922393 | 1.695540 |
| H | -2.056375 | 2.170637 | 0.514431 |
| C | -4.523481 | -0.230805 | 0.192026 |
| H | -4.007660 | -2.205598 | -0.554242 |
| H | -3.677225 | -0.885321 | -1.676694 |
| H | -4.529735 | 1.870883 | 0.746481 |
| H | -3.970369 | 1.547491 | -0.898060 |
| H | -5.549528 | -0.244169 | -0.181684 |
| H | -4.552530 | -0.566709 | 1.235504 |
| H | 0.380105 | -1.585167 | -0.058341 |
| N | -1.683499 | 0.228580 | -0.130819 |
| H | -0.042167 | 1.456538 | 0.052920 |
| C | 2.077745 | -0.231219 | -0.051598 |
| C | 2.605354 | 1.016824 | -0.419812 |
| C | 2.983272 | -1.229296 | 0.339216 |
| C | 3.971574 | 1.261585 | -0.363354 |
| H | 1.944268 | 1.798559 | -0.776169 |
| C | 4.350811 | -0.987363 | 0.386028 |
| H | 2.600736 | -2.205990 | 0.617425 |
| C | 4.854984 | 0.263271 | 0.040933 |
| H | 4.350834 | 2.234789 | -0.653816 |
| H | 5.024439 | -1.778554 | 0.694907 |
| H | 5.920567 | 0.454864 | 0.075299 |

**10F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -560.070510
Free energies: -559.834495
Corrected Free energies: -559.832868

| | | | |
|---|---|---|---|
| C | 0.608562 | 0.509869 | -0.281855 |
| C | -0.408624 | -0.447653 | -0.374094 |
| C | -2.297850 | 1.129184 | -0.657719 |
| C | -2.669955 | -1.300882 | -0.562209 |
| C | -3.237864 | 1.345475 | 0.530392 |
| H | -2.858575 | 1.142250 | -1.596319 |
| H | -1.528036 | 1.891330 | -0.710995 |
| C | -3.625490 | -1.136979 | 0.620585 |
| H | -3.214267 | -1.237270 | -1.508421 |
| H | -2.132824 | -2.246442 | -0.527293 |
| C | -4.290474 | 0.239049 | 0.593882 |
| H | -3.703948 | 2.325748 | 0.419098 |
| H | -2.645131 | 1.360850 | 1.449908 |
| H | -4.369261 | -1.933797 | 0.567952 |
| H | -3.062234 | -1.268001 | 1.549205 |
| H | -4.918751 | 0.368719 | 1.476486 |
| H | -4.942565 | 0.309086 | -0.283200 |
| H | 0.359453 | 1.560483 | -0.350536 |
| N | -1.688150 | -0.204091 | -0.555530 |
| H | -0.160949 | -1.499766 | -0.294029 |
| C | 1.988800 | 0.201020 | -0.090214 |
| C | 2.496317 | -1.115265 | 0.023856 |
| C | 2.896430 | 1.282514 | -0.009023 |
| C | 3.847868 | -1.326162 | 0.211684 |
| H | 1.836546 | -1.971237 | -0.033336 |
| C | 4.247547 | 1.061442 | 0.179170 |
| H | 2.516170 | 2.293716 | -0.096658 |
| C | 4.727782 | -0.243325 | 0.290631 |
| H | 4.226863 | -2.336553 | 0.298161 |
| H | 4.930140 | 1.899470 | 0.239635 |
| H | 5.786125 | -0.419677 | 0.438533 |

**10F-*Z***

Imaginary frequency: None
Electronic energies: -560.245802
Free energies: -560.009658
Corrected Free energies: -560.008101

| | | | |
|---|---|---|---|
| C | -0.754335 | 1.841295 | 0.151129 |
| C | 0.586106 | 1.770677 | -0.008028 |
| C | 1.034328 | -0.647965 | 0.378443 |

| | | | |
|---|---|---|---|
| C | 2.640864 | 0.766997 | -0.852206 |
| C | 2.193701 | -1.351843 | 1.083230 |
| H | 0.710471 | -1.254998 | -0.480647 |
| H | 0.182423 | -0.555639 | 1.051437 |
| C | 3.817512 | 0.071735 | -0.173560 |
| H | 2.459348 | 0.301568 | -1.833569 |
| H | 2.863576 | 1.820800 | -1.029563 |
| C | 3.443659 | -1.360394 | 0.205147 |
| H | 1.886397 | -2.370046 | 1.334559 |
| H | 2.409340 | -0.828906 | 2.020616 |
| H | 4.679297 | 0.087585 | -0.845227 |
| H | 4.087456 | 0.630492 | 0.728494 |
| H | 4.272430 | -1.851928 | 0.719547 |
| H | 3.241232 | -1.935510 | -0.706650 |
| H | -1.148499 | 2.831555 | 0.355646 |
| N | 1.429274 | 0.687125 | -0.042518 |
| H | 1.128823 | 2.712902 | -0.062004 |
| C | -1.754716 | 0.768902 | 0.024180 |
| C | -1.675738 | -0.181436 | -1.004517 |
| C | -2.865249 | 0.718235 | 0.878562 |
| C | -2.643371 | -1.169227 | -1.145440 |
| H | -0.852264 | -0.126301 | -1.708497 |
| C | -3.836757 | -0.266030 | 0.735864 |
| H | -2.956686 | 1.456451 | 1.668612 |
| C | -3.726781 | -1.220559 | -0.272364 |
| H | -2.558018 | -1.893356 | -1.947673 |
| H | -4.682170 | -0.288827 | 1.414016 |
| H | -4.483410 | -1.988038 | -0.384108 |

**10F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -560.061450

Free energies: -559.825932

Corrected Free energies: -559.824334

| | | | |
|---|---|---|---|
| C | 0.697685 | -1.624260 | 0.282678 |
| C | -0.634280 | -1.561912 | -0.181620 |
| C | -1.137239 | 0.829877 | 0.201738 |
| C | -2.703117 | -0.648125 | -1.033091 |
| C | -2.272214 | 1.210816 | 1.154759 |
| H | -1.077854 | 1.534383 | -0.632793 |
| H | -0.187041 | 0.817653 | 0.725276 |
| C | -3.846286 | -0.273658 | -0.094995 |
| H | -2.676174 | 0.028701 | -1.892192 |

| | | | |
|---|---|---|---|
| H | -2.789014 | -1.668531 | -1.400848 |
| C | -3.634421 | 1.127290 | 0.473050 |
| H | -2.070601 | 2.220956 | 1.515386 |
| H | -2.242358 | 0.539679 | 2.018338 |
| H | -4.778823 | -0.336125 | -0.658294 |
| H | -3.897751 | -1.007216 | 0.715034 |
| H | -4.425514 | 1.369978 | 1.184159 |
| H | -3.686309 | 1.862928 | -0.336787 |
| H | 0.956014 | -2.565696 | 0.755805 |
| N | -1.396545 | -0.509530 | -0.359551 |
| H | -1.110024 | -2.511578 | -0.412624 |
| C | 1.757267 | -0.681438 | 0.102190 |
| C | 1.718776 | 0.326784 | -0.887596 |
| C | 2.929123 | -0.825803 | 0.877194 |
| C | 2.792634 | 1.178724 | -1.058547 |
| H | 0.860013 | 0.407459 | -1.543519 |
| C | 3.992874 | 0.042187 | 0.710409 |
| H | 2.978835 | -1.617047 | 1.616318 |
| C | 3.926291 | 1.048319 | -0.253368 |
| H | 2.757512 | 1.941098 | -1.826481 |
| H | 4.879389 | -0.065239 | 1.322509 |
| H | 4.762956 | 1.722507 | -0.389237 |

**11F-*E***

Imaginary frequency: None

Electronic energies: -709.515178

Free energies: -709.298881

Corrected Free energies: -709.295647

| | | | |
|---|---|---|---|
| C | 3.733518 | -0.705643 | 0.134565 |
| C | 3.175287 | -2.108299 | 0.379191 |
| C | 1.731335 | -1.997730 | -0.110528 |
| C | 2.540737 | 0.207827 | 0.486814 |
| H | 4.614335 | -0.467279 | 0.727623 |
| H | 3.982689 | -0.583572 | -0.923314 |
| H | 3.184239 | -2.331924 | 1.448295 |
| H | 3.737088 | -2.881600 | -0.142875 |
| H | 1.646824 | -2.197269 | -1.186303 |
| H | 1.054442 | -2.676253 | 0.415841 |
| H | 2.576156 | 0.499087 | 1.543890 |
| N | 1.385963 | -0.614382 | 0.190404 |
| C | 0.106727 | -0.158199 | 0.241471 |
| C | -0.999657 | -0.865770 | -0.078325 |
| H | 0.022066 | 0.875874 | 0.562410 |

| | | | |
|---|---|---|---|
| H | -0.892662 | -1.870549 | -0.473680 |
| C | 2.596492 | 1.475965 | -0.343119 |
| O | 1.877566 | 1.751742 | -1.263936 |
| O | 3.598628 | 2.258477 | 0.074552 |
| H | 3.633384 | 3.040354 | -0.495494 |
| C | -2.366437 | -0.347289 | 0.010517 |
| C | -3.401453 | -1.029527 | -0.649206 |
| C | -2.711516 | 0.807617 | 0.733680 |
| C | -4.712575 | -0.570707 | -0.610341 |
| H | -3.163626 | -1.929610 | -1.206851 |
| C | -4.020088 | 1.270949 | 0.763848 |
| H | -1.953123 | 1.342833 | 1.293721 |
| C | -5.031898 | 0.588008 | 0.091528 |
| H | -5.487892 | -1.119499 | -1.133132 |
| H | -4.255373 | 2.166093 | 1.328650 |
| H | -6.052679 | 0.949035 | 0.122891 |

**11F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -709.328061

Free energies: -709.110577

Corrected Free energies: -709.107873

| | | | |
|---|---|---|---|
| C | 3.710914 | -0.762864 | 0.095002 |
| C | 3.116987 | -2.154141 | 0.308893 |
| C | 1.682017 | -2.001232 | -0.186635 |
| C | 2.555662 | 0.169708 | 0.493149 |
| H | 4.597694 | -0.565568 | 0.692305 |
| H | 3.958128 | -0.612401 | -0.958541 |
| H | 3.116813 | -2.408461 | 1.370426 |
| H | 3.650506 | -2.929016 | -0.237406 |
| H | 1.610105 | -2.097233 | -1.273602 |
| H | 0.980770 | -2.684982 | 0.288026 |
| H | 2.573671 | 0.380721 | 1.566676 |
| N | 1.348266 | -0.608898 | 0.179561 |
| C | 0.136514 | -0.105128 | 0.237795 |
| C | -1.015337 | -0.821370 | -0.108706 |
| H | 0.072563 | 0.924902 | 0.563804 |
| H | -0.900375 | -1.828534 | -0.491304 |
| C | 2.591317 | 1.492686 | -0.255991 |
| O | 1.740923 | 1.899403 | -0.995737 |
| O | 3.723649 | 2.127546 | 0.026494 |
| H | 3.746546 | 2.963966 | -0.462464 |
| C | -2.342223 | -0.312089 | -0.018657 |

| | | | |
|---|---|---|---|
| C | -3.400743 | -1.146773 | -0.449353 |
| C | -2.655181 | 0.975501 | 0.480326 |
| C | -4.711013 | -0.713596 | -0.388596 |
| H | -3.168997 | -2.134830 | -0.830264 |
| C | -3.967472 | 1.398603 | 0.537345 |
| H | -1.873983 | 1.639848 | 0.826388 |
| C | -4.998480 | 0.559714 | 0.104017 |
| H | -5.512041 | -1.361041 | -0.721571 |
| H | -4.198313 | 2.384386 | 0.920536 |
| H | -6.025295 | 0.900825 | 0.152471 |

**11F-*Z***

Imaginary frequency: None

Electronic energies: -709.511479

Free energies: -709.293939

Corrected Free energies: -709.291292

| | | | |
|---|---|---|---|
| C | 2.722515 | 1.542538 | 0.298090 |
| C | 1.550039 | 2.438711 | -0.101859 |
| C | 0.361747 | 1.478940 | -0.047506 |
| C | 2.384929 | 0.216171 | -0.412142 |
| H | 3.697513 | 1.922954 | -0.000174 |
| H | 2.724594 | 1.391056 | 1.381223 |
| H | 1.688315 | 2.800479 | -1.123607 |
| H | 1.428749 | 3.295158 | 0.560668 |
| H | -0.037840 | 1.406398 | 0.970019 |
| H | -0.458214 | 1.761158 | -0.710879 |
| H | 2.843109 | 0.187728 | -1.410200 |
| N | 0.938774 | 0.207977 | -0.493288 |
| C | 0.318185 | -0.643102 | -1.375176 |
| C | -1.000512 | -0.892010 | -1.503155 |
| H | 1.006168 | -1.139375 | -2.058328 |
| H | -1.294325 | -1.484470 | -2.362812 |
| C | 2.924364 | -0.965946 | 0.369406 |
| O | 2.272585 | -1.770211 | 0.977170 |
| O | 4.262780 | -0.989583 | 0.316584 |
| H | 4.575246 | -1.736440 | 0.847305 |
| C | -2.077946 | -0.498133 | -0.582911 |
| C | -3.365155 | -0.233973 | -1.071374 |
| C | -1.879230 | -0.456980 | 0.805348 |
| C | -4.405807 | 0.093338 | -0.210610 |
| H | -3.542855 | -0.281074 | -2.140739 |
| C | -2.920637 | -0.131661 | 1.666516 |
| H | -0.899961 | -0.702399 | 1.202281 |

| | | | |
|---|---|---|---|
| C | -4.187761 | 0.152483 | 1.163707 |
| H | -5.390727 | 0.301061 | -0.613129 |
| H | -2.744000 | -0.109582 | 2.735833 |
| H | -4.998501 | 0.407616 | 1.835507 |

**11F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -709.319708

Free energies: -709.101560

Corrected Free energies: -709.098930

| | | | |
|---|---|---|---|
| C | 2.800812 | 1.471538 | 0.423058 |
| C | 1.641995 | 2.433982 | 0.155638 |
| C | 0.434203 | 1.503010 | 0.127765 |
| C | 2.431795 | 0.237955 | -0.419803 |
| H | 3.772222 | 1.865874 | 0.135225 |
| H | 2.834645 | 1.203940 | 1.481231 |
| H | 1.760719 | 2.919540 | -0.814667 |
| H | 1.541461 | 3.197059 | 0.924853 |
| H | 0.144504 | 1.212432 | 1.139775 |
| H | -0.435108 | 1.885678 | -0.403853 |
| H | 2.908140 | 0.270299 | -1.403870 |
| N | 0.972356 | 0.327852 | -0.589721 |
| C | 0.344976 | -0.458571 | -1.431706 |
| C | -1.046154 | -0.553128 | -1.623153 |
| H | 0.987699 | -1.060437 | -2.068669 |
| H | -1.353127 | -0.871811 | -2.613445 |
| C | 2.793677 | -1.082696 | 0.243935 |
| O | 2.017449 | -1.961376 | 0.493366 |
| O | 4.095226 | -1.114490 | 0.504662 |
| H | 4.312625 | -1.958529 | 0.928170 |
| C | -2.061791 | -0.345469 | -0.640949 |
| C | -3.381086 | -0.064781 | -1.060552 |
| C | -1.801424 | -0.507848 | 0.738470 |
| C | -4.384279 | 0.122163 | -0.127992 |
| H | -3.590886 | 0.025551 | -2.119968 |
| C | -2.815908 | -0.340786 | 1.661314 |
| H | -0.814849 | -0.820487 | 1.062118 |
| C | -4.103412 | -0.009370 | 1.232882 |
| H | -5.388495 | 0.361343 | -0.453898 |
| H | -2.614811 | -0.481209 | 2.715721 |
| H | -4.893062 | 0.126728 | 1.961668 |

**12F-*E***

Imaginary frequency: None

Electronic energies: -1097.499743

Free energies: -1097.112476

Corrected Free energies: -1097.107441

| | | | |
|---|---|---|---|
| C | -1.047923 | 1.307231 | 0.453682 |
| C | -1.764269 | 2.668286 | 0.530435 |
| C | -1.100514 | 3.523098 | -0.558907 |
| C | 0.344937 | 3.029919 | -0.572042 |
| H | -1.581949 | 3.109605 | 1.512919 |
| H | -2.844825 | 2.584219 | 0.404350 |
| H | -1.162756 | 4.588804 | -0.341403 |
| H | -1.564204 | 3.347434 | -1.529271 |
| H | 0.978111 | 3.617647 | 0.107163 |
| H | 0.797799 | 3.070139 | -1.567133 |
| C | -1.799077 | 0.267043 | -0.434212 |
| O | -2.022836 | 0.821527 | -1.726234 |
| C | -3.139157 | -0.163316 | 0.168636 |
| C | -4.006751 | -0.892369 | -0.651415 |
| C | -3.531944 | 0.112837 | 1.478061 |
| C | -5.236105 | -1.329749 | -0.178379 |
| H | -3.704520 | -1.113940 | -1.669003 |
| C | -4.766041 | -0.327416 | 1.954840 |
| H | -2.892840 | 0.679775 | 2.143760 |
| C | -5.620797 | -1.047539 | 1.130738 |
| H | -5.893656 | -1.894342 | -0.828867 |
| H | -5.055372 | -0.099794 | 2.973961 |
| H | -6.579653 | -1.388102 | 1.502875 |
| C | -0.899382 | -0.948897 | -0.623999 |
| C | -0.743951 | -1.878185 | 0.406559 |
| C | -0.139460 | -1.087883 | -1.783008 |
| C | 0.167921 | -2.921320 | 0.284472 |
| H | -1.333857 | -1.784394 | 1.312897 |
| C | 0.768252 | -2.136043 | -1.908464 |
| H | -0.253533 | -0.363456 | -2.578358 |
| C | 0.928274 | -3.053168 | -0.875036 |
| H | 0.281790 | -3.634081 | 1.092796 |
| H | 1.356373 | -2.229809 | -2.813994 |
| H | 1.640934 | -3.864009 | -0.970320 |
| N | 0.261994 | 1.655024 | -0.096587 |
| H | -0.913863 | 0.866171 | 1.445005 |
| C | 1.389843 | 0.949740 | 0.195749 |
| C | 2.660045 | 1.324530 | -0.078339 |
| H | 2.852113 | 2.284893 | -0.545057 |

| | | | |
|---|---|---|---|
| H | 1.201279 | 0.003188 | 0.692973 |
| H | -2.772501 | 1.422676 | -1.666238 |
| C | 3.833620 | 0.504272 | 0.233170 |
| C | 5.109207 | 1.089811 | 0.218092 |
| C | 3.754853 | -0.866302 | 0.537555 |
| C | 6.249979 | 0.351929 | 0.512877 |
| H | 5.199860 | 2.143882 | -0.024007 |
| C | 4.893928 | -1.600131 | 0.840653 |
| H | 2.795897 | -1.372658 | 0.515539 |
| C | 6.151124 | -0.998946 | 0.832671 |
| H | 7.219904 | 0.836066 | 0.493673 |
| H | 4.800400 | -2.655663 | 1.071222 |
| H | 7.038118 | -1.576242 | 1.064166 |

**12F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1097.316349

Free energies: -1096.927571

Corrected Free energies: -1096.923239

| | | | |
|---|---|---|---|
| C | -1.142131 | 1.279494 | 0.707929 |
| C | -1.917363 | 2.599658 | 0.792471 |
| C | -1.256458 | 3.533617 | -0.236371 |
| C | 0.187235 | 3.037148 | -0.367426 |
| H | -1.805710 | 3.005807 | 1.798756 |
| H | -2.981033 | 2.461240 | 0.603989 |
| H | -1.282356 | 4.569309 | 0.096544 |
| H | -1.758306 | 3.480695 | -1.199928 |
| H | 0.900571 | 3.687925 | 0.141160 |
| H | 0.497045 | 2.904879 | -1.405473 |
| C | -1.686737 | 0.270741 | -0.361845 |
| O | -1.650329 | 0.903610 | -1.630170 |
| C | -3.103250 | -0.199644 | -0.034204 |
| C | -3.835005 | -0.797253 | -1.064330 |
| C | -3.671359 | -0.114479 | 1.236736 |
| C | -5.111388 | -1.291230 | -0.830457 |
| H | -3.392784 | -0.882885 | -2.050693 |
| C | -4.950006 | -0.614552 | 1.471027 |
| H | -3.135719 | 0.342747 | 2.060484 |
| C | -5.673083 | -1.202159 | 0.440390 |
| H | -5.664552 | -1.753019 | -1.639458 |
| H | -5.378267 | -0.538891 | 2.463150 |
| H | -6.667648 | -1.589902 | 0.624606 |
| C | -0.747581 | -0.931537 | -0.420733 |

| | | | |
|---|---|---|---|
| C | -0.730174 | -1.844546 | 0.635859 |
| C | 0.167041 | -1.077388 | -1.462860 |
| C | 0.196303 | -2.880099 | 0.658073 |
| H | -1.444581 | -1.748991 | 1.446890 |
| C | 1.094045 | -2.118180 | -1.440449 |
| H | 0.158852 | -0.370579 | -2.282517 |
| C | 1.113839 | -3.018643 | -0.381519 |
| H | 0.199099 | -3.580660 | 1.484266 |
| H | 1.804944 | -2.219082 | -2.251996 |
| H | 1.839145 | -3.823373 | -0.363296 |
| N | 0.204167 | 1.726043 | 0.308276 |
| H | -1.056887 | 0.774119 | 1.670462 |
| C | 1.286642 | 1.010317 | 0.511672 |
| C | 2.558905 | 1.375503 | 0.054920 |
| H | 2.676085 | 2.324876 | -0.454642 |
| H | 1.141913 | 0.090354 | 1.065819 |
| H | -2.474581 | 1.385032 | -1.759423 |
| C | 3.719810 | 0.559149 | 0.189409 |
| C | 4.948514 | 1.061461 | -0.299063 |
| C | 3.697907 | -0.734684 | 0.763335 |
| C | 6.103946 | 0.308637 | -0.211143 |
| H | 4.972682 | 2.049653 | -0.743950 |
| C | 4.857265 | -1.480386 | 0.843607 |
| H | 2.774356 | -1.161138 | 1.134523 |
| C | 6.062421 | -0.963886 | 0.359564 |
| H | 7.038528 | 0.705219 | -0.587343 |
| H | 4.829493 | -2.470970 | 1.279773 |
| H | 6.967133 | -1.555895 | 0.424186 |

**12F-*Z***

Imaginary frequency: None

Electronic energies: -1097.493059

Free energies: -1097.105455

Corrected Free energies: -1097.100592

| | | | |
|---|---|---|---|
| C | -0.812481 | -1.152830 | -0.758118 |
| C | -1.073809 | -2.654816 | -0.563127 |
| C | 0.141735 | -3.157422 | 0.225767 |
| C | 1.291838 | -2.264292 | -0.244708 |
| H | -1.107219 | -3.135010 | -1.543729 |
| H | -2.022125 | -2.861861 | -0.064229 |
| H | 0.349472 | -4.210657 | 0.038622 |
| H | -0.011205 | -3.030082 | 1.297416 |
| H | 1.845220 | -2.711513 | -1.080247 |

| | | | |
|---|---|---|---|
| H | 2.004413 | -2.076688 | 0.559705 |
| C | -1.484606 | -0.249867 | 0.320186 |
| O | -1.074168 | -0.677382 | 1.614451 |
| C | -3.013783 | -0.264717 | 0.242769 |
| C | -3.721366 | 0.260018 | 1.329054 |
| C | -3.731518 | -0.749081 | -0.850706 |
| C | -5.109043 | 0.296831 | 1.325492 |
| H | -3.168906 | 0.641477 | 2.180464 |
| C | -5.125065 | -0.710663 | -0.856188 |
| H | -3.222258 | -1.170899 | -1.708434 |
| C | -5.817514 | -0.189839 | 0.229183 |
| H | -5.638557 | 0.708040 | 2.176833 |
| H | -5.665660 | -1.094441 | -1.713236 |
| H | -6.900492 | -0.162928 | 0.223410 |
| C | -0.970606 | 1.173500 | 0.135327 |
| C | -1.371806 | 1.922584 | -0.972843 |
| C | -0.033113 | 1.713278 | 1.012554 |
| C | -0.829756 | 3.180455 | -1.209432 |
| H | -2.110250 | 1.519669 | -1.659532 |
| C | 0.507864 | 2.975036 | 0.778193 |
| H | 0.273459 | 1.139733 | 1.877116 |
| C | 0.117927 | 3.709392 | -0.336056 |
| H | -1.146762 | 3.748763 | -2.076096 |
| H | 1.240370 | 3.379843 | 1.467233 |
| H | 0.543098 | 4.688841 | -0.520665 |
| N | 0.642476 | -1.034615 | -0.708571 |
| H | -1.158316 | -0.810839 | -1.738084 |
| C | 1.270944 | -0.175884 | -1.581216 |
| C | 2.570314 | 0.186805 | -1.616302 |
| H | 2.875272 | 0.756395 | -2.488103 |
| H | 0.615731 | 0.226510 | -2.352096 |
| H | -1.577272 | -1.466561 | 1.841434 |
| C | 3.602794 | -0.007517 | -0.590105 |
| C | 4.955782 | -0.066219 | -0.954649 |
| C | 3.291078 | -0.033037 | 0.778315 |
| C | 5.955303 | -0.176792 | 0.004525 |
| H | 5.219421 | -0.025658 | -2.006699 |
| C | 4.290967 | -0.139189 | 1.738059 |
| H | 2.252728 | 0.053280 | 1.080293 |
| C | 5.628175 | -0.218902 | 1.357715 |
| H | 6.993054 | -0.227810 | -0.304955 |
| H | 4.024924 | -0.151947 | 2.789145 |
| H | 6.406331 | -0.305287 | 2.106693 |

**12F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1097.305022

Free energies: -1096.917578

Corrected Free energies: -1096.912542

| | | | |
|---|---|---|---|
| C | -0.860681 | -1.177388 | -0.804550 |
| C | -1.098403 | -2.673995 | -0.578211 |
| C | 0.104465 | -3.174021 | 0.250427 |
| C | 1.180969 | -2.079103 | 0.161742 |
| H | -1.127761 | -3.173846 | -1.546430 |
| H | -2.050667 | -2.859990 | -0.082080 |
| H | 0.479735 | -4.116486 | -0.143642 |
| H | -0.168450 | -3.331728 | 1.291924 |
| H | 2.129576 | -2.420696 | -0.251538 |
| H | 1.352732 | -1.625299 | 1.135944 |
| C | -1.484432 | -0.252278 | 0.285436 |
| O | -1.034985 | -0.695388 | 1.556820 |
| C | -3.012098 | -0.255768 | 0.233502 |
| C | -3.686608 | 0.285118 | 1.332459 |
| C | -3.753243 | -0.735365 | -0.845160 |
| C | -5.073233 | 0.339370 | 1.354545 |
| H | -3.114114 | 0.668740 | 2.169778 |
| C | -5.145450 | -0.677607 | -0.822864 |
| H | -3.269563 | -1.167447 | -1.712807 |
| C | -5.808096 | -0.143035 | 0.274252 |
| H | -5.580387 | 0.762760 | 2.213079 |
| H | -5.707824 | -1.056866 | -1.667411 |
| H | -6.890348 | -0.101231 | 0.289258 |
| C | -0.956817 | 1.165629 | 0.079703 |
| C | -1.306592 | 1.876312 | -1.071305 |
| C | -0.075202 | 1.739390 | 0.992430 |
| C | -0.759507 | 3.129529 | -1.317299 |
| H | -2.013186 | 1.452563 | -1.778772 |
| C | 0.471732 | 2.997042 | 0.744683 |
| H | 0.177315 | 1.202946 | 1.898120 |
| C | 0.138601 | 3.691039 | -0.411960 |
| H | -1.036227 | 3.669788 | -2.214612 |
| H | 1.160632 | 3.430213 | 1.460409 |
| H | 0.567558 | 4.666877 | -0.604964 |
| N | 0.610212 | -1.068046 | -0.750543 |
| H | -1.179709 | -0.840346 | -1.789900 |
| C | 1.263911 | -0.284065 | -1.576433 |
| C | 2.650400 | -0.045908 | -1.645246 |

| | | | |
|---|---|---|---|
| H | 2.995616 | 0.253563 | -2.629349 |
| H | 0.649469 | 0.188090 | -2.337351 |
| H | -1.632732 | -1.379190 | 1.878216 |
| C | 3.627913 | -0.096370 | -0.604660 |
| C | 4.988272 | -0.239580 | -0.958128 |
| C | 3.293386 | 0.091501 | 0.753853 |
| C | 5.965638 | -0.266319 | 0.018967 |
| H | 5.252679 | -0.349862 | -2.003402 |
| C | 4.278997 | 0.085105 | 1.722384 |
| H | 2.266018 | 0.301205 | 1.024525 |
| C | 5.613565 | -0.109544 | 1.360339 |
| H | 7.003907 | -0.398784 | -0.257352 |
| H | 4.017085 | 0.245571 | 2.760539 |
| H | 6.382112 | -0.119246 | 2.123628 |

**13F-*E***

Imaginary frequency: None

Electronic energies: -1506.169819

Free energies: -1505.687153

Corrected Free energies: -1505.681845

| | | | |
|---|---|---|---|
| Si | 0.002587 | -2.233712 | -0.759476 |
| O | -0.459454 | -0.616800 | -0.745435 |
| N | 0.602961 | 1.211756 | 1.127764 |
| C | -0.646439 | 0.506075 | 1.379122 |
| C | -1.417058 | 1.486176 | 2.281224 |
| C | -0.863119 | 2.879569 | 1.935956 |
| C | 0.577758 | 2.622815 | 1.486862 |
| C | -1.382812 | 0.111533 | 0.054250 |
| C | 1.597051 | -2.198737 | -1.733808 |
| C | 0.272190 | -2.932121 | 0.963502 |
| C | -1.236473 | -3.336095 | -1.626376 |
| C | -2.622932 | -0.752184 | 0.306248 |
| C | -2.971800 | -1.266128 | 1.554197 |
| C | -4.075851 | -2.107058 | 1.693518 |
| C | -4.848796 | -2.438089 | 0.588316 |
| C | -4.513131 | -1.924787 | -0.663148 |
| C | -3.410804 | -1.093953 | -0.798768 |
| C | -1.732324 | 1.387276 | -0.708932 |
| C | -0.742491 | 2.014438 | -1.468313 |
| C | -0.985321 | 3.246332 | -2.066857 |
| C | -2.223709 | 3.865687 | -1.920658 |
| C | -3.221615 | 3.237643 | -1.182532 |
| C | -2.977456 | 2.006153 | -0.581701 |

| | | | |
|---|---|---|---|
| C | 1.765665 | 0.585135 | 0.822361 |
| C | 2.962430 | 1.178813 | 0.601935 |
| H | -0.419505 | -0.428250 | 1.901474 |
| H | -1.202526 | 1.243431 | 3.324450 |
| H | -2.496330 | 1.425956 | 2.138345 |
| H | -1.432734 | 3.331992 | 1.123944 |
| H | -0.902260 | 3.552674 | 2.791878 |
| H | 0.859441 | 3.247211 | 0.632208 |
| H | 1.306217 | 2.801686 | 2.288266 |
| H | 1.400433 | -1.900220 | -2.767003 |
| H | 2.059422 | -3.189398 | -1.752292 |
| H | 2.318405 | -1.494261 | -1.311231 |
| H | 1.060895 | -2.437293 | 1.534285 |
| H | 0.558325 | -3.983125 | 0.854929 |
| H | -0.648484 | -2.904237 | 1.552262 |
| H | -2.093786 | -3.569071 | -0.991019 |
| H | -0.740907 | -4.275616 | -1.889948 |
| H | -1.606569 | -2.879478 | -2.547446 |
| H | -2.394819 | -1.022673 | 2.438166 |
| H | -4.329088 | -2.497526 | 2.671928 |
| H | -5.707164 | -3.090066 | 0.698035 |
| H | -5.107453 | -2.178746 | -1.533134 |
| H | -3.143583 | -0.705988 | -1.776194 |
| H | 0.221173 | 1.531174 | -1.576423 |
| H | -0.204899 | 3.724362 | -2.647721 |
| H | -2.411263 | 4.826207 | -2.386062 |
| H | -4.192927 | 3.705347 | -1.071058 |
| H | -3.763055 | 1.531495 | -0.004654 |
| H | 1.681996 | -0.492849 | 0.762257 |
| H | 3.032336 | 2.261342 | 0.591008 |
| C | 4.194500 | 0.440303 | 0.316856 |
| C | 4.349981 | -0.933064 | 0.577197 |
| C | 5.293117 | 1.119008 | -0.234663 |
| C | 5.529923 | -1.595271 | 0.264643 |
| H | 3.547622 | -1.490509 | 1.048719 |
| C | 6.478033 | 0.458415 | -0.535701 |
| H | 5.205294 | 2.181949 | -0.434994 |
| C | 6.604058 | -0.906871 | -0.295295 |
| H | 5.617146 | -2.655260 | 0.475436 |
| H | 7.305976 | 1.012672 | -0.963321 |
| H | 7.525903 | -1.424924 | -0.529913 |

**13F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1505.984006

Free energies: -1505.500871

Corrected Free energies: -1505.495686

| | | | |
|---|---|---|---|
| Si | -0.403018 | -2.435393 | -0.633036 |
| O | -0.469689 | -0.746670 | -0.583297 |
| N | 0.665347 | 1.057033 | 1.298799 |
| C | -0.659969 | 0.445031 | 1.482228 |
| C | -1.379418 | 1.434298 | 2.407357 |
| C | -0.688853 | 2.799990 | 2.219495 |
| C | 0.669688 | 2.507459 | 1.569056 |
| C | -1.314421 | 0.173832 | 0.079801 |
| C | 1.095410 | -2.723817 | -1.705143 |
| C | -0.148885 | -3.145494 | 1.083752 |
| C | -1.917312 | -3.213666 | -1.397350 |
| C | -2.718780 | -0.419148 | 0.228677 |
| C | -3.147047 | -1.059538 | 1.391833 |
| C | -4.383231 | -1.700325 | 1.434738 |
| C | -5.208301 | -1.704373 | 0.316666 |
| C | -4.791983 | -1.063225 | -0.847167 |
| C | -3.557409 | -0.429980 | -0.889945 |
| C | -1.313302 | 1.466776 | -0.737939 |
| C | -0.264680 | 1.728137 | -1.620981 |
| C | -0.207216 | 2.935217 | -2.311563 |
| C | -1.199641 | 3.893116 | -2.131985 |
| C | -2.257519 | 3.632146 | -1.266261 |
| C | -2.315796 | 2.425771 | -0.576977 |
| C | 1.724877 | 0.369020 | 0.940590 |
| C | 2.962931 | 0.951363 | 0.643884 |
| H | -0.505504 | -0.525756 | 1.955719 |
| H | -1.266479 | 1.090173 | 3.435791 |
| H | -2.445399 | 1.484331 | 2.192040 |
| H | -1.275787 | 3.450924 | 1.576238 |
| H | -0.554839 | 3.301477 | 3.175888 |
| H | 0.805575 | 3.042569 | 0.626126 |
| H | 1.509897 | 2.725427 | 2.228903 |
| H | 0.914497 | -2.355590 | -2.717984 |
| H | 1.325123 | -3.790448 | -1.767839 |
| H | 1.978612 | -2.210539 | -1.316393 |
| H | 0.745937 | -2.769468 | 1.586630 |
| H | -0.032620 | -4.229811 | 0.991601 |
| H | -1.010880 | -2.966325 | 1.731305 |
| H | -2.782039 | -3.180254 | -0.730384 |
| H | -1.692747 | -4.262724 | -1.613584 |

| | | | |
|---|---|---|---|
| H | -2.187900 | -2.724750 | -2.335990 |
| H | -2.534499 | -1.068684 | 2.285869 |
| H | -4.698571 | -2.191555 | 2.347208 |
| H | -6.170381 | -2.201078 | 0.352120 |
| H | -5.426526 | -1.062220 | -1.725359 |
| H | -3.234335 | 0.054073 | -1.804785 |
| H | 0.502097 | 0.977887 | -1.769831 |
| H | 0.612890 | 3.123506 | -2.994194 |
| H | -1.156032 | 4.831719 | -2.671182 |
| H | -3.043085 | 4.365766 | -1.130095 |
| H | -3.155038 | 2.229588 | 0.081635 |
| H | 1.582946 | -0.701070 | 0.871847 |
| H | 3.032581 | 2.032897 | 0.624852 |
| C | 4.142062 | 0.216899 | 0.322106 |
| C | 4.230809 | -1.193288 | 0.408531 |
| C | 5.283425 | 0.941144 | -0.093020 |
| C | 5.404681 | -1.839498 | 0.076242 |
| H | 3.389469 | -1.780017 | 0.755562 |
| C | 6.453888 | 0.285459 | -0.424838 |
| H | 5.226829 | 2.021925 | -0.153230 |
| C | 6.517674 | -1.105797 | -0.344137 |
| H | 5.463892 | -2.918097 | 0.148434 |
| H | 7.319706 | 0.851676 | -0.743834 |
| H | 7.434848 | -1.620986 | -0.601687 |

**13F-*Z***

Imaginary frequency: None

Electronic energies: -1506.162531

Free energies: -1505.680548

Corrected Free energies: -1505.674976

| | | | |
|---|---|---|---|
| Si | -1.693978 | -2.356274 | -0.909017 |
| O | -0.987955 | -0.836338 | -0.783089 |
| N | 1.011134 | -0.193921 | 1.102663 |
| C | -0.411164 | -0.005424 | 1.388501 |
| C | -0.436914 | 1.119087 | 2.435702 |
| C | 0.871175 | 1.893092 | 2.229229 |
| C | 1.853107 | 0.861122 | 1.669512 |
| C | -1.226269 | 0.266112 | 0.082817 |
| C | -0.435211 | -3.318856 | -1.896165 |
| C | -2.000897 | -3.190462 | 0.745242 |
| C | -3.328870 | -2.292314 | -1.817880 |
| C | -2.732687 | 0.394692 | 0.333237 |
| C | -3.346245 | 0.062084 | 1.540324 |

| | | | |
|---|---|---|---|
| C | -4.733433 | 0.117846 | 1.672755 |
| C | -5.524634 | 0.513522 | 0.602136 |
| C | -4.922413 | 0.853933 | -0.607364 |
| C | -3.542365 | 0.791319 | -0.736839 |
| C | -0.662905 | 1.512115 | -0.596120 |
| C | 0.441089 | 1.386080 | -1.439512 |
| C | 1.057539 | 2.512675 | -1.974689 |
| C | 0.569371 | 3.783037 | -1.681965 |
| C | -0.546140 | 3.916483 | -0.861311 |
| C | -1.158017 | 2.788345 | -0.322546 |
| C | 1.491925 | -1.453070 | 0.865467 |
| C | 2.749931 | -1.873374 | 0.598887 |
| H | -0.805416 | -0.938687 | 1.803387 |
| H | -0.455738 | 0.668141 | 3.430546 |
| H | -1.314103 | 1.760659 | 2.345972 |
| H | 0.729360 | 2.698068 | 1.507893 |
| H | 1.237957 | 2.331614 | 3.157075 |
| H | 2.505729 | 1.311309 | 0.919677 |
| H | 2.493673 | 0.422747 | 2.445420 |
| H | -0.286025 | -2.867123 | -2.880116 |
| H | -0.765688 | -4.350371 | -2.043154 |
| H | 0.529151 | -3.336162 | -1.381665 |
| H | -1.091661 | -3.404140 | 1.310562 |
| H | -2.490005 | -4.149028 | 0.543199 |
| H | -2.675578 | -2.608656 | 1.377582 |
| H | -4.130463 | -1.915371 | -1.178680 |
| H | -3.596496 | -3.303217 | -2.140081 |
| H | -3.272129 | -1.656987 | -2.705132 |
| H | -2.758332 | -0.246103 | 2.396709 |
| H | -5.190503 | -0.145998 | 2.619038 |
| H | -6.602046 | 0.558763 | 0.707862 |
| H | -5.529472 | 1.161177 | -1.450865 |
| H | -3.078298 | 1.044200 | -1.684181 |
| H | 0.805210 | 0.392688 | -1.669066 |
| H | 1.917652 | 2.397909 | -2.625276 |
| H | 1.047207 | 4.661327 | -2.099508 |
| H | -0.942946 | 4.899972 | -0.638397 |
| H | -2.024730 | 2.907838 | 0.318010 |
| H | 0.732778 | -2.224039 | 0.959505 |
| H | 2.882561 | -2.950450 | 0.615153 |
| C | 3.950579 | -1.099777 | 0.249684 |
| C | 5.213016 | -1.536834 | 0.679680 |
| C | 3.900740 | 0.023540 | -0.588230 |
| C | 6.371149 | -0.859946 | 0.318849 |

| | | | |
|---|---|---|---|
| H | 5.276258 | -2.416869 | 1.311541 |
| C | 5.058916 | 0.703352 | -0.949684 |
| H | 2.941724 | 0.351563 | -0.972103 |
| C | 6.300520 | 0.269606 | -0.494033 |
| H | 7.332650 | -1.214534 | 0.672584 |
| H | 4.990885 | 1.569284 | -1.598865 |
| H | 7.202872 | 0.798561 | -0.776432 |

**13F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1505.974744

Free energies: -1505.491226

Corrected Free energies: -1505.486099

| | | | |
|---|---|---|---|
| Si | -1.927181 | -2.331360 | -0.859494 |
| O | -1.008663 | -0.924298 | -0.677313 |
| N | 0.957444 | -0.268255 | 1.261425 |
| C | -0.489641 | -0.053173 | 1.472994 |
| C | -0.546184 | 1.036998 | 2.553089 |
| C | 0.857706 | 1.676953 | 2.629214 |
| C | 1.733698 | 0.937568 | 1.611113 |
| C | -1.178517 | 0.244981 | 0.097427 |
| C | -0.832889 | -3.370900 | -1.954885 |
| C | -2.210443 | -3.189541 | 0.783896 |
| C | -3.578454 | -2.006381 | -1.668808 |
| C | -2.666663 | 0.561038 | 0.267972 |
| C | -3.399190 | 0.166732 | 1.387977 |
| C | -4.777548 | 0.363627 | 1.437826 |
| C | -5.438025 | 0.959057 | 0.369921 |
| C | -4.713774 | 1.362713 | -0.748796 |
| C | -3.340719 | 1.164043 | -0.797720 |
| C | -0.436997 | 1.382501 | -0.607309 |
| C | 0.466008 | 1.098176 | -1.629607 |
| C | 1.226315 | 2.114954 | -2.204473 |
| C | 1.091953 | 3.425927 | -1.762340 |
| C | 0.168393 | 3.721211 | -0.762567 |
| C | -0.598113 | 2.709033 | -0.196890 |
| C | 1.427994 | -1.462594 | 0.984976 |
| C | 2.762362 | -1.868517 | 0.783044 |
| H | -0.903032 | -0.997045 | 1.830450 |
| H | -0.800640 | 0.571836 | 3.504916 |
| H | -1.320210 | 1.770220 | 2.339573 |
| H | 0.828725 | 2.738885 | 2.389804 |
| H | 1.271222 | 1.567200 | 3.630135 |

| | | | |
|---|---|---|---|
| H | 1.886946 | 1.537918 | 0.713030 |
| H | 2.701542 | 0.630344 | 2.003951 |
| H | -0.681382 | -2.888589 | -2.923485 |
| H | -1.287258 | -4.349480 | -2.129752 |
| H | 0.147165 | -3.530032 | -1.497512 |
| H | -1.286978 | -3.449285 | 1.307702 |
| H | -2.738909 | -4.127246 | 0.585276 |
| H | -2.839558 | -2.601080 | 1.455818 |
| H | -4.292452 | -1.554547 | -0.975624 |
| H | -3.992501 | -2.958822 | -2.013455 |
| H | -3.477033 | -1.347272 | -2.534176 |
| H | -2.914362 | -0.293292 | 2.241260 |
| H | -5.330351 | 0.053791 | 2.316446 |
| H | -6.509537 | 1.113124 | 0.410217 |
| H | -5.219424 | 1.829276 | -1.585708 |
| H | -2.784320 | 1.468604 | -1.677237 |
| H | 0.572551 | 0.075382 | -1.968675 |
| H | 1.926852 | 1.877325 | -2.997133 |
| H | 1.687685 | 4.215273 | -2.204433 |
| H | 0.036804 | 4.742942 | -0.427459 |
| H | -1.335525 | 2.962243 | 0.556162 |
| H | 0.682351 | -2.250658 | 0.997228 |
| H | 2.929257 | -2.917249 | 1.006526 |
| C | 3.890869 | -1.128284 | 0.313637 |
| C | 5.186614 | -1.609774 | 0.607010 |
| C | 3.760357 | 0.012700 | -0.506096 |
| C | 6.303442 | -0.931957 | 0.154903 |
| H | 5.293981 | -2.505143 | 1.208345 |
| C | 4.881224 | 0.672061 | -0.972431 |
| H | 2.775953 | 0.340684 | -0.812325 |
| C | 6.154657 | 0.212007 | -0.630812 |
| H | 7.292869 | -1.294450 | 0.403019 |
| H | 4.769104 | 1.538548 | -1.612508 |
| H | 7.031600 | 0.734834 | -0.992534 |

**14F-*E***

Imaginary frequency: None

Electronic energies: -2854.348597

Free energies: -2853.870812

Corrected Free energies: -2853.858111

| | | | |
|---|---|---|---|
| Si | -0.397695 | -2.520781 | 1.310728 |
| O | -0.508266 | -0.945615 | 0.707163 |
| N | -1.831258 | -0.307851 | -1.734332 |

| | | | |
|---|---|---|---|
| C | -0.412300 | -0.612861 | -1.683401 |
| C | 0.154759 | 0.171861 | -2.879428 |
| C | -0.830850 | 1.330544 | -3.116471 |
| C | -2.176904 | 0.817033 | -2.594257 |
| C | 0.210784 | -0.246146 | -0.290033 |
| C | -1.996081 | -2.695476 | 2.253757 |
| C | -0.253712 | -3.801276 | -0.052619 |
| C | 1.068347 | -2.734283 | 2.452495 |
| C | 1.689902 | -0.618794 | -0.180119 |
| C | 2.340524 | -1.435379 | -1.096024 |
| C | 3.653044 | -1.845924 | -0.865040 |
| C | 4.343720 | -1.443677 | 0.263777 |
| C | 3.693131 | -0.614655 | 1.173203 |
| C | 2.385754 | -0.211668 | 0.962656 |
| C | -0.022146 | 1.239747 | -0.043325 |
| C | -1.277835 | 1.644303 | 0.404351 |
| C | -1.588657 | 2.995760 | 0.482296 |
| C | -0.657669 | 3.969642 | 0.148747 |
| C | 0.603006 | 3.559152 | -0.262500 |
| C | 0.923861 | 2.209720 | -0.363626 |
| C | -2.788349 | -1.079497 | -1.151793 |
| C | -4.108095 | -0.795140 | -1.088604 |
| H | -0.277991 | -1.692005 | -1.807569 |
| H | 0.173501 | -0.488028 | -3.748699 |
| H | 1.173236 | 0.526506 | -2.712868 |
| H | -0.527084 | 2.219698 | -2.564163 |
| H | -0.885502 | 1.599550 | -4.170362 |
| H | -2.718023 | 1.587585 | -2.034142 |
| H | -2.835240 | 0.464143 | -3.397246 |
| H | -2.018161 | -1.997026 | 3.094009 |
| H | -2.101511 | -3.707614 | 2.652725 |
| H | -2.862060 | -2.487337 | 1.619435 |
| H | -1.080516 | -3.793424 | -0.766140 |
| H | -0.243784 | -4.787271 | 0.422914 |
| H | 0.683811 | -3.704256 | -0.607244 |
| H | 2.008646 | -2.847587 | 1.907325 |
| H | 0.914210 | -3.644289 | 3.040595 |
| H | 1.171142 | -1.898684 | 3.149000 |
| H | 1.844809 | -1.772758 | -1.998863 |
| H | 5.363624 | -1.763007 | 0.434680 |
| H | 1.891843 | 0.416793 | 1.696287 |
| H | -2.015893 | 0.893904 | 0.666148 |
| H | -0.908128 | 5.020911 | 0.204179 |
| H | 1.909684 | 1.925077 | -0.714755 |

| | | | |
|---|---|---|---|
| H | -2.409910 | -1.991378 | -0.705098 |
| H | -4.473855 | 0.156140 | -1.461093 |
| C | -5.094757 | -1.681093 | -0.464059 |
| C | -4.878877 | -3.056477 | -0.274162 |
| C | -6.318053 | -1.149765 | -0.026798 |
| C | -5.825109 | -3.849643 | 0.362581 |
| H | -3.970063 | -3.517709 | -0.646020 |
| C | -7.269549 | -1.946227 | 0.598288 |
| H | -6.511367 | -0.091638 | -0.170797 |
| C | -7.026752 | -3.301456 | 0.805181 |
| H | -5.629592 | -4.907260 | 0.499017 |
| H | -8.203286 | -1.505838 | 0.929398 |
| H | -7.766318 | -3.923884 | 1.293980 |
| C | 1.656967 | 4.577703 | -0.582873 |
| C | -2.972820 | 3.372524 | 0.922424 |
| C | 4.385360 | -0.221779 | 2.445858 |
| C | 4.293302 | -2.744580 | -1.882525 |
| F | 1.132490 | 5.772287 | -0.879560 |
| F | 2.495780 | 4.763533 | 0.448856 |
| F | 2.410685 | 4.200229 | -1.625911 |
| F | -3.184272 | 4.691799 | 0.873694 |
| F | -3.906750 | 2.790612 | 0.149483 |
| F | -3.220282 | 2.974644 | 2.178951 |
| F | 3.999826 | 0.986904 | 2.872595 |
| F | 5.715946 | -0.195921 | 2.306965 |
| F | 4.114044 | -1.087721 | 3.436681 |
| F | 5.527529 | -3.116544 | -1.532008 |
| F | 3.573269 | -3.863126 | -2.063898 |
| F | 4.378709 | -2.149102 | -3.081356 |

**14F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -2854.157307

Free energies: -2853.677703

Corrected Free energies: -2853.665794

| | | | |
|---|---|---|---|
| Si | -0.225902 | -2.557074 | 1.411889 |
| O | -0.478946 | -1.039721 | 0.684769 |
| N | -1.799419 | -0.452745 | -1.749915 |
| C | -0.354140 | -0.730015 | -1.693870 |
| C | 0.191765 | 0.022665 | -2.914809 |
| C | -0.799523 | 1.168035 | -3.191527 |
| C | -2.135105 | 0.707397 | -2.601809 |
| C | 0.218091 | -0.306766 | -0.293503 |

| | | | |
|---|---|---|---|
| C | -1.764263 | -2.727337 | 2.447661 |
| C | -0.090005 | -3.894079 | 0.107559 |
| C | 1.302319 | -2.604009 | 2.484543 |
| C | 1.716834 | -0.594855 | -0.183561 |
| C | 2.390724 | -1.459727 | -1.033305 |
| C | 3.724346 | -1.789273 | -0.786117 |
| C | 4.402386 | -1.262417 | 0.296087 |
| C | 3.722730 | -0.388147 | 1.142237 |
| C | 2.401247 | -0.056786 | 0.912258 |
| C | -0.090769 | 1.171978 | -0.056377 |
| C | -1.300833 | 1.519533 | 0.538859 |
| C | -1.666160 | 2.854467 | 0.650708 |
| C | -0.830792 | 3.869245 | 0.205192 |
| C | 0.390261 | 3.516499 | -0.350685 |
| C | 0.763902 | 2.183968 | -0.485313 |
| C | -2.698483 | -1.206184 | -1.154131 |
| C | -4.062173 | -0.894319 | -1.116284 |
| H | -0.227688 | -1.811323 | -1.776893 |
| H | 0.217961 | -0.665411 | -3.760410 |
| H | 1.205634 | 0.388866 | -2.756201 |
| H | -0.478505 | 2.094915 | -2.721559 |
| H | -0.894776 | 1.353786 | -4.259162 |
| H | -2.620476 | 1.476537 | -1.996883 |
| H | -2.834722 | 0.363745 | -3.365501 |
| H | -1.736914 | -2.016931 | 3.277486 |
| H | -1.840682 | -3.734044 | 2.865452 |
| H | -2.671454 | -2.529404 | 1.871036 |
| H | -0.946963 | -3.954971 | -0.567554 |
| H | -0.018410 | -4.857246 | 0.622012 |
| H | 0.816701 | -3.787060 | -0.494411 |
| H | 2.222823 | -2.699168 | 1.903748 |
| H | 1.228918 | -3.479487 | 3.136856 |
| H | 1.378510 | -1.718773 | 3.120755 |
| H | 1.904167 | -1.901249 | -1.895381 |
| H | 5.434077 | -1.530494 | 0.488395 |
| H | 1.886616 | 0.604436 | 1.599867 |
| H | -1.954166 | 0.741666 | 0.916718 |
| H | -1.119965 | 4.907896 | 0.294707 |
| H | 1.722950 | 1.946061 | -0.934354 |
| H | -2.318254 | -2.094160 | -0.667858 |
| H | -4.386364 | 0.055373 | -1.526292 |
| C | -5.062571 | -1.717882 | -0.526059 |
| C | -4.818760 | -3.031324 | -0.056252 |
| C | -6.369261 | -1.187504 | -0.409775 |

| | | | |
|---|---|---|---|
| C | -5.836518 | -3.762438 | 0.521527 |
| H | -3.841683 | -3.485476 | -0.166268 |
| C | -7.380964 | -1.926624 | 0.171446 |
| H | -6.562973 | -0.185594 | -0.775302 |
| C | -7.117183 | -3.213400 | 0.641792 |
| H | -5.644061 | -4.766891 | 0.876181 |
| H | -8.375107 | -1.508027 | 0.261700 |
| H | -7.909775 | -3.793893 | 1.097735 |
| C | 1.329949 | 4.567991 | -0.866309 |
| C | -3.025007 | 3.167431 | 1.206304 |
| C | 4.453456 | 0.165294 | 2.332228 |
| C | 4.400221 | -2.737725 | -1.734551 |
| F | 0.877849 | 5.805573 | -0.647854 |
| F | 2.539246 | 4.475017 | -0.296552 |
| F | 1.518937 | 4.439084 | -2.189658 |
| F | -3.174390 | 4.463526 | 1.491718 |
| F | -3.988841 | 2.840433 | 0.326487 |
| F | -3.277552 | 2.473950 | 2.323612 |
| F | 3.642860 | 0.833907 | 3.158152 |
| F | 5.432009 | 1.003983 | 1.964847 |
| F | 5.030414 | -0.813894 | 3.043452 |
| F | 5.622789 | -3.082666 | -1.323616 |
| F | 3.689425 | -3.866354 | -1.880601 |
| F | 4.522853 | -2.202536 | -2.957633 |

**14F-*Z***

Imaginary frequency: None

Electronic energies: -2854.342824

Free energies: -2853.862255

Corrected Free energies: -2853.850584

| | | | |
|---|---|---|---|
| Si | 0.790360 | -2.563452 | 1.917734 |
| O | 0.057256 | -1.252204 | 1.142914 |
| N | -1.687623 | -1.502815 | -1.044579 |
| C | -0.252021 | -1.309730 | -1.238779 |
| C | -0.139035 | -0.621522 | -2.608890 |
| C | -1.498778 | 0.052991 | -2.833985 |
| C | -2.493830 | -0.811784 | -2.056446 |
| C | 0.373167 | -0.534434 | -0.033432 |
| C | -0.583706 | -3.225895 | 2.988164 |
| C | 1.408467 | -3.874429 | 0.726248 |
| C | 2.235560 | -2.006891 | 2.969799 |
| C | 1.893402 | -0.386538 | -0.134603 |
| C | 2.672463 | -1.052977 | -1.071468 |

| | | | |
|---|---|---|---|
| C | 4.063187 | -0.958748 | -1.024308 |
| C | 4.700033 | -0.196111 | -0.061684 |
| C | 3.915406 | 0.482038 | 0.866314 |
| C | 2.534601 | 0.388223 | 0.836455 |
| C | -0.304018 | 0.826956 | 0.066799 |
| C | -1.510210 | 0.929082 | 0.761024 |
| C | -2.209506 | 2.126598 | 0.762649 |
| C | -1.730090 | 3.244365 | 0.086110 |
| C | -0.522626 | 3.139722 | -0.582736 |
| C | 0.192539 | 1.944663 | -0.593157 |
| C | -2.120316 | -2.665936 | -0.452961 |
| C | -3.369728 | -3.118412 | -0.215037 |
| H | 0.235318 | -2.290271 | -1.247899 |
| H | 0.027938 | -1.388567 | -3.367955 |
| H | 0.690354 | 0.084785 | -2.668441 |
| H | -1.498286 | 1.071866 | -2.444818 |
| H | -1.756145 | 0.104061 | -3.891305 |
| H | -3.276271 | -0.199907 | -1.604068 |
| H | -2.983153 | -1.559621 | -2.692417 |
| H | -0.915195 | -2.466872 | 3.701102 |
| H | -0.246079 | -4.098155 | 3.553639 |
| H | -1.444199 | -3.519310 | 2.381460 |
| H | 0.621939 | -4.334632 | 0.125054 |
| H | 1.863505 | -4.668172 | 1.327672 |
| H | 2.183753 | -3.496629 | 0.055295 |
| H | 3.149626 | -1.872437 | 2.387033 |
| H | 2.432406 | -2.773860 | 3.725150 |
| H | 2.020044 | -1.071245 | 3.491547 |
| H | 2.220561 | -1.659230 | -1.848243 |
| H | 5.779506 | -0.124792 | -0.033001 |
| H | 1.943496 | 0.913528 | 1.579348 |
| H | -1.878336 | 0.065499 | 1.299567 |
| H | -2.281184 | 4.176826 | 0.094066 |
| H | 1.137113 | 1.900118 | -1.124254 |
| H | -1.307293 | -3.331209 | -0.179640 |
| H | -3.417150 | -4.144640 | 0.135321 |
| C | -4.668060 | -2.434655 | -0.314475 |
| C | -4.844684 | -1.097864 | 0.066676 |
| C | -5.804107 | -3.159425 | -0.705177 |
| C | -6.100136 | -0.500344 | 0.031363 |
| H | -3.989141 | -0.535654 | 0.423503 |
| C | -7.058162 | -2.564275 | -0.744657 |
| H | -5.692099 | -4.202211 | -0.983191 |
| C | -7.212086 | -1.228254 | -0.381083 |

| | | | |
|---|---|---|---|
| H | -6.208216 | 0.532697 | 0.338651 |
| H | -7.919071 | -3.144682 | -1.056392 |
| H | -8.190288 | -0.763370 | -0.407809 |
| C | 0.001499 | 4.297285 | -1.379417 |
| C | -3.532913 | 2.233985 | 1.460524 |
| C | 4.572435 | 1.259537 | 1.969322 |
| C | 4.850717 | -1.730458 | -2.042520 |
| F | -0.513371 | 5.465350 | -0.980078 |
| F | 1.335194 | 4.395925 | -1.300411 |
| F | -0.296969 | 4.163763 | -2.683250 |
| F | -3.625048 | 3.346663 | 2.198959 |
| F | -4.544343 | 2.279835 | 0.572462 |
| F | -3.773200 | 1.193933 | 2.267091 |
| F | 3.844657 | 2.321617 | 2.335366 |
| F | 5.785978 | 1.701864 | 1.619429 |
| F | 4.735128 | 0.505016 | 3.068919 |
| F | 6.167365 | -1.538645 | -1.924877 |
| F | 4.627423 | -3.050369 | -1.930331 |
| F | 4.504968 | -1.391490 | -3.293091 |

**14F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -2854.148797

Free energies: -2853.666400

Corrected Free energies: -2853.655301

| | | | |
|---|---|---|---|
| Si | 1.120992 | -2.505926 | 1.950065 |
| O | 0.185498 | -1.383790 | 1.077785 |
| N | -1.475535 | -1.752767 | -1.196494 |
| C | -0.026573 | -1.489950 | -1.294255 |
| C | 0.145529 | -0.902265 | -2.701384 |
| C | -1.248280 | -0.422473 | -3.165403 |
| C | -2.248185 | -0.860710 | -2.086077 |
| C | 0.430649 | -0.619058 | -0.075663 |
| C | -0.089675 | -3.094091 | 3.234479 |
| C | 1.682650 | -3.915850 | 0.851437 |
| C | 2.618584 | -1.711747 | 2.734967 |
| C | 1.917077 | -0.260521 | -0.163308 |
| C | 2.823153 | -1.003278 | -0.912040 |
| C | 4.186765 | -0.733074 | -0.833788 |
| C | 4.671815 | 0.281941 | -0.026047 |
| C | 3.760489 | 1.031870 | 0.708165 |
| C | 2.401514 | 0.767847 | 0.647136 |
| C | -0.433078 | 0.639679 | 0.008114 |

| | | | |
|---|---|---|---|
| C | -1.459771 | 0.716904 | 0.946358 |
| C | -2.308797 | 1.817897 | 0.958506 |
| C | -2.158630 | 2.854094 | 0.045605 |
| C | -1.115931 | 2.781710 | -0.865654 |
| C | -0.247746 | 1.696505 | -0.880227 |
| C | -1.923512 | -2.811877 | -0.558518 |
| C | -3.250791 | -3.252003 | -0.398054 |
| H | 0.480501 | -2.450166 | -1.191536 |
| H | 0.510378 | -1.688706 | -3.361245 |
| H | 0.884914 | -0.103958 | -2.721124 |
| H | -1.283029 | 0.658820 | -3.288807 |
| H | -1.503625 | -0.874210 | -4.121585 |
| H | -2.617869 | -0.007495 | -1.515461 |
| H | -3.101802 | -1.414175 | -2.475056 |
| H | -0.423508 | -2.260832 | 3.857332 |
| H | 0.376410 | -3.838862 | 3.884200 |
| H | -0.969115 | -3.549914 | 2.773190 |
| H | 0.860846 | -4.440176 | 0.357748 |
| H | 2.188991 | -4.647320 | 1.489209 |
| H | 2.404826 | -3.604885 | 0.092514 |
| H | 3.421480 | -1.530324 | 2.015856 |
| H | 3.005794 | -2.394734 | 3.497023 |
| H | 2.370815 | -0.767813 | 3.226064 |
| H | 2.494146 | -1.798853 | -1.570355 |
| H | 5.732483 | 0.489804 | 0.027214 |
| H | 1.716273 | 1.359364 | 1.244831 |
| H | -1.586012 | -0.088085 | 1.659885 |
| H | -2.829807 | 3.703374 | 0.053402 |
| H | 0.580508 | 1.696374 | -1.580396 |
| H | -1.148358 | -3.468811 | -0.179375 |
| H | -3.331936 | -4.322749 | -0.241783 |
| C | -4.468285 | -2.507970 | -0.384124 |
| C | -4.520139 | -1.145561 | -0.018502 |
| C | -5.679112 | -3.186643 | -0.652434 |
| C | -5.728099 | -0.478371 | 0.031193 |
| H | -3.611306 | -0.642000 | 0.283509 |
| C | -6.881467 | -2.506044 | -0.627434 |
| H | -5.649922 | -4.241466 | -0.900028 |
| C | -6.909113 | -1.151298 | -0.291110 |
| H | -5.759288 | 0.560976 | 0.334250 |
| H | -7.802330 | -3.026542 | -0.857202 |
| H | -7.854233 | -0.623401 | -0.258389 |
| C | -0.925633 | 3.861099 | -1.892795 |
| C | -3.376995 | 1.921716 | 2.010849 |

| | | | |
|---|---|---|---|
| C | 4.250850 | 2.095370 | 1.648703 |
| C | 5.124089 | -1.605724 | -1.618538 |
| F | -1.618814 | 4.964887 | -1.603414 |
| F | 0.361784 | 4.208404 | -2.012010 |
| F | -1.326557 | 3.448416 | -3.107405 |
| F | -2.950345 | 2.593317 | 3.086506 |
| F | -4.461895 | 2.562165 | 1.552814 |
| F | -3.778067 | 0.714290 | 2.434241 |
| F | 3.422875 | 3.146354 | 1.685934 |
| F | 5.463214 | 2.545949 | 1.311067 |
| F | 4.340539 | 1.627679 | 2.904125 |
| F | 6.378701 | -1.150331 | -1.599744 |
| F | 5.144268 | -2.854917 | -1.125254 |
| F | 4.748133 | -1.707248 | -2.900476 |

**15F-*E***

Imaginary frequency: None

Electronic energies: -846.855550

Free energies: -846.520904

Corrected Free energies: -846.517604

| | | | |
|---|---|---|---|
| C | 2.725927 | -1.487948 | 0.109992 |
| C | 1.229292 | -1.585958 | 0.381929 |
| C | 1.798932 | 0.552447 | -0.595535 |
| H | 1.055145 | -1.531137 | 1.466706 |
| H | 1.709244 | 0.922234 | -1.625913 |
| N | 0.733407 | -0.412704 | -0.317184 |
| C | -0.590129 | -0.084217 | -0.421987 |
| C | -1.608897 | -0.640816 | 0.263089 |
| H | -0.782856 | 0.698550 | -1.151503 |
| H | -1.395307 | -1.352453 | 1.054096 |
| N | 2.976700 | -0.299580 | -0.479752 |
| O | 3.545655 | -2.361179 | 0.325432 |
| C | 4.261387 | -0.046121 | -1.110911 |
| H | 5.020406 | 0.247729 | -0.383800 |
| H | 4.592087 | -0.960561 | -1.605387 |
| H | 4.149451 | 0.745586 | -1.849495 |
| C | 0.709036 | -2.911913 | -0.166745 |
| H | -0.348762 | -3.056466 | 0.042863 |
| H | 0.862611 | -2.949211 | -1.247125 |
| H | 1.274986 | -3.720162 | 0.297464 |
| C | 1.831751 | 1.772525 | 0.372524 |
| C | 1.789516 | 1.295427 | 1.825694 |
| H | 2.621138 | 0.621205 | 2.049992 |

| | | | |
|---|---|---|---|
| H | 1.866586 | 2.153247 | 2.498370 |
| H | 0.849130 | 0.781888 | 2.043828 |
| C | 3.114268 | 2.578005 | 0.129003 |
| H | 3.218972 | 2.858008 | -0.923843 |
| H | 3.080216 | 3.498927 | 0.715505 |
| H | 4.003710 | 2.025750 | 0.434878 |
| C | 0.634944 | 2.695022 | 0.101435 |
| H | 0.762241 | 3.622432 | 0.664828 |
| H | 0.564297 | 2.956289 | -0.959194 |
| H | -0.310187 | 2.249679 | 0.415048 |
| C | -3.019987 | -0.304330 | 0.052979 |
| C | -3.951393 | -0.601071 | 1.059610 |
| C | -3.497169 | 0.306727 | -1.117676 |
| C | -5.295383 | -0.279604 | 0.916508 |
| H | -3.607374 | -1.083296 | 1.968822 |
| C | -4.839482 | 0.636677 | -1.255710 |
| H | -2.817836 | 0.505492 | -1.938872 |
| C | -5.748483 | 0.347649 | -0.240669 |
| H | -5.991191 | -0.518849 | 1.712583 |
| H | -5.181344 | 1.107816 | -2.170308 |
| H | -6.796146 | 0.597711 | -0.355618 |

**15F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -846.662808

Free energies: -846.326217

Corrected Free energies: -846.323188

| | | | |
|---|---|---|---|
| C | -2.596799 | -1.590926 | -0.030683 |
| C | -1.127507 | -1.586910 | -0.453421 |
| C | -1.797947 | 0.543436 | 0.547144 |
| H | -1.052368 | -1.566246 | -1.544885 |
| H | -1.586268 | 0.927960 | 1.550804 |
| N | -0.665030 | -0.306616 | 0.110854 |
| C | 0.584672 | 0.071151 | 0.280413 |
| C | 1.685358 | -0.539180 | -0.328697 |
| H | 0.718137 | 0.942676 | 0.910837 |
| H | 1.500102 | -1.286176 | -1.091018 |
| N | -2.876285 | -0.422923 | 0.586155 |
| O | -3.348703 | -2.530159 | -0.163505 |
| C | -4.115810 | -0.255779 | 1.332672 |
| H | -4.949953 | -0.007521 | 0.675439 |
| H | -4.336034 | -1.194740 | 1.840219 |
| H | -3.986146 | 0.534473 | 2.069720 |

| | | | |
|---|---|---|---|
| C | -0.449636 | -2.819901 | 0.140128 |
| H | 0.560322 | -2.973584 | -0.230570 |
| H | -0.428469 | -2.746628 | 1.228851 |
| H | -1.054268 | -3.681962 | -0.140981 |
| C | -2.038893 | 1.731037 | -0.432446 |
| C | -2.263083 | 1.217933 | -1.856380 |
| H | -3.099747 | 0.516381 | -1.905632 |
| H | -2.498659 | 2.060814 | -2.509341 |
| H | -1.367836 | 0.735298 | -2.258297 |
| C | -3.279663 | 2.496965 | 0.046669 |
| H | -3.190328 | 2.792991 | 1.095675 |
| H | -3.384074 | 3.405591 | -0.549160 |
| H | -4.192146 | 1.914574 | -0.079491 |
| C | -0.841894 | 2.688934 | -0.408151 |
| H | -1.097271 | 3.583326 | -0.979550 |
| H | -0.596341 | 3.004559 | 0.610395 |
| H | 0.048816 | 2.260439 | -0.873451 |
| C | 3.042231 | -0.195829 | -0.073655 |
| C | 4.038741 | -0.812742 | -0.867523 |
| C | 3.442955 | 0.716312 | 0.933466 |
| C | 5.374558 | -0.522554 | -0.672502 |
| H | 3.737030 | -1.515104 | -1.635965 |
| C | 4.780288 | 0.998368 | 1.120489 |
| H | 2.710035 | 1.190133 | 1.574032 |
| C | 5.748794 | 0.383772 | 0.320462 |
| H | 6.128450 | -0.998021 | -1.286556 |
| H | 5.081311 | 1.693786 | 1.893451 |
| H | 6.796347 | 0.610510 | 0.476533 |

**15F-*Z***

Imaginary frequency: None

Electronic energies: -846.855675

Free energies: -846.518991

Corrected Free energies: -846.516262

| | | | |
|---|---|---|---|
| C | -1.455246 | 1.862654 | 0.326716 |
| C | -0.092412 | 1.248632 | 0.037489 |
| C | -1.887435 | -0.246863 | -0.608975 |
| H | 0.413323 | 1.071096 | 0.995968 |
| H | -2.252729 | -0.420378 | -1.632248 |
| N | -0.446376 | 0.000473 | -0.634337 |
| C | 0.305319 | -0.583999 | -1.636909 |
| C | 1.640218 | -0.745028 | -1.687035 |
| H | -0.286212 | -0.943230 | -2.477633 |

| | | | |
|---|---|---|---|
| H | 2.039544 | -1.113562 | -2.625914 |
| N | -2.409901 | 1.016426 | -0.108114 |
| O | -1.641997 | 2.957479 | 0.827410 |
| C | -3.811575 | 1.387710 | -0.085905 |
| H | -4.289105 | 1.123857 | 0.861109 |
| H | -3.875415 | 2.467644 | -0.216449 |
| H | -4.333052 | 0.889434 | -0.902886 |
| C | 0.730384 | 2.232432 | -0.788939 |
| H | 1.754846 | 1.890493 | -0.925171 |
| H | 0.269962 | 2.381093 | -1.768546 |
| H | 0.743814 | 3.183871 | -0.255834 |
| C | -2.272224 | -1.476432 | 0.262288 |
| C | -1.957337 | -1.193087 | 1.731601 |
| H | -2.563071 | -0.369409 | 2.118408 |
| H | -2.165574 | -2.079087 | 2.336477 |
| H | -0.902245 | -0.936047 | 1.864682 |
| C | -3.761599 | -1.806383 | 0.093920 |
| H | -4.027185 | -1.903902 | -0.963220 |
| H | -3.978276 | -2.760293 | 0.580949 |
| H | -4.411182 | -1.056960 | 0.545752 |
| C | -1.461623 | -2.686956 | -0.216705 |
| H | -1.781900 | -3.577251 | 0.329476 |
| H | -1.619675 | -2.874021 | -1.283767 |
| H | -0.392099 | -2.548803 | -0.047049 |
| C | 2.618368 | -0.491329 | -0.621188 |
| C | 3.928484 | -0.114711 | -0.950867 |
| C | 2.305259 | -0.670070 | 0.734003 |
| C | 4.880481 | 0.106925 | 0.036389 |
| H | 4.192926 | 0.010801 | -1.995719 |
| C | 3.259981 | -0.454319 | 1.721784 |
| H | 1.311263 | -1.006667 | 1.006778 |
| C | 4.549137 | -0.056258 | 1.379401 |
| H | 5.884385 | 0.405702 | -0.242440 |
| H | 2.997415 | -0.605068 | 2.762598 |
| H | 5.291078 | 0.115043 | 2.150131 |

**15F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -846.656212

Free energies: -846.318903

Corrected Free energies: -846.316247

| | | | |
|---|---|---|---|
| C | -1.536867 | 1.839402 | 0.335532 |
| C | -0.150298 | 1.218595 | 0.139499 |

| | | | |
|---|---|---|---|
| C | -1.936563 | -0.267146 | -0.622190 |
| H | 0.227499 | 0.916670 | 1.120288 |
| H | -2.286783 | -0.459415 | -1.641823 |
| N | -0.481093 | 0.028950 | -0.676748 |
| C | 0.271166 | -0.587041 | -1.567154 |
| C | 1.671598 | -0.595551 | -1.680666 |
| H | -0.282762 | -1.146356 | -2.317116 |
| H | 2.037762 | -0.809342 | -2.679291 |
| N | -2.470445 | 0.986072 | -0.132785 |
| O | -1.734116 | 2.938326 | 0.802749 |
| C | -3.863927 | 1.392178 | -0.250676 |
| H | -4.399143 | 1.260061 | 0.690749 |
| H | -3.887393 | 2.446636 | -0.524509 |
| H | -4.344810 | 0.801958 | -1.028793 |
| C | 0.781373 | 2.224879 | -0.521542 |
| H | 1.827366 | 1.939975 | -0.449018 |
| H | 0.510002 | 2.367008 | -1.569158 |
| H | 0.642874 | 3.168646 | 0.006117 |
| C | -2.242255 | -1.501950 | 0.270781 |
| C | -1.797005 | -1.254721 | 1.713083 |
| H | -2.270180 | -0.364714 | 2.134639 |
| H | -2.081066 | -2.109423 | 2.330189 |
| H | -0.712163 | -1.146780 | 1.794830 |
| C | -3.756282 | -1.753943 | 0.235203 |
| H | -4.126748 | -1.834788 | -0.790558 |
| H | -3.969668 | -2.696568 | 0.742796 |
| H | -4.311854 | -0.970889 | 0.751029 |
| C | -1.531725 | -2.735766 | -0.295550 |
| H | -1.835591 | -3.613435 | 0.277883 |
| H | -1.801102 | -2.912744 | -1.341001 |
| H | -0.443654 | -2.665122 | -0.219286 |
| C | 2.640907 | -0.430981 | -0.649143 |
| C | 3.965973 | -0.098578 | -1.012481 |
| C | 2.337063 | -0.635619 | 0.715020 |
| C | 4.926404 | 0.100521 | -0.038788 |
| H | 4.209893 | 0.026858 | -2.060891 |
| C | 3.308064 | -0.454835 | 1.679856 |
| H | 1.353117 | -0.987901 | 0.999191 |
| C | 4.598521 | -0.068797 | 1.307285 |
| H | 5.933390 | 0.380056 | -0.320841 |
| H | 3.072907 | -0.625286 | 2.722620 |
| H | 5.354916 | 0.079249 | 2.068264 |

**16F-*E***

Imaginary frequency: None

Electronic energies: -1077.873300

Free energies: -1077.460361

Corrected Free energies: -1077.456004

| | | | |
|---|---|---|---|
| C | 2.587529 | 0.650613 | -1.620966 |
| C | 1.203110 | 0.889770 | -1.044768 |
| C | 2.196157 | -1.113091 | -0.108948 |
| H | 0.484887 | 0.875612 | -1.874644 |
| H | 1.957080 | -2.128060 | -0.455588 |
| N | 0.988419 | -0.269172 | -0.186422 |
| C | -0.233205 | -0.923507 | -0.188070 |
| C | -1.425988 | -0.424917 | -0.555336 |
| H | -0.170760 | -1.940159 | 0.186924 |
| H | -1.517094 | 0.614459 | -0.848620 |
| N | 3.082298 | -0.480331 | -1.077413 |
| O | 3.145423 | 1.363738 | -2.434761 |
| C | 4.334238 | -1.047569 | -1.543247 |
| H | 5.182444 | -0.711160 | -0.943118 |
| H | 4.277449 | -2.135517 | -1.508986 |
| H | 4.485553 | -0.721838 | -2.571898 |
| C | 1.151211 | 2.268348 | -0.360778 |
| H | 1.919055 | 2.310377 | 0.414907 |
| H | 1.413463 | 3.004697 | -1.124859 |
| C | 2.774707 | -1.225924 | 1.326975 |
| C | 1.662800 | -1.730473 | 2.255220 |
| H | 0.825533 | -1.030397 | 2.294647 |
| H | 1.288190 | -2.707316 | 1.932808 |
| H | 2.060284 | -1.844529 | 3.266261 |
| C | 3.918518 | -2.250124 | 1.357353 |
| H | 3.627999 | -3.186565 | 0.871358 |
| H | 4.825068 | -1.878721 | 0.879638 |
| H | 4.168836 | -2.478403 | 2.396213 |
| C | 3.274936 | 0.129778 | 1.822735 |
| H | 2.448468 | 0.836506 | 1.917695 |
| H | 3.733241 | 0.017268 | 2.808341 |
| H | 4.022612 | 0.554538 | 1.147105 |
| C | -0.206003 | 2.566504 | 0.215042 |
| C | -0.551163 | 2.118156 | 1.490603 |
| C | -1.173376 | 3.212025 | -0.556912 |
| C | -1.843818 | 2.286552 | 1.975102 |
| H | 0.193769 | 1.615934 | 2.098903 |
| C | -2.468137 | 3.382185 | -0.076165 |
| H | -0.912306 | 3.568752 | -1.548403 |

| | | | |
|---|---|---|---|
| C | -2.808062 | 2.912463 | 1.189740 |
| H | -2.101091 | 1.925854 | 2.964153 |
| H | -3.210914 | 3.879995 | -0.688648 |
| H | -3.816983 | 3.038204 | 1.564616 |
| C | -2.683782 | -1.182103 | -0.503306 |
| C | -3.894412 | -0.474292 | -0.496449 |
| C | -2.744656 | -2.583686 | -0.468699 |
| C | -5.115855 | -1.134975 | -0.437281 |
| H | -3.865415 | 0.610566 | -0.528409 |
| C | -3.965046 | -3.243184 | -0.400015 |
| H | -1.831919 | -3.167215 | -0.514887 |
| C | -5.158977 | -2.524901 | -0.383194 |
| H | -6.036043 | -0.561946 | -0.431393 |
| H | -3.985206 | -4.326681 | -0.374037 |
| H | -6.108962 | -3.043519 | -0.336965 |

**16F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1077.678998

Free energies: -1077.265265

Corrected Free energies: -1077.260977

| | | | |
|---|---|---|---|
| C | 2.745938 | 1.160854 | -1.252489 |
| C | 1.283415 | 1.153496 | -0.831492 |
| C | 2.361237 | -1.008661 | -0.397247 |
| H | 0.675873 | 1.395879 | -1.707031 |
| H | 2.264776 | -1.893838 | -1.036505 |
| N | 1.076615 | -0.256365 | -0.481913 |
| C | -0.077380 | -0.898637 | -0.530380 |
| C | -1.313842 | -0.317061 | -0.814632 |
| H | -0.011027 | -1.966006 | -0.360469 |
| H | -1.348077 | 0.717413 | -1.133021 |
| N | 3.275248 | -0.058419 | -1.006543 |
| O | 3.315569 | 2.113477 | -1.735486 |
| C | 4.600116 | -0.401439 | -1.505508 |
| H | 5.378919 | -0.150496 | -0.784112 |
| H | 4.637427 | -1.466705 | -1.727628 |
| H | 4.770952 | 0.167613 | -2.418617 |
| C | 1.031359 | 2.197500 | 0.277886 |
| H | 1.678755 | 1.990159 | 1.129627 |
| H | 1.358253 | 3.144523 | -0.158820 |
| C | 2.740173 | -1.472251 | 1.037445 |
| C | 1.638788 | -2.377673 | 1.603547 |
| H | 0.710519 | -1.834751 | 1.796455 |

| | | | |
|---|---|---|---|
| H | 1.429433 | -3.225310 | 0.944025 |
| H | 1.977068 | -2.782006 | 2.559409 |
| C | 4.032867 | -2.298363 | 0.943949 |
| H | 3.955100 | -3.086870 | 0.190247 |
| H | 4.901479 | -1.680616 | 0.718630 |
| H | 4.212996 | -2.775986 | 1.908801 |
| C | 2.955741 | -0.286525 | 1.976319 |
| H | 2.013980 | 0.216578 | 2.202682 |
| H | 3.364611 | -0.646782 | 2.922593 |
| H | 3.659929 | 0.439233 | 1.561413 |
| C | -0.412610 | 2.276111 | 0.691570 |
| C | -0.895251 | 1.514386 | 1.757470 |
| C | -1.310649 | 3.050921 | -0.047260 |
| C | -2.254217 | 1.498276 | 2.058763 |
| H | -0.207870 | 0.924976 | 2.355497 |
| C | -2.668654 | 3.034076 | 0.250251 |
| H | -0.943471 | 3.658878 | -0.868181 |
| C | -3.144910 | 2.247659 | 1.297846 |
| H | -2.615112 | 0.896045 | 2.883865 |
| H | -3.355669 | 3.633946 | -0.334800 |
| H | -4.204238 | 2.228195 | 1.524150 |
| C | -2.559700 | -1.002216 | -0.731625 |
| C | -3.716734 | -0.312515 | -1.164616 |
| C | -2.701626 | -2.312375 | -0.214143 |
| C | -4.959241 | -0.913169 | -1.102823 |
| H | -3.612405 | 0.695381 | -1.549866 |
| C | -3.947296 | -2.902824 | -0.155654 |
| H | -1.841619 | -2.858105 | 0.153736 |
| C | -5.077313 | -2.209790 | -0.600937 |
| H | -5.838001 | -0.378613 | -1.440167 |
| H | -4.050548 | -3.903966 | 0.242918 |
| H | -6.050885 | -2.681776 | -0.549198 |

**16F-*Z***

Imaginary frequency: None

Electronic energies: -1077.863250

Free energies: -1077.449585

Corrected Free energies: -1077.445716

| | | | |
|---|---|---|---|
| C | -1.376436 | -1.661541 | -0.766954 |
| C | -0.476085 | -0.467407 | -0.481943 |
| C | -2.802821 | 0.179535 | -0.442312 |
| H | 0.220305 | -0.337604 | -1.315533 |
| H | -3.362961 | 0.623993 | -1.276575 |

| | | | |
|---|---|---|---|
| N | -1.414003 | 0.659812 | -0.473224 |
| C | -1.165801 | 1.749459 | -1.307808 |
| C | 0.003611 | 2.348488 | -1.570139 |
| H | -2.053471 | 2.129968 | -1.806695 |
| H | -0.024556 | 3.123702 | -2.329179 |
| N | -2.658443 | -1.250275 | -0.689443 |
| O | -1.006843 | -2.800159 | -0.999170 |
| C | -3.750915 | -2.142726 | -1.033821 |
| H | -4.556073 | -1.571363 | -1.495183 |
| H | -3.373244 | -2.879181 | -1.742637 |
| H | -4.138262 | -2.667919 | -0.158296 |
| C | 0.318374 | -0.693560 | 0.821982 |
| H | 0.390070 | 0.261482 | 1.342974 |
| H | -0.248202 | -1.364851 | 1.477254 |
| C | -3.540149 | 0.559576 | 0.865344 |
| C | -2.859073 | -0.068926 | 2.079323 |
| H | -1.842281 | 0.311960 | 2.194624 |
| H | -3.417232 | 0.177268 | 2.986124 |
| H | -2.819866 | -1.158891 | 1.992424 |
| C | -3.503180 | 2.088107 | 0.982599 |
| H | -3.974258 | 2.562491 | 0.115465 |
| H | -4.050588 | 2.401589 | 1.874623 |
| H | -2.477610 | 2.454806 | 1.062108 |
| C | -5.006377 | 0.112709 | 0.799799 |
| H | -5.556884 | 0.554120 | 1.634152 |
| H | -5.483803 | 0.444171 | -0.127563 |
| H | -5.110484 | -0.970144 | 0.876432 |
| C | 1.713387 | -1.250791 | 0.635243 |
| C | 2.070370 | -2.039393 | -0.461147 |
| C | 2.679167 | -0.995582 | 1.611750 |
| C | 3.365347 | -2.536700 | -0.586730 |
| H | 1.326782 | -2.288287 | -1.209269 |
| C | 3.969464 | -1.498816 | 1.494488 |
| H | 2.416997 | -0.383330 | 2.468769 |
| C | 4.320356 | -2.267188 | 0.387651 |
| H | 3.624877 | -3.142505 | -1.447521 |
| H | 4.704085 | -1.283446 | 2.262127 |
| H | 5.327047 | -2.655962 | 0.288730 |
| C | 1.308676 | 2.139282 | -0.897809 |
| C | 2.448161 | 1.768879 | -1.618256 |
| C | 1.444502 | 2.418278 | 0.466366 |
| C | 3.686795 | 1.670831 | -0.991693 |
| H | 2.358626 | 1.557810 | -2.678755 |
| C | 2.681626 | 2.324487 | 1.093580 |

| | | | |
|---|---|---|---|
| H | 0.568309 | 2.723230 | 1.030321 |
| C | 3.807308 | 1.949562 | 0.365810 |
| H | 4.558341 | 1.376223 | -1.565226 |
| H | 2.767335 | 2.546032 | 2.151433 |
| H | 4.771036 | 1.869763 | 0.854955 |

**16F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1077.658961

Free energies: -1077.244621

Corrected Free energies: -1077.240948

| | | | |
|---|---|---|---|
| C | 1.400584 | 1.505780 | -1.038240 |
| C | 0.473427 | 0.404289 | -0.532277 |
| C | 2.824138 | -0.270424 | -0.412793 |
| H | -0.273427 | 0.166924 | -1.290044 |
| H | 3.382953 | -0.843390 | -1.160372 |
| N | 1.407471 | -0.737717 | -0.462014 |
| C | 1.159934 | -1.944047 | -0.946730 |
| C | -0.082785 | -2.497179 | -1.285386 |
| H | 2.043475 | -2.522040 | -1.199583 |
| H | -0.031620 | -3.233220 | -2.082201 |
| N | 2.679829 | 1.101308 | -0.869229 |
| O | 1.029873 | 2.573065 | -1.473885 |
| C | 3.786246 | 1.897625 | -1.384800 |
| H | 4.577048 | 1.235139 | -1.734737 |
| H | 3.411812 | 2.490415 | -2.218347 |
| H | 4.183181 | 2.569516 | -0.623356 |
| C | -0.207161 | 0.867515 | 0.774137 |
| H | -0.227470 | 0.047476 | 1.489544 |
| H | 0.398143 | 1.655858 | 1.230803 |
| C | 3.504686 | -0.481320 | 0.960671 |
| C | 2.822816 | 0.319247 | 2.067349 |
| H | 1.824377 | -0.065089 | 2.283455 |
| H | 3.409255 | 0.236166 | 2.984750 |
| H | 2.752655 | 1.379484 | 1.810546 |
| C | 3.468520 | -1.977929 | 1.293255 |
| H | 3.951479 | -2.573366 | 0.512336 |
| H | 4.012613 | -2.149229 | 2.223796 |
| H | 2.449721 | -2.344791 | 1.439591 |
| C | 4.972915 | -0.047363 | 0.838547 |
| H | 5.504123 | -0.348251 | 1.743587 |
| H | 5.465190 | -0.525614 | -0.012888 |
| H | 5.075047 | 1.033833 | 0.743241 |

| | | | |
|---|---|---|---|
| C | -1.621025 | 1.378976 | 0.580864 |
| C | -2.095120 | 1.872270 | -0.634005 |
| C | -2.478580 | 1.375445 | 1.684374 |
| C | -3.410570 | 2.318714 | -0.749859 |
| H | -1.438372 | 1.938197 | -1.493766 |
| C | -3.785407 | 1.830364 | 1.573787 |
| H | -2.118176 | 0.997674 | 2.636198 |
| C | -4.260262 | 2.295467 | 0.349110 |
| H | -3.765287 | 2.691980 | -1.703360 |
| H | -4.436338 | 1.813446 | 2.439993 |
| H | -5.282205 | 2.642652 | 0.256066 |
| C | -1.369915 | -2.220019 | -0.719805 |
| C | -2.517196 | -2.276491 | -1.539483 |
| C | -1.519852 | -1.999235 | 0.663801 |
| C | -3.765019 | -2.026705 | -0.999121 |
| H | -2.404262 | -2.482796 | -2.597202 |
| C | -2.778033 | -1.801263 | 1.202267 |
| H | -0.650170 | -2.053840 | 1.308376 |
| C | -3.897573 | -1.788751 | 0.370387 |
| H | -4.640811 | -2.031838 | -1.635426 |
| H | -2.892804 | -1.653268 | 2.268631 |
| H | -4.878835 | -1.611482 | 0.793861 |

**17F-*E***

Imaginary frequency: None

Electronic energies: -999.272401

Free energies: -998.914645

Corrected Free energies: -998.910703

| | | | |
|---|---|---|---|
| C | -2.284813 | -1.398662 | 1.108143 |
| C | -0.876892 | -0.871622 | 1.329940 |
| C | -1.243703 | -1.421623 | -1.020400 |
| H | -0.351825 | -1.540401 | 2.024824 |
| N | -0.308007 | -0.928150 | 0.003490 |
| C | 1.008159 | -0.700040 | -0.262830 |
| C | 1.979368 | -0.452999 | 0.641706 |
| H | 1.254237 | -0.724766 | -1.320652 |
| H | 1.752873 | -0.495387 | 1.701794 |
| N | -2.433512 | -1.667066 | -0.202861 |
| O | -3.132292 | -1.511982 | 1.977053 |
| C | -3.693506 | -2.093621 | -0.775275 |
| H | -4.085732 | -1.335046 | -1.456295 |
| H | -3.578716 | -3.036884 | -1.311671 |
| H | -4.393061 | -2.232078 | 0.046444 |

| | | | |
|---|---|---|---|
| C | -0.942904 | 0.546344 | 1.945351 |
| H | -1.562651 | 0.467531 | 2.841757 |
| H | 0.055052 | 0.858644 | 2.253551 |
| C | -1.519738 | 1.543718 | 0.974398 |
| C | -2.901274 | 1.659232 | 0.799964 |
| C | -0.674624 | 2.317740 | 0.177468 |
| C | -3.424932 | 2.523677 | -0.157253 |
| H | -3.565904 | 1.060509 | 1.415014 |
| C | -1.195088 | 3.186134 | -0.777333 |
| H | 0.400052 | 2.226522 | 0.303173 |
| C | -2.572629 | 3.287767 | -0.950227 |
| H | -4.498764 | 2.602795 | -0.281699 |
| H | -0.526313 | 3.780980 | -1.388678 |
| H | -2.980005 | 3.962423 | -1.693952 |
| C | -0.747202 | -2.726412 | -1.645836 |
| H | 0.175643 | -2.552299 | -2.202048 |
| H | -0.559144 | -3.464208 | -0.864090 |
| H | -1.484605 | -3.122389 | -2.346383 |
| C | -1.524286 | -0.363729 | -2.088162 |
| H | -1.956055 | 0.527922 | -1.630221 |
| H | -0.594134 | -0.090146 | -2.590421 |
| H | -2.207785 | -0.755758 | -2.844307 |
| C | 3.373878 | -0.171671 | 0.288192 |
| C | 4.374051 | -0.335259 | 1.259254 |
| C | 3.769678 | 0.272228 | -0.984269 |
| C | 5.711066 | -0.093435 | 0.967836 |
| H | 4.091370 | -0.665232 | 2.253549 |
| C | 5.107354 | 0.503997 | -1.277684 |
| H | 3.023802 | 0.459464 | -1.748643 |
| C | 6.088884 | 0.322310 | -0.305697 |
| H | 6.460836 | -0.231664 | 1.738637 |
| H | 5.384406 | 0.844777 | -2.268828 |
| H | 7.130308 | 0.512609 | -0.535397 |

**17F-*Z***

Imaginary frequency: None

Electronic energies: -999.267668

Free energies: -998.909371

Corrected Free energies: -998.905910

| | | | |
|---|---|---|---|
| C | 0.903419 | -1.389387 | -1.346916 |
| C | -0.207128 | -0.586772 | -0.695783 |
| C | 1.266459 | -1.567033 | 0.984040 |
| H | -1.159145 | -1.012960 | -1.028800 |

| | | | |
|---|---|---|---|
| N | 0.035291 | -0.796601 | 0.718895 |
| C | -0.592964 | -0.125705 | 1.739732 |
| C | -1.817227 | 0.440833 | 1.768509 |
| H | 0.018267 | -0.019756 | 2.631375 |
| H | -2.029695 | 1.048885 | 2.641546 |
| N | 1.670733 | -1.920111 | -0.377848 |
| O | 1.064924 | -1.506256 | -2.550611 |
| C | 2.869026 | -2.681973 | -0.663865 |
| H | 3.767133 | -2.086578 | -0.480558 |
| H | 2.902709 | -3.584154 | -0.052041 |
| H | 2.836909 | -2.961610 | -1.715022 |
| C | -0.159210 | 0.884280 | -1.162039 |
| H | -0.228566 | 0.858250 | -2.252751 |
| H | -1.040233 | 1.405691 | -0.783615 |
| C | 1.098829 | 1.590350 | -0.723830 |
| C | 1.091547 | 2.422752 | 0.396779 |
| C | 2.307363 | 1.382025 | -1.395975 |
| C | 2.264993 | 3.019034 | 0.849847 |
| H | 0.157572 | 2.591780 | 0.922534 |
| C | 3.482318 | 1.974645 | -0.944324 |
| H | 2.324455 | 0.745316 | -2.274654 |
| C | 3.465467 | 2.791288 | 0.183907 |
| H | 2.242420 | 3.659731 | 1.723888 |
| H | 4.411461 | 1.801360 | -1.474756 |
| H | 4.380874 | 3.251346 | 0.536906 |
| C | 0.935508 | -2.818566 | 1.797362 |
| H | 0.509387 | -2.523466 | 2.758588 |
| H | 0.207128 | -3.426610 | 1.258500 |
| H | 1.831034 | -3.410818 | 1.994422 |
| C | 2.369036 | -0.748710 | 1.663398 |
| H | 3.273701 | -1.355216 | 1.745239 |
| H | 2.590982 | 0.150659 | 1.086667 |
| H | 2.080493 | -0.467349 | 2.676995 |
| C | -2.902631 | 0.326933 | 0.783879 |
| C | -3.211335 | -0.893975 | 0.168636 |
| C | -3.711010 | 1.435291 | 0.489794 |
| C | -4.264667 | -0.995138 | -0.734691 |
| H | -2.630167 | -1.774090 | 0.425075 |
| C | -4.762881 | 1.335349 | -0.411876 |
| H | -3.499367 | 2.384189 | 0.972091 |
| C | -5.040944 | 0.120063 | -1.034357 |
| H | -4.484291 | -1.950443 | -1.197352 |
| H | -5.367624 | 2.207642 | -0.631911 |
| H | -5.860799 | 0.041727 | -1.738167 |

**17F-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -999.069485

Free energies: -998.709594

Corrected Free energies: -998.706607

| | | | |
|---|---|---|---|
| C | 0.928456 | -1.427199 | -1.324325 |
| C | -0.186672 | -0.577189 | -0.739089 |
| C | 1.245374 | -1.546441 | 1.024606 |
| H | -1.139605 | -1.009486 | -1.041346 |
| N | 0.031734 | -0.713425 | 0.709393 |
| C | -0.603922 | -0.085133 | 1.671727 |
| C | -1.811347 | 0.635817 | 1.591602 |
| H | -0.109436 | -0.098420 | 2.638979 |
| H | -1.912639 | 1.422121 | 2.332887 |
| N | 1.668028 | -1.927385 | -0.317366 |
| O | 1.105797 | -1.580668 | -2.514748 |
| C | 2.872641 | -2.704411 | -0.553294 |
| H | 3.763933 | -2.110864 | -0.339351 |
| H | 2.873210 | -3.604481 | 0.061355 |
| H | 2.873304 | -2.986655 | -1.603787 |
| C | -0.086723 | 0.877328 | -1.245731 |
| H | -0.106629 | 0.797760 | -2.335078 |
| H | -0.973851 | 1.433703 | -0.939979 |
| C | 1.170472 | 1.566166 | -0.775760 |
| C | 1.134388 | 2.443241 | 0.309477 |
| C | 2.400437 | 1.295737 | -1.384093 |
| C | 2.304246 | 3.019078 | 0.797672 |
| H | 0.183190 | 2.685972 | 0.772945 |
| C | 3.569830 | 1.870484 | -0.897966 |
| H | 2.439570 | 0.632395 | -2.241819 |
| C | 3.525479 | 2.727177 | 0.199523 |
| H | 2.259704 | 3.695814 | 1.642505 |
| H | 4.515980 | 1.652774 | -1.378912 |
| H | 4.437484 | 3.171862 | 0.579153 |
| C | 0.809099 | -2.761314 | 1.839208 |
| H | 0.418589 | -2.448715 | 2.808970 |
| H | 0.042121 | -3.320163 | 1.301484 |
| H | 1.668037 | -3.408311 | 2.019931 |
| C | 2.324430 | -0.729255 | 1.730268 |
| H | 3.197772 | -1.365917 | 1.880089 |
| H | 2.610062 | 0.136299 | 1.130900 |
| H | 1.993168 | -0.401884 | 2.715938 |

| | | | |
|---|---|---|---|
| C | -2.915174 | 0.413007 | 0.712576 |
| C | -3.184931 | -0.857865 | 0.159375 |
| C | -3.810180 | 1.475472 | 0.456142 |
| C | -4.277233 | -1.039415 | -0.667189 |
| H | -2.563467 | -1.704783 | 0.429498 |
| C | -4.886808 | 1.290062 | -0.390930 |
| H | -3.627241 | 2.443216 | 0.908970 |
| C | -5.118525 | 0.036596 | -0.958896 |
| H | -4.485793 | -2.018881 | -1.078264 |
| H | -5.554268 | 2.114701 | -0.605692 |
| H | -5.967922 | -0.108710 | -1.614987 |

**17F-*E*** radical cation

Imaginary frequency: None

Electronic energies: -999.079575

Free energies: -998.721178

Corrected Free energies: -998.717571

| | | | |
|---|---|---|---|
| C | -2.335552 | -1.294014 | 1.177109 |
| C | -0.889604 | -0.862836 | 1.376117 |
| C | -1.347547 | -1.449975 | -0.977373 |
| H | -0.395426 | -1.546278 | 2.071975 |
| N | -0.327411 | -1.020627 | 0.032561 |
| C | 0.932488 | -0.839843 | -0.295305 |
| C | 1.952723 | -0.565849 | 0.621344 |
| H | 1.160456 | -0.939838 | -1.350498 |
| H | 1.720366 | -0.605579 | 1.679135 |
| N | -2.526830 | -1.568534 | -0.127889 |
| O | -3.163264 | -1.318850 | 2.063317 |
| C | -3.834523 | -1.889496 | -0.671597 |
| H | -4.191618 | -1.081699 | -1.313445 |
| H | -3.800039 | -2.821049 | -1.236898 |
| H | -4.512948 | -2.005021 | 0.170665 |
| C | -0.848129 | 0.586425 | 1.913872 |
| H | -1.470249 | 0.576368 | 2.811507 |
| H | 0.165790 | 0.844363 | 2.219689 |
| C | -1.362672 | 1.584283 | 0.907150 |
| C | -2.735749 | 1.764517 | 0.717707 |
| C | -0.469858 | 2.300873 | 0.108840 |
| C | -3.203980 | 2.631344 | -0.264327 |
| H | -3.437558 | 1.221021 | 1.342263 |
| C | -0.936935 | 3.169276 | -0.873652 |
| H | 0.599111 | 2.183569 | 0.260498 |
| C | -2.305386 | 3.330913 | -1.066064 |

| | | | |
|---|---|---|---|
| H | -4.270668 | 2.763479 | -0.401247 |
| H | -0.232684 | 3.719692 | -1.485807 |
| H | -2.671140 | 4.006071 | -1.830245 |
| C | -0.950655 | -2.804194 | -1.560992 |
| H | -0.040488 | -2.717994 | -2.155729 |
| H | -0.798405 | -3.530248 | -0.761906 |
| H | -1.742768 | -3.157239 | -2.221933 |
| C | -1.530656 | -0.387831 | -2.057966 |
| H | -1.871512 | 0.552252 | -1.623956 |
| H | -0.594364 | -0.223748 | -2.593189 |
| H | -2.266131 | -0.741119 | -2.782262 |
| C | 3.301382 | -0.282411 | 0.267496 |
| C | 4.245179 | -0.151147 | 1.314759 |
| C | 3.741183 | -0.114362 | -1.068955 |
| C | 5.570787 | 0.118754 | 1.038672 |
| H | 3.912125 | -0.271446 | 2.339061 |
| C | 5.067167 | 0.157737 | -1.333360 |
| H | 3.044579 | -0.183612 | -1.894486 |
| C | 5.985703 | 0.272324 | -0.285052 |
| H | 6.285315 | 0.213216 | 1.846153 |
| H | 5.396839 | 0.286940 | -2.356177 |
| H | 7.025025 | 0.485902 | -0.502937 |

## Calculated Cartesian coordinates for butanone derived enamines

**1G-*E***

Imaginary frequency: None

Electronic energies: -660.895036

Free energies: -660.517588

Corrected Free energies: -660.514313

| | | | |
|---|---|---|---|
| C | -2.657648 | -0.188991 | -0.075196 |
| C | -3.025639 | -1.609198 | 0.376120 |
| H | -2.835124 | -1.735033 | 1.446102 |
| H | -4.089352 | -1.790624 | 0.200189 |
| H | -2.466415 | -2.377697 | -0.161178 |
| C | -3.513999 | 0.797548 | 0.728126 |
| H | -3.258108 | 0.753252 | 1.791040 |
| H | -3.366753 | 1.823982 | 0.390949 |
| H | -4.572535 | 0.544911 | 0.619479 |
| C | -2.973682 | -0.035063 | -1.569419 |

| | | | |
|---|---|---|---|
| H | -2.726384 | 0.963871 | -1.940635 |
| H | -2.431874 | -0.766817 | -2.173799 |
| H | -4.042809 | -0.187650 | -1.739757 |
| C | -1.156018 | 0.058851 | 0.216971 |
| H | -0.995253 | -0.233377 | 1.259174 |
| C | -0.200452 | -0.769635 | -0.665479 |
| H | -0.026768 | -0.207988 | -1.589641 |
| H | -0.649640 | -1.730567 | -0.959281 |
| N | -0.844738 | 1.496197 | 0.116900 |
| N | 1.078843 | -0.968564 | 0.009710 |
| C | 2.228423 | -0.926882 | -0.888825 |
| H | 2.169710 | 0.024256 | -1.426025 |
| H | 3.136917 | -0.879173 | -0.281696 |
| C | 1.030222 | -2.137584 | 0.880794 |
| H | 0.146783 | -2.033415 | 1.519179 |
| H | 0.878556 | -3.067240 | 0.303774 |
| C | 2.261936 | -2.275584 | 1.766229 |
| H | 3.149403 | -2.546227 | 1.190454 |
| H | 2.460670 | -1.333891 | 2.283598 |
| H | 2.101572 | -3.055289 | 2.513032 |
| C | 2.336422 | -2.086013 | -1.884498 |
| H | 1.432521 | -2.164308 | -2.494717 |
| H | 3.183347 | -1.930551 | -2.556180 |
| H | 2.485456 | -3.041279 | -1.374942 |
| H | -1.153084 | 1.839081 | -0.788505 |
| C | 0.488645 | 1.916951 | 0.336866 |
| C | 1.152109 | 2.619873 | -0.591971 |
| C | 2.497360 | 3.264493 | -0.416177 |
| H | 2.450668 | 4.340827 | -0.609513 |
| H | 3.229917 | 2.850566 | -1.117222 |
| H | 0.672958 | 2.761190 | -1.559532 |
| H | 2.889799 | 3.129942 | 0.592327 |
| C | 1.039651 | 1.643351 | 1.714511 |
| H | 2.085717 | 1.342580 | 1.663743 |
| H | 0.964306 | 2.539520 | 2.338470 |
| H | 0.493069 | 0.841013 | 2.206533 |

**1G-*Z***

Imaginary frequency: None

Electronic energies: -660.899315

Free energies: -660.522093

Corrected Free energies: -660.518429

| | | | |
|---|---|---|---|
| C | -2.252798 | -1.158666 | -0.052530 |

| | | | |
|---|---|---|---|
| C | -2.090124 | -2.618410 | 0.394717 |
| H | -1.739970 | -2.672100 | 1.430406 |
| H | -3.054896 | -3.129842 | 0.339893 |
| H | -1.390537 | -3.173633 | -0.232260 |
| C | -3.375440 | -0.530135 | 0.780956 |
| H | -3.108062 | -0.521417 | 1.842798 |
| H | -3.566820 | 0.497967 | 0.473114 |
| H | -4.296830 | -1.107867 | 0.667054 |
| C | -2.639264 | -1.122232 | -1.536002 |
| H | -2.775474 | -0.096837 | -1.892169 |
| H | -1.885304 | -1.608112 | -2.161091 |
| H | -3.586045 | -1.647658 | -1.687967 |
| C | -0.934479 | -0.383621 | 0.208338 |
| H | -0.710411 | -0.522317 | 1.269117 |
| C | 0.264768 | -0.889442 | -0.614351 |
| H | 0.166609 | -0.487751 | -1.628149 |
| H | 0.254242 | -1.985521 | -0.706674 |
| N | -1.120479 | 1.051680 | -0.008388 |
| N | 1.526461 | -0.420867 | -0.044394 |
| C | 2.526771 | -0.087995 | -1.059088 |
| H | 2.065844 | 0.639225 | -1.733662 |
| H | 3.352928 | 0.434007 | -0.569613 |
| C | 2.002896 | -1.347190 | 0.980402 |
| H | 1.192567 | -1.477929 | 1.705261 |
| H | 2.197883 | -2.348364 | 0.558851 |
| C | 3.242435 | -0.848766 | 1.712144 |
| H | 4.126296 | -0.861576 | 1.071093 |
| H | 3.092746 | 0.174027 | 2.066869 |
| H | 3.448912 | -1.486633 | 2.573272 |
| C | 3.070786 | -1.267299 | -1.870299 |
| H | 2.261181 | -1.815742 | -2.359009 |
| H | 3.750876 | -0.908214 | -2.645491 |
| H | 3.624510 | -1.967361 | -1.240178 |
| H | -1.258591 | 1.265455 | -0.988760 |
| C | -0.332143 | 2.009233 | 0.634240 |
| C | 0.011041 | 3.162747 | 0.034583 |
| C | -0.305523 | 3.486573 | -1.402003 |
| H | 0.222384 | 4.384575 | -1.724271 |
| H | -1.375208 | 3.663581 | -1.568937 |
| H | 0.525112 | 3.909324 | 0.627460 |
| H | -0.007302 | 2.676698 | -2.078916 |
| C | 0.024625 | 1.727415 | 2.067298 |
| H | 0.452829 | 2.618181 | 2.525714 |
| H | -0.859968 | 1.427931 | 2.637376 |

| | | | |
|---|---|---|---|
| H | 0.757322 | 0.918950 | 2.127919 |

**1G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -660.718314

Free energies: -660.339611

Corrected Free energies: -660.336698

| | | | |
|---|---|---|---|
| C | 1.789395 | -1.682229 | -0.074618 |
| C | 1.352143 | -2.997123 | -0.733619 |
| H | 1.086036 | -2.840693 | -1.782655 |
| H | 2.179902 | -3.709103 | -0.698697 |
| H | 0.502721 | -3.455828 | -0.225116 |
| C | 3.048312 | -1.176761 | -0.791121 |
| H | 2.836815 | -0.954674 | -1.841361 |
| H | 3.452696 | -0.274286 | -0.326020 |
| H | 3.823940 | -1.944802 | -0.757123 |
| C | 2.097056 | -1.932781 | 1.406455 |
| H | 2.402524 | -1.024533 | 1.935444 |
| H | 1.241257 | -2.364295 | 1.930034 |
| H | 2.926553 | -2.638855 | 1.487438 |
| C | 0.653965 | -0.644181 | -0.262118 |
| H | 0.421684 | -0.600152 | -1.326854 |
| C | -0.636263 | -0.919973 | 0.530526 |
| H | -0.430237 | -0.756077 | 1.591898 |
| H | -0.910038 | -1.977257 | 0.416764 |
| N | 1.109606 | 0.693163 | 0.131230 |
| N | -1.700657 | -0.022291 | 0.101828 |
| C | -2.546388 | 0.430909 | 1.210934 |
| H | -1.880203 | 0.865739 | 1.961003 |
| H | -3.172633 | 1.248764 | 0.848206 |
| C | -2.443968 | -0.597264 | -1.023670 |
| H | -1.719443 | -0.828411 | -1.812092 |
| H | -2.909275 | -1.556288 | -0.744989 |
| C | -3.501605 | 0.343735 | -1.584111 |
| H | -4.336525 | 0.471592 | -0.892708 |
| H | -3.076144 | 1.329065 | -1.790389 |
| H | -3.900163 | -0.061313 | -2.515371 |
| C | -3.420356 | -0.646712 | 1.854456 |
| H | -2.816737 | -1.484067 | 2.214608 |
| H | -3.960648 | -0.230301 | 2.706663 |
| H | -4.157572 | -1.037274 | 1.149320 |
| H | 1.529136 | 0.751827 | 1.056111 |
| C | 0.949469 | 1.822278 | -0.525898 |

| | | | |
|---|---|---|---|
| C | 1.403450 | 3.022923 | 0.071554 |
| C | 0.316110 | 1.830373 | -1.879925 |
| H | 0.258069 | 2.847266 | -2.259547 |
| H | 0.901386 | 1.227246 | -2.577712 |
| H | -0.687835 | 1.409517 | -1.807177 |
| H | 1.261992 | 3.930424 | -0.499878 |
| C | 2.044307 | 3.089541 | 1.408335 |
| H | 2.950983 | 2.474131 | 1.442851 |
| H | 2.317738 | 4.111645 | 1.655907 |
| H | 1.367619 | 2.718477 | 2.186952 |

**1G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -660.717438

Free energies: -660.339072

Corrected Free energies: -660.336079

| | | | |
|---|---|---|---|
| C | -2.450498 | -0.918702 | 0.094156 |
| C | -2.570193 | -2.206922 | 0.919874 |
| H | -2.242751 | -2.045971 | 1.950984 |
| H | -3.615243 | -2.523964 | 0.943710 |
| H | -1.987962 | -3.026226 | 0.495121 |
| C | -3.412054 | 0.125181 | 0.677171 |
| H | -3.141501 | 0.372010 | 1.708006 |
| H | -3.414461 | 1.049256 | 0.094197 |
| H | -4.429870 | -0.270726 | 0.678440 |
| C | -2.826688 | -1.215969 | -1.362411 |
| H | -2.786001 | -0.328681 | -2.001516 |
| H | -2.186434 | -1.985948 | -1.797939 |
| H | -3.855631 | -1.580951 | -1.398075 |
| C | -1.000618 | -0.391138 | 0.229621 |
| H | -0.799760 | -0.281692 | 1.295480 |
| C | 0.095522 | -1.264927 | -0.413166 |
| H | -0.030429 | -1.232935 | -1.498598 |
| H | -0.046640 | -2.307553 | -0.100879 |
| N | -0.874697 | 0.936332 | -0.377380 |
| N | 1.412816 | -0.755896 | -0.062386 |
| C | 2.363757 | -0.789174 | -1.177364 |
| H | 1.890138 | -0.268450 | -2.014086 |
| H | 3.234908 | -0.191497 | -0.900088 |
| C | 1.904114 | -1.371861 | 1.171829 |
| H | 1.130067 | -1.240689 | 1.935824 |
| H | 2.029727 | -2.459967 | 1.053309 |
| C | 3.202739 | -0.753149 | 1.669526 |

| | | | |
|---|---|---|---|
| H | 4.045039 | -1.003646 | 1.021963 |
| H | 3.117634 | 0.335064 | 1.716243 |
| H | 3.430700 | -1.125942 | 2.669124 |
| C | 2.807136 | -2.185077 | -1.618375 |
| H | 1.946413 | -2.807549 | -1.877326 |
| H | 3.449544 | -2.115354 | -2.498193 |
| H | 3.370926 | -2.693334 | -0.832717 |
| H | -1.294148 | 1.025625 | -1.300358 |
| C | -0.155661 | 1.964747 | 0.032253 |
| C | -0.086497 | 3.089283 | -0.821767 |
| C | 0.660432 | 4.324400 | -0.490572 |
| H | 0.327444 | 5.153980 | -1.110686 |
| H | 1.730930 | 4.174253 | -0.683671 |
| H | -0.587904 | 3.023222 | -1.781503 |
| H | 0.560044 | 4.594270 | 0.562368 |
| C | 0.519369 | 1.995620 | 1.364690 |
| H | 1.517649 | 2.419365 | 1.250190 |
| H | -0.047920 | 2.652244 | 2.031144 |
| H | 0.613494 | 1.014863 | 1.815103 |

**2G-*E***

Imaginary frequency: None

Electronic energies: -447.156168

Free energies: -446.916853

Corrected Free energies: -446.915622

| | | | |
|---|---|---|---|
| N | -0.700982 | -0.982349 | -0.269520 |
| C | -1.888956 | -0.327382 | 0.129536 |
| C | -2.859724 | -0.053227 | -0.754014 |
| C | -4.226549 | 0.505966 | -0.480916 |
| H | -5.006891 | -0.178356 | -0.828103 |
| H | -4.375803 | 1.448466 | -1.016441 |
| H | -2.652440 | -0.284031 | -1.798048 |
| H | -0.683429 | -1.097938 | -1.278905 |
| C | 0.579497 | -0.423706 | 0.182038 |
| C | 1.714497 | -1.331710 | -0.287781 |
| C | 0.812004 | 1.014361 | -0.296342 |
| H | 0.578174 | -0.431961 | 1.278312 |
| C | 3.077043 | -0.805396 | 0.169311 |
| H | 1.693142 | -1.378745 | -1.384912 |
| H | 1.541105 | -2.344948 | 0.083701 |
| C | 2.169546 | 1.546248 | 0.168468 |
| H | 0.770903 | 1.019072 | -1.393841 |
| H | 0.001317 | 1.660699 | 0.054552 |

| | | | |
|---|---|---|---|
| C | 3.303969 | 0.633218 | -0.301383 |
| H | 3.871749 | -1.458237 | -0.200386 |
| H | 3.124018 | -0.836109 | 1.264475 |
| H | 2.321311 | 2.564378 | -0.198987 |
| H | 2.179300 | 1.597891 | 1.264087 |
| H | 4.266103 | 1.003324 | 0.062428 |
| H | 3.346922 | 0.650449 | -1.397123 |
| H | -4.403973 | 0.700146 | 0.576143 |
| C | -1.969646 | -0.056258 | 1.608020 |
| H | -1.652118 | -0.941779 | 2.164279 |
| H | -1.305509 | 0.764631 | 1.894006 |
| H | -2.977091 | 0.206813 | 1.919775 |

**2G-*Z***

Imaginary frequency: None

Electronic energies: -447.158641

Free energies: -446.918831

Corrected Free energies: -446.917583

| | | | |
|---|---|---|---|
| N | 0.920152 | -0.353138 | -0.663245 |
| C | 1.996529 | 0.456667 | -0.271917 |
| C | 3.109569 | -0.048140 | 0.282808 |
| H | 1.029499 | -1.309786 | -0.344273 |
| C | -0.450993 | 0.110183 | -0.435505 |
| C | -1.427560 | -0.854912 | -1.105488 |
| C | -0.787394 | 0.266563 | 1.052569 |
| H | -0.558229 | 1.085840 | -0.923229 |
| C | -2.877292 | -0.407522 | -0.905344 |
| H | -1.290835 | -1.852348 | -0.666283 |
| H | -1.184326 | -0.932668 | -2.168227 |
| C | -2.233494 | 0.723794 | 1.254105 |
| H | -0.638101 | -0.707118 | 1.538024 |
| H | -0.087905 | 0.967462 | 1.518880 |
| C | -3.208799 | -0.243729 | 0.579956 |
| H | -3.557230 | -1.125424 | -1.370792 |
| H | -3.029384 | 0.552017 | -1.413885 |
| H | -2.456481 | 0.811076 | 2.320488 |
| H | -2.359277 | 1.723116 | 0.819593 |
| H | -4.237188 | 0.106094 | 0.701604 |
| H | -3.141068 | -1.221170 | 1.072933 |
| C | 1.864711 | 1.919283 | -0.600303 |
| H | 1.583673 | 2.053339 | -1.648593 |
| H | 1.095561 | 2.403745 | 0.007878 |
| H | 2.809886 | 2.429766 | -0.420587 |

| | | | |
|---|---|---|---|
| H | 3.939550 | 0.626711 | 0.455516 |
| C | 3.286928 | -1.500395 | 0.640266 |
| H | 3.359864 | -2.142091 | -0.245748 |
| H | 4.196699 | -1.649967 | 1.221795 |
| H | 2.450989 | -1.877385 | 1.240740 |

**2G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -446.974453

Free energies: -446.735686

Corrected Free energies: -446.734254

| | | | |
|---|---|---|---|
| N | 0.934091 | -0.257684 | 0.009578 |
| C | 1.996637 | 0.483479 | -0.225418 |
| C | 3.278668 | -0.039817 | 0.064206 |
| H | 1.081078 | -1.178330 | 0.417885 |
| C | -0.469699 | 0.110755 | -0.205076 |
| C | -1.211378 | -1.073126 | -0.828127 |
| C | -1.103830 | 0.538013 | 1.124977 |
| H | -0.485173 | 0.950671 | -0.901913 |
| C | -2.688833 | -0.725889 | -1.025386 |
| H | -1.126836 | -1.937155 | -0.158213 |
| H | -0.742056 | -1.340211 | -1.777482 |
| C | -2.581410 | 0.877721 | 0.914676 |
| H | -1.009985 | -0.288054 | 1.839046 |
| H | -0.560896 | 1.393000 | 1.535425 |
| C | -3.336445 | -0.298007 | 0.292522 |
| H | -3.207931 | -1.588442 | -1.447926 |
| H | -2.773648 | 0.087756 | -1.754462 |
| H | -3.026068 | 1.157703 | 1.871846 |
| H | -2.660224 | 1.750588 | 0.256734 |
| H | -4.381969 | -0.028804 | 0.127467 |
| H | -3.327041 | -1.143372 | 0.990063 |
| C | 1.840652 | 1.854618 | -0.801735 |
| H | 1.433294 | 1.791575 | -1.813567 |
| H | 1.157742 | 2.452575 | -0.196043 |
| H | 2.805357 | 2.352999 | -0.844162 |
| C | 3.516337 | -1.392071 | 0.625213 |
| H | 3.036559 | -1.501780 | 1.604646 |
| H | 3.104779 | -2.168956 | -0.028876 |
| H | 4.580004 | -1.577766 | 0.746633 |
| H | 4.120193 | 0.605728 | -0.149264 |

**2G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -446.974373

Free energies: -446.734792

Corrected Free energies: -446.733609

| | | | |
|---|---|---|---|
| N | -0.751870 | -0.502682 | -0.337230 |
| C | -1.913593 | -0.013118 | 0.055932 |
| C | -3.082550 | -0.526272 | -0.542991 |
| C | -4.454611 | -0.099840 | -0.180721 |
| H | -5.193099 | -0.759728 | -0.629230 |
| H | -4.642871 | 0.918560 | -0.542472 |
| H | -2.953292 | -1.273505 | -1.318770 |
| H | -0.766883 | -1.204001 | -1.075191 |
| C | 0.579770 | -0.122141 | 0.145597 |
| C | 1.469843 | -1.364873 | 0.193335 |
| C | 1.177378 | 0.962197 | -0.761400 |
| H | 0.461344 | 0.269950 | 1.157990 |
| C | 2.875839 | -0.987174 | 0.665697 |
| H | 1.527569 | -1.798742 | -0.812299 |
| H | 1.023972 | -2.111146 | 0.854651 |
| C | 2.584318 | 1.329118 | -0.283389 |
| H | 1.220205 | 0.573682 | -1.784888 |
| H | 0.526577 | 1.840210 | -0.770130 |
| C | 3.486894 | 0.095381 | -0.225484 |
| H | 3.505125 | -1.879344 | 0.673975 |
| H | 2.823173 | -0.622795 | 1.697786 |
| H | 3.005809 | 2.083143 | -0.951253 |
| H | 2.519688 | 1.781607 | 0.712685 |
| H | 4.477378 | 0.371236 | 0.142761 |
| H | 3.618242 | -0.303206 | -1.238014 |
| H | -4.598037 | -0.085015 | 0.902761 |
| C | -1.955865 | 1.033137 | 1.123065 |
| H | -1.776216 | 0.570669 | 2.097663 |
| H | -1.191655 | 1.792014 | 0.958118 |
| H | -2.928484 | 1.516704 | 1.146621 |

**3G-*E***

Imaginary frequency: None

Electronic energies: -330.436379

Free energies: -330.260445

Corrected Free energies: -330.259717

| | | | |
|---|---|---|---|
| C | -1.580338 | -0.090638 | 0.288821 |
| H | -1.272567 | 0.108986 | 1.323589 |

| | | | |
|---|---|---|---|
| N | -0.391898 | -0.385234 | -0.536207 |
| C | 0.874784 | 0.085757 | -0.126225 |
| C | 1.941568 | -0.728216 | -0.132336 |
| C | 3.380040 | -0.373182 | 0.113387 |
| H | 3.998585 | -0.642998 | -0.748266 |
| H | 3.779716 | -0.923886 | 0.970485 |
| H | 1.759133 | -1.772761 | -0.381144 |
| H | -0.341750 | -1.375818 | -0.742967 |
| C | -2.482314 | -1.321055 | 0.292683 |
| H | -3.395521 | -1.126404 | 0.857059 |
| H | -2.762974 | -1.579032 | -0.733066 |
| H | -1.975276 | -2.178836 | 0.740469 |
| C | -2.340725 | 1.119747 | -0.249872 |
| H | -2.677902 | 0.912854 | -1.269045 |
| H | -3.215269 | 1.330791 | 0.370923 |
| H | -1.716140 | 2.012984 | -0.273758 |
| H | 3.531817 | 0.688485 | 0.304084 |
| C | 0.919475 | 1.549428 | 0.217203 |
| H | 0.610686 | 2.147102 | -0.644780 |
| H | 0.232172 | 1.779364 | 1.035410 |
| H | 1.913642 | 1.864756 | 0.522495 |

**3G-*Z***

Imaginary frequency: -4.9367

Electronic energies: -330.438824

Free energies: -330.262030

Corrected Free energies: -330.261577

| | | | |
|---|---|---|---|
| C | 1.431672 | -0.172306 | -0.281827 |
| H | 1.324498 | 0.213941 | -1.303011 |
| N | 0.106495 | -0.267306 | 0.354668 |
| C | -0.946365 | 0.574231 | -0.024055 |
| C | -2.217320 | 0.142412 | -0.076246 |
| H | -0.193441 | -1.228891 | 0.445304 |
| C | 2.023787 | -1.575375 | -0.367649 |
| H | 3.022037 | -1.543055 | -0.806522 |
| H | 2.105036 | -2.007768 | 0.634136 |
| H | 1.397820 | -2.229025 | -0.979461 |
| C | 2.362653 | 0.748350 | 0.505321 |
| H | 2.496940 | 0.352518 | 1.515440 |
| H | 3.340146 | 0.807203 | 0.020035 |
| H | 1.961672 | 1.758757 | 0.585262 |
| C | -0.594875 | 2.014982 | -0.275677 |
| H | -0.203419 | 2.479663 | 0.633340 |

| | | | |
|---|---|---|---|
| H | 0.169138 | 2.119213 | -1.050446 |
| H | -1.480115 | 2.564244 | -0.593512 |
| C | -2.634387 | -1.281464 | 0.179891 |
| H | -2.035849 | -1.992733 | -0.400771 |
| H | -2.532505 | -1.563687 | 1.234568 |
| H | -3.677463 | -1.437364 | -0.095806 |
| H | -2.990943 | 0.873148 | -0.279780 |

**3G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -330.257665

Free energies: -330.082063

Corrected Free energies: -330.081301

| | | | |
|---|---|---|---|
| C | 1.524030 | 0.052920 | -0.150369 |
| H | 1.588341 | 0.975575 | -0.726221 |
| N | 0.093654 | -0.283011 | -0.040109 |
| C | -0.923951 | 0.546787 | -0.128357 |
| C | -2.237840 | 0.043733 | 0.024266 |
| H | -0.107571 | -1.258812 | 0.166909 |
| C | 2.226836 | -1.067850 | -0.905548 |
| H | 3.279591 | -0.811617 | -1.024829 |
| H | 2.166967 | -2.007120 | -0.349647 |
| H | 1.787815 | -1.209935 | -1.893525 |
| C | 2.099804 | 0.269314 | 1.248356 |
| H | 2.011442 | -0.644295 | 1.839479 |
| H | 3.156175 | 0.527122 | 1.162579 |
| H | 1.584802 | 1.077800 | 1.769232 |
| C | -0.685160 | 1.997962 | -0.398403 |
| H | 0.021276 | 2.413809 | 0.321725 |
| H | -0.267215 | 2.128825 | -1.399396 |
| H | -1.620564 | 2.547622 | -0.336602 |
| H | -3.039765 | 0.766487 | -0.046344 |
| C | -2.556074 | -1.383277 | 0.272197 |
| H | -3.630701 | -1.543372 | 0.281143 |
| H | -2.117150 | -2.029221 | -0.495923 |
| H | -2.154892 | -1.709322 | 1.239339 |

**3G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -330.257576

Free energies: -330.083050

Corrected Free energies: -330.082289

| | | | |
|---|---|---|---|
| C | -1.660160 | 0.108705 | 0.191583 |
| H | -1.486113 | 0.814070 | 1.003668 |
| N | -0.358523 | -0.492056 | -0.142957 |
| C | 0.838630 | 0.024834 | 0.061596 |
| C | 1.958821 | -0.729609 | -0.346574 |
| C | 3.363285 | -0.297360 | -0.156933 |
| H | 3.584155 | 0.575760 | -0.782393 |
| H | 4.050724 | -1.094120 | -0.428881 |
| H | 1.762992 | -1.681031 | -0.829729 |
| H | -0.401171 | -1.395543 | -0.609795 |
| C | -2.592340 | -0.996385 | 0.671716 |
| H | -3.551327 | -0.558129 | 0.948341 |
| H | -2.768442 | -1.726413 | -0.122489 |
| H | -2.178215 | -1.508230 | 1.540833 |
| C | -2.208049 | 0.843097 | -1.031793 |
| H | -2.369828 | 0.141527 | -1.852825 |
| H | -3.163122 | 1.301951 | -0.773038 |
| H | -1.524800 | 1.624594 | -1.366825 |
| H | 3.551417 | -0.001808 | 0.879256 |
| C | 0.968225 | 1.358147 | 0.725428 |
| H | 0.280765 | 2.080296 | 0.284912 |
| H | 0.730813 | 1.264252 | 1.788493 |
| H | 1.981341 | 1.738636 | 0.631033 |

**4G-*E***

Imaginary frequency: None

Electronic energies: -482.841038

Free energies: -482.643471

Corrected Free energies: -482.641749

| | | | |
|---|---|---|---|
| C | -3.494625 | 1.562645 | 0.514202 |
| C | -2.643611 | 0.699345 | -0.371786 |
| C | -1.924001 | -0.377958 | -0.027563 |
| H | -2.635568 | 0.978643 | -1.424873 |
| H | -3.161510 | 2.604219 | 0.477519 |
| H | -4.538393 | 1.555263 | 0.184875 |
| N | -1.275988 | -1.161463 | -1.007717 |
| H | -3.475675 | 1.249704 | 1.557461 |
| C | -1.775238 | -0.911429 | 1.370544 |
| H | -2.436595 | -0.407881 | 2.070259 |
| H | -2.000642 | -1.981093 | 1.387858 |
| H | -0.747515 | -0.786362 | 1.725434 |
| C | 0.061153 | -1.669100 | -0.723057 |
| H | 0.393224 | -2.205878 | -1.615713 |

| | | | |
|---|---|---|---|
| H | -1.333349 | -0.737477 | -1.925439 |
| H | 0.002528 | -2.413834 | 0.074883 |
| C | 1.104371 | -0.629748 | -0.348581 |
| C | 2.152169 | -0.969644 | 0.508411 |
| C | 1.051583 | 0.666128 | -0.862719 |
| C | 3.136239 | -0.041845 | 0.833921 |
| H | 2.196085 | -1.971518 | 0.924832 |
| C | 2.032048 | 1.598187 | -0.536206 |
| H | 0.234899 | 0.952922 | -1.515785 |
| C | 3.078673 | 1.246974 | 0.311093 |
| H | 3.944279 | -0.322745 | 1.499328 |
| H | 1.976573 | 2.601504 | -0.942475 |
| H | 3.841019 | 1.973438 | 0.566305 |

**4G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -482.655815

Free energies: -482.457742

Corrected Free energies: -482.456199

| | | | |
|---|---|---|---|
| C | -3.961373 | 1.237478 | 0.257538 |
| C | -3.122785 | 0.241622 | -0.446847 |
| C | -1.905314 | -0.258370 | 0.060814 |
| H | -3.459937 | -0.147565 | -1.401898 |
| H | -4.692911 | 1.671388 | -0.420053 |
| H | -4.508134 | 0.752097 | 1.076559 |
| N | -1.242391 | -1.130492 | -0.678849 |
| H | -3.359516 | 2.033298 | 0.701381 |
| C | -1.353671 | 0.181526 | 1.375957 |
| H | -2.153895 | 0.527524 | 2.026020 |
| H | -0.815688 | -0.624853 | 1.872388 |
| H | -0.651149 | 1.005498 | 1.215498 |
| C | 0.051655 | -1.735016 | -0.347895 |
| H | 0.271408 | -2.437522 | -1.151077 |
| H | -1.659423 | -1.400411 | -1.564338 |
| H | -0.055502 | -2.309672 | 0.574738 |
| C | 1.155583 | -0.707326 | -0.213103 |
| C | 2.038465 | -0.776205 | 0.861230 |
| C | 1.309581 | 0.297115 | -1.168681 |
| C | 3.070412 | 0.149832 | 0.980513 |
| H | 1.916381 | -1.550706 | 1.611214 |
| C | 2.335924 | 1.226090 | -1.045104 |
| H | 0.625923 | 0.356545 | -2.009095 |
| C | 3.218491 | 1.153696 | 0.029571 |

| | | | |
|---|---|---|---|
| H | 3.751555 | 0.090985 | 1.820674 |
| H | 2.448941 | 2.004735 | -1.789749 |
| H | 4.016873 | 1.879452 | 0.125722 |

**4G-*Z***

Imaginary frequency: None

Electronic energies: -482.841385

Free energies: -482.645120

Corrected Free energies: -482.642860

| | | | |
|---|---|---|---|
| C | -3.479894 | 0.581234 | -0.147363 |
| C | -2.529597 | -0.321043 | 0.140992 |
| N | -1.168781 | 0.015261 | 0.130959 |
| C | -0.175750 | -0.988414 | -0.244379 |
| H | -0.282499 | -1.846912 | 0.424331 |
| H | -0.318055 | -1.357821 | -1.268957 |
| C | 1.222006 | -0.430421 | -0.105113 |
| C | 2.169007 | -0.626689 | -1.108432 |
| C | 1.589330 | 0.275852 | 1.042777 |
| C | 3.464589 | -0.134744 | -0.967726 |
| H | 1.890660 | -1.166382 | -2.007625 |
| C | 2.880461 | 0.770435 | 1.184372 |
| H | 0.850380 | 0.438793 | 1.819225 |
| C | 3.823062 | 0.565425 | 0.178949 |
| H | 4.190367 | -0.293004 | -1.756834 |
| H | 3.153270 | 1.316911 | 2.079703 |
| H | 4.828888 | 0.953151 | 0.288746 |
| H | -0.989502 | 0.897685 | -0.333611 |
| C | -2.858870 | -1.723169 | 0.571365 |
| H | -3.937084 | -1.838462 | 0.671676 |
| H | -2.500363 | -2.460177 | -0.152433 |
| H | -2.390450 | -1.953237 | 1.532694 |
| C | -3.184592 | 1.996849 | -0.567386 |
| H | -2.683533 | 2.565033 | 0.225069 |
| H | -2.533498 | 2.036305 | -1.448691 |
| H | -4.101109 | 2.529568 | -0.819742 |
| H | -4.514514 | 0.279840 | -0.038596 |

**4G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -482.654757

Free energies: -482.460451

Corrected Free energies: -482.457745

| | | | |
|---|---|---|---|
| C | -3.344553 | 0.789373 | -0.032331 |
| C | -2.465574 | -0.315125 | 0.055960 |
| N | -1.191983 | -0.148287 | -0.233130 |
| C | -0.155614 | -1.189474 | -0.191528 |
| H | -0.368187 | -1.843818 | 0.654933 |
| H | -0.225986 | -1.780331 | -1.108501 |
| C | 1.204546 | -0.554748 | -0.059475 |
| C | 2.096199 | -0.566198 | -1.128659 |
| C | 1.567711 | 0.064539 | 1.138058 |
| C | 3.345496 | 0.035146 | -1.003324 |
| H | 1.814449 | -1.046999 | -2.058953 |
| C | 2.812927 | 0.668238 | 1.261091 |
| H | 0.876000 | 0.068482 | 1.974279 |
| C | 3.703433 | 0.652373 | 0.190081 |
| H | 4.036129 | 0.020241 | -1.837505 |
| H | 3.091710 | 1.145633 | 2.192577 |
| H | 4.676069 | 1.119353 | 0.288691 |
| H | -0.878486 | 0.769144 | -0.540138 |
| C | -2.952396 | -1.663093 | 0.475395 |
| H | -4.036750 | -1.667819 | 0.545093 |
| H | -2.633147 | -2.425709 | -0.237145 |
| H | -2.538088 | -1.919464 | 1.454299 |
| C | -2.923384 | 2.155700 | -0.424786 |
| H | -2.157527 | 2.542565 | 0.256829 |
| H | -2.495049 | 2.160890 | -1.433644 |
| H | -3.768506 | 2.838404 | -0.411377 |
| H | -4.381494 | 0.597049 | 0.209581 |

**5G-*E***

Imaginary frequency: None

Electronic energies: -443.541095

Free energies: -443.370966

Corrected Free energies: -443.369932

| | | | |
|---|---|---|---|
| N | -0.522865 | -0.966259 | 0.242650 |
| C | -1.698465 | -0.181033 | 0.211510 |
| C | -2.721715 | -0.518857 | -0.579811 |
| C | -4.073081 | 0.131823 | -0.572051 |
| H | -4.842754 | -0.561184 | -0.217495 |
| H | -4.362736 | 0.436341 | -1.581292 |
| H | -2.584163 | -1.353914 | -1.262782 |
| H | -0.636574 | -1.911851 | -0.095206 |
| C | 0.757867 | -0.437681 | 0.056014 |
| C | 1.868623 | -1.277162 | 0.227969 |

| | | | |
|---|---|---|---|
| C | 0.974244 | 0.900456 | -0.294581 |
| C | 3.155178 | -0.787244 | 0.062419 |
| H | 1.706564 | -2.315282 | 0.497783 |
| C | 2.270897 | 1.386066 | -0.436016 |
| H | 0.130822 | 1.554776 | -0.477075 |
| C | 3.369072 | 0.552436 | -0.260248 |
| H | 3.998007 | -1.455493 | 0.196334 |
| H | 2.417672 | 2.426223 | -0.703644 |
| H | 4.374856 | 0.935716 | -0.378434 |
| H | -4.099365 | 1.015746 | 0.065772 |
| C | -1.755462 | 0.947285 | 1.218860 |
| H | -0.815986 | 1.026019 | 1.764144 |
| H | -1.958761 | 1.909522 | 0.744361 |
| H | -2.550474 | 0.760653 | 1.944593 |

**5G-*Z***

Imaginary frequency: None

Electronic energies: -443.541851

Free energies: -443.372777

Corrected Free energies: -443.371200

| | | | |
|---|---|---|---|
| N | 0.770822 | -0.545330 | -0.246735 |
| C | 1.790524 | 0.427459 | -0.291090 |
| C | 3.027028 | 0.127814 | 0.127890 |
| H | 1.031456 | -1.483427 | -0.510060 |
| C | -0.588216 | -0.309377 | -0.076076 |
| C | -1.524208 | -1.177501 | -0.657517 |
| C | -1.055521 | 0.753923 | 0.708391 |
| C | -2.884430 | -0.974803 | -0.471224 |
| H | -1.172321 | -2.007526 | -1.260830 |
| C | -2.420664 | 0.960625 | 0.867977 |
| H | -0.346230 | 1.394481 | 1.217659 |
| C | -3.346331 | 0.102844 | 0.281163 |
| H | -3.589633 | -1.660119 | -0.927531 |
| H | -2.760099 | 1.791443 | 1.475999 |
| H | -4.408417 | 0.264995 | 0.415761 |
| C | 1.462107 | 1.744707 | -0.948221 |
| H | 0.965477 | 1.571006 | -1.906608 |
| H | 0.800526 | 2.370268 | -0.348148 |
| H | 2.381253 | 2.303007 | -1.123138 |
| C | 3.423095 | -1.166684 | 0.775455 |
| H | 3.820429 | -1.883120 | 0.047790 |
| H | 4.204737 | -1.003497 | 1.519903 |
| H | 2.571155 | -1.637041 | 1.271127 |

| | | | |
|---|---|---|---|
| H | 3.805618 | 0.862799 | -0.045272 |

**5G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -443.349221

Free energies: -443.178275

Corrected Free energies: -443.177516

| | | | |
|---|---|---|---|
| N | -0.798262 | -0.403931 | -0.096327 |
| C | -1.740621 | 0.485038 | 0.194498 |
| C | -3.088146 | 0.097721 | 0.050507 |
| H | -1.112940 | -1.344438 | -0.322458 |
| C | 0.614172 | -0.244301 | -0.075024 |
| C | 1.374609 | -1.299896 | 0.427501 |
| C | 1.220817 | 0.899967 | -0.589795 |
| C | 2.757155 | -1.190069 | 0.444806 |
| H | 0.883912 | -2.186180 | 0.812118 |
| C | 2.605878 | 0.994868 | -0.566806 |
| H | 0.626851 | 1.687382 | -1.033359 |
| C | 3.373836 | -0.042200 | -0.046396 |
| H | 3.352348 | -2.002106 | 0.842322 |
| H | 3.083419 | 1.878504 | -0.970281 |
| H | 4.453438 | 0.039253 | -0.033080 |
| C | -1.401235 | 1.852001 | 0.693268 |
| H | -0.468524 | 1.849780 | 1.256284 |
| H | -1.301457 | 2.549376 | -0.141563 |
| H | -2.211432 | 2.206203 | 1.327884 |
| C | -3.537337 | -1.215438 | -0.471609 |
| H | -3.027667 | -1.482155 | -1.401821 |
| H | -3.328931 | -2.007779 | 0.258978 |
| H | -4.608851 | -1.208991 | -0.653297 |
| H | -3.827111 | 0.822523 | 0.366870 |

**5G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -443.350087

Free energies: -443.179659

Corrected Free energies: -443.178702

| | | | |
|---|---|---|---|
| N | -0.587739 | -0.726535 | -0.323265 |
| C | -1.682415 | -0.049127 | 0.018002 |
| C | -2.919980 | -0.621958 | -0.320250 |
| C | -4.227339 | -0.007892 | -0.000158 |
| H | -4.998085 | -0.379940 | -0.672494 |

| | | | |
|---|---|---|---|
| H | -4.196286 | 1.081300 | -0.044637 |
| H | -2.907677 | -1.582025 | -0.826166 |
| H | -0.735043 | -1.648954 | -0.726951 |
| C | 0.773412 | -0.344804 | -0.176897 |
| C | 1.678296 | -1.313098 | 0.256482 |
| C | 1.196310 | 0.941000 | -0.509950 |
| C | 3.017012 | -0.974575 | 0.390759 |
| H | 1.329448 | -2.309694 | 0.499731 |
| C | 2.539211 | 1.264581 | -0.371613 |
| H | 0.493935 | 1.665915 | -0.900567 |
| C | 3.447856 | 0.313212 | 0.082727 |
| H | 3.723209 | -1.717819 | 0.738338 |
| H | 2.875648 | 2.259614 | -0.633211 |
| H | 4.494020 | 0.572011 | 0.187177 |
| H | -4.521444 | -0.286921 | 1.021000 |
| C | -1.599659 | 1.244254 | 0.760849 |
| H | -0.654086 | 1.340885 | 1.289934 |
| H | -1.706969 | 2.087526 | 0.073750 |
| H | -2.418723 | 1.294280 | 1.477246 |

**6G-*E***

Imaginary frequency: None

Electronic energies: -1622.956563

Free energies: -1622.547573

Corrected Free energies: -1622.540207

| | | | |
|---|---|---|---|
| S | -2.349433 | 0.711534 | -0.123183 |
| F | -3.893650 | -1.383972 | -0.412658 |
| F | -4.529776 | -0.034453 | 1.147117 |
| F | -4.841597 | 0.488478 | -0.923390 |
| O | -1.932527 | 0.517981 | -1.511759 |
| O | -1.587651 | -0.085474 | 0.852406 |
| O | -2.611153 | 2.090234 | 0.276762 |
| C | -4.004263 | -0.099326 | -0.073265 |
| N | 1.643633 | 0.676051 | 0.463397 |
| H | 1.899140 | 0.701639 | 1.445088 |
| N | 0.512082 | -1.770848 | 0.202104 |
| H | 0.169766 | -0.812955 | 0.417311 |
| C | 2.443099 | -0.285843 | -0.287474 |
| H | 2.176969 | -0.186667 | -1.343877 |
| C | 2.003647 | -1.683977 | 0.181462 |
| H | 2.382023 | -2.471004 | -0.466777 |
| H | 2.361795 | -1.874898 | 1.192789 |
| C | -0.075952 | -2.113761 | -1.138537 |

| | | | |
|---|---|---|---|
| H | -1.130314 | -1.848905 | -1.071366 |
| H | 0.383996 | -1.438618 | -1.861389 |
| C | 0.109931 | -3.566778 | -1.535048 |
| H | -0.431467 | -4.240484 | -0.870681 |
| H | 1.159002 | -3.864616 | -1.561829 |
| H | -0.294876 | -3.695519 | -2.539145 |
| C | -0.024807 | -2.646191 | 1.296070 |
| H | -1.084981 | -2.778036 | 1.077612 |
| H | 0.477736 | -3.611244 | 1.222883 |
| C | 0.152690 | -2.008988 | 2.663270 |
| H | -0.332227 | -2.643712 | 3.405467 |
| H | -0.322803 | -1.027838 | 2.685710 |
| H | 1.200270 | -1.911868 | 2.950217 |
| C | 3.984524 | -0.092030 | -0.188918 |
| C | 4.702266 | -1.293546 | -0.817923 |
| H | 4.610436 | -2.194400 | -0.206157 |
| H | 5.767498 | -1.073038 | -0.918920 |
| H | 4.307920 | -1.509736 | -1.815846 |
| C | 4.437912 | 0.074534 | 1.266355 |
| H | 4.055225 | 1.001905 | 1.701039 |
| H | 5.528844 | 0.125467 | 1.301990 |
| H | 4.130623 | -0.761028 | 1.901561 |
| C | 4.367885 | 1.170554 | -0.970489 |
| H | 4.129431 | 1.059590 | -2.032285 |
| H | 5.443071 | 1.347168 | -0.884600 |
| H | 3.848554 | 2.051489 | -0.585261 |
| C | 1.311355 | 1.961222 | -0.027320 |
| C | 1.232525 | 2.996428 | 0.820590 |
| C | 0.767562 | 4.392143 | 0.523370 |
| H | 0.540724 | 4.549344 | -0.530145 |
| H | 1.531110 | 5.122274 | 0.807299 |
| H | 1.508190 | 2.807338 | 1.857155 |
| H | -0.131398 | 4.636592 | 1.097896 |
| C | 0.985604 | 2.016273 | -1.493473 |
| H | 0.457526 | 2.933019 | -1.743054 |
| H | 1.892338 | 1.971088 | -2.102898 |
| H | 0.338797 | 1.179990 | -1.768298 |

**6G-*Z***

Imaginary frequency: None

Electronic energies: -1622.959669

Free energies: -1622.549616

Corrected Free energies: -1622.543044

| | | | |
|---|---|---|---|
| S | -2.518749 | 0.894825 | -0.512457 |
| F | -3.592468 | -1.408832 | 0.119537 |
| F | -4.207491 | 0.226813 | 1.387718 |
| F | -5.007972 | 0.050080 | -0.609129 |
| O | -2.345852 | 0.390592 | -1.874043 |
| O | -1.434312 | 0.528613 | 0.412674 |
| O | -2.981370 | 2.273141 | -0.396537 |
| C | -3.919336 | -0.113393 | 0.135384 |
| N | 1.826374 | 0.799240 | 0.347887 |
| H | 2.189314 | 0.978407 | 1.275734 |
| N | 0.371130 | -1.548443 | 0.323177 |
| H | 0.112021 | -0.543309 | 0.349217 |
| C | 2.443759 | -0.351660 | -0.297437 |
| H | 2.128297 | -0.351597 | -1.344057 |
| C | 1.864474 | -1.606250 | 0.370812 |
| H | 2.185009 | -2.524232 | -0.117201 |
| H | 2.162670 | -1.650271 | 1.417874 |
| C | -0.194991 | -2.080229 | -0.964767 |
| H | -1.208992 | -1.686919 | -1.028405 |
| H | 0.385173 | -1.628334 | -1.770601 |
| C | -0.180050 | -3.595150 | -1.060786 |
| H | -0.849970 | -4.054256 | -0.333781 |
| H | 0.819431 | -4.013656 | -0.933637 |
| H | -0.529427 | -3.872500 | -2.055456 |
| C | -0.296108 | -2.149997 | 1.526554 |
| H | -1.350833 | -2.248320 | 1.267019 |
| H | 0.127306 | -3.144081 | 1.674677 |
| C | -0.138488 | -1.265999 | 2.751119 |
| H | -0.690300 | -1.717623 | 3.576045 |
| H | -0.553851 | -0.276297 | 2.556293 |
| H | 0.900558 | -1.165249 | 3.066498 |
| C | 3.997946 | -0.335075 | -0.307907 |
| C | 4.520720 | -1.583601 | -1.030727 |
| H | 4.367317 | -2.493768 | -0.446267 |
| H | 5.595012 | -1.485314 | -1.204339 |
| H | 4.033652 | -1.709751 | -2.002672 |
| C | 4.580460 | -0.287379 | 1.109256 |
| H | 4.271956 | 0.612177 | 1.649028 |
| H | 5.671335 | -0.266286 | 1.049329 |
| H | 4.304488 | -1.162167 | 1.703253 |
| C | 4.453061 | 0.909657 | -1.078999 |
| H | 4.098714 | 0.878668 | -2.113642 |
| H | 5.544509 | 0.955702 | -1.099783 |
| H | 4.081691 | 1.827070 | -0.615341 |

| | | | |
|---|---|---|---|
| C | 1.430406 | 1.959749 | -0.336417 |
| C | 1.422228 | 3.153589 | 0.273505 |
| C | 1.911229 | 3.377137 | 1.679295 |
| H | 2.927323 | 2.990782 | 1.825766 |
| H | 1.270314 | 2.888681 | 2.423091 |
| H | 1.010712 | 3.994741 | -0.270176 |
| H | 1.933470 | 4.439554 | 1.920669 |
| C | 0.930780 | 1.771342 | -1.740469 |
| H | 0.462157 | 2.691709 | -2.087150 |
| H | 1.740230 | 1.524254 | -2.432919 |
| H | 0.185284 | 0.971629 | -1.787584 |

**6G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1622.768490

Free energies: -1622.355389

Corrected Free energies: -1622.350057

| | | | |
|---|---|---|---|
| S | 2.026085 | -0.733139 | -0.247300 |
| F | 3.360570 | 1.511536 | -0.334954 |
| F | 4.445817 | -0.126982 | 0.560939 |
| F | 4.177102 | -0.054875 | -1.579221 |
| O | 1.196568 | -0.223529 | -1.344602 |
| O | 1.510950 | -0.302387 | 1.069435 |
| O | 2.409937 | -2.135753 | -0.331450 |
| C | 3.606215 | 0.204794 | -0.410525 |
| N | -1.480873 | -1.059263 | 0.404889 |
| H | -1.500955 | -1.010561 | 1.420779 |
| N | -0.407026 | 1.777622 | 0.392897 |
| H | 0.205391 | 0.949178 | 0.500408 |
| C | -2.146280 | 0.054999 | -0.284370 |
| H | -1.723434 | 0.112149 | -1.287616 |
| C | -1.831023 | 1.331326 | 0.499424 |
| H | -2.451098 | 2.154847 | 0.155622 |
| H | -2.045285 | 1.180056 | 1.556526 |
| C | -0.083622 | 2.396440 | -0.949097 |
| H | 1.002906 | 2.468373 | -0.979854 |
| H | -0.376551 | 1.675437 | -1.708801 |
| C | -0.734383 | 3.748290 | -1.172422 |
| H | -0.390719 | 4.496603 | -0.458724 |
| H | -1.823812 | 3.703379 | -1.148762 |
| H | -0.446873 | 4.085111 | -2.168683 |
| C | -0.030192 | 2.699946 | 1.528865 |
| H | 0.913809 | 3.159641 | 1.234367 |

| | | | |
|---|---|---|---|
| H | -0.795370 | 3.474832 | 1.578375 |
| C | 0.124084 | 1.969870 | 2.851397 |
| H | 0.470866 | 2.690965 | 3.591975 |
| H | 0.862884 | 1.173128 | 2.770634 |
| H | -0.815632 | 1.555337 | 3.217634 |
| C | -3.685581 | -0.173694 | -0.420230 |
| C | -4.270908 | 0.950151 | -1.287299 |
| H | -4.283133 | 1.914845 | -0.777214 |
| H | -5.306319 | 0.705812 | -1.532979 |
| H | -3.719860 | 1.056721 | -2.226021 |
| C | -4.369690 | -0.191396 | 0.951128 |
| H | -3.962379 | -0.972151 | 1.599963 |
| H | -5.432596 | -0.401533 | 0.815693 |
| H | -4.291096 | 0.768703 | 1.465976 |
| C | -3.937776 | -1.509123 | -1.128214 |
| H | -3.476965 | -1.529480 | -2.118690 |
| H | -5.013190 | -1.643039 | -1.258850 |
| H | -3.573837 | -2.359369 | -0.546624 |
| C | -0.876861 | -2.117717 | -0.107057 |
| C | -0.266978 | -3.034216 | 0.786892 |
| C | -0.808791 | -2.397983 | -1.572058 |
| H | 0.185576 | -2.780240 | -1.801568 |
| H | -1.541733 | -3.174270 | -1.809786 |
| H | -0.996669 | -1.525537 | -2.189620 |
| H | 0.220747 | -3.884351 | 0.329261 |
| C | -0.228884 | -2.863121 | 2.257387 |
| H | 0.346302 | -1.961951 | 2.505016 |
| H | -1.233880 | -2.748542 | 2.678964 |
| H | 0.243818 | -3.717531 | 2.734055 |

**6G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1622.768871

Free energies: -1622.355229

Corrected Free energies: -1622.350104

| | | | |
|---|---|---|---|
| S | -2.000403 | 0.580479 | -0.099655 |
| F | -3.350898 | -1.608039 | -0.571034 |
| F | -4.492071 | -0.053963 | 0.403452 |
| F | -4.022014 | 0.108024 | -1.696986 |
| O | -1.087847 | 0.216466 | -1.188833 |
| O | -1.595655 | -0.032171 | 1.181164 |
| O | -2.373740 | 1.986740 | -0.021386 |
| C | -3.568732 | -0.295743 | -0.517616 |

| | | | |
|---|---|---|---|
| N | 1.509449 | 1.006377 | 0.611923 |
| H | 1.615505 | 0.877047 | 1.615578 |
| N | 0.482080 | -1.874467 | 0.452998 |
| H | -0.158290 | -1.075792 | 0.614243 |
| C | 2.105008 | -0.044264 | -0.225901 |
| H | 1.565176 | -0.036209 | -1.173984 |
| C | 1.891936 | -1.378938 | 0.497208 |
| H | 2.517721 | -2.153413 | 0.061258 |
| H | 2.175192 | -1.285140 | 1.545151 |
| C | 0.117217 | -2.464975 | -0.890701 |
| H | -0.970098 | -2.533411 | -0.893298 |
| H | 0.395972 | -1.730849 | -1.643364 |
| C | 0.753799 | -3.815785 | -1.160052 |
| H | 0.396901 | -4.585402 | -0.476453 |
| H | 1.843671 | -3.785451 | -1.125902 |
| H | 0.470294 | -4.112566 | -2.170118 |
| C | 0.187589 | -2.840868 | 1.574795 |
| H | -0.762126 | -3.309541 | 1.314606 |
| H | 0.968995 | -3.600806 | 1.556755 |
| C | 0.088261 | -2.156441 | 2.926267 |
| H | -0.236618 | -2.899469 | 3.654936 |
| H | -0.648633 | -1.353806 | 2.899987 |
| H | 1.043062 | -1.759577 | 3.272162 |
| C | 3.621447 | 0.209834 | -0.512541 |
| C | 4.098184 | -0.819766 | -1.546971 |
| H | 4.149766 | -1.833364 | -1.146031 |
| H | 5.106249 | -0.553580 | -1.871014 |
| H | 3.452915 | -0.824580 | -2.429925 |
| C | 4.452114 | 0.095853 | 0.770559 |
| H | 4.123296 | 0.812205 | 1.528763 |
| H | 5.496287 | 0.318864 | 0.541864 |
| H | 4.420592 | -0.908239 | 1.198691 |
| C | 3.812838 | 1.608409 | -1.108629 |
| H | 3.267807 | 1.722924 | -2.048227 |
| H | 4.873193 | 1.757191 | -1.320902 |
| H | 3.507919 | 2.397434 | -0.417295 |
| C | 0.893019 | 2.124142 | 0.249958 |
| C | 0.396249 | 2.943535 | 1.289970 |
| C | -0.293283 | 4.228484 | 1.052919 |
| H | 0.179281 | 4.803785 | 0.254228 |
| H | -0.327133 | 4.823506 | 1.962644 |
| H | 0.505207 | 2.581820 | 2.307315 |
| H | -1.323395 | 4.015579 | 0.736696 |
| C | 0.720028 | 2.543280 | -1.171426 |

| | | | |
|---|---|---|---|
| H | -0.298647 | 2.908168 | -1.304612 |
| H | 1.409554 | 3.367300 | -1.377458 |
| H | 0.894855 | 1.741309 | -1.879753 |

**7G-*E***

Imaginary frequency: None

Electronic energies: -581.093340

Free energies: -580.785004

Corrected Free energies: -580.782771

| | | | |
|---|---|---|---|
| N | 0.939406 | -0.238740 | -0.846460 |
| C | 2.200148 | -0.448361 | -0.240639 |
| C | 3.106917 | 0.540435 | -0.199907 |
| H | 0.845839 | 0.741532 | -1.101259 |
| C | -0.264882 | -0.610675 | -0.093131 |
| C | -1.352983 | 0.452560 | -0.335663 |
| C | -0.813977 | -1.983738 | -0.495389 |
| H | -0.050219 | -0.632988 | 0.986408 |
| C | -2.591442 | 0.123450 | 0.511018 |
| H | -1.639520 | 0.373036 | -1.394098 |
| C | -2.067812 | -2.335318 | 0.307010 |
| H | -1.045232 | -1.956595 | -1.566620 |
| H | -0.046680 | -2.747462 | -0.355263 |
| C | -3.142036 | -1.258364 | 0.147280 |
| H | -3.360203 | 0.885677 | 0.358681 |
| H | -2.323907 | 0.138994 | 1.573869 |
| H | -2.453907 | -3.308177 | -0.007355 |
| H | -1.802686 | -2.424901 | 1.367416 |
| H | -4.013368 | -1.492120 | 0.764305 |
| H | -3.483149 | -1.243357 | -0.894720 |
| N | -0.812064 | 1.809457 | -0.185842 |
| C | -1.726905 | 2.834486 | -0.664252 |
| H | -2.598017 | 2.981392 | -0.006781 |
| H | -1.197301 | 3.787298 | -0.733908 |
| H | -2.088335 | 2.568675 | -1.659836 |
| C | -0.327561 | 2.124902 | 1.150874 |
| H | 0.119550 | 3.121310 | 1.134541 |
| H | -1.122629 | 2.124872 | 1.912665 |
| H | 0.448700 | 1.418274 | 1.451040 |
| C | 2.434209 | -1.845999 | 0.262690 |
| H | 1.710505 | -2.103315 | 1.041347 |
| H | 2.303490 | -2.564648 | -0.550757 |
| H | 3.429352 | -1.969565 | 0.682297 |
| H | 2.786568 | 1.510996 | -0.577344 |

| | | | |
|---|---|---|---|
| C | 4.534839 | 0.471762 | 0.260552 |
| H | 4.827950 | -0.522427 | 0.595329 |
| H | 5.217444 | 0.762102 | -0.544162 |
| H | 4.713278 | 1.165540 | 1.087658 |

**7G-*Z***

Imaginary frequency: None

Electronic energies: -581.097068

Free energies: -580.786919

Corrected Free energies: -580.785437

| | | | |
|---|---|---|---|
| N | 1.028745 | -0.529262 | -0.694955 |
| C | 2.171527 | -0.998475 | -0.024204 |
| C | 3.289357 | -0.263001 | 0.089307 |
| H | 1.138980 | 0.445300 | -0.956208 |
| C | -0.282248 | -0.680084 | -0.052332 |
| C | -1.119761 | 0.582292 | -0.327455 |
| C | -1.046116 | -1.910306 | -0.550563 |
| H | -0.163429 | -0.775275 | 1.037615 |
| C | -2.467533 | 0.476267 | 0.403716 |
| H | -1.326563 | 0.593015 | -1.407286 |
| C | -2.404093 | -2.032792 | 0.142109 |
| H | -1.180592 | -1.814015 | -1.634338 |
| H | -0.450426 | -2.809338 | -0.380351 |
| C | -3.236261 | -0.765391 | -0.056574 |
| H | -3.061809 | 1.374363 | 0.215358 |
| H | -2.297588 | 0.419293 | 1.485014 |
| H | -2.942121 | -2.905571 | -0.236065 |
| H | -2.246515 | -2.196272 | 1.215064 |
| H | -4.184546 | -0.840700 | 0.481477 |
| H | -3.479938 | -0.659410 | -1.120335 |
| N | -0.340096 | 1.800394 | -0.073051 |
| C | -1.003213 | 3.004315 | -0.548662 |
| H | -1.868144 | 3.298701 | 0.065745 |
| H | -0.292023 | 3.833436 | -0.543048 |
| H | -1.346511 | 2.853361 | -1.574354 |
| C | 0.114340 | 1.956940 | 1.301599 |
| H | 0.725646 | 2.860069 | 1.365371 |
| H | -0.708743 | 2.055345 | 2.025506 |
| H | 0.741932 | 1.111437 | 1.593680 |
| C | 2.098981 | -2.409275 | 0.492763 |
| H | 1.304368 | -2.524725 | 1.235622 |
| H | 1.885058 | -3.105633 | -0.322798 |
| H | 3.041903 | -2.691428 | 0.959795 |

| | | | |
|---|---|---|---|
| C | 3.434557 | 1.157101 | -0.388476 |
| H | 3.706051 | 1.212861 | -1.449139 |
| H | 2.508132 | 1.726621 | -0.260587 |
| H | 4.217413 | 1.673830 | 0.169195 |
| H | 4.161688 | -0.738739 | 0.523749 |

**7G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -580.914234

Free energies: -580.606340

Corrected Free energies: -580.604528

| | | | |
|---|---|---|---|
| N | 1.131858 | -0.160174 | -0.111500 |
| C | 2.287687 | -0.711814 | 0.184963 |
| C | 3.472390 | -0.023335 | -0.170766 |
| H | 1.118278 | 0.805996 | -0.453054 |
| C | -0.220198 | -0.640792 | 0.184967 |
| C | -1.184198 | 0.473248 | -0.266762 |
| C | -0.582930 | -1.951367 | -0.521141 |
| H | -0.293469 | -0.784481 | 1.269649 |
| C | -2.611157 | 0.099108 | 0.146539 |
| H | -1.145146 | 0.482494 | -1.364051 |
| C | -2.023101 | -2.335906 | -0.165058 |
| H | -0.480527 | -1.806633 | -1.601581 |
| H | 0.094047 | -2.754403 | -0.230614 |
| C | -3.014537 | -1.223739 | -0.511415 |
| H | -3.299269 | 0.896751 | -0.143881 |
| H | -2.666531 | -0.001529 | 1.236144 |
| H | -2.287355 | -3.257641 | -0.686936 |
| H | -2.077541 | -2.549287 | 0.908400 |
| H | -4.020756 | -1.507821 | -0.196457 |
| H | -3.044227 | -1.089756 | -1.598431 |
| N | -0.679460 | 1.781156 | 0.154201 |
| C | -1.247322 | 2.878239 | -0.621140 |
| H | -2.317437 | 3.033537 | -0.420152 |
| H | -0.719714 | 3.800206 | -0.371002 |
| H | -1.115421 | 2.684118 | -1.686758 |
| C | -0.804399 | 2.038016 | 1.585643 |
| H | -0.271187 | 2.959088 | 1.825919 |
| H | -1.850015 | 2.153486 | 1.904326 |
| H | -0.352428 | 1.229301 | 2.162935 |
| C | 2.364634 | -2.030623 | 0.885064 |
| H | 1.527315 | -2.172853 | 1.567527 |
| H | 2.357396 | -2.840777 | 0.151804 |

| | | | |
|---|---|---|---|
| H | 3.296995 | -2.091478 | 1.443294 |
| C | 3.485068 | 1.276869 | -0.884895 |
| H | 2.908308 | 1.225941 | -1.814234 |
| H | 3.032276 | 2.062361 | -0.266993 |
| H | 4.501274 | 1.579344 | -1.123146 |
| H | 4.406724 | -0.490254 | 0.112379 |

**7G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -580.914379

Free energies: -580.605079

Corrected Free energies: -580.603640

| | | | |
|---|---|---|---|
| N | -1.000752 | -0.167105 | -0.261331 |
| C | -2.252165 | 0.139404 | 0.019778 |
| C | -3.262962 | -0.686714 | -0.514895 |
| C | -4.710696 | -0.463931 | -0.298630 |
| H | -5.016616 | -0.910832 | 0.656799 |
| H | -5.292146 | -0.944586 | -1.083269 |
| H | -2.947538 | -1.543026 | -1.101462 |
| H | -0.812114 | -1.056925 | -0.729245 |
| C | 0.222996 | 0.523540 | 0.150181 |
| C | 1.405153 | -0.349185 | -0.308790 |
| C | 0.354578 | 1.926890 | -0.452592 |
| H | 0.216645 | 0.598002 | 1.243785 |
| C | 2.707944 | 0.266707 | 0.215202 |
| H | 1.422973 | -0.288022 | -1.405025 |
| C | 1.667795 | 2.560558 | 0.017893 |
| H | 0.343802 | 1.838158 | -1.543755 |
| H | -0.489048 | 2.555715 | -0.166556 |
| C | 2.874320 | 1.687271 | -0.332282 |
| H | 3.555063 | -0.357174 | -0.080240 |
| H | 2.688608 | 0.294629 | 1.310361 |
| H | 1.771551 | 3.550674 | -0.430371 |
| H | 1.625312 | 2.703962 | 1.103433 |
| H | 3.788712 | 2.135163 | 0.062384 |
| H | 2.983721 | 1.641452 | -1.421597 |
| N | 1.150112 | -1.755820 | 0.001459 |
| C | 1.971476 | -2.662060 | -0.792976 |
| H | 3.038143 | -2.616075 | -0.527885 |
| H | 1.628744 | -3.685773 | -0.632281 |
| H | 1.863750 | -2.425503 | -1.852752 |
| C | 1.247007 | -2.081605 | 1.420634 |
| H | 0.898804 | -3.104669 | 1.571042 |

| | | | |
|---|---|---|---|
| H | 2.275692 | -2.009619 | 1.801727 |
| H | 0.610581 | -1.421562 | 2.012835 |
| H | -4.963639 | 0.596532 | -0.256670 |
| C | -2.587853 | 1.316255 | 0.878766 |
| H | -1.751461 | 1.609650 | 1.509113 |
| H | -2.871514 | 2.166154 | 0.251945 |
| H | -3.439105 | 1.071365 | 1.513052 |

**8G-*E***

Imaginary frequency: None

Electronic energies: -887.099985

Free energies: -886.729931

Corrected Free energies: -886.726146

| | | | |
|---|---|---|---|
| N | 1.929547 | -0.288739 | 0.641003 |
| C | 3.095474 | -0.133708 | -0.145508 |
| C | 4.021265 | -1.103764 | -0.179724 |
| C | 5.369754 | -1.073007 | -0.839424 |
| H | 5.463208 | -1.880122 | -1.572108 |
| H | 6.166834 | -1.222493 | -0.104561 |
| H | 3.789309 | -2.019809 | 0.362215 |
| H | 1.887308 | -1.217481 | 1.052410 |
| C | 0.639169 | -0.012019 | 0.010789 |
| C | -0.427713 | -0.894978 | 0.707721 |
| H | 0.665689 | -0.262940 | -1.058648 |
| H | -0.523077 | -0.502864 | 1.726767 |
| N | 0.049736 | -2.274723 | 0.876128 |
| C | -0.799881 | -3.041352 | 1.775776 |
| H | -1.794380 | -3.246803 | 1.349603 |
| H | -0.317293 | -3.995861 | 1.995091 |
| H | -0.932408 | -2.496969 | 2.713182 |
| C | 0.299713 | -3.010665 | -0.356040 |
| H | 0.804664 | -3.945597 | -0.103838 |
| H | -0.619809 | -3.258557 | -0.906179 |
| H | 0.961751 | -2.441636 | -1.013014 |
| C | 0.224667 | 1.445008 | 0.135428 |
| C | 0.412921 | 2.126676 | 1.337666 |
| C | -0.384468 | 2.108554 | -0.928070 |
| C | -0.005626 | 3.445503 | 1.476030 |
| H | 0.909071 | 1.617512 | 2.156615 |
| C | -0.805192 | 3.428994 | -0.793478 |
| H | -0.529229 | 1.589299 | -1.870479 |
| C | -0.617904 | 4.100931 | 0.410103 |
| H | 0.149010 | 3.964218 | 2.415108 |

| | | | |
|---|---|---|---|
| H | -1.275756 | 3.932798 | -1.629823 |
| H | -0.942590 | 5.129212 | 0.516323 |
| C | -1.792177 | -0.771630 | 0.046632 |
| C | -2.910964 | -0.480131 | 0.828269 |
| C | -1.974484 | -0.971377 | -1.325346 |
| C | -4.179332 | -0.388904 | 0.261921 |
| H | -2.783635 | -0.316637 | 1.893994 |
| C | -3.240556 | -0.884912 | -1.895372 |
| H | -1.125357 | -1.186995 | -1.964058 |
| C | -4.347450 | -0.593001 | -1.103408 |
| H | -5.033537 | -0.154688 | 0.886438 |
| H | -3.361823 | -1.041416 | -2.960876 |
| H | -5.332712 | -0.520682 | -1.548528 |
| H | 5.569616 | -0.135467 | -1.356492 |
| C | 3.205316 | 1.192890 | -0.845684 |
| H | 2.426524 | 1.298738 | -1.606741 |
| H | 3.059389 | 2.005671 | -0.129394 |
| H | 4.169054 | 1.319150 | -1.332618 |

**8G-*Z***

Imaginary frequency: None

Electronic energies: -887.103050

Free energies: -886.733679

Corrected Free energies: -886.729692

| | | | |
|---|---|---|---|
| N | 2.047764 | 0.007934 | 0.361439 |
| C | 3.120330 | 0.360305 | -0.473982 |
| C | 4.228418 | -0.391809 | -0.561413 |
| H | 2.155866 | -0.916061 | 0.767495 |
| C | 0.683078 | 0.143295 | -0.140412 |
| C | -0.192818 | -0.894360 | 0.606108 |
| H | 0.641614 | -0.065043 | -1.218169 |
| H | -0.235265 | -0.555766 | 1.647777 |
| N | 0.470660 | -2.205870 | 0.661103 |
| C | -0.188184 | -3.111786 | 1.591620 |
| H | -1.184830 | -3.425822 | 1.245094 |
| H | 0.428026 | -4.004233 | 1.717247 |
| H | -0.298630 | -2.627382 | 2.564094 |
| C | 0.685503 | -2.852907 | -0.626846 |
| H | 1.302406 | -3.740244 | -0.468462 |
| H | -0.248646 | -3.171188 | -1.112033 |
| H | 1.227073 | -2.187375 | -1.304110 |
| C | 0.108474 | 1.532937 | 0.082880 |
| C | 0.339096 | 2.206628 | 1.282209 |

| | | | |
|---|---|---|---|
| C | -0.685509 | 2.137566 | -0.889609 |
| C | -0.218973 | 3.460769 | 1.506394 |
| H | 0.976641 | 1.746940 | 2.029279 |
| C | -1.244900 | 3.393173 | -0.669370 |
| H | -0.865045 | 1.622651 | -1.828184 |
| C | -1.013889 | 4.057676 | 0.530874 |
| H | -0.030397 | 3.975094 | 2.441674 |
| H | -1.856829 | 3.853166 | -1.436439 |
| H | -1.446031 | 5.036430 | 0.703285 |
| C | -1.621304 | -0.925242 | 0.083741 |
| C | -2.679534 | -0.824299 | 0.987990 |
| C | -1.919929 | -1.076126 | -1.274210 |
| C | -4.001565 | -0.867798 | 0.555488 |
| H | -2.463344 | -0.701937 | 2.044832 |
| C | -3.240035 | -1.123481 | -1.710916 |
| H | -1.121729 | -1.145867 | -2.005037 |
| C | -4.285335 | -1.018211 | -0.797645 |
| H | -4.807423 | -0.780205 | 1.274732 |
| H | -3.451813 | -1.237332 | -2.767587 |
| H | -5.312843 | -1.049702 | -1.140082 |
| C | 2.980156 | 1.665695 | -1.207599 |
| H | 2.142812 | 1.640606 | -1.911194 |
| H | 2.781571 | 2.481664 | -0.507199 |
| H | 3.889758 | 1.884474 | -1.765713 |
| C | 4.423165 | -1.712074 | 0.134926 |
| H | 4.747168 | -1.590620 | 1.174923 |
| H | 3.503642 | -2.306904 | 0.151611 |
| H | 5.185196 | -2.306520 | -0.371107 |
| H | 5.054615 | -0.002970 | -1.145884 |

**8G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -886.917420

Free energies: -886.549892

Corrected Free energies: -886.545674

| | | | |
|---|---|---|---|
| N | 1.895193 | -0.596881 | -0.126317 |
| C | 3.043435 | -0.184530 | -0.620750 |
| C | 4.215430 | -0.902098 | -0.283892 |
| H | 1.839616 | -1.479692 | 0.397405 |
| C | 0.563297 | -0.043732 | -0.382040 |
| C | -0.422073 | -0.906531 | 0.447423 |
| H | 0.362842 | -0.150699 | -1.452815 |
| H | -0.276461 | -0.606613 | 1.490746 |

| | | | |
|---|---|---|---|
| N | -0.019597 | -2.318005 | 0.396292 |
| C | -0.643391 | -3.100792 | 1.459066 |
| H | -1.730134 | -3.196582 | 1.321795 |
| H | -0.205937 | -4.100017 | 1.465123 |
| H | -0.452395 | -2.630857 | 2.425314 |
| C | -0.202044 | -2.965948 | -0.900005 |
| H | 0.254651 | -3.955715 | -0.856683 |
| H | -1.260176 | -3.082885 | -1.169372 |
| H | 0.301125 | -2.400942 | -1.687897 |
| C | 0.447190 | 1.417461 | -0.002727 |
| C | 0.948034 | 1.874882 | 1.216327 |
| C | -0.200395 | 2.304261 | -0.858472 |
| C | 0.809188 | 3.212125 | 1.569093 |
| H | 1.457197 | 1.189898 | 1.887033 |
| C | -0.346555 | 3.640770 | -0.500964 |
| H | -0.587911 | 1.949356 | -1.807803 |
| C | 0.160223 | 4.096633 | 0.711500 |
| H | 1.205738 | 3.563451 | 2.514032 |
| H | -0.850696 | 4.325319 | -1.172124 |
| H | 0.052032 | 5.138370 | 0.987923 |
| C | -1.868494 | -0.611681 | 0.090079 |
| C | -2.784558 | -0.390120 | 1.119327 |
| C | -2.324249 | -0.584365 | -1.230947 |
| C | -4.125982 | -0.147204 | 0.841411 |
| H | -2.440644 | -0.402117 | 2.148717 |
| C | -3.664502 | -0.339991 | -1.511816 |
| H | -1.640912 | -0.754430 | -2.055801 |
| C | -4.568570 | -0.121010 | -0.476732 |
| H | -4.822310 | 0.025904 | 1.653116 |
| H | -4.001855 | -0.319861 | -2.541168 |
| H | -5.611602 | 0.071877 | -0.697375 |
| C | 3.099495 | 1.009323 | -1.516438 |
| H | 2.324356 | 0.951158 | -2.283358 |
| H | 2.922812 | 1.919160 | -0.936437 |
| H | 4.074436 | 1.075165 | -1.993167 |
| C | 4.224483 | -2.088110 | 0.606443 |
| H | 3.853346 | -1.828092 | 1.604403 |
| H | 3.573256 | -2.879351 | 0.216527 |
| H | 5.228254 | -2.491582 | 0.707126 |
| H | 5.142413 | -0.542077 | -0.710393 |

**8G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -886.917185

Free energies: -886.548691

Corrected Free energies: -886.544487

| | | | |
|---|---|---|---|
| N | 1.739490 | -0.895389 | 0.057512 |
| C | 2.959834 | -0.588831 | -0.341960 |
| C | 4.019676 | -1.387494 | 0.136220 |
| C | 5.442636 | -1.154638 | -0.202500 |
| H | 5.638409 | -1.457640 | -1.239059 |
| H | 6.093491 | -1.736852 | 0.445390 |
| H | 3.759314 | -2.223329 | 0.776538 |
| H | 1.577738 | -1.750074 | 0.603918 |
| C | 0.486308 | -0.224795 | -0.296065 |
| C | -0.628069 | -0.939663 | 0.510421 |
| H | 0.329202 | -0.360099 | -1.370939 |
| H | -0.494705 | -0.622101 | 1.550081 |
| N | -0.394458 | -2.388348 | 0.519121 |
| C | -1.145960 | -3.054329 | 1.578675 |
| H | -2.230759 | -3.025876 | 1.400784 |
| H | -0.832037 | -4.097732 | 1.632339 |
| H | -0.934955 | -2.577876 | 2.537540 |
| C | -0.605695 | -3.055873 | -0.762252 |
| H | -0.256359 | -4.085654 | -0.676676 |
| H | -1.662127 | -3.070762 | -1.062577 |
| H | -0.024936 | -2.570719 | -1.549777 |
| C | 0.504868 | 1.257153 | 0.018809 |
| C | 0.973216 | 1.711267 | 1.251930 |
| C | 0.013162 | 2.170118 | -0.910654 |
| C | 0.957244 | 3.069778 | 1.546300 |
| H | 1.361899 | 1.006085 | 1.980261 |
| C | -0.009610 | 3.528747 | -0.612283 |
| H | -0.349290 | 1.818293 | -1.871168 |
| C | 0.464512 | 3.980301 | 0.615066 |
| H | 1.328373 | 3.417498 | 2.502784 |
| H | -0.393625 | 4.233171 | -1.340171 |
| H | 0.452108 | 5.038679 | 0.845704 |
| C | -2.011496 | -0.487462 | 0.075466 |
| C | -2.933637 | -0.104751 | 1.050041 |
| C | -2.403916 | -0.462889 | -1.265762 |
| C | -4.219258 | 0.294830 | 0.698900 |
| H | -2.638525 | -0.112943 | 2.094668 |
| C | -3.688255 | -0.063285 | -1.619899 |
| H | -1.712657 | -0.752676 | -2.049445 |
| C | -4.599051 | 0.316587 | -0.638641 |
| H | -4.920183 | 0.592809 | 1.469400 |

| | | | |
|---|---|---|---|
| H | -3.976126 | -0.047358 | -2.664359 |
| H | -5.598049 | 0.630117 | -0.916680 |
| H | 5.706480 | -0.097072 | -0.124942 |
| C | 3.191924 | 0.567648 | -1.258652 |
| H | 2.375627 | 0.672992 | -1.972267 |
| H | 3.249756 | 1.492467 | -0.676463 |
| H | 4.126115 | 0.438304 | -1.800261 |

**9G-*E***

Imaginary frequency: None

Electronic energies: -368.531636

Free energies: -368.349014

Corrected Free energies: -368.347489

| | | | |
|---|---|---|---|
| C | -2.621994 | 0.376015 | 0.460643 |
| C | -2.468196 | -0.960134 | -0.269065 |
| C | -0.977250 | -1.239225 | -0.109424 |
| C | -1.348474 | 1.139789 | 0.076865 |
| H | -3.528003 | 0.918881 | 0.191630 |
| H | -2.635586 | 0.201183 | 1.539504 |
| H | -2.711267 | -0.844741 | -1.328668 |
| H | -3.091171 | -1.752429 | 0.145682 |
| H | -0.763821 | -1.687869 | 0.874493 |
| H | -0.583277 | -1.915445 | -0.873437 |
| H | -1.008010 | 1.779258 | 0.895259 |
| H | -1.520421 | 1.777687 | -0.797440 |
| N | -0.377187 | 0.079760 | -0.233935 |
| C | 0.992821 | 0.256978 | -0.090514 |
| C | 1.838953 | -0.778839 | 0.089934 |
| C | 3.338985 | -0.711488 | 0.190231 |
| H | 3.826781 | -1.144311 | -0.690432 |
| H | 3.715543 | 0.304061 | 0.308658 |
| H | 3.690140 | -1.285036 | 1.053104 |
| H | 1.419207 | -1.776751 | 0.155758 |
| C | 1.442145 | 1.693510 | -0.203588 |
| H | 1.233668 | 2.248578 | 0.715103 |
| H | 2.507026 | 1.766921 | -0.407071 |
| H | 0.907554 | 2.192064 | -1.015090 |

**9G-*Z***

Imaginary frequency: None

Electronic energies: -368.529357

Free energies: -368.344077

Corrected Free energies: -368.343625

| | | | |
|---|---|---|---|
| C | -2.490112 | 0.071348 | 0.482006 |
| C | -2.125090 | -0.889900 | -0.650679 |
| C | -0.632241 | -1.132944 | -0.413797 |
| C | -1.284592 | 1.006399 | 0.501184 |
| H | -3.427214 | 0.602969 | 0.317367 |
| H | -2.557571 | -0.471549 | 1.428724 |
| H | -2.276627 | -0.395081 | -1.613879 |
| H | -2.704411 | -1.813257 | -0.643080 |
| H | -0.484500 | -2.003292 | 0.233744 |
| H | -0.079204 | -1.310957 | -1.340822 |
| H | -1.158040 | 1.513074 | 1.461105 |
| H | -1.399480 | 1.773855 | -0.275893 |
| N | -0.159641 | 0.106559 | 0.229012 |
| C | 1.114695 | 0.604798 | -0.056559 |
| C | 2.206831 | -0.180230 | -0.067980 |
| C | 1.217039 | 2.079021 | -0.359549 |
| H | 0.862574 | 2.681971 | 0.481031 |
| H | 2.254325 | 2.347825 | -0.554610 |
| H | 0.613990 | 2.350321 | -1.230725 |
| H | 3.140546 | 0.273701 | -0.380729 |
| C | 2.249762 | -1.612711 | 0.390208 |
| H | 1.539816 | -1.774629 | 1.205612 |
| H | 2.008422 | -2.334220 | -0.398136 |
| H | 3.247113 | -1.861323 | 0.758208 |

**9G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -368.351651

Free energies: -368.166398

Corrected Free energies: -368.166008

| | | | |
|---|---|---|---|
| C | -2.535618 | 0.156488 | 0.338851 |
| C | -2.110025 | -1.114002 | -0.395600 |
| C | -0.630983 | -1.222933 | -0.040897 |
| C | -1.360782 | 1.094367 | 0.090645 |
| H | -3.467183 | 0.578580 | -0.032825 |
| H | -2.640833 | -0.039043 | 1.407903 |
| H | -2.226597 | -0.987985 | -1.474100 |
| H | -2.659633 | -2.000216 | -0.084611 |
| H | -0.502734 | -1.672848 | 0.946383 |
| H | -0.039660 | -1.764493 | -0.774377 |
| H | -1.209125 | 1.840666 | 0.869053 |
| H | -1.453323 | 1.600957 | -0.874655 |

| | | | |
|---|---|---|---|
| N | -0.188250 | 0.189526 | 0.024292 |
| C | 1.051931 | 0.642867 | -0.050257 |
| C | 2.202765 | -0.176419 | -0.058927 |
| C | 1.244481 | 2.132113 | -0.108750 |
| H | 0.612962 | 2.579028 | -0.878016 |
| H | 0.976521 | 2.581896 | 0.850609 |
| H | 2.283149 | 2.371146 | -0.320004 |
| H | 3.118978 | 0.367058 | -0.253289 |
| C | 2.352901 | -1.633996 | 0.184135 |
| H | 1.638914 | -2.030554 | 0.902414 |
| H | 2.236160 | -2.191570 | -0.753692 |
| H | 3.362142 | -1.830209 | 0.543958 |

**9G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -368.356601

Free energies: -368.172316

Corrected Free energies: -368.171835

| | | | |
|---|---|---|---|
| C | -2.635977 | 0.435165 | 0.355497 |
| C | -2.468254 | -0.951452 | -0.267002 |
| C | -0.999313 | -1.272798 | -0.005801 |
| C | -1.344668 | 1.141470 | -0.041304 |
| H | -3.512448 | 0.967489 | -0.008358 |
| H | -2.697754 | 0.359122 | 1.443062 |
| H | -2.652825 | -0.908266 | -1.342124 |
| H | -3.124513 | -1.701956 | 0.168967 |
| H | -0.848037 | -1.708816 | 0.985213 |
| H | -0.555519 | -1.922130 | -0.758743 |
| H | -1.038064 | 1.931527 | 0.642183 |
| H | -1.402436 | 1.548872 | -1.055499 |
| N | -0.342698 | 0.055103 | -0.036010 |
| C | 0.963179 | 0.263199 | -0.039933 |
| C | 1.848063 | -0.828279 | 0.058222 |
| C | 3.324498 | -0.681718 | 0.086087 |
| H | 3.692712 | -0.293587 | -0.870558 |
| H | 3.637773 | 0.028498 | 0.857244 |
| H | 3.803032 | -1.639582 | 0.273397 |
| H | 1.430865 | -1.823350 | 0.133585 |
| C | 1.463006 | 1.673423 | -0.117282 |
| H | 0.886719 | 2.250309 | -0.840318 |
| H | 1.366065 | 2.155111 | 0.860009 |
| H | 2.510107 | 1.696984 | -0.406889 |

**10G-*E***

Imaginary frequency: None

Electronic energies: -407.841680

Free energies: -407.629006

Corrected Free energies: -407.627995

| | | | |
|---|---|---|---|
| C | 3.614621 | -0.691657 | 0.271788 |
| C | 2.110311 | -0.788154 | 0.217047 |
| C | 1.298894 | 0.221645 | -0.135526 |
| H | 4.072224 | -0.813611 | -0.716629 |
| H | 4.019736 | -1.477856 | 0.910393 |
| C | -0.655989 | -1.236864 | -0.081924 |
| C | -0.857663 | 1.106433 | 0.500447 |
| C | -2.123834 | -1.287124 | -0.496057 |
| H | -0.557283 | -1.562219 | 0.969550 |
| H | -0.077756 | -1.930217 | -0.695267 |
| C | -2.328088 | 1.124232 | 0.098582 |
| H | -0.774238 | 0.888823 | 1.580250 |
| H | -0.416113 | 2.087937 | 0.331277 |
| C | -2.947739 | -0.259576 | 0.275553 |
| H | -2.505188 | -2.297856 | -0.331123 |
| H | -2.193036 | -1.079188 | -1.568866 |
| H | -2.854278 | 1.870025 | 0.699544 |
| H | -2.402582 | 1.430018 | -0.950296 |
| H | -3.987646 | -0.266106 | -0.059290 |
| H | -2.947273 | -0.521157 | 1.340564 |
| H | 1.686631 | -1.752472 | 0.468130 |
| N | -0.105000 | 0.101371 | -0.264140 |
| H | 3.956287 | 0.264466 | 0.673362 |
| C | 1.847615 | 1.585083 | -0.490235 |
| H | 1.918973 | 2.239437 | 0.383623 |
| H | 2.844965 | 1.496484 | -0.919587 |
| H | 1.202803 | 2.069778 | -1.224698 |

**10G-*Z***

Imaginary frequency: None

Electronic energies: -407.835998

Free energies: -407.623251

Corrected Free energies: -407.622447

| | | | |
|---|---|---|---|
| C | 2.471912 | -0.216911 | -0.035269 |
| C | 1.400219 | 0.587887 | -0.158160 |
| C | -0.363478 | -1.175650 | -0.167307 |
| C | -0.841576 | 1.018448 | 0.771263 |

| | | | |
|---|---|---|---|
| C | -1.773990 | -1.264448 | -0.749016 |
| H | -0.360653 | -1.671806 | 0.816613 |
| H | 0.342619 | -1.698904 | -0.811797 |
| C | -2.273182 | 0.979924 | 0.241357 |
| H | -0.824942 | 0.636086 | 1.806227 |
| H | -0.483781 | 2.046394 | 0.800012 |
| C | -2.757524 | -0.462542 | 0.102127 |
| H | -2.074313 | -2.314328 | -0.802760 |
| H | -1.759977 | -0.868238 | -1.769531 |
| H | -2.923377 | 1.546294 | 0.913219 |
| H | -2.296376 | 1.471541 | -0.737040 |
| H | -3.760004 | -0.493671 | -0.331239 |
| H | -2.822326 | -0.916657 | 1.098452 |
| N | 0.048496 | 0.218202 | -0.067905 |
| C | 1.615977 | 2.047851 | -0.501751 |
| H | 1.546580 | 2.686799 | 0.382644 |
| H | 2.609021 | 2.189729 | -0.926988 |
| H | 0.868816 | 2.390610 | -1.221420 |
| H | 3.420001 | 0.235231 | -0.310054 |
| C | 2.573540 | -1.636759 | 0.459736 |
| H | 1.759956 | -1.910893 | 1.128166 |
| H | 2.602093 | -2.369488 | -0.354424 |
| H | 3.505806 | -1.752912 | 1.017384 |

**10G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -407.655165

Free energies: -407.441437

Corrected Free energies: -407.440695

| | | | |
|---|---|---|---|
| C | 2.385478 | -0.100677 | -0.346789 |
| C | 1.209112 | 0.653595 | -0.124499 |
| C | -0.286248 | -1.283949 | 0.278836 |
| C | -1.011918 | 0.983365 | 0.864281 |
| C | -1.498757 | -1.425384 | -0.649575 |
| H | -0.521281 | -1.627605 | 1.289365 |
| H | 0.539567 | -1.861098 | -0.116200 |
| C | -2.222222 | 0.899861 | -0.065034 |
| H | -1.268551 | 0.578673 | 1.847781 |
| H | -0.660554 | 2.000278 | 1.001390 |
| C | -2.669298 | -0.553620 | -0.202761 |
| H | -1.776927 | -2.480795 | -0.666674 |
| H | -1.189923 | -1.148690 | -1.662300 |
| H | -3.016001 | 1.521795 | 0.351607 |

| | | | |
|---|---|---|---|
| H | -1.956374 | 1.311339 | -1.043855 |
| H | -3.488393 | -0.633670 | -0.919259 |
| H | -3.043910 | -0.910269 | 0.762384 |
| N | 0.088893 | 0.140124 | 0.362489 |
| C | 1.277935 | 2.131358 | -0.404798 |
| H | 1.428842 | 2.686923 | 0.524054 |
| H | 2.123965 | 2.337578 | -1.055925 |
| H | 0.366400 | 2.490190 | -0.882126 |
| H | 3.125449 | 0.392613 | -0.964677 |
| C | 2.800774 | -1.384488 | 0.273555 |
| H | 2.233084 | -1.633997 | 1.168260 |
| H | 2.714294 | -2.210851 | -0.442576 |
| H | 3.858923 | -1.313652 | 0.532035 |

**10G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -407.659821

Free energies: -407.446799

Corrected Free energies: -407.445765

| | | | |
|---|---|---|---|
| C | 3.453858 | -0.725023 | -0.406839 |
| C | 2.023686 | -0.830254 | -0.019663 |
| C | 1.177295 | 0.282211 | 0.160932 |
| H | 3.561920 | -0.242480 | -1.384055 |
| H | 3.906514 | -1.711906 | -0.459632 |
| C | -0.751418 | -1.160272 | 0.802791 |
| C | -1.058312 | 1.238338 | 0.558682 |
| C | -1.734154 | -1.454985 | -0.333112 |
| H | -1.288158 | -1.037736 | 1.746575 |
| H | -0.024484 | -1.950987 | 0.940861 |
| C | -2.059281 | 1.031184 | -0.583975 |
| H | -1.566397 | 1.198719 | 1.525169 |
| H | -0.547898 | 2.190762 | 0.478756 |
| C | -2.755508 | -0.323950 | -0.458735 |
| H | -2.227199 | -2.405321 | -0.122181 |
| H | -1.172539 | -1.571435 | -1.265040 |
| H | -2.782340 | 1.847908 | -0.552198 |
| H | -1.524658 | 1.099039 | -1.536430 |
| H | -3.402071 | -0.494828 | -1.320966 |
| H | -3.394213 | -0.318660 | 0.430684 |
| H | 1.622211 | -1.824305 | 0.103095 |
| N | -0.088313 | 0.129398 | 0.540515 |
| H | 4.015418 | -0.119455 | 0.311149 |
| C | 1.696777 | 1.669598 | -0.089687 |

| | | | |
|---|---|---|---|
| H | 1.153239 | 2.141726 | -0.910532 |
| H | 1.582083 | 2.288231 | 0.801855 |
| H | 2.749106 | 1.643856 | -0.353072 |

**11G-*E***

Imaginary frequency: None

Electronic energies: -557.104585

Free energies: -556.910023

Corrected Free energies: -556.908055

| | | | |
|---|---|---|---|
| C | 2.248031 | 0.985940 | -0.239710 |
| C | 1.494937 | 2.312906 | -0.083335 |
| C | 0.114738 | 1.872102 | 0.391843 |
| C | 1.137109 | -0.053686 | -0.567506 |
| H | 3.010760 | 1.011278 | -1.015922 |
| H | 2.737216 | 0.724090 | 0.701155 |
| H | 1.401093 | 2.813585 | -1.048710 |
| H | 1.987921 | 2.989370 | 0.614221 |
| H | 0.109624 | 1.660314 | 1.471987 |
| H | -0.661079 | 2.611567 | 0.184522 |
| H | 1.242079 | -0.443226 | -1.582430 |
| N | -0.111425 | 0.673111 | -0.398756 |
| C | -1.339804 | -0.000479 | -0.372478 |
| C | -2.375043 | 0.434416 | 0.366509 |
| C | -3.769484 | -0.125857 | 0.401433 |
| H | -4.497533 | 0.595287 | 0.015647 |
| H | -3.879136 | -1.044509 | -0.172983 |
| H | -4.065747 | -0.349111 | 1.430548 |
| H | -2.211716 | 1.290724 | 1.012419 |
| C | 1.283372 | -1.214981 | 0.399331 |
| O | 0.714009 | -1.321011 | 1.452516 |
| O | 2.176350 | -2.109579 | -0.047180 |
| H | 2.280571 | -2.796802 | 0.627152 |
| C | -1.393525 | -1.185563 | -1.302865 |
| H | -1.016764 | -0.904049 | -2.289233 |
| H | -0.776554 | -2.012639 | -0.938258 |
| H | -2.405617 | -1.561733 | -1.420839 |

**11G-*Z***

Imaginary frequency: None

Electronic energies: -557.102549

Free energies: -556.906833

Corrected Free energies: -556.905231

| | | | |
|---|---|---|---|
| C | 1.542753 | 1.628000 | 0.010568 |
| C | 0.373038 | 2.519970 | -0.402047 |
| C | -0.841710 | 1.705090 | 0.044785 |
| C | 1.019644 | 0.230590 | -0.363790 |
| H | 2.481083 | 1.858008 | -0.490950 |
| H | 1.697766 | 1.685256 | 1.091956 |
| H | 0.366498 | 2.639146 | -1.488445 |
| H | 0.408731 | 3.507796 | 0.056760 |
| H | -1.105216 | 1.943409 | 1.080501 |
| H | -1.723729 | 1.880789 | -0.576216 |
| H | 1.252264 | 0.030835 | -1.418588 |
| N | -0.401352 | 0.307539 | -0.096233 |
| C | -1.283738 | -0.686187 | -0.542006 |
| C | -2.518822 | -0.812272 | -0.031389 |
| C | 1.706273 | -0.846075 | 0.451636 |
| O | 1.200259 | -1.528356 | 1.300354 |
| O | 2.999228 | -0.943581 | 0.106755 |
| H | 3.407357 | -1.626214 | 0.658216 |
| C | -0.786473 | -1.599946 | -1.632903 |
| H | -0.482414 | -1.036405 | -2.519666 |
| H | 0.077090 | -2.184632 | -1.301188 |
| H | -1.571080 | -2.300224 | -1.915365 |
| H | -3.175452 | -1.542690 | -0.490749 |
| C | -3.031679 | -0.070161 | 1.171755 |
| H | -2.219092 | 0.110908 | 1.880283 |
| H | -3.477743 | 0.900821 | 0.930749 |
| H | -3.798216 | -0.658141 | 1.679785 |

**11G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -556.915783

Free energies: -556.719646

Corrected Free energies: -556.718285

| | | | |
|---|---|---|---|
| C | 1.528828 | 1.696688 | -0.119752 |
| C | 0.276679 | 2.530997 | -0.372421 |
| C | -0.828608 | 1.639533 | 0.177538 |
| C | 1.065047 | 0.268845 | -0.464655 |
| H | 2.384266 | 1.983761 | -0.726295 |
| H | 1.811876 | 1.751971 | 0.934151 |
| H | 0.129313 | 2.693134 | -1.441723 |
| H | 0.301504 | 3.494442 | 0.132657 |
| H | -0.857222 | 1.686830 | 1.268706 |
| H | -1.811139 | 1.849940 | -0.234217 |

| | | | |
|---|---|---|---|
| H | 1.268286 | 0.048025 | -1.514546 |
| N | -0.390811 | 0.283778 | -0.231689 |
| C | -1.172095 | -0.756702 | -0.468383 |
| C | -2.544117 | -0.797870 | -0.117289 |
| C | 1.752873 | -0.758476 | 0.418230 |
| O | 1.224762 | -1.372524 | 1.301594 |
| O | 3.038767 | -0.838464 | 0.093317 |
| H | 3.476913 | -1.459764 | 0.694306 |
| C | -0.599733 | -1.985347 | -1.115538 |
| H | -0.210795 | -2.652666 | -0.343248 |
| H | -1.387570 | -2.510023 | -1.651737 |
| H | 0.204500 | -1.756246 | -1.812796 |
| H | -3.084294 | -1.625305 | -0.560939 |
| C | -3.310363 | 0.058119 | 0.821214 |
| H | -2.694511 | 0.519588 | 1.589398 |
| H | -3.835635 | 0.852373 | 0.275802 |
| H | -4.079111 | -0.549328 | 1.299354 |

**11G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -556.920927

Free energies: -556.724564

Corrected Free energies: -556.723590

| | | | |
|---|---|---|---|
| C | -2.129860 | 1.171473 | 0.084991 |
| C | -1.277026 | 2.433617 | 0.177570 |
| C | 0.069097 | 1.975366 | -0.367763 |
| C | -1.148875 | 0.054286 | 0.490866 |
| H | -3.002885 | 1.177922 | 0.732986 |
| H | -2.459618 | 1.016059 | -0.945130 |
| H | -1.168072 | 2.748605 | 1.216897 |
| H | -1.684296 | 3.260573 | -0.400446 |
| H | 0.077660 | 1.946103 | -1.460908 |
| H | 0.905274 | 2.569075 | -0.007158 |
| H | -1.199847 | -0.138568 | 1.564722 |
| N | 0.177711 | 0.587801 | 0.140279 |
| C | 1.305921 | -0.096403 | 0.248264 |
| C | 2.500021 | 0.438490 | -0.282437 |
| C | 3.804672 | -0.257602 | -0.193446 |
| H | 4.228976 | -0.127091 | 0.810804 |
| H | 3.708124 | -1.332223 | -0.361263 |
| H | 4.511097 | 0.158344 | -0.908214 |
| H | 2.463061 | 1.393964 | -0.787449 |
| C | -1.449410 | -1.220565 | -0.280129 |

| | | | |
|---|---|---|---|
| O | -0.798815 | -1.642045 | -1.193762 |
| O | -2.569508 | -1.768396 | 0.179063 |
| H | -2.779782 | -2.549448 | -0.354899 |
| C | 1.331643 | -1.435249 | 0.918805 |
| H | 1.399348 | -2.222977 | 0.165150 |
| H | 2.213391 | -1.495843 | 1.556948 |
| H | 0.453076 | -1.616040 | 1.533281 |

**12G-*E***

Imaginary frequency: None

Electronic energies: -945.083750

Free energies: -944.718601

Corrected Free energies: -944.715301

| | | | |
|---|---|---|---|
| C | 0.078914 | -1.198255 | -0.533681 |
| C | -0.445529 | -2.645449 | -0.474366 |
| C | 0.394779 | -3.330933 | 0.620584 |
| C | 1.673309 | -2.481519 | 0.740263 |
| H | -0.260412 | -3.117643 | -1.440764 |
| H | -1.517348 | -2.704443 | -0.280464 |
| H | 0.629551 | -4.359842 | 0.348375 |
| H | -0.135416 | -3.368612 | 1.572519 |
| H | 2.565562 | -3.035250 | 0.429444 |
| H | 1.835804 | -2.144938 | 1.771746 |
| C | -0.707777 | -0.242878 | 0.430450 |
| O | -0.583141 | -0.723889 | 1.768474 |
| C | -2.189428 | -0.137188 | 0.061183 |
| C | -3.086114 | 0.288236 | 1.045170 |
| C | -2.680532 | -0.397728 | -1.219318 |
| C | -4.437251 | 0.446367 | 0.759851 |
| H | -2.713036 | 0.500683 | 2.040277 |
| C | -4.033970 | -0.238856 | -1.507062 |
| H | -2.018930 | -0.729944 | -2.009702 |
| C | -4.916971 | 0.182787 | -0.519802 |
| H | -5.115144 | 0.778998 | 1.537165 |
| H | -4.395635 | -0.448352 | -2.506799 |
| H | -5.969668 | 0.305465 | -0.744598 |
| C | -0.059285 | 1.136876 | 0.418112 |
| C | -0.498874 | 2.144827 | -0.441533 |
| C | 1.052809 | 1.376200 | 1.226590 |
| C | 0.172770 | 3.362198 | -0.507649 |
| H | -1.367136 | 1.981321 | -1.069528 |
| C | 1.725126 | 2.591685 | 1.159680 |
| H | 1.399342 | 0.596168 | 1.892591 |

| | | | |
|---|---|---|---|
| C | 1.291298 | 3.587144 | 0.288090 |
| H | -0.180579 | 4.133733 | -1.181658 |
| H | 2.593043 | 2.760393 | 1.786930 |
| H | 1.817225 | 4.533161 | 0.235114 |
| N | 1.475074 | -1.365409 | -0.170156 |
| H | 0.008938 | -0.784422 | -1.540170 |
| C | 2.549630 | -0.604633 | -0.608418 |
| C | 3.765908 | -0.688373 | -0.029187 |
| C | 4.991448 | 0.063512 | -0.493066 |
| H | 5.285355 | -0.190254 | -1.516836 |
| H | 5.840645 | -0.173805 | 0.149170 |
| H | 3.884404 | -1.309886 | 0.850156 |
| H | 4.855679 | 1.149848 | -0.457978 |
| H | -1.147876 | -1.498294 | 1.859643 |
| C | 2.309135 | 0.278935 | -1.804788 |
| H | 1.842155 | -0.283623 | -2.617607 |
| H | 1.655963 | 1.119775 | -1.558031 |
| H | 3.250748 | 0.681013 | -2.172308 |

**12G-*Z***

Imaginary frequency: None

Electronic energies: -945.084304

Free energies: -944.717942

Corrected Free energies: -944.715208

| | | | |
|---|---|---|---|
| C | -0.122266 | -1.264784 | 0.386531 |
| C | 0.310499 | -2.718357 | 0.100170 |
| C | -0.806392 | -3.278935 | -0.787497 |
| C | -2.038101 | -2.590552 | -0.217945 |
| H | 0.343642 | -3.275056 | 1.040205 |
| H | 1.302664 | -2.788941 | -0.350330 |
| H | -0.875439 | -4.365974 | -0.743724 |
| H | -0.664351 | -2.978361 | -1.827027 |
| H | -2.383315 | -3.112444 | 0.688726 |
| H | -2.872470 | -2.546390 | -0.922071 |
| C | 0.631027 | -0.223502 | -0.492053 |
| O | 0.488805 | -0.558725 | -1.868207 |
| C | 2.124837 | -0.131748 | -0.156995 |
| C | 2.945439 | 0.561934 | -1.052726 |
| C | 2.703799 | -0.678089 | 0.988615 |
| C | 4.304657 | 0.707621 | -0.811517 |
| H | 2.502141 | 0.988958 | -1.945253 |
| C | 4.068817 | -0.531134 | 1.233531 |
| H | 2.107432 | -1.231718 | 1.703342 |

| | | | |
|---|---|---|---|
| C | 4.872754 | 0.160623 | 0.337242 |
| H | 4.921871 | 1.250900 | -1.517408 |
| H | 4.499630 | -0.964047 | 2.128629 |
| H | 5.933072 | 0.273672 | 0.529161 |
| C | -0.021366 | 1.139988 | -0.294807 |
| C | 0.170096 | 1.834565 | 0.900791 |
| C | -0.859750 | 1.683239 | -1.264706 |
| C | -0.479709 | 3.041596 | 1.131637 |
| H | 0.835961 | 1.431365 | 1.657988 |
| C | -1.507428 | 2.894454 | -1.037423 |
| H | -1.008776 | 1.149509 | -2.193336 |
| C | -1.325717 | 3.574581 | 0.161912 |
| H | -0.322162 | 3.567171 | 2.066266 |
| H | -2.161562 | 3.303584 | -1.799095 |
| H | -1.832185 | 4.516099 | 0.338954 |
| N | -1.558916 | -1.239334 | 0.097655 |
| H | 0.070295 | -1.008609 | 1.431780 |
| C | -2.434063 | -0.480419 | 0.927598 |
| C | -3.532565 | 0.075180 | 0.404215 |
| H | 1.045191 | -1.324489 | -2.043594 |
| C | -2.137103 | -0.409593 | 2.405719 |
| H | -1.927632 | -1.407206 | 2.806666 |
| H | -1.268851 | 0.220362 | 2.617567 |
| H | -2.989143 | 0.009573 | 2.941040 |
| C | -3.883779 | 0.073614 | -1.052390 |
| H | -4.710906 | -0.611353 | -1.269163 |
| H | -4.199053 | 1.070810 | -1.372441 |
| H | -3.021299 | -0.227756 | -1.648331 |
| H | -4.224909 | 0.563771 | 1.084108 |

**12G-*Z*** radical cation

Imaginary frequency: -30.1962

Electronic energies: -944.899533

Free energies: -944.531130

Corrected Free energies: -944.528874

| | | | |
|---|---|---|---|
| C | -0.122492 | -1.123807 | 0.698133 |
| C | 0.252994 | -2.609303 | 0.673881 |
| C | -0.720490 | -3.274695 | -0.315451 |
| C | -1.886550 | -2.291970 | -0.489373 |
| H | 0.117771 | -3.019038 | 1.675106 |
| H | 1.295199 | -2.757168 | 0.394504 |
| H | -1.074550 | -4.229070 | 0.069375 |
| H | -0.248767 | -3.461191 | -1.278380 |

| | | | |
|---|---|---|---|
| H | -2.840814 | -2.711988 | -0.181381 |
| H | -1.945137 | -1.938448 | -1.517106 |
| C | 0.619127 | -0.257218 | -0.376460 |
| O | 0.326289 | -0.785301 | -1.662684 |
| C | 2.129981 | -0.243750 | -0.143684 |
| C | 2.939965 | 0.144388 | -1.214464 |
| C | 2.728730 | -0.547274 | 1.078833 |
| C | 4.319298 | 0.217832 | -1.069094 |
| H | 2.480849 | 0.396153 | -2.163591 |
| C | 4.111610 | -0.470142 | 1.224688 |
| H | 2.135928 | -0.850048 | 1.933818 |
| C | 4.910148 | -0.090040 | 0.152962 |
| H | 4.931981 | 0.519495 | -1.910117 |
| H | 4.561236 | -0.711104 | 2.180263 |
| H | 5.985679 | -0.033116 | 0.268963 |
| C | 0.061506 | 1.163253 | -0.336513 |
| C | 0.557156 | 2.096459 | 0.575721 |
| C | -1.007088 | 1.518936 | -1.160864 |
| C | -0.018428 | 3.358311 | 0.675395 |
| H | 1.396365 | 1.840864 | 1.213029 |
| C | -1.588939 | 2.778813 | -1.053729 |
| H | -1.380253 | 0.808513 | -1.888897 |
| C | -1.099272 | 3.700354 | -0.132430 |
| H | 0.377272 | 4.073556 | 1.386471 |
| H | -2.423781 | 3.040148 | -1.693094 |
| H | -1.551449 | 4.681340 | -0.049683 |
| N | -1.569692 | -1.144554 | 0.396960 |
| H | 0.035070 | -0.678657 | 1.675659 |
| C | -2.472740 | -0.320864 | 0.902779 |
| C | -3.814758 | -0.261480 | 0.439810 |
| H | 0.938263 | -1.506361 | -1.847861 |
| C | -2.138632 | 0.648120 | 2.002548 |
| H | -1.272883 | 0.363617 | 2.592758 |
| H | -1.961121 | 1.637404 | 1.571424 |
| H | -3.000497 | 0.722687 | 2.664929 |
| H | -4.473853 | 0.295778 | 1.094236 |
| C | -4.413809 | -0.737014 | -0.832570 |
| H | -3.701731 | -0.793607 | -1.652488 |
| H | -4.865481 | -1.728503 | -0.704140 |
| H | -5.221668 | -0.060434 | -1.111757 |

**12G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -944.905760

Free energies: -944.537972

Corrected Free energies: -944.535592

| | | | |
|---|---|---|---|
| C | -0.018658 | 1.247375 | -0.601664 |
| C | 0.497570 | 2.688493 | -0.519365 |
| C | -0.330072 | 3.363354 | 0.587500 |
| C | -1.620147 | 2.542907 | 0.696665 |
| H | 0.319780 | 3.176068 | -1.478709 |
| H | 1.567731 | 2.725901 | -0.321190 |
| H | -0.552041 | 4.398245 | 0.334348 |
| H | 0.196029 | 3.360720 | 1.539293 |
| H | -2.492894 | 3.105703 | 0.369668 |
| H | -1.784996 | 2.163894 | 1.706136 |
| C | 0.691195 | 0.264621 | 0.394934 |
| O | 0.537198 | 0.777477 | 1.711805 |
| C | 2.175218 | 0.105042 | 0.062914 |
| C | 2.995669 | -0.438546 | 1.055678 |
| C | 2.734815 | 0.424679 | -1.173486 |
| C | 4.348659 | -0.645731 | 0.821758 |
| H | 2.563597 | -0.705789 | 2.013487 |
| C | 4.091682 | 0.213986 | -1.408321 |
| H | 2.132874 | 0.844185 | -1.970521 |
| C | 4.901791 | -0.318065 | -0.413060 |
| H | 4.970298 | -1.067013 | 1.602550 |
| H | 4.511645 | 0.471216 | -2.373093 |
| H | 5.956978 | -0.478807 | -0.597842 |
| C | -0.005549 | -1.094365 | 0.368152 |
| C | 0.330144 | -2.053153 | -0.588362 |
| C | -1.027997 | -1.369132 | 1.277964 |
| C | -0.356138 | -3.261288 | -0.645010 |
| H | 1.132784 | -1.860277 | -1.291768 |
| C | -1.718213 | -2.576306 | 1.217306 |
| H | -1.277412 | -0.637956 | 2.037020 |
| C | -1.386697 | -3.524057 | 0.253637 |
| H | -0.083926 | -3.998271 | -1.390918 |
| H | -2.511828 | -2.775906 | 1.927551 |
| H | -1.921663 | -4.465016 | 0.208405 |
| N | -1.437836 | 1.393187 | -0.223576 |
| H | 0.045611 | 0.844889 | -1.608516 |
| C | -2.438681 | 0.620621 | -0.621834 |
| C | -3.706373 | 0.759638 | -0.008452 |
| C | -4.875989 | -0.066145 | -0.392325 |
| H | -5.282519 | 0.277609 | -1.352278 |
| H | -5.664073 | 0.013919 | 0.352640 |

| | | | |
|---|---|---|---|
| H | -3.831481 | 1.485534 | 0.782531 |
| H | -4.604123 | -1.116748 | -0.522010 |
| H | 1.254393 | 1.396044 | 1.887942 |
| C | -2.289607 | -0.403093 | -1.705352 |
| H | -1.350247 | -0.337277 | -2.241843 |
| H | -2.375961 | -1.407288 | -1.281371 |
| H | -3.107023 | -0.270720 | -2.416593 |

**13G-*E***

Imaginary frequency: None

Electronic energies: -1353.749916

Free energies: -1353.289125

Corrected Free energies: -1353.285461

| | | | |
|---|---|---|---|
| C | -0.455378 | 0.376231 | -1.488358 |
| C | 0.369202 | 1.484723 | -2.176102 |
| C | -0.143601 | 2.817326 | -1.599674 |
| C | -1.441784 | 2.474965 | -0.854244 |
| H | 0.189051 | 1.436732 | -3.251679 |
| H | 1.439069 | 1.365256 | -2.014271 |
| H | -0.327857 | 3.540208 | -2.394692 |
| H | 0.588592 | 3.259329 | -0.924952 |
| H | -2.290878 | 3.071140 | -1.201704 |
| H | -1.338475 | 2.637022 | 0.227232 |
| C | 0.281727 | -0.225436 | -0.248170 |
| O | 0.546359 | 0.855556 | 0.629638 |
| Si | 1.856581 | 1.654708 | 1.292914 |
| C | 2.588920 | 0.745301 | 2.765003 |
| H | 3.033392 | 1.478598 | 3.444379 |
| H | 3.365921 | 0.031884 | 2.485568 |
| H | 1.810354 | 0.211091 | 3.317528 |
| C | 1.114408 | 3.241084 | 1.953331 |
| H | 0.650780 | 3.851867 | 1.176643 |
| H | 1.889200 | 3.840339 | 2.439780 |
| H | 0.351016 | 3.011819 | 2.702257 |
| C | 3.209194 | 1.996621 | 0.041000 |
| H | 4.046229 | 2.476529 | 0.557806 |
| H | 2.885287 | 2.667818 | -0.757802 |
| H | 3.580345 | 1.072078 | -0.410165 |
| C | 1.572578 | -0.965978 | -0.627651 |
| C | 2.313522 | -1.531627 | 0.414696 |
| C | 2.033396 | -1.138287 | -1.932113 |
| C | 3.511196 | -2.189745 | 0.174432 |
| H | 1.931738 | -1.464449 | 1.427322 |

| | | | |
|---|---|---|---|
| C | 3.230462 | -1.810385 | -2.180358 |
| H | 1.474218 | -0.756455 | -2.776454 |
| C | 3.980922 | -2.323131 | -1.130731 |
| H | 4.071410 | -2.609472 | 1.001980 |
| H | 3.572701 | -1.928631 | -3.201600 |
| H | 4.914224 | -2.837503 | -1.326004 |
| C | -0.647897 | -1.211619 | 0.466852 |
| C | -0.751138 | -2.534987 | 0.030722 |
| C | -1.441682 | -0.790274 | 1.531012 |
| C | -1.626936 | -3.420419 | 0.648000 |
| H | -0.137387 | -2.880492 | -0.794581 |
| C | -2.323731 | -1.673895 | 2.147526 |
| H | -1.371443 | 0.237705 | 1.863701 |
| C | -2.419427 | -2.991227 | 1.709425 |
| H | -1.690794 | -4.444761 | 0.299977 |
| H | -2.938097 | -1.331325 | 2.972443 |
| H | -3.103032 | -3.679369 | 2.192806 |
| N | -1.691606 | 1.077145 | -1.164869 |
| H | -0.659088 | -0.447141 | -2.175612 |
| C | -2.925274 | 0.517187 | -0.857996 |
| C | -3.869209 | 1.182691 | -0.159731 |
| C | -5.238332 | 0.610023 | 0.107373 |
| H | -5.853360 | 0.536932 | -0.797861 |
| H | -5.783523 | 1.236427 | 0.814674 |
| H | -3.648041 | 2.156076 | 0.258765 |
| H | -5.186942 | -0.397575 | 0.535295 |
| C | -3.245745 | -0.852054 | -1.407592 |
| H | -2.504896 | -1.209417 | -2.119098 |
| H | -3.321825 | -1.584146 | -0.599256 |
| H | -4.212020 | -0.821020 | -1.916137 |

**13G-*Z***

Imaginary frequency: None

Electronic energies: -1353.749875

Free energies: -1353.291087

Corrected Free energies: -1353.286561

| | | | |
|---|---|---|---|
| C | 0.548435 | -0.196086 | -1.455821 |
| C | -0.145034 | -1.325050 | -2.243915 |
| C | 0.515105 | -2.635541 | -1.768408 |
| C | 1.705177 | -2.215030 | -0.879934 |
| H | 0.033817 | -1.168884 | -3.309814 |
| H | -1.222945 | -1.335892 | -2.087020 |
| H | 0.855267 | -3.227149 | -2.619026 |

| | | | |
|---|---|---|---|
| H | -0.190135 | -3.246637 | -1.204726 |
| H | 2.642585 | -2.690380 | -1.178259 |
| H | 1.501344 | -2.475129 | 0.163455 |
| C | -0.265274 | 0.251727 | -0.201618 |
| O | -0.572430 | -0.930400 | 0.515298 |
| Si | -1.908285 | -1.743583 | 1.099810 |
| C | -2.666472 | -0.919400 | 2.607484 |
| H | -3.168001 | -1.683243 | 3.209184 |
| H | -3.401926 | -0.154166 | 2.354357 |
| H | -1.892040 | -0.461879 | 3.230024 |
| C | -1.194011 | -3.380723 | 1.656665 |
| H | -0.720716 | -3.924811 | 0.836784 |
| H | -1.977718 | -4.015844 | 2.078446 |
| H | -0.440333 | -3.218056 | 2.432392 |
| C | -3.215662 | -1.989400 | -0.219669 |
| H | -4.082561 | -2.488296 | 0.223945 |
| H | -2.852889 | -2.617340 | -1.037702 |
| H | -3.551545 | -1.035565 | -0.636224 |
| C | -1.536205 | 1.031215 | -0.557963 |
| C | -2.284785 | 1.567594 | 0.494096 |
| C | -1.994664 | 1.223426 | -1.861090 |
| C | -3.482407 | 2.229676 | 0.261108 |
| H | -1.914158 | 1.466970 | 1.508548 |
| C | -3.191254 | 1.898508 | -2.100704 |
| H | -1.433798 | 0.851721 | -2.709060 |
| C | -3.945034 | 2.391008 | -1.043204 |
| H | -4.049462 | 2.628157 | 1.094456 |
| H | -3.531874 | 2.034670 | -3.120289 |
| H | -4.877941 | 2.908664 | -1.231747 |
| C | 0.649573 | 1.121738 | 0.661392 |
| C | 0.960243 | 2.422924 | 0.261935 |
| C | 1.250750 | 0.605524 | 1.805622 |
| C | 1.870073 | 3.186884 | 0.984306 |
| H | 0.487496 | 2.843489 | -0.620814 |
| C | 2.155277 | 1.371872 | 2.535935 |
| H | 1.011831 | -0.405509 | 2.111203 |
| C | 2.474208 | 2.661140 | 2.124112 |
| H | 2.105896 | 4.193761 | 0.659712 |
| H | 2.618086 | 0.955010 | 3.423317 |
| H | 3.182213 | 3.256015 | 2.688971 |
| N | 1.821874 | -0.774684 | -1.077276 |
| H | 0.710422 | 0.689008 | -2.073102 |
| C | 3.041732 | -0.106542 | -1.157948 |
| C | 4.106862 | -0.419322 | -0.397271 |

| | | | |
|---|---|---|---|
| C | 3.147527 | 0.982926 | -2.200350 |
| H | 2.782710 | 0.635323 | -3.171407 |
| H | 2.564964 | 1.864545 | -1.920882 |
| H | 4.186375 | 1.294003 | -2.304211 |
| H | 5.040699 | 0.076556 | -0.640096 |
| C | 4.119666 | -1.346964 | 0.786135 |
| H | 3.128373 | -1.421093 | 1.234735 |
| H | 4.454226 | -2.361153 | 0.540684 |
| H | 4.801086 | -0.963339 | 1.550007 |

**13G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1353.568083

Free energies: -1353.107669

Corrected Free energies: -1353.103672

| | | | |
|---|---|---|---|
| C | 0.494704 | -0.269019 | -1.551974 |
| C | -0.173574 | -1.496666 | -2.210629 |
| C | 0.845604 | -2.640102 | -2.124058 |
| C | 1.758908 | -2.247831 | -0.969787 |
| H | -0.435701 | -1.287028 | -3.246299 |
| H | -1.088216 | -1.748277 | -1.676625 |
| H | 1.430939 | -2.699610 | -3.042687 |
| H | 0.376574 | -3.607486 | -1.949885 |
| H | 2.755133 | -2.671736 | -1.051939 |
| H | 1.311482 | -2.487962 | -0.005456 |
| C | -0.278166 | 0.249259 | -0.285883 |
| O | -0.373951 | -0.869081 | 0.567463 |
| Si | -1.571702 | -1.717930 | 1.396912 |
| C | -2.069864 | -0.822425 | 2.965534 |
| H | -2.384498 | -1.554356 | 3.714692 |
| H | -2.898969 | -0.130734 | 2.806872 |
| H | -1.225925 | -0.262650 | 3.378288 |
| C | -0.684915 | -3.304708 | 1.828860 |
| H | -0.433694 | -3.876542 | 0.931289 |
| H | -1.316156 | -3.935379 | 2.460349 |
| H | 0.239425 | -3.098842 | 2.375768 |
| C | -3.072379 | -2.090903 | 0.341488 |
| H | -3.770417 | -2.678056 | 0.947068 |
| H | -2.815717 | -2.693747 | -0.533270 |
| H | -3.592785 | -1.190474 | 0.007049 |
| C | -1.661890 | 0.808128 | -0.634415 |
| C | -2.396046 | 1.364065 | 0.419051 |
| C | -2.234316 | 0.782335 | -1.903077 |

| | | | |
|---|---|---|---|
| C | -3.689607 | 1.824295 | 0.225279 |
| H | -1.939793 | 1.442894 | 1.399907 |
| C | -3.531847 | 1.253938 | -2.103368 |
| H | -1.691032 | 0.402845 | -2.757575 |
| C | -4.267933 | 1.760128 | -1.041315 |
| H | -4.243095 | 2.241436 | 1.058173 |
| H | -3.961539 | 1.220685 | -3.097228 |
| H | -5.277934 | 2.118692 | -1.198674 |
| C | 0.548369 | 1.339036 | 0.405086 |
| C | 0.504891 | 2.658226 | -0.051738 |
| C | 1.389901 | 1.016944 | 1.468286 |
| C | 1.299651 | 3.634878 | 0.536593 |
| H | -0.155456 | 2.926561 | -0.869598 |
| C | 2.194727 | 1.992767 | 2.051684 |
| H | 1.408418 | -0.001472 | 1.837898 |
| C | 2.153441 | 3.303126 | 1.586171 |
| H | 1.254063 | 4.654734 | 0.174011 |
| H | 2.847231 | 1.727930 | 2.875330 |
| H | 2.775257 | 4.063573 | 2.042936 |
| N | 1.820694 | -0.776052 | -1.114724 |
| H | 0.628805 | 0.552448 | -2.252081 |
| C | 2.922673 | -0.060570 | -0.979226 |
| C | 4.052308 | -0.537055 | -0.261649 |
| C | 3.067512 | 1.318270 | -1.556354 |
| H | 2.275121 | 1.595754 | -2.243314 |
| H | 3.110538 | 2.052695 | -0.749025 |
| H | 4.021067 | 1.350858 | -2.086816 |
| H | 4.963636 | 0.023688 | -0.434236 |
| C | 4.102073 | -1.580539 | 0.791648 |
| H | 3.121444 | -1.869834 | 1.162704 |
| H | 4.618168 | -2.477054 | 0.427411 |
| H | 4.698847 | -1.200979 | 1.624349 |

**13G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1353.572815

Free energies: -1353.111808

Corrected Free energies: -1353.108080

| | | | |
|---|---|---|---|
| C | -0.440509 | 0.353255 | -1.506201 |
| C | 0.334516 | 1.486635 | -2.194974 |
| C | -0.190750 | 2.803704 | -1.598384 |
| C | -1.461877 | 2.450011 | -0.820625 |
| H | 0.143441 | 1.444797 | -3.267677 |

| | | | |
|---|---|---|---|
| H | 1.406200 | 1.382625 | -2.040690 |
| H | -0.411065 | 3.525174 | -2.383074 |
| H | 0.544368 | 3.251801 | -0.933733 |
| H | -2.324111 | 3.015650 | -1.166450 |
| H | -1.337421 | 2.585787 | 0.256086 |
| C | 0.294831 | -0.220882 | -0.244015 |
| O | 0.556998 | 0.892199 | 0.581347 |
| Si | 1.877851 | 1.656579 | 1.294142 |
| C | 2.546925 | 0.714694 | 2.770349 |
| H | 2.974312 | 1.433993 | 3.474978 |
| H | 3.327106 | -0.001126 | 2.507591 |
| H | 1.744603 | 0.181508 | 3.288589 |
| C | 1.131976 | 3.245233 | 1.938903 |
| H | 0.736167 | 3.891015 | 1.152845 |
| H | 1.891214 | 3.812184 | 2.484612 |
| H | 0.319880 | 3.020398 | 2.636010 |
| C | 3.237247 | 1.978979 | 0.049183 |
| H | 4.074107 | 2.462194 | 0.562611 |
| H | 2.916031 | 2.646432 | -0.754471 |
| H | 3.608061 | 1.050911 | -0.394530 |
| C | 1.575607 | -0.967245 | -0.638649 |
| C | 2.313041 | -1.541961 | 0.400904 |
| C | 2.033277 | -1.127542 | -1.945182 |
| C | 3.508545 | -2.200486 | 0.153115 |
| H | 1.932102 | -1.485219 | 1.414075 |
| C | 3.228675 | -1.799865 | -2.198837 |
| H | 1.477852 | -0.740891 | -2.790030 |
| C | 3.977162 | -2.322728 | -1.153297 |
| H | 4.067082 | -2.629788 | 0.976481 |
| H | 3.569701 | -1.910282 | -3.221013 |
| H | 4.908864 | -2.837854 | -1.353147 |
| C | -0.639446 | -1.178175 | 0.504680 |
| C | -0.746382 | -2.516230 | 0.118904 |
| C | -1.439021 | -0.708253 | 1.546965 |
| C | -1.643578 | -3.365631 | 0.755272 |
| H | -0.123728 | -2.900205 | -0.681970 |
| C | -2.344941 | -1.556804 | 2.178775 |
| H | -1.347339 | 0.324579 | 1.862849 |
| C | -2.451022 | -2.886787 | 1.783994 |
| H | -1.712692 | -4.401833 | 0.446698 |
| H | -2.963515 | -1.177716 | 2.983698 |
| H | -3.152098 | -3.548081 | 2.278829 |
| N | -1.694891 | 1.012849 | -1.091282 |
| H | -0.665189 | -0.463117 | -2.188116 |

| | | | |
|---|---|---|---|
| C | -2.873182 | 0.425376 | -0.923951 |
| C | -3.903249 | 1.131272 | -0.260528 |
| C | -5.257308 | 0.599863 | 0.008521 |
| H | -6.004280 | 1.281218 | -0.412123 |
| H | -5.429867 | 0.593685 | 1.090080 |
| H | -3.690710 | 2.117632 | 0.129020 |
| H | -5.427941 | -0.399834 | -0.381173 |
| C | -3.153950 | -0.963427 | -1.411380 |
| H | -2.337201 | -1.400839 | -1.972535 |
| H | -3.378709 | -1.613565 | -0.562305 |
| H | -4.036411 | -0.928900 | -2.053070 |

**14G-*E***

Imaginary frequency: None

Electronic energies: -2701.932684

Free energies: -2701.472881

Corrected Free energies: -2701.463030

| | | | |
|---|---|---|---|
| C | 0.047667 | -1.582920 | -1.666731 |
| C | -0.677466 | -2.940290 | -1.758885 |
| C | 0.354831 | -3.974226 | -1.252631 |
| C | 1.696729 | -3.218076 | -1.180653 |
| H | -0.928884 | -3.123745 | -2.804908 |
| H | -1.594926 | -2.973980 | -1.172522 |
| H | 0.423521 | -4.817495 | -1.940179 |
| H | 0.076235 | -4.355278 | -0.271874 |
| H | 2.514139 | -3.744158 | -1.680166 |
| H | 1.994587 | -3.052367 | -0.136132 |
| C | -0.217481 | -0.887868 | -0.269815 |
| O | -0.302646 | -1.917263 | 0.692058 |
| Si | -1.197718 | -2.193112 | 2.090649 |
| C | -0.714995 | -1.003060 | 3.454709 |
| H | -1.104780 | -1.381849 | 4.404494 |
| H | -1.126256 | -0.001888 | 3.311267 |
| H | 0.371166 | -0.921348 | 3.550446 |
| C | -0.692158 | -3.930270 | 2.546392 |
| H | -1.071326 | -4.651695 | 1.818344 |
| H | -1.087702 | -4.201481 | 3.528490 |
| H | 0.396963 | -4.018581 | 2.580588 |
| C | -3.042770 | -2.113779 | 1.773213 |
| H | -3.560593 | -2.598097 | 2.606627 |
| H | -3.314162 | -2.648681 | 0.858617 |
| H | -3.419493 | -1.090841 | 1.696927 |
| C | -1.517310 | -0.071784 | -0.272611 |

| | | | |
|---|---|---|---|
| C | -1.696516 | 0.934694 | 0.677468 |
| C | -2.581342 | -0.371492 | -1.120896 |
| C | -2.914942 | 1.589576 | 0.799170 |
| H | -0.876921 | 1.215692 | 1.330402 |
| C | -3.796267 | 0.291940 | -0.989409 |
| H | -2.484993 | -1.126104 | -1.891500 |
| C | -3.984447 | 1.271892 | -0.026085 |
| H | -4.934600 | 1.780340 | 0.072358 |
| C | 0.980094 | 0.000036 | 0.056796 |
| C | 1.176933 | 1.203097 | -0.618137 |
| C | 1.949689 | -0.433524 | 0.951627 |
| C | 2.351540 | 1.920032 | -0.440770 |
| H | 0.416155 | 1.581777 | -1.293137 |
| C | 3.112882 | 0.304368 | 1.133921 |
| H | 1.805022 | -1.361633 | 1.489603 |
| C | 3.338355 | 1.476894 | 0.430690 |
| H | 4.251188 | 2.042849 | 0.568540 |
| N | 1.426052 | -1.980253 | -1.891745 |
| H | -0.263072 | -0.885983 | -2.449134 |
| C | 2.445520 | -1.111658 | -2.310726 |
| C | 3.688587 | -1.196374 | -1.810139 |
| H | 3.860084 | -1.908740 | -1.008596 |
| C | -4.933616 | -0.127631 | -1.874439 |
| C | -3.066533 | 2.613579 | 1.885755 |
| C | 4.176143 | -0.236769 | 2.040994 |
| C | 2.589393 | 3.155278 | -1.256510 |
| F | 4.947280 | -1.141066 | 1.409588 |
| F | 3.656929 | -0.857649 | 3.109872 |
| F | 4.996597 | 0.720106 | 2.491898 |
| F | 3.392599 | 4.027121 | -0.634957 |
| F | 1.449552 | 3.794709 | -1.549462 |
| F | 3.176793 | 2.860399 | -2.431447 |
| F | -3.095802 | 2.032460 | 3.097809 |
| F | -2.041997 | 3.476788 | 1.902277 |
| F | -4.190900 | 3.324825 | 1.763326 |
| F | -5.936598 | 0.756294 | -1.868062 |
| F | -4.542140 | -0.284498 | -3.146637 |
| F | -5.443949 | -1.306789 | -1.482996 |
| C | 4.885435 | -0.380833 | -2.214111 |
| H | 5.564784 | -0.932643 | -2.873001 |
| H | 4.611870 | 0.549508 | -2.712233 |
| H | 5.458431 | -0.112550 | -1.321918 |
| C | 2.054352 | -0.194448 | -3.444038 |
| H | 2.920623 | 0.310302 | -3.864217 |

| | | | |
|---|---|---|---|
| H | 1.580914 | -0.784027 | -4.233838 |
| H | 1.339783 | 0.573539 | -3.142447 |

**14G-*Z***

Imaginary frequency: -28.6735

Electronic energies: -2701.931539

Free energies: -2701.471947

Corrected Free energies: -2701.462143

| | | | |
|---|---|---|---|
| C | 0.114006 | -1.686891 | -1.495635 |
| C | -0.673378 | -3.013966 | -1.522393 |
| C | 0.330139 | -4.103974 | -1.085626 |
| C | 1.687181 | -3.390698 | -0.926785 |
| H | -1.023497 | -3.194853 | -2.540284 |
| H | -1.542496 | -2.991240 | -0.866074 |
| H | 0.395852 | -4.886791 | -1.841849 |
| H | 0.026927 | -4.568684 | -0.148056 |
| H | 2.509370 | -3.923827 | -1.408632 |
| H | 1.924245 | -3.277120 | 0.136374 |
| C | -0.152057 | -0.871761 | -0.177828 |
| O | -0.147595 | -1.805614 | 0.879847 |
| Si | -1.083029 | -2.087186 | 2.250884 |
| C | -0.795530 | -0.768411 | 3.553162 |
| H | -1.027724 | -1.184009 | 4.538076 |
| H | -1.428613 | 0.109649 | 3.412246 |
| H | 0.248787 | -0.444059 | 3.567805 |
| C | -0.436443 | -3.732143 | 2.847835 |
| H | -0.681872 | -4.529838 | 2.142905 |
| H | -0.877567 | -3.988584 | 3.814525 |
| H | 0.649720 | -3.703063 | 2.966087 |
| C | -2.909169 | -2.207645 | 1.846277 |
| H | -3.422344 | -2.670977 | 2.694484 |
| H | -3.094171 | -2.832540 | 0.968123 |
| H | -3.368064 | -1.230555 | 1.674574 |
| C | -1.479184 | -0.104246 | -0.212322 |
| C | -1.685123 | 0.919880 | 0.714475 |
| C | -2.523827 | -0.434658 | -1.071241 |
| C | -2.914180 | 1.557008 | 0.808314 |
| H | -0.875617 | 1.227990 | 1.368385 |
| C | -3.751462 | 0.212675 | -0.967729 |
| H | -2.404732 | -1.199551 | -1.828359 |
| C | -3.968015 | 1.205501 | -0.024922 |
| H | -4.926769 | 1.701410 | 0.050873 |
| C | 1.012576 | 0.097653 | -0.004028 |

| | | | |
|---|---|---|---|
| C | 1.119160 | 1.212885 | -0.831008 |
| C | 2.036428 | -0.178835 | 0.893729 |
| C | 2.255049 | 2.009713 | -0.785854 |
| H | 0.319587 | 1.459694 | -1.522331 |
| C | 3.158280 | 0.640075 | 0.943290 |
| H | 1.960628 | -1.047024 | 1.536808 |
| C | 3.289726 | 1.732098 | 0.097451 |
| H | 4.174930 | 2.355390 | 0.127737 |
| N | 1.493553 | -2.111299 | -1.595213 |
| H | -0.139170 | -1.040761 | -2.339104 |
| C | 2.478513 | -1.433778 | -2.316290 |
| C | 3.789070 | -1.455067 | -2.013175 |
| C | -4.866914 | -0.238503 | -1.864860 |
| C | -3.096364 | 2.605960 | 1.866329 |
| C | 4.236198 | 0.366505 | 1.950468 |
| C | 2.397797 | 3.139406 | -1.761274 |
| F | 4.258130 | -0.915530 | 2.337822 |
| F | 4.075779 | 1.103549 | 3.061498 |
| F | 5.454037 | 0.658672 | 1.469371 |
| F | 3.163667 | 4.127904 | -1.282949 |
| F | 1.214397 | 3.671306 | -2.093021 |
| F | 2.969885 | 2.728098 | -2.907180 |
| F | -3.179175 | 2.052728 | 3.089520 |
| F | -2.063880 | 3.458424 | 1.903830 |
| F | -4.207737 | 3.325009 | 1.685813 |
| F | -5.900663 | 0.609048 | -1.858392 |
| F | -4.460973 | -0.369803 | -3.135599 |
| F | -5.336790 | -1.439007 | -1.487935 |
| C | 2.003942 | -0.696931 | -3.548065 |
| H | 2.860682 | -0.381731 | -4.142300 |
| H | 1.361073 | -1.335191 | -4.160984 |
| H | 1.435398 | 0.202271 | -3.297496 |
| C | 4.444958 | -2.017591 | -0.783466 |
| H | 5.228393 | -1.336261 | -0.438577 |
| H | 3.738701 | -2.142772 | 0.035473 |
| H | 4.924769 | -2.985554 | -0.965060 |
| H | 4.453507 | -0.995941 | -2.738023 |

**14G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -2701.741458

Free energies: -2701.283139

Corrected Free energies: -2701.272685

| | | | |
|---|---|---|---|
| C | 0.277541 | -1.413095 | -1.687556 |
| C | -0.541982 | -2.682223 | -1.966736 |
| C | 0.361683 | -3.880819 | -1.626436 |
| C | 1.740172 | -3.306531 | -1.291376 |
| H | -0.825483 | -2.699511 | -3.018913 |
| H | -1.455009 | -2.696967 | -1.375268 |
| H | 0.430018 | -4.561393 | -2.472863 |
| H | -0.026913 | -4.444114 | -0.779435 |
| H | 2.541030 | -3.803820 | -1.830036 |
| H | 1.931239 | -3.338499 | -0.218796 |
| C | -0.024311 | -0.790702 | -0.281990 |
| O | 0.184955 | -1.814548 | 0.651087 |
| Si | -0.651694 | -2.650750 | 1.864382 |
| C | -0.823210 | -1.612923 | 3.413069 |
| H | -0.825605 | -2.278931 | 4.280444 |
| H | -1.748323 | -1.035357 | 3.442117 |
| H | 0.022604 | -0.928780 | 3.525719 |
| C | 0.492996 | -4.079673 | 2.219329 |
| H | 0.612664 | -4.751208 | 1.366498 |
| H | 0.100849 | -4.668173 | 3.052972 |
| H | 1.480937 | -3.710389 | 2.507961 |
| C | -2.324597 | -3.225408 | 1.258344 |
| H | -2.822231 | -3.754831 | 2.076580 |
| H | -2.245302 | -3.921589 | 0.419789 |
| H | -2.971773 | -2.394812 | 0.963416 |
| C | -1.446912 | -0.222586 | -0.209490 |
| C | -1.819232 | 0.390542 | 0.988967 |
| C | -2.368753 | -0.265231 | -1.248572 |
| C | -3.102150 | 0.883834 | 1.160774 |
| H | -1.090917 | 0.501054 | 1.785014 |
| C | -3.653966 | 0.242095 | -1.064846 |
| H | -2.118917 | -0.682085 | -2.216225 |
| C | -4.040979 | 0.806326 | 0.137888 |
| H | -5.040809 | 1.198244 | 0.271476 |
| C | 0.979789 | 0.334868 | -0.012509 |
| C | 0.776394 | 1.616868 | -0.519984 |
| C | 2.153103 | 0.061202 | 0.681479 |
| C | 1.745832 | 2.596280 | -0.350390 |
| H | -0.136699 | 1.858782 | -1.053138 |
| C | 3.123751 | 1.047443 | 0.824970 |
| H | 2.304747 | -0.923435 | 1.110132 |
| C | 2.934888 | 2.323443 | 0.314902 |
| H | 3.691262 | 3.087957 | 0.436366 |
| N | 1.680024 | -1.889026 | -1.719982 |

| | | | |
|---|---|---|---|
| H | 0.127518 | -0.654799 | -2.450992 |
| C | 2.728301 | -1.183844 | -2.116999 |
| C | 4.073695 | -1.598516 | -1.923838 |
| C | -4.630659 | 0.121270 | -2.200104 |
| C | -3.483291 | 1.477485 | 2.487091 |
| C | 4.410350 | 0.674099 | 1.502079 |
| C | 1.530265 | 3.939562 | -0.985691 |
| F | 5.116831 | -0.183381 | 0.740448 |
| F | 4.197360 | 0.057586 | 2.670783 |
| F | 5.191830 | 1.730071 | 1.735453 |
| F | 2.293660 | 4.888645 | -0.436071 |
| F | 0.255898 | 4.336953 | -0.890501 |
| F | 1.827766 | 3.902505 | -2.295277 |
| F | -3.812641 | 0.520535 | 3.371597 |
| F | -2.475036 | 2.171205 | 3.028122 |
| F | -4.534378 | 2.295930 | 2.388883 |
| F | -5.721546 | 0.868477 | -2.012783 |
| F | -4.079595 | 0.493027 | -3.363682 |
| F | -5.038713 | -1.147329 | -2.356572 |
| C | 2.585958 | 0.145457 | -2.808226 |
| H | 2.993761 | 0.933372 | -2.170686 |
| H | 3.193225 | 0.113738 | -3.714505 |
| H | 1.570968 | 0.408807 | -3.082199 |
| H | 4.786560 | -0.981879 | -2.459222 |
| C | 4.660519 | -2.665076 | -1.074457 |
| H | 4.824266 | -3.574468 | -1.666846 |
| H | 5.640506 | -2.333499 | -0.731916 |
| H | 4.055635 | -2.926228 | -0.209379 |

**14G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -2701.747559

Free energies: -2701.285944

Corrected Free energies: -2701.276604

| | | | |
|---|---|---|---|
| C | 0.225354 | -1.515665 | -1.654731 |
| C | -0.609856 | -2.782147 | -1.893726 |
| C | 0.241852 | -3.966306 | -1.404797 |
| C | 1.658341 | -3.424523 | -1.189771 |
| H | -0.820246 | -2.868890 | -2.959859 |
| H | -1.560029 | -2.738582 | -1.364804 |
| H | 0.247933 | -4.767584 | -2.141089 |
| H | -0.150919 | -4.372388 | -0.475485 |
| H | 2.397808 | -3.966449 | -1.774523 |

| | | | |
|---|---|---|---|
| H | 1.944711 | -3.427778 | -0.135871 |
| C | -0.074527 | -0.847994 | -0.266664 |
| O | 0.081277 | -1.863738 | 0.686107 |
| Si | -0.769397 | -2.580117 | 1.963691 |
| C | -0.895670 | -1.440779 | 3.445455 |
| H | -0.911285 | -2.054244 | 4.350793 |
| H | -1.800194 | -0.831023 | 3.448047 |
| H | -0.025378 | -0.781314 | 3.511461 |
| C | 0.333330 | -4.014433 | 2.419289 |
| H | 0.447667 | -4.744431 | 1.615747 |
| H | -0.081128 | -4.535084 | 3.286635 |
| H | 1.326529 | -3.648354 | 2.693992 |
| C | -2.460400 | -3.130549 | 1.387709 |
| H | -2.970583 | -3.629229 | 2.217056 |
| H | -2.399792 | -3.844473 | 0.562295 |
| H | -3.084111 | -2.288679 | 1.074238 |
| C | -1.477379 | -0.228294 | -0.234444 |
| C | -1.843702 | 0.446992 | 0.932442 |
| C | -2.389888 | -0.284148 | -1.281289 |
| C | -3.110810 | 0.990514 | 1.066707 |
| H | -1.122260 | 0.568117 | 1.733041 |
| C | -3.658863 | 0.274142 | -1.136131 |
| H | -2.144527 | -0.748775 | -2.228159 |
| C | -4.040173 | 0.902085 | 0.036259 |
| H | -5.027451 | 1.332713 | 0.140976 |
| C | 0.966258 | 0.242249 | 0.009967 |
| C | 0.819901 | 1.534204 | -0.493410 |
| C | 2.119557 | -0.080287 | 0.716981 |
| C | 1.824594 | 2.473212 | -0.302274 |
| H | -0.073792 | 1.815434 | -1.040428 |
| C | 3.126821 | 0.865078 | 0.880501 |
| H | 2.232468 | -1.076999 | 1.129539 |
| C | 2.993335 | 2.150860 | 0.378117 |
| H | 3.776935 | 2.885279 | 0.513109 |
| N | 1.612525 | -2.021083 | -1.666495 |
| H | 0.095204 | -0.779240 | -2.443602 |
| C | 2.694095 | -1.338327 | -2.022002 |
| C | 3.974503 | -1.865972 | -1.731412 |
| H | 4.045181 | -2.804381 | -1.199206 |
| C | -4.621119 | 0.144125 | -2.282534 |
| C | -3.484739 | 1.652656 | 2.362223 |
| C | 4.372442 | 0.441167 | 1.603717 |
| C | 1.677945 | 3.828587 | -0.931408 |
| F | 4.937084 | -0.622677 | 1.001832 |

| | | | |
|---|---|---|---|
| F | 4.113342 | 0.069754 | 2.863774 |
| F | 5.291718 | 1.407063 | 1.648055 |
| F | 2.438140 | 4.749001 | -0.330182 |
| F | 0.412307 | 4.261190 | -0.897480 |
| F | 2.043475 | 3.798929 | -2.223818 |
| F | -3.834715 | 0.744195 | 3.289000 |
| F | -2.464845 | 2.351100 | 2.874800 |
| F | -4.519408 | 2.485661 | 2.222191 |
| F | -5.712638 | 0.895252 | -2.116804 |
| F | -4.053832 | 0.504167 | -3.442261 |
| F | -5.028967 | -1.125230 | -2.433142 |
| C | 5.236877 | -1.191331 | -2.114532 |
| H | 5.469516 | -1.414217 | -3.164423 |
| H | 5.174721 | -0.105477 | -2.023171 |
| H | 6.061751 | -1.556831 | -1.506760 |
| C | 2.618652 | -0.014760 | -2.720600 |
| H | 3.034436 | 0.770107 | -2.084461 |
| H | 3.239534 | -0.068703 | -3.617351 |
| H | 1.615643 | 0.272828 | -3.014361 |

**15G-*E***

Imaginary frequency: None

Electronic energies: -694.444468

Free energies: -694.131962

Corrected Free energies: -694.129811

| | | | |
|---|---|---|---|
| C | -1.449812 | 1.592541 | 0.203227 |
| C | 0.051239 | 1.560755 | 0.449464 |
| C | -0.679145 | -0.481278 | -0.579681 |
| H | 0.214001 | 1.395249 | 1.525267 |
| H | -0.699019 | -0.849032 | -1.612616 |
| N | 0.456665 | 0.432822 | -0.378103 |
| C | 1.796661 | 0.007021 | -0.436687 |
| C | 2.690826 | 0.340977 | 0.505293 |
| C | 4.170621 | 0.095415 | 0.440546 |
| H | 4.503786 | -0.512011 | 1.287483 |
| H | 4.470835 | -0.412684 | -0.475424 |
| H | 4.724976 | 1.037722 | 0.492443 |
| H | 2.339956 | 0.874051 | 1.384230 |
| N | -1.802033 | 0.435042 | -0.391882 |
| O | -2.198813 | 2.520261 | 0.454964 |
| C | -3.115836 | 0.281345 | -0.993930 |
| H | -3.877462 | 0.038321 | -0.250727 |
| H | -3.392189 | 1.219386 | -1.478042 |

| | | | |
|---|---|---|---|
| H | -3.080110 | -0.512575 | -1.737792 |
| C | 0.680729 | 2.883618 | 0.032330 |
| H | 1.748358 | 2.901600 | 0.246758 |
| H | 0.532725 | 3.039636 | -1.038289 |
| H | 0.194437 | 3.693916 | 0.576999 |
| C | -0.743155 | -1.710526 | 0.376634 |
| C | -0.538853 | -1.273844 | 1.828880 |
| H | -1.270176 | -0.515454 | 2.122953 |
| H | -0.666368 | -2.132561 | 2.493182 |
| H | 0.466918 | -0.874515 | 1.981515 |
| C | -2.110476 | -2.392420 | 0.236935 |
| H | -2.331846 | -2.640185 | -0.805916 |
| H | -2.109112 | -3.324944 | 0.806245 |
| H | -2.915903 | -1.768473 | 0.626861 |
| C | 0.331253 | -2.738273 | -0.004260 |
| H | 0.205596 | -3.631889 | 0.612654 |
| H | 0.237088 | -3.041258 | -1.051389 |
| H | 1.340340 | -2.360538 | 0.162587 |
| C | 2.174823 | -0.703527 | -1.717232 |
| H | 2.596979 | 0.015389 | -2.425168 |
| H | 2.911523 | -1.488243 | -1.546911 |
| H | 1.309493 | -1.158875 | -2.195844 |

**15G-*Z***

Imaginary frequency: None

Electronic energies: -694.447276

Free energies: -694.132949

Corrected Free energies: -694.131348

| | | | |
|---|---|---|---|
| C | -0.618112 | 1.913904 | 0.255288 |
| C | 0.768950 | 1.336631 | 0.486033 |
| C | -0.699477 | -0.303686 | -0.516231 |
| H | 0.949120 | 1.303576 | 1.568912 |
| H | -0.735160 | -0.604208 | -1.571550 |
| N | 0.666570 | -0.001838 | -0.095797 |
| C | 1.780908 | -0.604133 | -0.718195 |
| C | 2.902229 | -0.818864 | -0.016746 |
| N | -1.367581 | 0.985189 | -0.368262 |
| O | -0.971690 | 3.045737 | 0.541321 |
| C | -2.697529 | 1.299244 | -0.852135 |
| H | -3.459110 | 1.150456 | -0.082452 |
| H | -2.710170 | 2.347575 | -1.150660 |
| H | -2.930081 | 0.672531 | -1.712718 |
| C | 1.798508 | 2.256118 | -0.165076 |

| | | | |
|---|---|---|---|
| H | 2.815210 | 1.908399 | 0.012135 |
| H | 1.629307 | 2.308352 | -1.243793 |
| H | 1.684234 | 3.254883 | 0.258260 |
| C | -1.341236 | -1.438109 | 0.333662 |
| C | -1.475442 | -0.988136 | 1.788783 |
| H | -2.164554 | -0.144675 | 1.885610 |
| H | -1.859272 | -1.808356 | 2.400744 |
| H | -0.503114 | -0.691031 | 2.192110 |
| C | -2.714274 | -1.826782 | -0.229408 |
| H | -2.653734 | -2.046169 | -1.300114 |
| H | -3.072837 | -2.727684 | 0.274959 |
| H | -3.462863 | -1.048988 | -0.078171 |
| C | -0.429677 | -2.668975 | 0.259462 |
| H | -0.888284 | -3.495701 | 0.807864 |
| H | -0.288887 | -2.996333 | -0.775562 |
| H | 0.550324 | -2.466948 | 0.695219 |
| C | 1.681141 | -0.942871 | -2.183885 |
| H | 1.337991 | -0.077504 | -2.759184 |
| H | 2.655993 | -1.253281 | -2.558540 |
| H | 0.980411 | -1.760453 | -2.371210 |
| C | 3.023122 | -0.594712 | 1.461642 |
| H | 3.333636 | 0.427476 | 1.711622 |
| H | 2.060706 | -0.769951 | 1.950893 |
| H | 3.762796 | -1.269305 | 1.895936 |
| H | 3.774266 | -1.179789 | -0.551638 |

**15G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -694.247988

Free energies: -693.932300

Corrected Free energies: -693.931220

| | | | |
|---|---|---|---|
| C | -0.697784 | 1.887121 | 0.153395 |
| C | 0.683283 | 1.310512 | 0.486760 |
| C | -0.766229 | -0.351818 | -0.528903 |
| H | 0.724908 | 1.147002 | 1.566561 |
| H | -0.852015 | -0.751733 | -1.541484 |
| N | 0.641321 | 0.018885 | -0.242557 |
| C | 1.681121 | -0.610148 | -0.787247 |
| C | 2.968511 | -0.571804 | -0.213031 |
| N | -1.435571 | 0.930046 | -0.441340 |
| O | -1.029750 | 3.032449 | 0.360724 |
| C | -2.708451 | 1.246266 | -1.075767 |
| H | -3.514488 | 1.307255 | -0.343766 |

| | | | |
|---|---|---|---|
| H | -2.612966 | 2.209682 | -1.576635 |
| H | -2.942332 | 0.476011 | -1.808277 |
| C | 1.759996 | 2.278543 | 0.020246 |
| H | 2.747504 | 2.036692 | 0.402140 |
| H | 1.787345 | 2.318810 | -1.070145 |
| H | 1.480886 | 3.262541 | 0.397206 |
| C | -1.284023 | -1.410291 | 0.492842 |
| C | -1.086767 | -0.933225 | 1.934165 |
| H | -1.529499 | 0.052154 | 2.102370 |
| H | -1.580821 | -1.633302 | 2.610766 |
| H | -0.029619 | -0.906962 | 2.211964 |
| C | -2.779039 | -1.629806 | 0.226500 |
| H | -2.972348 | -1.866778 | -0.823469 |
| H | -3.123255 | -2.473295 | 0.828257 |
| H | -3.372143 | -0.759046 | 0.508299 |
| C | -0.550532 | -2.739082 | 0.290622 |
| H | -0.934351 | -3.465493 | 1.009778 |
| H | -0.723714 | -3.142935 | -0.710226 |
| H | 0.525416 | -2.652423 | 0.465180 |
| C | 1.495398 | -1.418966 | -2.043089 |
| H | 2.470030 | -1.616049 | -2.483419 |
| H | 1.021997 | -2.379014 | -1.839076 |
| H | 0.885472 | -0.873803 | -2.764346 |
| C | 3.321888 | -0.302690 | 1.197140 |
| H | 4.130893 | 0.430518 | 1.261465 |
| H | 2.487136 | 0.007318 | 1.819014 |
| H | 3.729764 | -1.233004 | 1.609595 |
| H | 3.769713 | -0.923918 | -0.852075 |

**15G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -694.252213

Free energies: -693.937807

Corrected Free energies: -693.936398

| | | | |
|---|---|---|---|
| C | -1.205983 | 1.726638 | 0.181185 |
| C | 0.257232 | 1.500457 | 0.560464 |
| C | -0.701960 | -0.441740 | -0.558995 |
| H | 0.340818 | 1.370363 | 1.643338 |
| H | -0.611612 | -0.812070 | -1.581269 |
| N | 0.556796 | 0.227548 | -0.136498 |
| C | 1.783496 | -0.226773 | -0.374908 |
| C | 2.853539 | 0.240602 | 0.415569 |
| C | 4.268202 | -0.120806 | 0.184559 |

| | | | |
|---|---|---|---|
| H | 4.508380 | -1.016751 | 0.773529 |
| H | 4.487256 | -0.340401 | -0.859087 |
| H | 4.923027 | 0.674479 | 0.540100 |
| H | 2.618219 | 0.817338 | 1.301090 |
| N | -1.640963 | 0.660733 | -0.518738 |
| O | -1.827886 | 2.739884 | 0.410806 |
| C | -2.908342 | 0.703511 | -1.236036 |
| H | -3.753216 | 0.576795 | -0.558078 |
| H | -2.993826 | 1.672779 | -1.727519 |
| H | -2.923624 | -0.086775 | -1.983948 |
| C | 1.066006 | 2.697593 | 0.066161 |
| H | 2.091417 | 2.703155 | 0.426931 |
| H | 1.066525 | 2.723379 | -1.024890 |
| H | 0.566444 | 3.592566 | 0.436593 |
| C | -1.072209 | -1.610204 | 0.407806 |
| C | -1.148303 | -1.116203 | 1.854933 |
| H | -1.848000 | -0.283820 | 1.965812 |
| H | -1.504039 | -1.930123 | 2.489656 |
| H | -0.168424 | -0.813791 | 2.233736 |
| C | -2.439574 | -2.161248 | -0.020001 |
| H | -2.451432 | -2.431714 | -1.079635 |
| H | -2.651864 | -3.063834 | 0.556445 |
| H | -3.243842 | -1.451445 | 0.173978 |
| C | -0.045693 | -2.742872 | 0.311851 |
| H | -0.367456 | -3.558322 | 0.962479 |
| H | 0.028220 | -3.139237 | -0.703552 |
| H | 0.946202 | -2.437757 | 0.652257 |
| C | 2.068157 | -1.210334 | -1.470339 |
| H | 2.669184 | -0.691610 | -2.222620 |
| H | 2.656905 | -2.046870 | -1.092911 |
| H | 1.179595 | -1.595108 | -1.955725 |

**16G-*E***

Imaginary frequency: None

Electronic energies: -925.458447

Free energies: -925.068975

Corrected Free energies: -925.065906

| | | | |
|---|---|---|---|
| C | 1.588898 | -1.788939 | 0.709981 |
| C | 0.194209 | -1.202639 | 0.622619 |
| C | 1.842782 | 0.497750 | 0.216318 |
| H | -0.276360 | -1.340458 | 1.604816 |
| H | 2.170397 | 1.225752 | 0.971510 |
| N | 0.399709 | 0.224400 | 0.352586 |

| | | | |
|---|---|---|---|
| C | -0.288868 | 1.076021 | 1.297127 |
| C | -1.433459 | 1.643842 | 0.918901 |
| C | -2.345992 | 2.482326 | 1.760489 |
| H | -2.521567 | 3.450183 | 1.282597 |
| H | -3.322050 | 1.995226 | 1.854244 |
| H | -1.955510 | 2.668016 | 2.760469 |
| H | -1.754348 | 1.460166 | -0.102678 |
| N | 2.470467 | -0.789064 | 0.508853 |
| O | 1.861083 | -2.956997 | 0.934583 |
| C | 3.893658 | -1.004232 | 0.688372 |
| H | 4.023524 | -1.804949 | 1.416305 |
| H | 4.383784 | -1.298883 | -0.242564 |
| H | 4.355701 | -0.091346 | 1.064077 |
| C | -0.648047 | -1.952070 | -0.423653 |
| H | -0.109281 | -1.975337 | -1.373726 |
| H | -0.746761 | -2.984886 | -0.076435 |
| C | 2.191175 | 1.092208 | -1.173170 |
| C | 1.335586 | 2.350342 | -1.360466 |
| H | 1.595091 | 2.835625 | -2.304768 |
| H | 0.274016 | 2.099470 | -1.373545 |
| H | 1.508436 | 3.068880 | -0.552226 |
| C | 3.668750 | 1.501495 | -1.237098 |
| H | 3.945748 | 2.125557 | -0.381480 |
| H | 4.339255 | 0.642476 | -1.269822 |
| H | 3.843718 | 2.084994 | -2.144594 |
| C | 1.875758 | 0.089439 | -2.280632 |
| H | 2.445157 | -0.836773 | -2.158564 |
| H | 0.810795 | -0.151069 | -2.277375 |
| H | 2.126739 | 0.515643 | -3.255401 |
| C | -2.000948 | -1.316713 | -0.609412 |
| C | -2.312243 | -0.619161 | -1.775201 |
| C | -2.944227 | -1.354497 | 0.419745 |
| C | -3.530691 | 0.044435 | -1.905881 |
| H | -1.591354 | -0.586155 | -2.585693 |
| C | -4.158651 | -0.690870 | 0.297216 |
| H | -2.717569 | -1.898791 | 1.331621 |
| C | -4.453518 | 0.017779 | -0.866303 |
| H | -3.755185 | 0.585355 | -2.817939 |
| H | -4.876513 | -0.724856 | 1.108719 |
| H | -5.399567 | 0.537338 | -0.962643 |
| C | 0.320335 | 1.192562 | 2.678124 |
| H | -0.441435 | 1.319881 | 3.446252 |
| H | 0.891931 | 0.291594 | 2.919261 |
| H | 1.006268 | 2.041500 | 2.750388 |

**16G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -925.264619

Free energies: -924.871828

Corrected Free energies: -924.869249

| | | | |
|---|---|---|---|
| C | 1.519871 | -1.880158 | 0.697870 |
| C | 0.158127 | -1.210461 | 0.607446 |
| C | 1.970208 | 0.415534 | 0.398675 |
| H | -0.385776 | -1.472245 | 1.516510 |
| H | 2.367011 | 1.084547 | 1.164409 |
| N | 0.508483 | 0.223802 | 0.659167 |
| C | -0.287596 | 1.152717 | 1.192522 |
| C | -1.616241 | 0.833130 | 1.551161 |
| C | -2.603501 | 1.839082 | 2.005068 |
| H | -3.611878 | 1.480530 | 1.799433 |
| H | -2.520687 | 1.967887 | 3.093142 |
| H | -2.459170 | 2.815522 | 1.543115 |
| H | -1.939675 | -0.196377 | 1.547642 |
| N | 2.471059 | -0.926824 | 0.642589 |
| O | 1.690665 | -3.073044 | 0.821134 |
| C | 3.868584 | -1.250337 | 0.889407 |
| H | 3.898065 | -2.070766 | 1.605250 |
| H | 4.377268 | -1.562993 | -0.023997 |
| H | 4.371633 | -0.380605 | 1.309388 |
| C | -0.619987 | -1.721421 | -0.624656 |
| H | -0.027143 | -1.569119 | -1.524580 |
| H | -0.695620 | -2.800078 | -0.467787 |
| C | 2.337355 | 0.985866 | -1.009449 |
| C | 1.587704 | 2.291480 | -1.297979 |
| H | 1.834196 | 2.607878 | -2.313566 |
| H | 0.503013 | 2.165880 | -1.253811 |
| H | 1.885661 | 3.096778 | -0.625103 |
| C | 3.843423 | 1.297904 | -1.003733 |
| H | 4.127417 | 1.899855 | -0.136176 |
| H | 4.454489 | 0.396109 | -1.021331 |
| H | 4.084608 | 1.871898 | -1.900613 |
| C | 2.032666 | -0.005976 | -2.133960 |
| H | 2.396390 | -1.012750 | -1.915134 |
| H | 0.964726 | -0.047026 | -2.352750 |
| H | 2.528168 | 0.334008 | -3.045632 |
| C | -1.988987 | -1.115039 | -0.769028 |
| C | -2.159798 | 0.113552 | -1.412789 |

| | | | |
|---|---|---|---|
| C | -3.098705 | -1.734518 | -0.191237 |
| C | -3.410165 | 0.722807 | -1.457667 |
| H | -1.310112 | 0.598623 | -1.883089 |
| C | -4.348771 | -1.126063 | -0.231789 |
| H | -2.978180 | -2.693409 | 0.302561 |
| C | -4.505724 | 0.107238 | -0.859789 |
| H | -3.527361 | 1.676764 | -1.957619 |
| H | -5.200944 | -1.615522 | 0.224197 |
| H | -5.478918 | 0.582008 | -0.890179 |
| C | 0.178608 | 2.550724 | 1.465355 |
| H | -0.176768 | 2.844762 | 2.453485 |
| H | 1.255202 | 2.667863 | 1.439303 |
| H | -0.260149 | 3.239111 | 0.739006 |

**16G-*Z***

Imaginary frequency: None

Electronic energies: -925.455113

Free energies: -925.066097

Corrected Free energies: -925.062340

| | | | |
|---|---|---|---|
| C | -0.308229 | -1.699492 | -0.359180 |
| C | 0.275259 | -0.298814 | -0.319926 |
| C | -2.134276 | -0.218882 | -0.348468 |
| H | 0.865498 | -0.173996 | -1.237546 |
| H | -2.740809 | -0.015680 | -1.240171 |
| N | -0.898896 | 0.582972 | -0.353350 |
| C | -0.800868 | 1.609685 | -1.355218 |
| C | -0.317789 | 2.813775 | -1.040473 |
| N | -1.648368 | -1.594247 | -0.417519 |
| O | 0.326293 | -2.743339 | -0.352452 |
| C | -2.475657 | -2.766875 | -0.636028 |
| H | -3.381343 | -2.478432 | -1.168463 |
| H | -1.906643 | -3.473874 | -1.239536 |
| H | -2.748653 | -3.254232 | 0.302514 |
| C | 1.204214 | -0.081050 | 0.896757 |
| H | 0.984051 | 0.903190 | 1.309232 |
| H | 0.955941 | -0.812364 | 1.674128 |
| C | -3.011593 | 0.100465 | 0.889560 |
| C | -2.244561 | -0.200779 | 2.176149 |
| H | -1.334651 | 0.401549 | 2.230064 |
| H | -2.863485 | 0.032588 | 3.046255 |
| H | -1.966447 | -1.257664 | 2.232609 |
| C | -3.363179 | 1.591496 | 0.820457 |
| H | -3.899806 | 1.823014 | -0.105811 |

| | | | |
|---|---|---|---|
| H | -4.010080 | 1.858361 | 1.659889 |
| H | -2.467678 | 2.212546 | 0.860800 |
| C | -4.320350 | -0.698665 | 0.856305 |
| H | -5.000642 | -0.310650 | 1.618648 |
| H | -4.819716 | -0.603959 | -0.113215 |
| H | -4.166628 | -1.757444 | 1.065726 |
| C | 2.679756 | -0.162436 | 0.580514 |
| C | 3.201144 | -1.202207 | -0.194762 |
| C | 3.553663 | 0.811304 | 1.067496 |
| C | 4.563025 | -1.263553 | -0.472885 |
| H | 2.528106 | -1.966313 | -0.570147 |
| C | 4.917201 | 0.749447 | 0.793769 |
| H | 3.161882 | 1.626394 | 1.667655 |
| C | 5.426293 | -0.288804 | 0.020822 |
| H | 4.951804 | -2.075885 | -1.076209 |
| H | 5.579992 | 1.515044 | 1.180168 |
| H | 6.486615 | -0.337618 | -0.197027 |
| C | -1.166609 | 1.237755 | -2.772858 |
| H | -2.248382 | 1.169583 | -2.913423 |
| H | -0.789955 | 1.982265 | -3.473664 |
| H | -0.741965 | 0.264029 | -3.038468 |
| H | -0.187311 | 3.520662 | -1.855458 |
| C | 0.066752 | 3.293602 | 0.325913 |
| H | -0.303001 | 2.619189 | 1.098219 |
| H | 1.154816 | 3.365809 | 0.425998 |
| H | -0.336173 | 4.293705 | 0.505277 |

**16G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -925.253203

Free energies: -924.861541

Corrected Free energies: -924.858549

| | | | |
|---|---|---|---|
| C | -0.389369 | -1.533183 | -0.856362 |
| C | 0.209228 | -0.174888 | -0.512418 |
| C | -2.227354 | -0.146385 | -0.358425 |
| H | 0.831103 | 0.130038 | -1.353214 |
| H | -2.957857 | 0.187316 | -1.095579 |
| N | -0.993907 | 0.689840 | -0.495475 |
| C | -1.007609 | 1.952846 | -0.905245 |
| C | 0.155777 | 2.750629 | -1.081182 |
| N | -1.729575 | -1.448018 | -0.764997 |
| O | 0.254190 | -2.516614 | -1.154770 |
| C | -2.581499 | -2.551972 | -1.184674 |

| | | | |
|---|---|---|---|
| H | -3.530715 | -2.157964 | -1.544861 |
| H | -2.073735 | -3.077154 | -1.992536 |
| H | -2.761946 | -3.251744 | -0.367312 |
| C | 1.037554 | -0.243071 | 0.794947 |
| H | 0.792140 | 0.615203 | 1.422376 |
| H | 0.734189 | -1.131200 | 1.355337 |
| C | -2.874384 | -0.110097 | 1.059108 |
| C | -1.979506 | -0.772233 | 2.107267 |
| H | -1.095616 | -0.170962 | 2.323488 |
| H | -2.540492 | -0.866294 | 3.039298 |
| H | -1.667155 | -1.775095 | 1.805561 |
| C | -3.163694 | 1.333469 | 1.487182 |
| H | -3.908019 | 1.810065 | 0.846813 |
| H | -3.569989 | 1.315482 | 2.500324 |
| H | -2.260849 | 1.948780 | 1.510388 |
| C | -4.211266 | -0.863925 | 0.983767 |
| H | -4.753661 | -0.706083 | 1.918140 |
| H | -4.838420 | -0.495591 | 0.167124 |
| H | -4.072976 | -1.938396 | 0.864663 |
| C | 2.533475 | -0.298411 | 0.567385 |
| C | 3.088488 | -1.056858 | -0.464702 |
| C | 3.384272 | 0.404024 | 1.422381 |
| C | 4.468447 | -1.096898 | -0.644568 |
| H | 2.442245 | -1.631206 | -1.120219 |
| C | 4.762808 | 0.359069 | 1.246300 |
| H | 2.964034 | 0.997000 | 2.228581 |
| C | 5.309105 | -0.389582 | 0.208104 |
| H | 4.885908 | -1.687946 | -1.451099 |
| H | 5.408460 | 0.914849 | 1.915808 |
| H | 6.382494 | -0.420965 | 0.065407 |
| C | -2.287061 | 2.670990 | -1.242250 |
| H | -2.447281 | 3.475342 | -0.520992 |
| H | -2.158760 | 3.129769 | -2.223827 |
| H | -3.173090 | 2.049862 | -1.264543 |
| C | 1.552749 | 2.577616 | -0.612507 |
| H | 1.594659 | 2.351073 | 0.454623 |
| H | 2.084191 | 1.774799 | -1.133251 |
| H | 2.102076 | 3.499773 | -0.787883 |
| H | -0.061045 | 3.684566 | -1.585801 |

**17G-*E***

Imaginary frequency: None

Electronic energies: -846.856185

Free energies: -846.520249

Corrected Free energies: -846.517660

| | | | |
|---|---|---|---|
| C | -0.626331 | 1.639161 | -1.204474 |
| C | 0.413940 | 0.553284 | -1.380728 |
| C | 0.446825 | 1.399796 | 0.893856 |
| H | 1.151238 | 0.933384 | -2.101327 |
| N | 0.948516 | 0.377219 | -0.047496 |
| C | 2.122795 | -0.364834 | 0.152171 |
| C | 2.928476 | -0.714919 | -0.866551 |
| C | 4.126319 | -1.627172 | -0.752427 |
| H | 3.850481 | -2.635740 | -0.428875 |
| H | 4.615699 | -1.722830 | -1.721930 |
| H | 4.872895 | -1.252494 | -0.046925 |
| H | 2.707720 | -0.350173 | -1.862427 |
| N | -0.559374 | 2.076101 | 0.062726 |
| O | -1.391716 | 2.030513 | -2.071958 |
| C | -1.467103 | 3.079432 | 0.580896 |
| H | -0.933446 | 3.788177 | 1.214676 |
| H | -1.893133 | 3.608429 | -0.269406 |
| H | -2.276251 | 2.621396 | 1.155478 |
| C | -0.238127 | -0.728780 | -1.943075 |
| H | -0.781776 | -0.446531 | -2.847649 |
| H | 0.544284 | -1.437171 | -2.219826 |
| C | -1.161142 | -1.341156 | -0.921500 |
| C | -0.693663 | -2.326648 | -0.049920 |
| C | -2.464420 | -0.867032 | -0.758662 |
| C | -1.505497 | -2.826333 | 0.963021 |
| H | 0.322771 | -2.692444 | -0.163855 |
| C | -3.279474 | -1.361671 | 0.256190 |
| H | -2.834966 | -0.095924 | -1.426367 |
| C | -2.801773 | -2.341762 | 1.121297 |
| H | -1.125709 | -3.589979 | 1.632226 |
| H | -4.288488 | -0.982233 | 0.369343 |
| H | -3.435603 | -2.727231 | 1.911122 |
| C | 1.535097 | 2.403059 | 1.286921 |
| H | 1.126666 | 3.190045 | 1.923884 |
| H | 2.336645 | 1.913557 | 1.839978 |
| H | 1.955914 | 2.854429 | 0.386429 |
| C | -0.258078 | 0.797712 | 2.112923 |
| H | -0.779446 | 1.584101 | 2.663742 |
| H | -0.981670 | 0.049926 | 1.777441 |
| H | 0.448818 | 0.335141 | 2.797989 |
| C | 2.353024 | -0.905172 | 1.541590 |
| H | 1.476058 | -1.475474 | 1.860003 |

| | | | |
|---|---|---|---|
| H | 3.217235 | -1.565618 | 1.553614 |
| H | 2.528594 | -0.123877 | 2.282541 |

**17G-*Z***

Imaginary frequency: None

Electronic energies: -846.854759

Free energies: -846.519283

Corrected Free energies: -846.516453

| | | | |
|---|---|---|---|
| C | 0.347519 | 1.634555 | -1.120448 |
| C | 0.814017 | 0.200318 | -1.240977 |
| C | 0.883891 | 0.937964 | 1.081146 |
| H | 1.670841 | 0.214354 | -1.919652 |
| N | 1.161063 | -0.148908 | 0.124172 |
| C | 1.686253 | -1.402737 | 0.471079 |
| C | 2.561760 | -2.063798 | -0.308174 |
| N | 0.445345 | 2.002903 | 0.167209 |
| O | -0.045705 | 2.325469 | -2.048138 |
| C | 0.021710 | 3.311095 | 0.623584 |
| H | 0.713237 | 3.693755 | 1.374658 |
| H | 0.022425 | 3.976326 | -0.237801 |
| H | -0.986989 | 3.278833 | 1.043667 |
| C | -0.267709 | -0.693282 | -1.879559 |
| H | -0.501280 | -0.259854 | -2.855712 |
| H | 0.160870 | -1.685220 | -2.043683 |
| C | -1.503994 | -0.794906 | -1.024909 |
| C | -1.717865 | -1.909576 | -0.214594 |
| C | -2.425348 | 0.255730 | -0.975177 |
| C | -2.814876 | -1.971115 | 0.641209 |
| H | -1.010754 | -2.732901 | -0.250633 |
| C | -3.522532 | 0.198558 | -0.121573 |
| H | -2.272033 | 1.125901 | -1.605242 |
| C | -3.717706 | -0.913360 | 0.693759 |
| H | -2.963019 | -2.843779 | 1.267031 |
| H | -4.226578 | 1.022160 | -0.093991 |
| H | -4.571141 | -0.957410 | 1.360010 |
| C | 2.166411 | 1.351616 | 1.804754 |
| H | 2.905995 | 1.687740 | 1.075930 |
| H | 1.977331 | 2.149128 | 2.526186 |
| H | 2.573473 | 0.497548 | 2.349241 |
| C | -0.248509 | 0.658978 | 2.080308 |
| H | -1.110660 | 0.230461 | 1.564924 |
| H | 0.073238 | -0.013210 | 2.872498 |
| H | -0.545793 | 1.596986 | 2.554882 |

| | | | |
|---|---|---|---|
| C | 1.201014 | -2.047373 | 1.749490 |
| H | 1.588561 | -1.533048 | 2.632849 |
| H | 0.111375 | -2.044534 | 1.812712 |
| H | 1.558562 | -3.075801 | 1.792934 |
| H | 2.784366 | -3.085574 | -0.020594 |
| C | 3.306433 | -1.527757 | -1.497751 |
| H | 4.228274 | -2.093526 | -1.640326 |
| H | 2.739246 | -1.600179 | -2.434140 |
| H | 3.578421 | -0.479329 | -1.353318 |

**17G-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -846.657926

Free energies: -846.320666

Corrected Free energies: -846.318934

| | | | |
|---|---|---|---|
| C | 0.321026 | 1.632597 | -1.222358 |
| C | 0.906401 | 0.235925 | -1.247202 |
| C | 0.756269 | 1.111421 | 1.058602 |
| H | 1.820141 | 0.264381 | -1.837775 |
| N | 1.186624 | -0.040178 | 0.176733 |
| C | 1.658724 | -1.201532 | 0.606273 |
| C | 2.352741 | -2.099426 | -0.248717 |
| N | 0.249881 | 2.045862 | 0.052636 |
| O | -0.049145 | 2.230062 | -2.212271 |
| C | -0.360070 | 3.317928 | 0.404154 |
| H | 0.203247 | 3.804493 | 1.199173 |
| H | -0.339483 | 3.944100 | -0.485070 |
| H | -1.396583 | 3.179460 | 0.719175 |
| C | -0.113580 | -0.749575 | -1.859848 |
| H | -0.367370 | -0.333858 | -2.837584 |
| H | 0.355426 | -1.720239 | -2.024645 |
| C | -1.341502 | -0.910787 | -0.997493 |
| C | -1.473812 | -2.025517 | -0.167480 |
| C | -2.335273 | 0.071661 | -0.970580 |
| C | -2.559820 | -2.146061 | 0.695162 |
| H | -0.726513 | -2.813143 | -0.203452 |
| C | -3.422709 | -0.048193 | -0.111294 |
| H | -2.257073 | 0.931909 | -1.627521 |
| C | -3.532828 | -1.152243 | 0.730313 |
| H | -2.645269 | -3.016655 | 1.334483 |
| H | -4.185654 | 0.721067 | -0.100226 |
| H | -4.377991 | -1.241941 | 1.401938 |
| C | 1.993689 | 1.701499 | 1.736530 |

| | | | |
|---|---|---|---|
| H | 2.718942 | 2.008417 | 0.982387 |
| H | 1.697950 | 2.571703 | 2.323900 |
| H | 2.460636 | 0.991646 | 2.416860 |
| C | -0.358374 | 0.765511 | 2.045686 |
| H | -1.133446 | 0.161241 | 1.571458 |
| H | 0.019535 | 0.264918 | 2.932311 |
| H | -0.805969 | 1.703043 | 2.378591 |
| C | 1.469383 | -1.656810 | 2.027640 |
| H | 1.831633 | -0.928681 | 2.749613 |
| H | 0.406014 | -1.829260 | 2.211711 |
| H | 2.010285 | -2.584884 | 2.188993 |
| H | 2.406797 | -3.115417 | 0.122558 |
| C | 3.138576 | -1.789862 | -1.470446 |
| H | 3.938641 | -2.522697 | -1.564250 |
| H | 2.533622 | -1.866759 | -2.381582 |
| H | 3.577068 | -0.792359 | -1.432112 |

**17G-*E*** radical cation

Imaginary frequency: None

Electronic energies: -846.664870

Free energies: -846.328356

Corrected Free energies: -846.326151

| | | | |
|---|---|---|---|
| C | -0.888505 | 1.546322 | -1.254336 |
| C | 0.352569 | 0.695186 | -1.433641 |
| C | 0.124023 | 1.474075 | 0.897642 |
| H | 1.014396 | 1.181468 | -2.153745 |
| N | 0.963438 | 0.700810 | -0.090761 |
| C | 2.117918 | 0.099552 | 0.170026 |
| C | 2.891554 | -0.407928 | -0.901401 |
| C | 4.102734 | -1.239313 | -0.713150 |
| H | 3.999739 | -1.944713 | 0.112805 |
| H | 4.333643 | -1.780479 | -1.628506 |
| H | 4.963125 | -0.594646 | -0.487614 |
| H | 2.632601 | -0.127185 | -1.912599 |
| N | -0.979458 | 1.903821 | 0.036809 |
| O | -1.676226 | 1.790757 | -2.144970 |
| C | -2.131674 | 2.624993 | 0.551441 |
| H | -1.817595 | 3.463242 | 1.172506 |
| H | -2.681416 | 3.002243 | -0.308000 |
| H | -2.778999 | 1.961129 | 1.127739 |
| C | -0.067086 | -0.708703 | -1.929872 |
| H | -0.682711 | -0.525350 | -2.813115 |
| H | 0.806757 | -1.276027 | -2.249867 |

| | | | |
|---|---|---|---|
| C | -0.833948 | -1.477681 | -0.883278 |
| C | -0.180442 | -2.414006 | -0.080189 |
| C | -2.190918 | -1.226848 | -0.662427 |
| C | -0.861883 | -3.074692 | 0.938089 |
| H | 0.867144 | -2.639343 | -0.259532 |
| C | -2.874041 | -1.887381 | 0.354050 |
| H | -2.711435 | -0.510721 | -1.290387 |
| C | -2.209323 | -2.807584 | 1.160382 |
| H | -0.341591 | -3.799560 | 1.552484 |
| H | -3.926286 | -1.685083 | 0.514423 |
| H | -2.741308 | -3.320707 | 1.952492 |
| C | 0.891546 | 2.708334 | 1.377680 |
| H | 0.237705 | 3.304293 | 2.015026 |
| H | 1.773579 | 2.456964 | 1.961405 |
| H | 1.191312 | 3.308904 | 0.518182 |
| C | -0.421700 | 0.600159 | 2.025516 |
| H | -1.138735 | 1.193684 | 2.595153 |
| H | -0.932326 | -0.272222 | 1.616400 |
| H | 0.350728 | 0.277764 | 2.717314 |
| C | 2.639172 | -0.112610 | 1.560034 |
| H | 2.343596 | -1.115909 | 1.885870 |
| H | 3.726285 | -0.067570 | 1.553919 |
| H | 2.273758 | 0.600116 | 2.285687 |

## Calculated Cartesian coordinates for cyclohexanone derived enamines

**1H**

Imaginary frequency: None

Electronic energies: -738.311102

Free energies: -737.894684

Corrected Free energies: -737.891377

| | | | |
|---|---|---|---|
| C | 2.723753 | -1.067178 | 0.130534 |
| C | 3.608968 | -0.222487 | 1.059083 |
| H | 3.147883 | -0.114220 | 2.046013 |
| H | 4.576759 | -0.713018 | 1.193328 |
| H | 3.801744 | 0.775274 | 0.661237 |
| C | 2.689701 | -2.497123 | 0.682922 |
| H | 2.242708 | -2.512621 | 1.682378 |
| H | 2.102589 | -3.153119 | 0.040485 |
| H | 3.705482 | -2.894852 | 0.758348 |

| | | | |
|---|---|---|---|
| C | 3.334158 | -1.081927 | -1.276204 |
| H | 2.752678 | -1.705789 | -1.961061 |
| H | 3.402946 | -0.075568 | -1.697300 |
| H | 4.345456 | -1.496088 | -1.237612 |
| C | 1.281634 | -0.493878 | 0.117786 |
| H | 0.956437 | -0.477750 | 1.161740 |
| C | 1.186792 | 0.935272 | -0.450134 |
| H | 1.213944 | 0.862143 | -1.542465 |
| H | 2.057962 | 1.538475 | -0.153710 |
| N | 0.374783 | -1.397418 | -0.598610 |
| N | -0.061684 | 1.588105 | -0.061725 |
| C | -0.572876 | 2.495402 | -1.089766 |
| H | -0.645424 | 1.918441 | -2.016081 |
| H | -1.596154 | 2.774754 | -0.824862 |
| C | 0.063349 | 2.201406 | 1.258813 |
| H | 0.401753 | 1.424296 | 1.951459 |
| H | 0.845854 | 2.980023 | 1.269219 |
| C | -1.246361 | 2.783986 | 1.774720 |
| H | -1.542658 | 3.674408 | 1.216453 |
| H | -2.050694 | 2.047743 | 1.695456 |
| H | -1.140578 | 3.069197 | 2.822746 |
| C | 0.258353 | 3.757569 | -1.338252 |
| H | 1.292531 | 3.505719 | -1.587851 |
| H | -0.161050 | 4.325386 | -2.171313 |
| H | 0.269720 | 4.410167 | -0.461884 |
| H | 0.584211 | -1.401867 | -1.591623 |
| C | -1.012317 | -1.331984 | -0.386860 |
| C | -1.890288 | -1.454053 | -1.395274 |
| C | -3.386529 | -1.486197 | -1.210171 |
| H | -3.771542 | -2.505854 | -1.348873 |
| C | -1.454979 | -1.239178 | 1.054948 |
| H | -1.305844 | -0.209702 | 1.396848 |
| H | -0.803703 | -1.874540 | 1.664665 |
| C | -2.918104 | -1.640654 | 1.239648 |
| H | -3.014865 | -2.728933 | 1.153822 |
| C | -3.789375 | -0.979792 | 0.174173 |
| H | -3.643802 | 0.106053 | 0.219124 |
| H | -3.250465 | -1.365113 | 2.243527 |
| H | -4.848209 | -1.176812 | 0.359522 |
| H | -3.864876 | -0.878226 | -1.984706 |
| H | -1.507768 | -1.537923 | -2.410480 |

**1H** radical cation

Imaginary frequency: None
Electronic energies: -738.131754
Free energies: -737.716837
Corrected Free energies: -737.713038

| | | | |
|---|---|---|---|
| C | -2.261782 | -1.743079 | -0.181431 |
| C | -3.316531 | -1.333096 | -1.217618 |
| H | -2.860612 | -1.168809 | -2.198127 |
| H | -4.052854 | -2.133552 | -1.319179 |
| H | -3.852436 | -0.427612 | -0.928696 |
| C | -1.659032 | -3.088587 | -0.606449 |
| H | -1.151538 | -3.000803 | -1.571873 |
| H | -0.939822 | -3.463199 | 0.125703 |
| H | -2.451641 | -3.833074 | -0.707961 |
| C | -2.924155 | -1.881316 | 1.194090 |
| H | -2.216645 | -2.182109 | 1.972933 |
| H | -3.408645 | -0.953619 | 1.506153 |
| H | -3.691454 | -2.657495 | 1.146308 |
| C | -1.139008 | -0.676340 | -0.180133 |
| H | -0.777887 | -0.578664 | -1.204304 |
| C | -1.536674 | 0.718391 | 0.342461 |
| H | -1.719285 | 0.647632 | 1.418198 |
| H | -2.482746 | 1.019384 | -0.127038 |
| N | -0.003622 | -1.113710 | 0.636368 |
| N | -0.467061 | 1.677378 | 0.100424 |
| C | -0.308502 | 2.645856 | 1.190143 |
| H | -0.195899 | 2.071141 | 2.113199 |
| H | 0.637163 | 3.171969 | 1.041187 |
| C | -0.595855 | 2.284380 | -1.227458 |
| H | -0.628458 | 1.470820 | -1.959997 |
| H | -1.551088 | 2.824039 | -1.328340 |
| C | 0.558198 | 3.215606 | -1.572800 |
| H | 0.532479 | 4.130100 | -0.977343 |
| H | 1.520889 | 2.726842 | -1.401383 |
| H | 0.500174 | 3.501674 | -2.623932 |
| C | -1.446973 | 3.656208 | 1.342263 |
| H | -2.409264 | 3.152963 | 1.467872 |
| H | -1.276741 | 4.282234 | 2.220176 |
| H | -1.516713 | 4.312887 | 0.472043 |
| H | -0.229959 | -1.376019 | 1.593562 |
| C | 1.279992 | -1.015310 | 0.337728 |
| C | 2.217014 | -1.292590 | 1.352412 |
| C | 3.678423 | -1.120527 | 1.171953 |
| H | 4.124787 | -2.124892 | 1.114279 |
| C | 1.719556 | -0.618076 | -1.043258 |

| | | | |
|---|---|---|---|
| H | 1.456245 | 0.437198 | -1.164910 |
| H | 1.138753 | -1.183348 | -1.775835 |
| C | 3.217609 | -0.836491 | -1.265813 |
| H | 3.416999 | -1.903934 | -1.401730 |
| C | 4.025314 | -0.316861 | -0.080858 |
| H | 3.794093 | 0.739980 | 0.087063 |
| H | 3.508945 | -0.332670 | -2.187811 |
| H | 5.095025 | -0.390565 | -0.277997 |
| H | 4.093474 | -0.671659 | 2.078899 |
| H | 1.843884 | -1.641533 | 2.309953 |

**2H**

Imaginary frequency: None

Electronic energies: -524.569654

Free energies: -524.292796

Corrected Free energies: -524.291392

| | | | |
|---|---|---|---|
| N | 0.029716 | -1.157796 | -0.246917 |
| C | 1.280960 | -0.536123 | -0.057637 |
| C | 2.143254 | -0.944898 | 0.884327 |
| C | 1.633157 | 0.541990 | -1.055353 |
| C | 3.564093 | -0.454288 | 1.000211 |
| C | 2.918910 | 1.279566 | -0.680147 |
| H | 1.728633 | 0.077652 | -2.044661 |
| H | 0.810934 | 1.258644 | -1.134240 |
| C | 4.004160 | 0.292605 | -0.258608 |
| H | 4.232105 | -1.300640 | 1.188940 |
| H | 3.664027 | 0.207246 | 1.870819 |
| H | 3.248992 | 1.892653 | -1.521914 |
| H | 2.713708 | 1.960074 | 0.154064 |
| H | 4.951960 | 0.807196 | -0.083710 |
| H | 4.167314 | -0.426795 | -1.069195 |
| H | 1.816466 | -1.705764 | 1.590083 |
| H | -0.122161 | -1.863604 | 0.468229 |
| C | -1.171065 | -0.321317 | -0.374483 |
| C | -2.387138 | -1.234329 | -0.523557 |
| C | -1.364830 | 0.642832 | 0.800975 |
| H | -1.081243 | 0.262836 | -1.297856 |
| C | -3.678682 | -0.427446 | -0.670803 |
| H | -2.456950 | -1.868043 | 0.370923 |
| H | -2.237269 | -1.897327 | -1.379584 |
| C | -2.651704 | 1.457316 | 0.650010 |
| H | -1.407672 | 0.049952 | 1.724306 |
| H | -0.495895 | 1.303373 | 0.887027 |

| | | | |
|---|---|---|---|
| C | -3.865697 | 0.537468 | 0.502053 |
| H | -4.533542 | -1.103914 | -0.748184 |
| H | -3.640045 | 0.145802 | -1.604659 |
| H | -2.778299 | 2.125346 | 1.505703 |
| H | -2.572683 | 2.092372 | -0.240908 |
| H | -4.776132 | 1.126840 | 0.365238 |
| H | -3.992764 | -0.039579 | 1.426062 |

**2H** radical cation

Imaginary frequency: None

Electronic energies: -524.388142

Free energies: -524.111145

Corrected Free energies: -524.109941

| | | | |
|---|---|---|---|
| N | 0.082096 | -0.826865 | 0.304891 |
| C | 1.313444 | -0.376407 | 0.142248 |
| C | 2.378557 | -1.148714 | 0.643042 |
| C | 1.558947 | 0.919369 | -0.579059 |
| C | 3.802109 | -0.773733 | 0.469538 |
| C | 2.979956 | 1.441832 | -0.354386 |
| H | 1.387381 | 0.738568 | -1.647023 |
| H | 0.821249 | 1.657871 | -0.259814 |
| C | 4.005611 | 0.332175 | -0.565840 |
| H | 4.375842 | -1.673331 | 0.228392 |
| H | 4.174606 | -0.448240 | 1.452639 |
| H | 3.158225 | 2.272184 | -1.037853 |
| H | 3.067879 | 1.832829 | 0.663834 |
| H | 5.019811 | 0.723944 | -0.485754 |
| H | 3.893309 | -0.083515 | -1.571748 |
| H | 2.137522 | -2.052403 | 1.193787 |
| H | -0.030387 | -1.706607 | 0.804675 |
| C | -1.161704 | -0.179897 | -0.125382 |
| C | -2.153026 | -1.249890 | -0.583189 |
| C | -1.736139 | 0.662505 | 1.022004 |
| H | -0.919170 | 0.466177 | -0.971834 |
| C | -3.472607 | -0.598894 | -1.004915 |
| H | -2.336660 | -1.941395 | 0.248012 |
| H | -1.719885 | -1.823407 | -1.405742 |
| C | -3.055285 | 1.307079 | 0.590561 |
| H | -1.905890 | 0.005534 | 1.882297 |
| H | -1.010852 | 1.421168 | 1.326477 |
| C | -4.058121 | 0.250523 | 0.124700 |
| H | -4.177410 | -1.375915 | -1.307436 |
| H | -3.296826 | 0.033058 | -1.882808 |

| | | | |
|---|---|---|---|
| H | -3.463686 | 1.884439 | 1.422528 |
| H | -2.862304 | 2.012115 | -0.225871 |
| H | -4.982730 | 0.728707 | -0.205937 |
| H | -4.315159 | -0.399426 | 0.968998 |

**3H**

Imaginary frequency: None

Electronic energies: -407.850559

Free energies: -407.637142

Corrected Free energies: -407.636422

| | | | |
|---|---|---|---|
| C | -2.157102 | 0.065241 | 0.275650 |
| H | -1.789046 | 0.350001 | 1.269591 |
| N | -1.078469 | -0.592733 | -0.484370 |
| C | 0.269168 | -0.348016 | -0.165869 |
| C | 1.175171 | -1.337015 | -0.117254 |
| C | 0.656878 | 1.099801 | 0.020554 |
| C | 2.660493 | -1.118859 | 0.024960 |
| C | 2.082931 | 1.254231 | 0.549650 |
| H | 0.548402 | 1.614030 | -0.942594 |
| H | -0.043546 | 1.585583 | 0.705980 |
| C | 3.039910 | 0.342328 | -0.212858 |
| H | 3.196293 | -1.765334 | -0.677542 |
| H | 2.992545 | -1.423740 | 1.026192 |
| H | 2.390749 | 2.299596 | 0.473995 |
| H | 2.106511 | 0.986204 | 1.611917 |
| H | 4.074122 | 0.521111 | 0.090718 |
| H | 2.969714 | 0.566956 | -1.283303 |
| H | 0.828395 | -2.362442 | -0.225814 |
| H | -1.246768 | -1.588103 | -0.569176 |
| C | -3.297084 | -0.930938 | 0.461636 |
| H | -4.133555 | -0.463492 | 0.983483 |
| H | -3.653340 | -1.275873 | -0.513670 |
| H | -2.970881 | -1.798863 | 1.039191 |
| C | -2.656832 | 1.313053 | -0.450391 |
| H | -3.064257 | 1.027864 | -1.424042 |
| H | -3.443842 | 1.805371 | 0.126677 |
| H | -1.853418 | 2.031299 | -0.617477 |

**3H** radical cation

Imaginary frequency: None

Electronic energies: -407.671430

Free energies: -407.458539

Corrected Free energies: -407.457656

| | | | |
|---|---|---|---|
| C | -2.191309 | 0.207118 | -0.214444 |
| H | -1.843076 | 0.954987 | -0.926728 |
| N | -1.036899 | -0.648943 | 0.106152 |
| C | 0.240030 | -0.317719 | 0.051765 |
| C | 1.198463 | -1.288144 | 0.402526 |
| C | 0.651102 | 1.057628 | -0.394092 |
| C | 2.659395 | -1.047717 | 0.332136 |
| C | 2.104871 | 1.365918 | -0.028153 |
| H | 0.518551 | 1.103716 | -1.481753 |
| H | -0.022412 | 1.798912 | 0.039030 |
| C | 3.020483 | 0.218761 | -0.444025 |
| H | 3.141722 | -1.937298 | -0.083546 |
| H | 3.026441 | -0.977899 | 1.367315 |
| H | 2.398175 | 2.295177 | -0.516828 |
| H | 2.182713 | 1.525896 | 1.051646 |
| H | 4.065159 | 0.471576 | -0.261702 |
| H | 2.910439 | 0.034340 | -1.516935 |
| H | 0.842521 | -2.251629 | 0.752778 |
| H | -1.262577 | -1.589878 | 0.423024 |
| C | -2.691816 | 0.885201 | 1.060612 |
| H | -3.529841 | 1.537368 | 0.811273 |
| H | -3.035138 | 0.135305 | 1.776228 |
| H | -1.909588 | 1.484271 | 1.528845 |
| C | -3.261277 | -0.656306 | -0.869405 |
| H | -3.611072 | -1.426204 | -0.176788 |
| H | -4.112198 | -0.030116 | -1.137785 |
| H | -2.881177 | -1.134370 | -1.772656 |

**4H**

Imaginary frequency: None

Electronic energies: -560.256542

Free energies: -560.022898

Corrected Free energies: -560.020660

| | | | |
|---|---|---|---|
| C | -3.745567 | -1.200437 | 0.505679 |
| C | -2.251687 | -1.041178 | 0.360029 |
| C | -1.669964 | 0.081190 | -0.092288 |
| C | -2.468866 | 1.273318 | -0.565272 |
| C | -3.940202 | 0.931180 | -0.791426 |
| C | -4.480381 | 0.135387 | 0.394408 |
| H | -1.638644 | -1.885331 | 0.656510 |
| H | -4.124259 | -1.889213 | -0.260940 |
| H | -3.970995 | -1.671877 | 1.467606 |

| | | | |
|---|---|---|---|
| H | -2.374155 | 2.073383 | 0.178053 |
| H | -2.021392 | 1.657887 | -1.488528 |
| H | -4.514083 | 1.847721 | -0.945506 |
| H | -4.038189 | 0.329355 | -1.701721 |
| H | -4.322192 | 0.714217 | 1.311520 |
| H | -5.555652 | -0.030747 | 0.295024 |
| N | -0.289188 | 0.300552 | -0.110592 |
| C | 0.608330 | -0.804893 | 0.175639 |
| H | 0.393097 | -1.157689 | 1.190899 |
| H | 0.442937 | -1.658526 | -0.497526 |
| C | 2.049814 | -0.362812 | 0.094861 |
| C | 2.987347 | -1.112450 | -0.612804 |
| C | 2.467117 | 0.800330 | 0.746437 |
| C | 4.321149 | -0.714389 | -0.665123 |
| H | 2.671682 | -2.012946 | -1.129221 |
| C | 3.796541 | 1.201865 | 0.692935 |
| H | 1.737482 | 1.389531 | 1.290603 |
| C | 4.728749 | 0.443647 | -0.012407 |
| H | 5.038719 | -1.307129 | -1.220206 |
| H | 4.107404 | 2.105777 | 1.203778 |
| H | 5.765320 | 0.756734 | -0.053948 |
| H | 0.012958 | 0.850452 | -0.906262 |

**4H** radical cation

Imaginary frequency: None

Electronic energies: -560.067317

Free energies: -559.833021

Corrected Free energies: -559.830931

| | | | |
|---|---|---|---|
| C | 3.769055 | -1.153881 | -0.401236 |
| C | 2.290883 | -1.064596 | -0.340156 |
| C | 1.616721 | 0.107963 | 0.060532 |
| C | 2.374919 | 1.355672 | 0.422801 |
| C | 3.830181 | 1.055623 | 0.783465 |
| C | 4.473168 | 0.199596 | -0.304605 |
| H | 1.714313 | -1.950193 | -0.578171 |
| H | 4.077364 | -1.803214 | 0.433131 |
| H | 4.050790 | -1.702997 | -1.304631 |
| H | 2.339125 | 2.016698 | -0.450773 |
| H | 1.855013 | 1.867013 | 1.235650 |
| H | 4.364979 | 1.997964 | 0.903468 |
| H | 3.872218 | 0.530329 | 1.742533 |
| H | 4.400683 | 0.718508 | -1.265094 |
| H | 5.532074 | 0.041898 | -0.099092 |

| | | | |
|---|---|---|---|
| N | 0.301262 | 0.142090 | 0.117172 |
| C | -0.627026 | -0.945341 | -0.241268 |
| H | -0.399211 | -1.261894 | -1.261492 |
| H | -0.452933 | -1.785020 | 0.434901 |
| C | -2.046562 | -0.454170 | -0.135098 |
| C | -2.835114 | -0.809094 | 0.957219 |
| C | -2.567566 | 0.386208 | -1.120059 |
| C | -4.137308 | -0.330716 | 1.064026 |
| H | -2.431192 | -1.463449 | 1.721765 |
| C | -3.866370 | 0.868375 | -1.009931 |
| H | -1.956984 | 0.658920 | -1.974968 |
| C | -4.652434 | 0.508873 | 0.082109 |
| H | -4.747229 | -0.613935 | 1.913286 |
| H | -4.266978 | 1.519050 | -1.777520 |
| H | -5.666015 | 0.882049 | 0.165139 |
| H | -0.130125 | 1.006565 | 0.434864 |

**5H**

Imaginary frequency: None

Electronic energies: -520.954859

Free energies: -520.747189

Corrected Free energies: -520.745842

| | | | |
|---|---|---|---|
| N | -0.174327 | -1.193370 | -0.363629 |
| C | 1.083730 | -0.581470 | -0.131162 |
| C | 1.932181 | -1.041985 | 0.791770 |
| C | 1.437326 | 0.543135 | -1.075288 |
| C | 3.330594 | -0.513592 | 0.979835 |
| C | 2.636512 | 1.341562 | -0.568630 |
| H | 1.661965 | 0.101858 | -2.053998 |
| H | 0.571232 | 1.191631 | -1.228859 |
| C | 3.766687 | 0.391477 | -0.174263 |
| H | 4.028659 | -1.349042 | 1.089674 |
| H | 3.377076 | 0.041537 | 1.925112 |
| H | 2.969554 | 2.043153 | -1.336555 |
| H | 2.338357 | 1.932718 | 0.305132 |
| H | 4.664201 | 0.947999 | 0.104759 |
| H | 4.024727 | -0.226300 | -1.041547 |
| H | 1.606497 | -1.849769 | 1.442638 |
| H | -0.211615 | -2.174210 | -0.120063 |
| C | -1.376812 | -0.511370 | -0.120482 |
| C | -2.586438 | -1.125121 | -0.474033 |
| C | -1.412267 | 0.758287 | 0.467170 |
| C | -3.794797 | -0.481767 | -0.250208 |

| | | | |
|---|---|---|---|
| H | -2.562378 | -2.109611 | -0.928818 |
| C | -2.628936 | 1.404634 | 0.665408 |
| H | -0.490214 | 1.228109 | 0.789242 |
| C | -3.826542 | 0.793685 | 0.311793 |
| H | -4.718730 | -0.976970 | -0.525937 |
| H | -2.635695 | 2.389674 | 1.117882 |
| H | -4.770772 | 1.297960 | 0.475285 |

**5H** radical cation

Imaginary frequency: None

Electronic energies: -520.761138

Free energies: -520.554963

Corrected Free energies: -520.553110

| | | | |
|---|---|---|---|
| N | -0.065891 | -1.078153 | 0.452445 |
| C | 1.090191 | -0.475544 | 0.217030 |
| C | 2.275478 | -1.173064 | 0.523649 |
| C | 1.125431 | 0.890918 | -0.403173 |
| C | 3.624679 | -0.626501 | 0.253558 |
| C | 2.500518 | 1.547935 | -0.271458 |
| H | 0.864383 | 0.758259 | -1.461029 |
| H | 0.344938 | 1.515326 | 0.031209 |
| C | 3.606935 | 0.581282 | -0.683042 |
| H | 4.262620 | -1.432078 | -0.121055 |
| H | 4.057111 | -0.347626 | 1.227200 |
| H | 2.517877 | 2.444892 | -0.890786 |
| H | 2.655112 | 1.864635 | 0.764528 |
| H | 4.578987 | 1.074061 | -0.658223 |
| H | 3.436354 | 0.244486 | -1.710056 |
| H | 2.187337 | -2.146399 | 0.995240 |
| H | -0.039110 | -2.031865 | 0.806357 |
| C | -1.368685 | -0.515603 | 0.220560 |
| C | -2.128687 | -0.992923 | -0.839904 |
| C | -1.846780 | 0.468606 | 1.078951 |
| C | -3.394841 | -0.457719 | -1.050722 |
| H | -1.729727 | -1.763857 | -1.487662 |
| C | -3.112530 | 0.995827 | 0.855625 |
| H | -1.238133 | 0.804391 | 1.910121 |
| C | -3.883915 | 0.534984 | -0.207418 |
| H | -3.996398 | -0.817024 | -1.876049 |
| H | -3.496387 | 1.762005 | 1.517157 |
| H | -4.870489 | 0.948671 | -0.376007 |

**6H**

Imaginary frequency: None

Electronic energies: -1700.373345

Free energies: -1699.924721

Corrected Free energies: -1699.918275

| | | | |
|---|---|---|---|
| S | -2.881188 | -0.327838 | 0.701851 |
| F | -2.527052 | 0.007589 | -1.877315 |
| F | -4.584552 | 0.157834 | -1.240428 |
| F | -3.210948 | 1.773205 | -0.841766 |
| O | -1.451562 | 0.000737 | 0.819179 |
| O | -3.149015 | -1.749886 | 0.475883 |
| O | -3.746924 | 0.335580 | 1.669003 |
| C | -3.331219 | 0.450366 | -0.908451 |
| N | 1.772360 | 0.345385 | 0.757455 |
| H | 2.262274 | 0.272069 | 1.642593 |
| N | 0.424895 | -2.010973 | 0.200308 |
| H | 0.110033 | -1.063698 | 0.487731 |
| C | 2.344757 | -0.528012 | -0.262818 |
| H | 1.872332 | -0.273626 | -1.216710 |
| C | 1.916862 | -1.953404 | 0.107915 |
| H | 2.237691 | -2.692325 | -0.622026 |
| H | 2.324783 | -2.231264 | 1.079687 |
| C | -0.228505 | -2.280879 | -1.127235 |
| H | -1.278941 | -2.030220 | -0.991991 |
| H | 0.206878 | -1.578183 | -1.839093 |
| C | -0.078989 | -3.715130 | -1.602616 |
| H | -0.590394 | -4.413767 | -0.940250 |
| H | 0.962759 | -4.022013 | -1.703929 |
| H | -0.541741 | -3.792480 | -2.586803 |
| C | -0.080510 | -2.931445 | 1.274893 |
| H | -1.145666 | -3.062611 | 1.079608 |
| H | 0.429173 | -3.887775 | 1.153876 |
| C | 0.133503 | -2.337111 | 2.655814 |
| H | -0.295053 | -3.013994 | 3.395343 |
| H | -0.370069 | -1.372335 | 2.734958 |
| H | 1.189065 | -2.207205 | 2.897457 |
| C | 3.878275 | -0.391155 | -0.479542 |
| C | 4.358275 | -1.453325 | -1.478282 |
| H | 4.371018 | -2.454469 | -1.041178 |
| H | 5.377983 | -1.222890 | -1.795829 |
| H | 3.724281 | -1.471701 | -2.370575 |
| C | 4.650942 | -0.540062 | 0.835825 |
| H | 4.422545 | 0.271318 | 1.532029 |
| H | 5.723849 | -0.498676 | 0.632614 |

| | | | |
|---|---|---|---|
| H | 4.450203 | -1.493436 | 1.332224 |
| C | 4.161830 | 0.995992 | -1.070017 |
| H | 3.679207 | 1.111208 | -2.045216 |
| H | 5.238134 | 1.124163 | -1.211705 |
| H | 3.808564 | 1.793089 | -0.412119 |
| C | 1.372894 | 1.669829 | 0.481592 |
| C | 1.572291 | 2.654212 | 1.367527 |
| H | 2.106821 | 2.426241 | 2.287300 |
| C | 1.071760 | 4.063741 | 1.186015 |
| C | 0.639191 | 4.329468 | -0.255813 |
| H | 0.226281 | 4.249316 | 1.861508 |
| H | 1.853128 | 4.770500 | 1.481851 |
| H | 1.527418 | 4.432087 | -0.889945 |
| C | -0.205736 | 3.165453 | -0.768193 |
| H | -0.610085 | 3.377300 | -1.760925 |
| C | 0.624006 | 1.882857 | -0.812135 |
| H | -0.031230 | 1.023868 | -0.986990 |
| H | 0.084924 | 5.268951 | -0.317136 |
| H | 1.333307 | 1.928144 | -1.647797 |
| H | -1.056031 | 3.011489 | -0.096339 |

**6H** radical cation

Imaginary frequency: None

Electronic energies: -1700.183464

Free energies: -1699.732291

Corrected Free energies: -1699.726820

| | | | |
|---|---|---|---|
| S | -2.534714 | -0.406067 | 0.580179 |
| F | -2.216680 | -0.982656 | -1.956564 |
| F | -4.277370 | -0.794952 | -1.337569 |
| F | -3.059985 | 0.968605 | -1.595557 |
| O | -1.151986 | 0.128397 | 0.535621 |
| O | -2.567135 | -1.839194 | 0.865451 |
| O | -3.482197 | 0.436127 | 1.291696 |
| C | -3.058321 | -0.295265 | -1.185717 |
| N | 1.766702 | 0.884429 | 0.698105 |
| H | 2.149751 | 0.834750 | 1.639234 |
| N | 0.653083 | -1.970523 | 0.503903 |
| H | 0.037713 | -1.134471 | 0.605113 |
| C | 2.240666 | -0.155399 | -0.221939 |
| H | 1.611128 | -0.115733 | -1.111664 |
| C | 2.074717 | -1.505843 | 0.483723 |
| H | 2.664042 | -2.275636 | -0.006653 |
| H | 2.417774 | -1.439807 | 1.516123 |

| | | | |
|---|---|---|---|
| C | 0.225712 | -2.611981 | -0.794038 |
| H | -0.855551 | -2.717174 | -0.712549 |
| H | 0.436548 | -1.896187 | -1.589447 |
| C | 0.884238 | -3.951407 | -1.066575 |
| H | 0.646624 | -4.685818 | -0.296971 |
| H | 1.967538 | -3.880454 | -1.170566 |
| H | 0.491490 | -4.324493 | -2.012778 |
| C | 0.353230 | -2.857206 | 1.685500 |
| H | -0.589730 | -3.350920 | 1.453164 |
| H | 1.146575 | -3.602740 | 1.745887 |
| C | 0.222393 | -2.052986 | 2.965629 |
| H | -0.096110 | -2.724528 | 3.762856 |
| H | -0.534704 | -1.274744 | 2.854155 |
| H | 1.162870 | -1.596639 | 3.277095 |
| C | 3.707446 | 0.109021 | -0.681718 |
| C | 4.086458 | -0.942448 | -1.734303 |
| H | 4.246603 | -1.931663 | -1.301813 |
| H | 5.023209 | -0.645617 | -2.209999 |
| H | 3.324145 | -1.020075 | -2.514961 |
| C | 4.683569 | 0.042113 | 0.497404 |
| H | 4.478013 | 0.811611 | 1.246554 |
| H | 5.697565 | 0.212638 | 0.129828 |
| H | 4.673924 | -0.935308 | 0.986097 |
| C | 3.780320 | 1.493961 | -1.333511 |
| H | 3.129102 | 1.551316 | -2.210156 |
| H | 4.803160 | 1.680048 | -1.666690 |
| H | 3.512589 | 2.291838 | -0.636543 |
| C | 0.950919 | 1.901794 | 0.461727 |
| C | 0.682276 | 2.770306 | 1.541587 |
| H | 1.117858 | 2.531584 | 2.506924 |
| C | -0.183833 | 3.965473 | 1.432712 |
| C | -0.493836 | 4.350270 | -0.012911 |
| H | -1.115416 | 3.730414 | 1.970895 |
| H | 0.273955 | 4.784896 | 1.994697 |
| H | 0.376391 | 4.841784 | -0.458332 |
| C | -0.846309 | 3.098735 | -0.809315 |
| H | -1.159975 | 3.352077 | -1.822393 |
| C | 0.352963 | 2.151649 | -0.891273 |
| H | 0.059736 | 1.205257 | -1.345929 |
| H | -1.317197 | 5.064536 | -0.030462 |
| H | 1.134842 | 2.594125 | -1.519252 |
| H | -1.676327 | 2.578523 | -0.325202 |

**7H**

Imaginary frequency: None

Electronic energies: -658.504886

Free energies: -658.159030

Corrected Free energies: -658.156943

| | | | |
|---|---|---|---|
| N | -0.369420 | -0.692804 | -0.386453 |
| C | -1.734836 | -0.384299 | -0.256928 |
| C | -2.604706 | -0.528333 | -1.267253 |
| C | -2.179652 | 0.012443 | 1.132375 |
| C | -4.099209 | -0.389212 | -1.123959 |
| C | -3.610028 | 0.550477 | 1.144496 |
| H | -2.095899 | -0.866268 | 1.784121 |
| H | -1.498773 | 0.761592 | 1.545617 |
| C | -4.530106 | -0.367060 | 0.343049 |
| H | -4.599743 | -1.208844 | -1.649567 |
| H | -4.436071 | 0.532208 | -1.617073 |
| H | -3.958314 | 0.652005 | 2.174877 |
| H | -3.624011 | 1.551219 | 0.697456 |
| H | -5.570998 | -0.045700 | 0.427236 |
| H | -4.466867 | -1.380118 | 0.756453 |
| H | -2.217931 | -0.791026 | -2.249577 |
| H | -0.141089 | -1.026354 | -1.316859 |
| C | 0.626203 | 0.276956 | 0.074471 |
| C | 2.031829 | -0.174162 | -0.348973 |
| C | 0.375508 | 1.703205 | -0.436966 |
| H | 0.597779 | 0.303978 | 1.170650 |
| C | 3.072703 | 0.791140 | 0.248556 |
| H | 2.081546 | -0.071317 | -1.443565 |
| C | 1.404649 | 2.682159 | 0.127486 |
| H | 0.426164 | 1.694697 | -1.533255 |
| H | -0.638840 | 2.014777 | -0.170442 |
| C | 2.823658 | 2.229423 | -0.214888 |
| H | 4.077276 | 0.477914 | -0.046171 |
| H | 3.027581 | 0.746562 | 1.342920 |
| H | 1.221144 | 3.688899 | -0.256325 |
| H | 1.293138 | 2.730298 | 1.217523 |
| H | 3.559714 | 2.902039 | 0.232848 |
| H | 2.963217 | 2.282192 | -1.301343 |
| N | 2.256818 | -1.597356 | -0.080529 |
| C | 3.525409 | -2.074246 | -0.606052 |
| H | 4.399994 | -1.740594 | -0.024560 |
| H | 3.526642 | -3.166985 | -0.608318 |
| H | 3.649765 | -1.730117 | -1.635704 |
| C | 2.084504 | -1.986501 | 1.309627 |

| | | | |
|---|---|---|---|
| H | 2.235735 | -3.065469 | 1.390995 |
| H | 2.795279 | -1.498070 | 1.995840 |
| H | 1.066228 | -1.768348 | 1.634844 |

**7H** radical cation

Imaginary frequency: None

Electronic energies: -658.326740

Free energies: -657.979874

Corrected Free energies: -657.978362

| | | | |
|---|---|---|---|
| N | -0.420966 | -0.192371 | -0.658174 |
| C | -1.695243 | -0.072581 | -0.334728 |
| C | -2.637663 | -0.846671 | -1.037169 |
| C | -2.117466 | 0.840019 | 0.783066 |
| C | -4.090451 | -0.820854 | -0.741940 |
| C | -3.616113 | 1.144902 | 0.736387 |
| H | -1.869121 | 0.329729 | 1.722481 |
| H | -1.530883 | 1.758498 | 0.759913 |
| C | -4.421846 | -0.142521 | 0.587015 |
| H | -4.478317 | -1.842592 | -0.789127 |
| H | -4.579210 | -0.288820 | -1.572086 |
| H | -3.894440 | 1.674639 | 1.647666 |
| H | -3.826571 | 1.811379 | -0.105862 |
| H | -5.491449 | 0.063246 | 0.633507 |
| H | -4.182763 | -0.819274 | 1.412901 |
| H | -2.280629 | -1.473440 | -1.848071 |
| H | -0.168063 | -0.909505 | -1.335879 |
| C | 0.712993 | 0.514342 | -0.062138 |
| C | 1.969982 | -0.342091 | -0.274953 |
| C | 0.913645 | 1.903367 | -0.685970 |
| H | 0.510504 | 0.626129 | 1.007041 |
| C | 3.153652 | 0.335622 | 0.428657 |
| H | 2.173124 | -0.328751 | -1.354742 |
| C | 2.110406 | 2.591600 | -0.024111 |
| H | 1.093720 | 1.778876 | -1.758694 |
| H | 0.010937 | 2.507334 | -0.575915 |
| C | 3.376578 | 1.740598 | -0.138960 |
| H | 4.052173 | -0.273386 | 0.302273 |
| H | 2.953081 | 0.402711 | 1.503700 |
| H | 2.264778 | 3.569758 | -0.484095 |
| H | 1.883095 | 2.766856 | 1.033325 |
| H | 4.204281 | 2.227733 | 0.380850 |
| H | 3.663103 | 1.660859 | -1.193608 |
| N | 1.701237 | -1.740708 | 0.057757 |

| | | | |
|---|---|---|---|
| C | 2.690651 | -2.646887 | -0.511729 |
| H | 3.681447 | -2.552913 | -0.042043 |
| H | 2.351329 | -3.675525 | -0.376230 |
| H | 2.793202 | -2.457238 | -1.581671 |
| C | 1.530845 | -1.997381 | 1.482987 |
| H | 1.191672 | -3.025964 | 1.616880 |
| H | 2.462398 | -1.868365 | 2.053577 |
| H | 0.770882 | -1.339194 | 1.908340 |

**8H**

Imaginary frequency: None

Electronic energies: -964.511209

Free energies: -964.105336

Corrected Free energies: -964.100780

| | | | |
|---|---|---|---|
| N | -1.195330 | -1.251110 | -0.235022 |
| C | -2.513512 | -0.840093 | 0.000916 |
| C | -3.488859 | -1.022974 | -0.901672 |
| C | -2.785015 | -0.275658 | 1.375396 |
| C | -4.950079 | -0.772122 | -0.627842 |
| C | -4.174191 | 0.354196 | 1.468017 |
| H | -2.680263 | -1.084909 | 2.109071 |
| H | -2.024338 | 0.468291 | 1.627321 |
| C | -5.222483 | -0.576934 | 0.864115 |
| H | -5.547734 | -1.604944 | -1.012360 |
| H | -5.284744 | 0.116645 | -1.179040 |
| H | -4.406685 | 0.584740 | 2.510227 |
| H | -4.176658 | 1.301644 | 0.916977 |
| H | -6.229607 | -0.181723 | 1.016800 |
| H | -5.170598 | -1.546115 | 1.373260 |
| H | -3.218983 | -1.400146 | -1.885772 |
| H | -1.051253 | -1.717621 | -1.121862 |
| C | -0.061261 | -0.422273 | 0.155032 |
| C | 1.202713 | -0.940488 | -0.575415 |
| H | 0.085223 | -0.512994 | 1.237073 |
| H | 1.109699 | -0.604410 | -1.615448 |
| N | 1.233821 | -2.404413 | -0.654610 |
| C | 2.286919 | -2.879171 | -1.539407 |
| H | 3.297654 | -2.710472 | -1.134590 |
| H | 2.159045 | -3.951621 | -1.701579 |
| H | 2.215399 | -2.373570 | -2.505321 |
| C | 1.283375 | -3.093880 | 0.625854 |
| H | 1.131482 | -4.161570 | 0.451824 |
| H | 2.245902 | -2.969510 | 1.145162 |

| | | | |
|---|---|---|---|
| H | 0.477444 | -2.741630 | 1.271864 |
| C | -0.225979 | 1.057453 | -0.166281 |
| C | -0.789250 | 1.452265 | -1.380454 |
| C | 0.195413 | 2.037210 | 0.732063 |
| C | -0.920569 | 2.801136 | -1.693874 |
| H | -1.136458 | 0.696295 | -2.077207 |
| C | 0.067902 | 3.387773 | 0.420892 |
| H | 0.627169 | 1.737412 | 1.682299 |
| C | -0.490892 | 3.772886 | -0.794044 |
| H | -1.361798 | 3.094944 | -2.639233 |
| H | 0.402087 | 4.138028 | 1.128054 |
| H | -0.595211 | 4.823771 | -1.036564 |
| C | 2.469298 | -0.304378 | -0.016358 |
| C | 3.380237 | 0.291967 | -0.889646 |
| C | 2.773564 | -0.322875 | 1.348535 |
| C | 4.561444 | 0.859049 | -0.420368 |
| H | 3.156445 | 0.317517 | -1.951800 |
| C | 3.954330 | 0.240281 | 1.822185 |
| H | 2.083979 | -0.768242 | 2.056757 |
| C | 4.852008 | 0.834044 | 0.939618 |
| H | 5.251911 | 1.320821 | -1.116483 |
| H | 4.170991 | 0.218865 | 2.883834 |
| H | 5.769789 | 1.274684 | 1.310591 |

**8H** radical cation

Imaginary frequency: None

Electronic energies: -964.329572

Free energies: -963.923477

Corrected Free energies: -963.919306

| | | | |
|---|---|---|---|
| N | -1.314788 | -0.811114 | -0.443985 |
| C | -2.559561 | -0.594843 | -0.056709 |
| C | -3.572768 | -1.386118 | -0.631642 |
| C | -2.869490 | 0.435148 | 0.989907 |
| C | -4.995147 | -1.297863 | -0.224279 |
| C | -4.364590 | 0.750996 | 1.067655 |
| H | -2.511117 | 0.035978 | 1.948064 |
| H | -2.289342 | 1.337847 | 0.792274 |
| C | -5.193076 | -0.529798 | 1.082869 |
| H | -5.411053 | -2.308364 | -0.175668 |
| H | -5.537257 | -0.800566 | -1.043008 |
| H | -4.551788 | 1.345677 | 1.961984 |
| H | -4.650389 | 1.361073 | 0.205276 |
| H | -6.251380 | -0.304088 | 1.215594 |

| | | | |
|---|---|---|---|
| H | -4.884622 | -1.156255 | 1.925491 |
| H | -3.290299 | -2.084786 | -1.412575 |
| H | -1.105685 | -1.616422 | -1.045281 |
| C | -0.100873 | -0.173696 | 0.069883 |
| C | 1.092088 | -0.898515 | -0.607275 |
| H | -0.082861 | -0.323013 | 1.153929 |
| H | 1.115405 | -0.532646 | -1.639427 |
| N | 0.818233 | -2.335850 | -0.718345 |
| C | 1.695652 | -2.983582 | -1.688399 |
| H | 2.743196 | -3.004766 | -1.354504 |
| H | 1.359581 | -4.010511 | -1.838424 |
| H | 1.642872 | -2.457680 | -2.643331 |
| C | 0.818242 | -3.064009 | 0.547192 |
| H | 0.457992 | -4.077056 | 0.362460 |
| H | 1.817531 | -3.128062 | 0.998574 |
| H | 0.139466 | -2.594287 | 1.262782 |
| C | -0.042497 | 1.313573 | -0.222216 |
| C | -0.413871 | 1.804016 | -1.473677 |
| C | 0.431497 | 2.191515 | 0.750163 |
| C | -0.319084 | 3.163917 | -1.745595 |
| H | -0.786524 | 1.125618 | -2.234338 |
| C | 0.533696 | 3.551148 | 0.473855 |
| H | 0.717618 | 1.811228 | 1.725253 |
| C | 0.156387 | 4.039249 | -0.772844 |
| H | -0.616248 | 3.539543 | -2.717163 |
| H | 0.902969 | 4.228297 | 1.234419 |
| H | 0.230079 | 5.098753 | -0.985790 |
| C | 2.416429 | -0.521473 | 0.034556 |
| C | 3.485287 | -0.157684 | -0.785516 |
| C | 2.613759 | -0.555717 | 1.417637 |
| C | 4.724103 | 0.166673 | -0.241699 |
| H | 3.342310 | -0.122473 | -1.860783 |
| C | 3.850504 | -0.230757 | 1.964458 |
| H | 1.805105 | -0.835023 | 2.083898 |
| C | 4.908550 | 0.131512 | 1.136219 |
| H | 5.541572 | 0.450964 | -0.893305 |
| H | 3.986668 | -0.259249 | 3.038843 |
| H | 5.870656 | 0.386872 | 1.563804 |

**9H**

Imaginary frequency: None

Electronic energies: -445.945703

Free energies: -445.724385

Corrected Free energies: -445.723530

| | | | |
|---|---|---|---|
| C | -2.578458 | -1.286594 | -0.275151 |
| C | -1.072470 | -1.185642 | -0.249891 |
| C | -0.401973 | -0.045269 | 0.010710 |
| C | -1.122018 | 1.268582 | 0.230272 |
| C | -2.594850 | 1.206176 | -0.172517 |
| C | -3.242034 | -0.067198 | 0.362804 |
| H | -0.519375 | -2.101934 | -0.423837 |
| H | -2.937065 | -1.393098 | -1.307938 |
| H | -2.893218 | -2.197447 | 0.244667 |
| H | -1.029057 | 1.537972 | 1.289826 |
| H | -0.622348 | 2.063497 | -0.328961 |
| H | -3.112286 | 2.096455 | 0.192510 |
| H | -2.672784 | 1.212352 | -1.265514 |
| H | -3.106990 | -0.105774 | 1.449890 |
| H | -4.316880 | -0.071252 | 0.166190 |
| C | 1.778382 | -1.204012 | 0.072272 |
| C | 1.768359 | 1.194536 | -0.146203 |
| C | 3.186432 | -0.699539 | 0.366701 |
| H | 1.720921 | -1.641067 | -0.938223 |
| H | 1.430427 | -1.959276 | 0.781962 |
| C | 3.195543 | 0.657871 | -0.343306 |
| H | 1.719393 | 1.927465 | 0.665334 |
| H | 1.407789 | 1.681091 | -1.058267 |
| H | 3.310232 | -0.568684 | 1.444727 |
| H | 3.962068 | -1.375540 | 0.006865 |
| H | 3.950981 | 1.342324 | 0.042173 |
| H | 3.387823 | 0.508103 | -1.408319 |
| N | 0.974127 | 0.001622 | 0.187538 |

**9H** radical cation

Imaginary frequency: None

Electronic energies: -445.769711

Free energies: -445.548243

Corrected Free energies: -445.547481

| | | | |
|---|---|---|---|
| C | -2.568165 | -1.302905 | -0.119531 |
| C | -1.088836 | -1.218363 | -0.206354 |
| C | -0.380862 | -0.010300 | -0.068660 |
| C | -1.109633 | 1.300382 | 0.078999 |
| C | -2.601398 | 1.186927 | -0.237957 |
| C | -3.209235 | -0.035533 | 0.440734 |
| H | -0.541904 | -2.130408 | -0.408709 |
| H | -2.945108 | -1.503404 | -1.133702 |

| | | | |
|---|---|---|---|
| H | -2.831365 | -2.190001 | 0.464505 |
| H | -0.963955 | 1.641975 | 1.111117 |
| H | -0.644630 | 2.048444 | -0.565018 |
| H | -3.098176 | 2.102406 | 0.084421 |
| H | -2.737928 | 1.106565 | -1.320826 |
| H | -3.034999 | 0.018262 | 1.519815 |
| H | -4.287686 | -0.070313 | 0.284649 |
| C | 1.787163 | -1.234018 | -0.063959 |
| C | 1.773888 | 1.202052 | 0.043121 |
| C | 3.161283 | -0.719609 | 0.355865 |
| H | 1.796469 | -1.634707 | -1.081261 |
| H | 1.376239 | -1.976913 | 0.616843 |
| C | 3.188805 | 0.696383 | -0.217616 |
| H | 1.663111 | 1.616770 | 1.049523 |
| H | 1.434542 | 1.940455 | -0.681185 |
| H | 3.227816 | -0.689908 | 1.445332 |
| H | 3.958382 | -1.355037 | -0.024802 |
| H | 3.934822 | 1.336271 | 0.249291 |
| H | 3.377271 | 0.665939 | -1.292499 |
| N | 0.942720 | -0.016642 | -0.049335 |

**10H**

Imaginary frequency: None

Electronic energies: -485.256032

Free energies: -485.004768

Corrected Free energies: -485.004122

| | | | |
|---|---|---|---|
| C | 3.562620 | -0.094455 | -0.354065 |
| C | 2.892486 | 1.275909 | -0.280935 |
| C | 1.387584 | 1.184261 | -0.212339 |
| C | 0.712954 | 0.052756 | 0.050692 |
| C | 1.441677 | -1.259245 | 0.273922 |
| C | 2.908022 | -1.045105 | 0.644509 |
| H | 3.265237 | 1.818336 | 0.598242 |
| H | 3.177829 | 1.881672 | -1.146626 |
| H | 3.444914 | -0.506389 | -1.362772 |
| H | 4.634545 | -0.002617 | -0.163647 |
| H | 0.922281 | -1.814201 | 1.060636 |
| H | 1.392644 | -1.874580 | -0.631883 |
| H | 2.973126 | -0.614194 | 1.649898 |
| H | 3.426851 | -2.006285 | 0.668155 |
| C | -1.408211 | 1.253669 | 0.127987 |
| C | -1.341451 | -1.066091 | -0.576737 |
| C | -2.857514 | 1.100324 | 0.580084 |

| | | | |
|---|---|---|---|
| H | -1.380256 | 1.649540 | -0.903303 |
| H | -0.902520 | 1.977046 | 0.769910 |
| C | -2.785837 | -1.281699 | -0.140093 |
| H | -1.317365 | -0.796224 | -1.647524 |
| H | -0.785406 | -1.995167 | -0.461397 |
| C | -3.575585 | 0.021427 | -0.226041 |
| H | -3.362226 | 2.064648 | 0.481338 |
| H | -2.866678 | 0.830171 | 1.641251 |
| H | -3.235253 | -2.055698 | -0.767259 |
| H | -2.789850 | -1.646869 | 0.892265 |
| H | -4.596976 | -0.117294 | 0.135881 |
| H | -3.641308 | 0.335541 | -1.274648 |
| H | 0.850746 | 2.112980 | -0.363743 |
| N | -0.690114 | -0.012990 | 0.214760 |

**10H** radical cation

Imaginary frequency: None

Electronic energies: -485.073484

Free energies: -484.823187

Corrected Free energies: -484.822126

| | | | |
|---|---|---|---|
| C | 3.495202 | -0.049597 | -0.068330 |
| C | 2.798972 | 1.276189 | 0.218094 |
| C | 1.332866 | 1.238951 | -0.018313 |
| C | 0.611074 | 0.051762 | -0.241129 |
| C | 1.307689 | -1.284349 | -0.105200 |
| C | 2.684163 | -1.178531 | 0.552620 |
| H | 2.952533 | 1.567568 | 1.267870 |
| H | 3.217574 | 2.098689 | -0.370259 |
| H | 3.571988 | -0.201966 | -1.149308 |
| H | 4.508774 | -0.027556 | 0.332569 |
| H | 0.676804 | -1.953677 | 0.482004 |
| H | 1.403380 | -1.722985 | -1.104668 |
| H | 2.562908 | -0.992722 | 1.624330 |
| H | 3.191927 | -2.137471 | 0.444944 |
| C | -1.525450 | 1.281906 | -0.616947 |
| C | -1.482333 | -1.139989 | -0.775093 |
| C | -2.495629 | 1.229642 | 0.567646 |
| H | -2.071755 | 1.246524 | -1.562122 |
| H | -0.926876 | 2.184044 | -0.614798 |
| C | -2.449285 | -1.286972 | 0.404070 |
| H | -2.037690 | -0.996405 | -1.704935 |
| H | -0.841792 | -2.005513 | -0.897133 |
| C | -3.336756 | -0.046920 | 0.522735 |

| | | | |
|---|---|---|---|
| H | -3.129948 | 2.116833 | 0.530894 |
| H | -1.916138 | 1.273527 | 1.494886 |
| H | -3.048916 | -2.184741 | 0.244960 |
| H | -1.869961 | -1.432565 | 1.321293 |
| H | -3.961053 | -0.115104 | 1.415180 |
| H | -4.008515 | -0.004367 | -0.341064 |
| H | 0.822866 | 2.190684 | -0.010166 |
| N | -0.677027 | 0.077807 | -0.577913 |

**11H**

Imaginary frequency: None

Electronic energies: -634.518858

Free energies: -634.286079

Corrected Free energies: -634.284101

| | | | |
|---|---|---|---|
| C | -3.137177 | 0.871681 | 0.735314 |
| C | -1.657020 | 1.139521 | 0.619508 |
| C | -0.822546 | 0.415848 | -0.146512 |
| C | -1.300220 | -0.787908 | -0.931364 |
| C | -2.683387 | -1.257967 | -0.484802 |
| C | -3.635201 | -0.072619 | -0.357255 |
| H | -1.267623 | 1.978192 | 1.185971 |
| H | -3.363106 | 0.439291 | 1.719187 |
| H | -3.685689 | 1.818002 | 0.692033 |
| H | -1.310611 | -0.523928 | -1.996193 |
| H | -0.593259 | -1.616914 | -0.834897 |
| H | -3.065493 | -1.997124 | -1.192504 |
| H | -2.596225 | -1.753497 | 0.488680 |
| H | -3.670142 | 0.461466 | -1.313695 |
| H | -4.650320 | -0.410056 | -0.135013 |
| C | 1.544444 | -0.228414 | -0.578806 |
| C | 1.079595 | 1.952074 | 0.276979 |
| C | 2.884172 | 0.542746 | -0.408670 |
| H | 1.466160 | -0.672086 | -1.573996 |
| C | 2.468189 | 2.016954 | -0.347794 |
| H | 1.136262 | 1.845004 | 1.371118 |
| H | 0.468030 | 2.827769 | 0.050383 |
| H | 3.359898 | 0.255698 | 0.532029 |
| H | 3.578419 | 0.319351 | -1.216697 |
| H | 3.166407 | 2.620907 | 0.230949 |
| H | 2.393762 | 2.434540 | -1.353625 |
| N | 0.511653 | 0.771329 | -0.355030 |
| C | 1.516107 | -1.349301 | 0.444682 |
| O | 1.053016 | -1.270486 | 1.551081 |

| | | | |
|---|---|---|---|
| O | 2.119803 | -2.450497 | -0.023360 |
| H | 2.127678 | -3.113742 | 0.682035 |

**11H** radical cation

Imaginary frequency: None

Electronic energies: -634.333313

Free energies: -634.100376

Corrected Free energies: -634.098791

| | | | |
|---|---|---|---|
| C | -3.273335 | 0.830812 | 0.533330 |
| C | -1.821274 | 1.124898 | 0.588972 |
| C | -0.845329 | 0.319877 | -0.030574 |
| C | -1.240449 | -0.956325 | -0.729734 |
| C | -2.655529 | -1.408737 | -0.369866 |
| C | -3.636615 | -0.247699 | -0.483833 |
| H | -1.504336 | 1.980283 | 1.171570 |
| H | -3.577647 | 0.521875 | 1.544769 |
| H | -3.807527 | 1.768590 | 0.350552 |
| H | -1.170407 | -0.761423 | -1.807507 |
| H | -0.529765 | -1.749349 | -0.502471 |
| H | -2.938004 | -2.227713 | -1.031628 |
| H | -2.662887 | -1.797461 | 0.653067 |
| H | -3.593430 | 0.169976 | -1.494277 |
| H | -4.659407 | -0.583458 | -0.311913 |
| C | 1.527552 | -0.130729 | -0.524214 |
| C | 0.926696 | 2.022662 | 0.411111 |
| C | 2.771505 | 0.783372 | -0.463251 |
| H | 1.317344 | -0.460477 | -1.544223 |
| C | 2.183894 | 2.192721 | -0.431467 |
| H | 1.154011 | 1.967142 | 1.479637 |
| H | 0.179761 | 2.790335 | 0.230063 |
| H | 3.327775 | 0.588630 | 0.456239 |
| H | 3.430342 | 0.600271 | -1.308399 |
| H | 2.865502 | 2.921435 | 0.002681 |
| H | 1.909575 | 2.518982 | -1.436101 |
| N | 0.423042 | 0.703996 | -0.030774 |
| C | 1.725501 | -1.345867 | 0.371902 |
| O | 1.148714 | -1.544229 | 1.403173 |
| O | 2.664603 | -2.131695 | -0.143965 |
| H | 2.815573 | -2.878131 | 0.455434 |

**11H'**

Imaginary frequency: None

Electronic energies: -634.042095
Free energies: -633.821819
Corrected Free energies: -633.820276

| | | | |
|---|---|---|---|
| C | 3.091137 | -0.996342 | 0.657351 |
| C | 1.604143 | -1.229193 | 0.537604 |
| C | 0.767053 | -0.431254 | -0.157761 |
| C | 1.269289 | 0.812074 | -0.863460 |
| C | 2.647160 | 1.239535 | -0.365005 |
| C | 3.595591 | 0.044440 | -0.341565 |
| H | 1.207676 | -2.099168 | 1.049380 |
| H | 3.340637 | -0.666012 | 1.675193 |
| H | 3.627959 | -1.940293 | 0.512907 |
| H | 1.307981 | 0.602079 | -1.940237 |
| H | 0.559278 | 1.632129 | -0.740843 |
| H | 3.037850 | 2.039968 | -0.998116 |
| H | 2.550245 | 1.643621 | 0.649218 |
| H | 3.631079 | -0.397230 | -1.344315 |
| H | 4.612422 | 0.354145 | -0.086802 |
| C | -1.587966 | 0.313745 | -0.551330 |
| C | -1.148788 | -1.936758 | 0.194095 |
| C | -2.917830 | -0.425045 | -0.278796 |
| H | -1.556507 | 0.696962 | -1.575902 |
| C | -2.566782 | -1.912804 | -0.364000 |
| H | -1.156907 | -1.914754 | 1.295760 |
| H | -0.576311 | -2.814663 | -0.118941 |
| H | -3.242789 | -0.195445 | 0.739672 |
| H | -3.706890 | -0.120742 | -0.966495 |
| H | -3.254708 | -2.545341 | 0.198299 |
| H | -2.555470 | -2.248409 | -1.404191 |
| N | -0.569409 | -0.729954 | -0.365109 |
| C | -1.481858 | 1.518009 | 0.422551 |
| O | -1.104685 | 1.264761 | 1.585273 |
| O | -1.828638 | 2.623288 | -0.051140 |

**11H'** radical cation
Imaginary frequency: None
Electronic energies: -633.875865
Free energies: -633.657397
Corrected Free energies: -633.655444

| | | | |
|---|---|---|---|
| C | 3.194905 | -0.889553 | 0.588949 |
| C | 1.729602 | -1.144142 | 0.598201 |
| C | 0.802276 | -0.339110 | -0.073600 |
| C | 1.253519 | 0.888847 | -0.825683 |

| | | | |
|---|---|---|---|
| C | 2.660661 | 1.326875 | -0.422909 |
| C | 3.622374 | 0.143901 | -0.450758 |
| H | 1.376267 | -1.975668 | 1.193886 |
| H | 3.475285 | -0.550414 | 1.596922 |
| H | 3.713484 | -1.843811 | 0.452911 |
| H | 1.225598 | 0.647120 | -1.895584 |
| H | 0.547376 | 1.697123 | -0.650057 |
| H | 2.992683 | 2.116865 | -1.097760 |
| H | 2.629150 | 1.751019 | 0.586252 |
| H | 3.610280 | -0.309861 | -1.446890 |
| H | 4.645528 | 0.464545 | -0.250564 |
| C | -1.546333 | 0.219986 | -0.549084 |
| C | -1.058315 | -1.906978 | 0.465378 |
| C | -2.819573 | -0.646018 | -0.548150 |
| H | -1.298563 | 0.598675 | -1.542433 |
| C | -2.318046 | -2.081633 | -0.373584 |
| H | -1.290145 | -1.733614 | 1.521603 |
| H | -0.356555 | -2.731120 | 0.372648 |
| H | -3.449653 | -0.355613 | 0.293790 |
| H | -3.398441 | -0.507984 | -1.459165 |
| H | -3.042439 | -2.731979 | 0.114185 |
| H | -2.048808 | -2.519147 | -1.337055 |
| N | -0.484981 | -0.668695 | -0.089169 |
| C | -1.719974 | 1.484373 | 0.407631 |
| O | -0.887902 | 1.624243 | 1.313610 |
| O | -2.704940 | 2.166438 | 0.095534 |

**11H''**

Imaginary frequency: None

Electronic energies: -673.809302

Free energies: -673.550453

Corrected Free energies: -673.548380

| | | | |
|---|---|---|---|
| C | 3.515710 | 0.346137 | -0.784515 |
| C | 2.172165 | 0.994084 | -0.562608 |
| C | 1.207087 | 0.465058 | 0.212682 |
| C | 1.414484 | -0.823414 | 0.980630 |
| C | 2.879852 | -1.257668 | 1.015305 |
| C | 3.514523 | -1.122354 | -0.365233 |
| H | 1.999411 | 1.939677 | -1.063190 |
| H | 3.789301 | 0.433773 | -1.840620 |
| H | 4.296709 | 0.881024 | -0.227179 |
| H | 1.046684 | -0.692525 | 2.002130 |
| H | 0.803216 | -1.615540 | 0.528512 |

| | | | |
|---|---|---|---|
| H | 3.427155 | -0.622704 | 1.720732 |
| H | 2.948070 | -2.283632 | 1.383870 |
| H | 4.531880 | -1.520708 | -0.364897 |
| H | 2.932491 | -1.707295 | -1.086569 |
| C | -1.199515 | 0.347285 | 0.829556 |
| C | -0.409001 | 2.227845 | -0.420313 |
| C | -2.260218 | 1.451987 | 0.945808 |
| H | -1.053064 | -0.167156 | 1.779762 |
| C | -1.932744 | 2.353468 | -0.250680 |
| H | -0.142890 | 2.049154 | -1.468733 |
| H | 0.127184 | 3.122831 | -0.088734 |
| H | -3.277043 | 1.060034 | 0.932735 |
| H | -2.099646 | 1.978707 | 1.887728 |
| H | -2.435484 | 1.981557 | -1.145145 |
| H | -2.249092 | 3.383736 | -0.092852 |
| N | -0.026160 | 1.084926 | 0.409938 |
| C | -1.644368 | -0.680731 | -0.204306 |
| O | -1.298075 | -0.694305 | -1.357609 |
| O | -2.500366 | -1.558394 | 0.324304 |
| C | -3.024708 | -2.541427 | -0.578481 |
| H | -3.568832 | -2.055363 | -1.388016 |
| H | -2.213365 | -3.139276 | -0.993332 |
| H | -3.691644 | -3.160806 | 0.013586 |

**11H''** radical cation

Imaginary frequency: None

Electronic energies: -673.624919

Free energies: -673.366904

Corrected Free energies: -673.364792

| | | | |
|---|---|---|---|
| C | 3.644081 | 0.361727 | -0.566850 |
| C | 2.318524 | 1.001871 | -0.392921 |
| C | 1.210577 | 0.340820 | 0.173419 |
| C | 1.347737 | -1.060045 | 0.709597 |
| C | 2.807309 | -1.478629 | 0.893557 |
| C | 3.621832 | -1.149876 | -0.352702 |
| H | 2.216663 | 2.035317 | -0.697828 |
| H | 4.033235 | 0.634126 | -1.552655 |
| H | 4.327613 | 0.839010 | 0.151955 |
| H | 0.810566 | -1.145743 | 1.655467 |
| H | 0.851797 | -1.728357 | -0.003976 |
| H | 3.231894 | -0.957823 | 1.757214 |
| H | 2.837521 | -2.546573 | 1.110674 |
| H | 4.642379 | -1.521494 | -0.259324 |

| | | | |
|---|---|---|---|
| H | 3.173397 | -1.638028 | -1.223379 |
| C | -1.180722 | 0.362508 | 0.787695 |
| C | -0.242696 | 2.291325 | -0.360225 |
| C | -2.128954 | 1.560428 | 0.923088 |
| H | -0.979431 | -0.118518 | 1.743823 |
| C | -1.762920 | 2.412450 | -0.292166 |
| H | 0.147133 | 2.335136 | -1.375692 |
| H | 0.254318 | 3.044127 | 0.256292 |
| H | -3.169768 | 1.244303 | 0.944322 |
| H | -1.900808 | 2.088262 | 1.850267 |
| H | -2.211494 | 2.001628 | -1.198621 |
| H | -2.075093 | 3.449588 | -0.191634 |
| N | 0.037722 | 0.954725 | 0.221840 |
| C | -1.734430 | -0.676528 | -0.189095 |
| O | -1.288137 | -0.885469 | -1.284720 |
| O | -2.781236 | -1.285115 | 0.341322 |
| C | -3.424215 | -2.268912 | -0.489539 |
| H | -3.773464 | -1.803877 | -1.410231 |
| H | -2.723725 | -3.070195 | -0.720736 |
| H | -4.258550 | -2.642125 | 0.095238 |

**12H**

Imaginary frequency: None

Electronic energies: -1022.499696

Free energies: -1022.095274

Corrected Free energies: -1022.091876

| | | | |
|---|---|---|---|
| C | -0.230980 | 1.120037 | 0.467375 |
| C | -0.842274 | 2.509982 | 0.717180 |
| C | -0.309649 | 3.374630 | -0.427093 |
| C | 1.092099 | 2.814315 | -0.668797 |
| H | -0.463761 | 2.882359 | 1.672832 |
| H | -1.929539 | 2.496935 | 0.765333 |
| H | -0.274780 | 4.433122 | -0.169528 |
| H | -0.934954 | 3.258160 | -1.311572 |
| H | 1.851277 | 3.362375 | -0.096324 |
| H | 1.380656 | 2.868986 | -1.723369 |
| C | -1.106373 | 0.206083 | -0.469250 |
| O | -1.141644 | 0.796285 | -1.760393 |
| C | -2.551575 | 0.089433 | -0.002282 |
| C | -3.558462 | -0.082179 | -0.953168 |
| C | -2.902883 | 0.107295 | 1.349470 |
| C | -4.885829 | -0.227920 | -0.564221 |
| H | -3.294022 | -0.094361 | -2.002783 |

| | | | |
|---|---|---|---|
| C | -4.230356 | -0.040330 | 1.739807 |
| H | -2.144509 | 0.245671 | 2.112339 |
| C | -5.227508 | -0.207237 | 0.784195 |
| H | -5.654216 | -0.357197 | -1.317635 |
| H | -4.483754 | -0.019279 | 2.793235 |
| H | -6.261340 | -0.318148 | 1.088538 |
| C | -0.459301 | -1.184839 | -0.546767 |
| C | -0.725567 | -2.171910 | 0.405581 |
| C | 0.501616 | -1.449228 | -1.524242 |
| C | -0.027507 | -3.375624 | 0.400091 |
| H | -1.475765 | -2.003081 | 1.168951 |
| C | 1.203223 | -2.650707 | -1.529937 |
| H | 0.724263 | -0.713487 | -2.286332 |
| C | 0.947791 | -3.616721 | -0.562752 |
| H | -0.246291 | -4.125455 | 1.151441 |
| H | 1.953793 | -2.827753 | -2.291672 |
| H | 1.496820 | -4.550764 | -0.564059 |
| N | 1.047663 | 1.422937 | -0.190207 |
| H | -0.069378 | 0.591639 | 1.407134 |
| C | 2.271160 | 0.806183 | 0.124173 |
| C | 3.416902 | 1.204530 | -0.460861 |
| C | 2.269796 | -0.276224 | 1.182807 |
| C | 4.780142 | 0.647846 | -0.132012 |
| C | 3.576375 | -1.068052 | 1.208915 |
| H | 2.099180 | 0.194787 | 2.160006 |
| H | 1.443087 | -0.966863 | 1.020973 |
| C | 4.779238 | -0.132196 | 1.180135 |
| H | 5.505666 | 1.465971 | -0.083617 |
| H | 5.122883 | -0.009155 | -0.942802 |
| H | 3.592277 | -1.708716 | 2.094059 |
| H | 3.609747 | -1.725332 | 0.332301 |
| H | 5.712802 | -0.688587 | 1.293998 |
| H | 4.709549 | 0.566805 | 2.021482 |
| H | 3.383698 | 1.968567 | -1.229447 |
| H | -0.234334 | 1.058954 | -1.958970 |

**12H** radical cation

Imaginary frequency: None

Electronic energies: -1022.319256

Free energies: -1021.915201

Corrected Free energies: -1021.911810

| | | | |
|---|---|---|---|
| C | -0.361827 | 1.166710 | 0.498175 |
| C | -1.032085 | 2.542449 | 0.593418 |

| | | | |
|---|---|---|---|
| C | -0.430405 | 3.366051 | -0.555161 |
| C | 0.947155 | 2.744327 | -0.816741 |
| H | -0.771961 | 2.983161 | 1.557098 |
| H | -2.116331 | 2.467255 | 0.534151 |
| H | -0.332712 | 4.415542 | -0.283235 |
| H | -1.048291 | 3.289329 | -1.444867 |
| H | 1.760018 | 3.391950 | -0.491070 |
| H | 1.090698 | 2.476776 | -1.864775 |
| C | -1.089607 | 0.189212 | -0.492369 |
| O | -1.109814 | 0.887578 | -1.725939 |
| C | -2.510739 | -0.040264 | 0.032149 |
| C | -3.595810 | 0.068019 | -0.835343 |
| C | -2.756116 | -0.343567 | 1.375594 |
| C | -4.894790 | -0.139896 | -0.378946 |
| H | -3.437399 | 0.332744 | -1.872480 |
| C | -4.052912 | -0.546251 | 1.832731 |
| H | -1.939307 | -0.432267 | 2.083119 |
| C | -5.128529 | -0.447694 | 0.955501 |
| H | -5.723576 | -0.052127 | -1.071187 |
| H | -4.221072 | -0.778886 | 2.877323 |
| H | -6.139231 | -0.603722 | 1.312530 |
| C | -0.307210 | -1.119268 | -0.664955 |
| C | -0.599514 | -2.278170 | 0.057214 |
| C | 0.773368 | -1.143066 | -1.555505 |
| C | 0.191303 | -3.415427 | -0.076819 |
| H | -1.446712 | -2.308274 | 0.728822 |
| C | 1.559742 | -2.281481 | -1.692153 |
| H | 1.005397 | -0.265329 | -2.147683 |
| C | 1.277476 | -3.420375 | -0.944561 |
| H | -0.052193 | -4.302809 | 0.495024 |
| H | 2.395122 | -2.275015 | -2.382302 |
| H | 1.892041 | -4.306777 | -1.045203 |
| N | 0.985202 | 1.510358 | 0.009474 |
| H | -0.276278 | 0.690415 | 1.470688 |
| C | 2.105488 | 0.878836 | 0.338247 |
| C | 3.312303 | 1.248531 | -0.290320 |
| C | 2.106707 | -0.195775 | 1.398837 |
| C | 4.630893 | 0.665307 | 0.057661 |
| C | 3.386428 | -1.033394 | 1.386594 |
| H | 2.006137 | 0.316067 | 2.364670 |
| H | 1.239510 | -0.843269 | 1.285814 |
| C | 4.619363 | -0.137958 | 1.355179 |
| H | 5.372294 | 1.470390 | 0.075248 |
| H | 4.927036 | 0.022605 | -0.785619 |

| | | | |
|---|---|---|---|
| H | 3.388913 | -1.674708 | 2.268726 |
| H | 3.381897 | -1.686261 | 0.508095 |
| H | 5.533164 | -0.728496 | 1.427324 |
| H | 4.600820 | 0.543429 | 2.211185 |
| H | 3.282994 | 1.961203 | -1.104343 |
| H | -1.292982 | 0.262810 | -2.436412 |

**13H**

Imaginary frequency: None

Electronic energies: -1431.167276

Free energies: -1430.668568

Corrected Free energies: -1430.664588

| | | | |
|---|---|---|---|
| C | -0.220940 | 0.558326 | -1.532383 |
| C | 0.243003 | 1.774661 | -2.354689 |
| C | -0.681136 | 2.948492 | -1.960949 |
| C | -1.779705 | 2.339438 | -1.071389 |
| H | 0.126666 | 1.541396 | -3.413929 |
| H | 1.296557 | 2.002839 | -2.192727 |
| H | -1.115700 | 3.405965 | -2.849961 |
| H | -0.136603 | 3.724789 | -1.423772 |
| H | -2.787299 | 2.586325 | -1.419610 |
| H | -1.691223 | 2.697439 | -0.037151 |
| C | 0.688155 | 0.225719 | -0.291231 |
| O | 0.186842 | -1.014998 | 0.187926 |
| Si | 0.845711 | -2.163515 | 1.222444 |
| C | -0.606092 | -3.289137 | 1.558707 |
| H | -0.314474 | -4.112190 | 2.216430 |
| H | -0.989394 | -3.716112 | 0.627957 |
| H | -1.419885 | -2.740017 | 2.040212 |
| C | 1.466959 | -1.420572 | 2.827409 |
| H | 2.237049 | -0.663636 | 2.665703 |
| H | 1.904446 | -2.217248 | 3.437066 |
| H | 0.656088 | -0.962443 | 3.397799 |
| C | 2.220925 | -3.131280 | 0.396992 |
| H | 2.482585 | -3.990558 | 1.021884 |
| H | 3.121011 | -2.530027 | 0.245734 |
| H | 1.896063 | -3.508519 | -0.576379 |
| C | 2.154819 | 0.022580 | -0.699590 |
| C | 3.209022 | 0.340454 | 0.159679 |
| C | 2.461515 | -0.627804 | -1.900052 |
| C | 4.525059 | 0.022995 | -0.167404 |
| H | 3.010904 | 0.839170 | 1.099980 |
| C | 3.774015 | -0.940187 | -2.233281 |

| | | | |
|---|---|---|---|
| H | 1.673480 | -0.910349 | -2.587017 |
| C | 4.813792 | -0.617842 | -1.365970 |
| H | 5.323149 | 0.278153 | 0.519788 |
| H | 3.982987 | -1.442988 | -3.170184 |
| H | 5.837315 | -0.864371 | -1.622619 |
| C | 0.484783 | 1.312780 | 0.762804 |
| C | 1.137773 | 2.544926 | 0.679146 |
| C | -0.473570 | 1.134227 | 1.761453 |
| C | 0.841025 | 3.571693 | 1.569722 |
| H | 1.886689 | 2.710253 | -0.087603 |
| C | -0.768497 | 2.156581 | 2.656976 |
| H | -1.015449 | 0.198267 | 1.811484 |
| C | -0.114304 | 3.381326 | 2.563472 |
| H | 1.358856 | 4.520105 | 1.486388 |
| H | -1.519255 | 1.999043 | 3.423076 |
| H | -0.344939 | 4.180122 | 3.258402 |
| N | -1.589876 | 0.900724 | -1.184306 |
| H | -0.226846 | -0.345683 | -2.141352 |
| C | -2.576102 | 0.010042 | -0.773113 |
| C | -3.618350 | 0.405951 | -0.014955 |
| C | -2.499714 | -1.389177 | -1.348493 |
| C | -4.821035 | -0.456663 | 0.282912 |
| C | -3.538054 | -2.330586 | -0.738250 |
| H | -2.647209 | -1.318064 | -2.434113 |
| H | -1.500479 | -1.793635 | -1.187267 |
| C | -4.903961 | -1.657294 | -0.657630 |
| H | -5.732923 | 0.144735 | 0.206750 |
| H | -4.785963 | -0.815446 | 1.320866 |
| H | -3.583342 | -3.251802 | -1.324881 |
| H | -3.222514 | -2.609259 | 0.273202 |
| H | -5.666583 | -2.360193 | -0.312520 |
| H | -5.197996 | -1.318526 | -1.657732 |
| H | -3.617643 | 1.408716 | 0.399240 |

**13H** radical cation

Imaginary frequency: None

Electronic energies: -1430.987562

Free energies: -1430.487731

Corrected Free energies: -1430.484023

| | | | |
|---|---|---|---|
| C | -0.263906 | 0.518036 | -1.498551 |
| C | 0.136796 | 1.714635 | -2.369774 |
| C | -0.748599 | 2.902206 | -1.939214 |
| C | -1.822009 | 2.328972 | -1.004216 |

| | | | |
|---|---|---|---|
| H | -0.049428 | 1.462923 | -3.413607 |
| H | 1.198700 | 1.935475 | -2.275279 |
| H | -1.214744 | 3.365605 | -2.806686 |
| H | -0.172605 | 3.665858 | -1.421139 |
| H | -2.827733 | 2.549796 | -1.354328 |
| H | -1.709937 | 2.684452 | 0.023024 |
| C | 0.679460 | 0.221304 | -0.270689 |
| O | 0.196687 | -0.997647 | 0.256478 |
| Si | 0.916893 | -2.149338 | 1.267812 |
| C | -0.528815 | -3.258133 | 1.674188 |
| H | -0.215245 | -4.066493 | 2.339802 |
| H | -0.945355 | -3.709974 | 0.769643 |
| H | -1.322662 | -2.697224 | 2.174669 |
| C | 1.613980 | -1.380832 | 2.824326 |
| H | 2.379084 | -0.631198 | 2.613400 |
| H | 2.079437 | -2.171264 | 3.421163 |
| H | 0.835374 | -0.913133 | 3.430422 |
| C | 2.242002 | -3.113310 | 0.367815 |
| H | 2.521076 | -3.981605 | 0.972270 |
| H | 3.141668 | -2.520289 | 0.186312 |
| H | 1.872208 | -3.476799 | -0.594378 |
| C | 2.123772 | 0.021554 | -0.751808 |
| C | 3.208095 | 0.362558 | 0.058839 |
| C | 2.378229 | -0.652401 | -1.950370 |
| C | 4.509741 | 0.041928 | -0.317257 |
| H | 3.045511 | 0.878886 | 0.996137 |
| C | 3.676830 | -0.966286 | -2.331537 |
| H | 1.565647 | -0.954132 | -2.600112 |
| C | 4.749323 | -0.622187 | -1.513938 |
| H | 5.334944 | 0.313996 | 0.329797 |
| H | 3.849036 | -1.486223 | -3.266167 |
| H | 5.761959 | -0.870374 | -1.808319 |
| C | 0.514138 | 1.337997 | 0.763200 |
| C | 1.147643 | 2.574228 | 0.615480 |
| C | -0.384964 | 1.167874 | 1.817616 |
| C | 0.878321 | 3.618976 | 1.493717 |
| H | 1.859649 | 2.728640 | -0.187698 |
| C | -0.652154 | 2.210380 | 2.699166 |
| H | -0.891407 | 0.218128 | 1.937788 |
| C | -0.025343 | 3.441741 | 2.536718 |
| H | 1.377866 | 4.571273 | 1.361882 |
| H | -1.355687 | 2.059987 | 3.509263 |
| H | -0.234623 | 4.255627 | 3.220267 |
| N | -1.623806 | 0.860217 | -1.037279 |

| | | | |
|---|---|---|---|
| H | -0.328485 | -0.401239 | -2.075531 |
| C | -2.586425 | -0.015572 | -0.768533 |
| C | -3.776774 | 0.441435 | -0.167396 |
| C | -2.442746 | -1.469804 | -1.147478 |
| C | -4.966167 | -0.416848 | 0.056873 |
| C | -3.500713 | -2.353810 | -0.487285 |
| H | -2.548786 | -1.517903 | -2.239142 |
| H | -1.443923 | -1.814287 | -0.894490 |
| C | -4.892468 | -1.758639 | -0.666392 |
| H | -5.858867 | 0.153795 | -0.219323 |
| H | -5.052490 | -0.571544 | 1.142961 |
| H | -3.440361 | -3.352385 | -0.922321 |
| H | -3.280001 | -2.451810 | 0.580627 |
| H | -5.659057 | -2.428423 | -0.275744 |
| H | -5.094470 | -1.614002 | -1.732139 |
| H | -3.823149 | 1.460233 | 0.195734 |

**14H**

Imaginary frequency: None

Electronic energies: -2779.348281

Free energies: -2778.854048

Corrected Free energies: -2778.842841

| | | | |
|---|---|---|---|
| C | -0.267253 | -1.240657 | -1.707595 |
| C | 0.139859 | -0.433623 | -2.955023 |
| C | -1.144906 | 0.249366 | -3.475293 |
| C | -2.296474 | -0.320945 | -2.630328 |
| H | 0.530425 | -1.125817 | -3.701372 |
| H | 0.934888 | 0.283121 | -2.745172 |
| H | -1.294196 | 0.024300 | -4.530842 |
| H | -1.093303 | 1.334196 | -3.379429 |
| H | -3.110881 | -0.722658 | -3.239962 |
| H | -2.731978 | 0.453278 | -1.983301 |
| C | 0.133784 | -0.565727 | -0.340664 |
| O | -0.121921 | -1.546198 | 0.646337 |
| Si | 0.403501 | -1.693575 | 2.246219 |
| C | -0.681325 | -3.063092 | 2.894312 |
| H | -0.561922 | -3.971968 | 2.299084 |
| H | -1.734287 | -2.769792 | 2.861426 |
| H | -0.427215 | -3.297586 | 3.931234 |
| C | 0.125966 | -0.127876 | 3.236873 |
| H | 0.744182 | 0.710794 | 2.908774 |
| H | 0.396143 | -0.340114 | 4.276547 |
| H | -0.920066 | 0.186671 | 3.224654 |

| | | | |
|---|---|---|---|
| C | 2.208908 | -2.183200 | 2.324402 |
| H | 2.436149 | -2.539955 | 3.333257 |
| H | 2.880080 | -1.348394 | 2.106630 |
| H | 2.429973 | -2.992020 | 1.622928 |
| C | 1.627601 | -0.224274 | -0.289121 |
| C | 2.108557 | 0.876841 | 0.413645 |
| C | 2.557687 | -1.125193 | -0.814349 |
| C | 3.475936 | 1.067066 | 0.590343 |
| H | 1.422247 | 1.592916 | 0.849850 |
| C | 3.917971 | -0.921600 | -0.636376 |
| H | 2.231327 | -2.006541 | -1.352892 |
| C | 4.398248 | 0.174401 | 0.069545 |
| H | 5.460429 | 0.322075 | 0.214049 |
| C | -0.777906 | 0.637526 | -0.121386 |
| C | -0.555743 | 1.862631 | -0.745243 |
| C | -1.945428 | 0.470808 | 0.618888 |
| C | -1.483383 | 2.892471 | -0.624007 |
| C | -2.857085 | 1.510182 | 0.741933 |
| H | -2.151403 | -0.487771 | 1.079020 |
| C | -2.643706 | 2.732792 | 0.119042 |
| N | -1.697704 | -1.414282 | -1.877486 |
| H | 0.213170 | -2.219825 | -1.694731 |
| C | -2.496573 | -2.318835 | -1.173797 |
| C | -3.794535 | -2.061677 | -0.927072 |
| C | -1.869978 | -3.656270 | -0.841815 |
| C | -4.758280 | -3.065507 | -0.345995 |
| C | -2.763190 | -4.504458 | 0.064166 |
| H | -1.677101 | -4.183516 | -1.784929 |
| H | -0.904573 | -3.501797 | -0.359005 |
| C | -4.208876 | -4.489045 | -0.422658 |
| H | -5.715932 | -3.002219 | -0.872678 |
| H | -4.975630 | -2.814518 | 0.701270 |
| H | -2.372489 | -5.524116 | 0.110061 |
| H | -2.729178 | -4.101719 | 1.082166 |
| H | -4.827090 | -5.168298 | 0.169579 |
| H | -4.241885 | -4.836828 | -1.461584 |
| H | -4.192339 | -1.079630 | -1.158535 |
| C | 4.871165 | -1.964049 | -1.144226 |
| C | 3.927646 | 2.277543 | 1.354312 |
| F | 4.517454 | -2.418212 | -2.353812 |
| F | 6.123353 | -1.503631 | -1.237270 |
| F | 4.904416 | -3.030728 | -0.327717 |
| F | 3.762678 | 3.401584 | 0.640944 |
| F | 5.217998 | 2.210708 | 1.695894 |

| | | | |
|---|---|---|---|
| F | 3.219741 | 2.434954 | 2.483647 |
| H | 0.342780 | 2.030958 | -1.330239 |
| H | -3.356609 | 3.540317 | 0.218772 |
| C | -1.199709 | 4.181123 | -1.337248 |
| C | -4.098807 | 1.267661 | 1.548431 |
| F | -4.950927 | 0.441125 | 0.920706 |
| F | -4.767393 | 2.397446 | 1.806099 |
| F | -3.812818 | 0.692933 | 2.727726 |
| F | 0.023479 | 4.648033 | -1.046033 |
| F | -1.236862 | 4.021980 | -2.671612 |
| F | -2.078283 | 5.140448 | -1.031037 |

**14H** radical cation

Imaginary frequency: None

Electronic energies: -2779.161750

Free energies: -2778.667017

Corrected Free energies: -2778.656047

| | | | |
|---|---|---|---|
| C | -0.308929 | -1.255127 | -1.626658 |
| C | 0.050003 | -0.492266 | -2.908490 |
| C | -1.230907 | 0.226195 | -3.380395 |
| C | -2.381134 | -0.331295 | -2.532622 |
| H | 0.380674 | -1.210434 | -3.657742 |
| H | 0.873550 | 0.201560 | -2.744449 |
| H | -1.411859 | 0.026600 | -4.434455 |
| H | -1.159479 | 1.305126 | -3.259167 |
| H | -3.162559 | -0.774466 | -3.145578 |
| H | -2.826990 | 0.426540 | -1.883202 |
| C | 0.105540 | -0.548416 | -0.278941 |
| O | -0.158874 | -1.489356 | 0.731873 |
| Si | 0.425517 | -1.639766 | 2.325618 |
| C | -0.665166 | -2.991981 | 2.995217 |
| H | -0.564531 | -3.909932 | 2.410291 |
| H | -1.714921 | -2.687098 | 2.982117 |
| H | -0.394642 | -3.220183 | 4.029293 |
| C | 0.190853 | -0.058872 | 3.296150 |
| H | 0.819019 | 0.763743 | 2.947854 |
| H | 0.475096 | -0.263204 | 4.333494 |
| H | -0.849248 | 0.274531 | 3.299652 |
| C | 2.221805 | -2.155220 | 2.332210 |
| H | 2.479394 | -2.512364 | 3.333482 |
| H | 2.898112 | -1.332145 | 2.088984 |
| H | 2.403136 | -2.970474 | 1.627159 |
| C | 1.606358 | -0.231263 | -0.280278 |

| | | | |
|---|---|---|---|
| C | 2.109093 | 0.868828 | 0.408574 |
| C | 2.512610 | -1.145374 | -0.820529 |
| C | 3.480887 | 1.046344 | 0.554292 |
| H | 1.439250 | 1.593035 | 0.856336 |
| C | 3.878365 | -0.953216 | -0.672516 |
| H | 2.171679 | -2.028283 | -1.348182 |
| C | 4.382392 | 0.142012 | 0.016758 |
| H | 5.448951 | 0.280769 | 0.137012 |
| C | -0.779940 | 0.682444 | -0.083154 |
| C | -0.540325 | 1.883590 | -0.747322 |
| C | -1.938199 | 0.561351 | 0.680115 |
| C | -1.449721 | 2.930742 | -0.651153 |
| C | -2.837434 | 1.615818 | 0.767020 |
| H | -2.148732 | -0.370343 | 1.192637 |
| C | -2.609555 | 2.812115 | 0.101858 |
| N | -1.775735 | -1.400653 | -1.700844 |
| H | 0.127666 | -2.251085 | -1.606972 |
| C | -2.479680 | -2.395233 | -1.166823 |
| C | -3.886456 | -2.295073 | -1.145112 |
| C | -1.805362 | -3.637839 | -0.640021 |
| C | -4.779045 | -3.369764 | -0.650530 |
| C | -2.732074 | -4.475946 | 0.241449 |
| H | -1.507165 | -4.220053 | -1.522112 |
| H | -0.903258 | -3.370192 | -0.097823 |
| C | -4.072883 | -4.707085 | -0.445743 |
| H | -5.631803 | -3.450474 | -1.332099 |
| H | -5.207526 | -3.011154 | 0.298215 |
| H | -2.237193 | -5.422255 | 0.463658 |
| H | -2.892250 | -3.961790 | 1.194444 |
| H | -4.706544 | -5.367971 | 0.146252 |
| H | -3.909524 | -5.188847 | -1.414478 |
| H | -4.352682 | -1.369104 | -1.456330 |
| C | 4.810909 | -2.007496 | -1.196880 |
| C | 3.961442 | 2.257371 | 1.301730 |
| F | 4.426679 | -2.458067 | -2.397995 |
| F | 6.064475 | -1.560166 | -1.314627 |
| F | 4.845817 | -3.071364 | -0.378236 |
| F | 3.812801 | 3.374152 | 0.575428 |
| F | 5.251782 | 2.167359 | 1.634548 |
| F | 3.263167 | 2.438929 | 2.432761 |
| H | 0.355852 | 2.016974 | -1.345235 |
| H | -3.314095 | 3.630179 | 0.170743 |
| C | -1.158187 | 4.186815 | -1.421389 |
| C | -4.080482 | 1.404725 | 1.582134 |

| | | | |
|---|---|---|---|
| F | -4.826375 | 0.406360 | 1.079518 |
| F | -4.851415 | 2.492881 | 1.631162 |
| F | -3.785593 | 1.060182 | 2.844241 |
| F | 0.078678 | 4.637787 | -1.176596 |
| F | -1.231548 | 3.968808 | -2.745822 |
| F | -2.013151 | 5.170653 | -1.133848 |

**15H**

Imaginary frequency: None

Electronic energies: -771.859458

Free energies: -771.506691

Corrected Free energies: -771.505285

| | | | |
|---|---|---|---|
| C | -2.092206 | 1.451281 | 0.041173 |
| C | -0.645390 | 1.611446 | 0.486644 |
| C | -0.981560 | -0.533383 | -0.538341 |
| H | -0.611368 | 1.493460 | 1.580420 |
| H | -0.813759 | -0.935274 | -1.544944 |
| N | -0.003336 | 0.521961 | -0.235510 |
| N | -2.220269 | 0.242909 | -0.544393 |
| O | -2.973445 | 2.285988 | 0.150464 |
| C | -3.412819 | -0.090304 | -1.304682 |
| H | -4.235539 | -0.398148 | -0.656778 |
| H | -3.727707 | 0.789177 | -1.868883 |
| H | -3.183969 | -0.900007 | -1.995069 |
| C | -0.125805 | 2.991554 | 0.106971 |
| H | 0.888132 | 3.148977 | 0.472220 |
| H | -0.132371 | 3.103371 | -0.979233 |
| H | -0.782006 | 3.745812 | 0.543051 |
| C | -1.031236 | -1.725584 | 0.467023 |
| C | -1.078332 | -1.213291 | 1.908392 |
| H | -1.923825 | -0.537250 | 2.064871 |
| H | -1.196811 | -2.056372 | 2.593983 |
| H | -0.154013 | -0.692499 | 2.170800 |
| C | -2.278764 | -2.574502 | 0.188566 |
| H | -2.328820 | -2.884376 | -0.859940 |
| H | -2.245263 | -3.479651 | 0.799842 |
| H | -3.195809 | -2.039552 | 0.440054 |
| C | 0.196306 | -2.629708 | 0.292324 |
| H | 0.103707 | -3.488571 | 0.962038 |
| H | 0.265725 | -3.012681 | -0.730168 |
| H | 1.125245 | -2.114862 | 0.541646 |
| C | 1.374826 | 0.273704 | -0.131412 |

| | | | |
|---|---|---|---|
| C | 1.995161 | -0.399086 | -1.336677 |
| C | 2.118332 | 0.715098 | 0.893019 |
| C | 3.413573 | -0.887639 | -1.051995 |
| H | 2.004426 | 0.330311 | -2.155780 |
| H | 1.371789 | -1.228174 | -1.677125 |
| C | 3.620180 | 0.599117 | 0.955937 |
| C | 4.228586 | 0.224485 | -0.395740 |
| H | 3.882761 | -1.220867 | -1.980406 |
| H | 3.375021 | -1.752927 | -0.379751 |
| H | 4.047749 | 1.540885 | 1.314358 |
| H | 3.893797 | -0.157178 | 1.703264 |
| H | 5.270569 | -0.077985 | -0.268738 |
| H | 4.222256 | 1.101490 | -1.052581 |
| H | 1.627761 | 1.201763 | 1.731236 |

**15H** radical cation

Imaginary frequency: None

Electronic energies: -771.665464

Free energies: -771.313309

Corrected Free energies: -771.311587

| | | | |
|---|---|---|---|
| C | -1.937410 | 1.558166 | 0.009386 |
| C | -0.526879 | 1.609278 | 0.600186 |
| C | -0.973384 | -0.517967 | -0.502221 |
| H | -0.582219 | 1.536561 | 1.690230 |
| H | -0.677423 | -0.915159 | -1.475491 |
| N | 0.077998 | 0.384595 | 0.028169 |
| N | -2.084340 | 0.398962 | -0.662208 |
| O | -2.745827 | 2.456817 | 0.079996 |
| C | -3.223014 | 0.181784 | -1.544285 |
| H | -4.120283 | -0.078773 | -0.981705 |
| H | -3.409518 | 1.101752 | -2.098309 |
| H | -2.986781 | -0.620699 | -2.240229 |
| C | 0.133228 | 2.910883 | 0.152863 |
| H | 1.072934 | 3.114191 | 0.660567 |
| H | 0.300674 | 2.895010 | -0.925475 |
| H | -0.563434 | 3.716061 | 0.385988 |
| C | -1.271956 | -1.682049 | 0.498339 |
| C | -1.615675 | -1.129075 | 1.884650 |
| H | -2.432493 | -0.403809 | 1.846148 |
| H | -1.940480 | -1.952505 | 2.523697 |
| H | -0.747310 | -0.668828 | 2.363546 |
| C | -2.464180 | -2.479588 | -0.047914 |
| H | -2.300708 | -2.790100 | -1.083672 |

| | | | |
|---|---|---|---|
| H | -2.589489 | -3.381453 | 0.554559 |
| H | -3.393362 | -1.912517 | 0.009887 |
| C | -0.075923 | -2.632102 | 0.623985 |
| H | -0.326883 | -3.407741 | 1.350301 |
| H | 0.149293 | -3.131387 | -0.321590 |
| H | 0.823650 | -2.131065 | 0.991480 |
| C | 1.386774 | 0.160186 | -0.074407 |
| C | 1.932464 | -0.754209 | -1.143687 |
| C | 2.265359 | 0.812933 | 0.806549 |
| C | 3.371190 | -1.184840 | -0.864405 |
| H | 1.892394 | -0.173169 | -2.074632 |
| H | 1.294486 | -1.620514 | -1.288746 |
| C | 3.740361 | 0.711217 | 0.719798 |
| C | 4.236429 | 0.032348 | -0.554593 |
| H | 3.749451 | -1.719633 | -1.735821 |
| H | 3.390891 | -1.880836 | -0.019200 |
| H | 4.163047 | 1.713913 | 0.846623 |
| H | 4.068951 | 0.153781 | 1.609853 |
| H | 5.281449 | -0.252333 | -0.431991 |
| H | 4.184754 | 0.736268 | -1.390600 |
| H | 1.845130 | 1.351763 | 1.647418 |

**16H**

Imaginary frequency: None

Electronic energies: -1002.876413

Free energies: -1002.449291

Corrected Free energies: -1002.445981

| | | | |
|---|---|---|---|
| C | 1.497104 | -1.636751 | 0.994486 |
| C | 0.544922 | -0.565740 | 1.516961 |
| C | 1.530898 | 0.103384 | -0.575032 |
| H | 0.995533 | -0.110692 | 2.412217 |
| H | 1.145243 | 0.092820 | -1.603458 |
| N | 0.454911 | 0.326586 | 0.381255 |
| N | 1.962009 | -1.243483 | -0.205393 |
| O | 1.741820 | -2.700569 | 1.539839 |
| C | 2.658853 | -2.177004 | -1.072646 |
| H | 2.674059 | -1.782639 | -2.086471 |
| H | 3.684074 | -2.350616 | -0.740126 |
| H | 2.125621 | -3.129934 | -1.064717 |
| C | -0.793818 | -1.217727 | 1.922639 |
| H | -0.534655 | -2.079735 | 2.543544 |
| H | -1.369069 | -0.525970 | 2.538089 |
| C | 2.690750 | 1.142310 | -0.483866 |

| | | | |
|---|---|---|---|
| C | 3.141207 | 1.298078 | 0.970444 |
| H | 3.455410 | 0.341257 | 1.397800 |
| H | 3.993874 | 1.979896 | 1.021991 |
| H | 2.337838 | 1.711482 | 1.585763 |
| C | 3.875436 | 0.686555 | -1.344175 |
| H | 4.359931 | -0.198916 | -0.929465 |
| H | 3.565351 | 0.468201 | -2.370868 |
| H | 4.622177 | 1.483374 | -1.385933 |
| C | 2.212588 | 2.499794 | -1.011548 |
| H | 1.382374 | 2.895009 | -0.422685 |
| H | 3.035024 | 3.217649 | -0.955987 |
| H | 1.902751 | 2.429961 | -2.058483 |
| C | -0.510336 | 1.330149 | 0.260424 |
| C | -1.062935 | 1.547575 | -1.134404 |
| C | -0.993252 | 1.974276 | 1.334019 |
| C | -2.385849 | 2.315116 | -1.120109 |
| H | -1.204939 | 0.561889 | -1.591559 |
| H | -0.336788 | 2.083349 | -1.753473 |
| C | -2.102841 | 2.990458 | 1.267897 |
| C | -2.316874 | 3.498130 | -0.156759 |
| H | -3.189701 | 1.644074 | -0.798856 |
| H | -2.628632 | 2.647161 | -2.132237 |
| H | -3.038692 | 2.555748 | 1.646185 |
| H | -1.869011 | 3.824684 | 1.936190 |
| H | -1.479124 | 4.145411 | -0.440443 |
| H | -3.228398 | 4.097853 | -0.213553 |
| H | -0.577409 | 1.747909 | 2.312177 |
| C | -1.618419 | -1.641144 | 0.730769 |
| C | -2.792810 | -0.959612 | 0.411689 |
| C | -1.213405 | -2.693710 | -0.096647 |
| C | -3.538628 | -1.303305 | -0.712762 |
| H | -3.117148 | -0.141328 | 1.046789 |
| C | -1.952504 | -3.036440 | -1.224619 |
| H | -0.322613 | -3.260718 | 0.153606 |
| C | -3.115559 | -2.338211 | -1.540139 |
| H | -4.448444 | -0.760305 | -0.943012 |
| H | -1.623503 | -3.855193 | -1.854160 |
| H | -3.691297 | -2.605953 | -2.418343 |

**16H** radical cation

Imaginary frequency: None

Electronic energies: -1002.681471

Free energies: -1002.251292

Corrected Free energies: -1002.248749

| | | | |
|---|---|---|---|
| C | 1.558622 | -1.564877 | 1.001672 |
| C | 0.574962 | -0.528906 | 1.551833 |
| C | 1.522315 | 0.157679 | -0.582601 |
| H | 1.006447 | -0.037474 | 2.428109 |
| H | 1.110140 | 0.176343 | -1.595069 |
| N | 0.453997 | 0.401977 | 0.412501 |
| N | 1.945798 | -1.182773 | -0.229561 |
| O | 1.846215 | -2.602021 | 1.558546 |
| C | 2.638551 | -2.105000 | -1.118652 |
| H | 2.585998 | -1.724886 | -2.136546 |
| H | 3.682525 | -2.229926 | -0.829502 |
| H | 2.140385 | -3.074355 | -1.067764 |
| C | -0.741236 | -1.252827 | 1.924047 |
| H | -0.423479 | -2.122046 | 2.505013 |
| H | -1.346425 | -0.631667 | 2.583295 |
| C | 2.666694 | 1.216069 | -0.447988 |
| C | 3.196034 | 1.263673 | 0.988040 |
| H | 3.526008 | 0.281777 | 1.336858 |
| H | 4.060834 | 1.929170 | 1.024604 |
| H | 2.450578 | 1.660387 | 1.682455 |
| C | 3.799473 | 0.810693 | -1.400888 |
| H | 4.305323 | -0.095895 | -1.068424 |
| H | 3.435083 | 0.662438 | -2.421144 |
| H | 4.540739 | 1.611809 | -1.424563 |
| C | 2.173527 | 2.608508 | -0.850578 |
| H | 1.375466 | 2.975390 | -0.199932 |
| H | 3.005187 | 3.310311 | -0.762124 |
| H | 1.834610 | 2.628652 | -1.889381 |
| C | -0.557547 | 1.254538 | 0.229797 |
| C | -0.993910 | 1.635474 | -1.165514 |
| C | -1.212110 | 1.773808 | 1.356808 |
| C | -2.390314 | 2.264364 | -1.171122 |
| H | -0.984907 | 0.728188 | -1.776794 |
| H | -0.282162 | 2.334128 | -1.607411 |
| C | -2.326635 | 2.747729 | 1.276825 |
| C | -2.496124 | 3.356707 | -0.114005 |
| H | -3.142126 | 1.492938 | -0.982013 |
| H | -2.580514 | 2.665276 | -2.167164 |
| H | -3.243826 | 2.216400 | 1.575849 |
| H | -2.175845 | 3.508360 | 2.047773 |
| H | -1.718003 | 4.108026 | -0.280110 |
| H | -3.458867 | 3.864211 | -0.175325 |
| H | -0.847334 | 1.498170 | 2.339075 |

| | | | |
|---|---|---|---|
| C | -1.547347 | -1.672835 | 0.716789 |
| C | -2.764150 | -1.050548 | 0.436513 |
| C | -1.082724 | -2.659509 | -0.159009 |
| C | -3.490097 | -1.379943 | -0.705771 |
| H | -3.160484 | -0.314304 | 1.129044 |
| C | -1.802530 | -2.985956 | -1.303179 |
| H | -0.168234 | -3.197219 | 0.067757 |
| C | -3.003480 | -2.339747 | -1.585505 |
| H | -4.435578 | -0.888288 | -0.902900 |
| H | -1.428681 | -3.753189 | -1.970605 |
| H | -3.562973 | -2.595564 | -2.477085 |

**17H**

Imaginary frequency: None

Electronic energies: -924.265017

Free energies: -923.893892

Corrected Free energies: -923.890629

| | | | |
|---|---|---|---|
| C | -2.392087 | -1.340079 | -0.698320 |
| C | -0.910798 | -1.039327 | -0.580066 |
| C | -2.205801 | 0.723258 | 0.451232 |
| H | -0.464371 | -1.101477 | -1.576805 |
| N | -0.886945 | 0.312410 | -0.056273 |
| N | -3.065321 | -0.322881 | -0.130381 |
| O | -2.869319 | -2.349989 | -1.189576 |
| C | -4.509034 | -0.315962 | -0.014370 |
| H | -4.867816 | -1.279373 | -0.371913 |
| H | -4.816098 | -0.183924 | 1.024690 |
| H | -4.949904 | 0.477024 | -0.621618 |
| C | -0.260465 | -2.120276 | 0.315940 |
| H | -0.735124 | -2.088540 | 1.300711 |
| H | -0.484531 | -3.090416 | -0.135794 |
| C | 0.209038 | 1.178481 | -0.225618 |
| C | 0.480339 | 2.193383 | 0.609298 |
| C | 1.068461 | 0.916977 | -1.449371 |
| C | 1.638990 | 3.144494 | 0.441100 |
| C | 1.976658 | 2.097331 | -1.791536 |
| C | 2.679447 | 2.608686 | -0.539107 |
| H | 2.097535 | 3.319720 | 1.419502 |
| H | 1.281482 | 4.124348 | 0.096848 |
| H | 2.699089 | 1.790028 | -2.551582 |
| H | 1.377882 | 2.907773 | -2.222385 |
| H | 3.406069 | 3.386164 | -0.786997 |
| H | 3.224677 | 1.779444 | -0.073868 |

| | | | |
|---|---|---|---|
| H | 1.679976 | 0.022643 | -1.282821 |
| C | 1.225991 | -1.930363 | 0.442794 |
| C | 2.096938 | -2.530471 | -0.469153 |
| C | 1.753175 | -1.083458 | 1.418280 |
| C | 3.463290 | -2.273124 | -0.422533 |
| H | 1.697034 | -3.196109 | -1.227845 |
| C | 3.118444 | -0.821742 | 1.467642 |
| H | 1.082002 | -0.608000 | 2.126348 |
| C | 3.976800 | -1.410811 | 0.542901 |
| H | 4.126993 | -2.743263 | -1.138902 |
| H | 3.512504 | -0.152242 | 2.223863 |
| H | 5.040081 | -1.204865 | 0.578530 |
| C | -2.647422 | 2.085854 | -0.080207 |
| H | -2.020979 | 2.885109 | 0.309197 |
| H | -2.593090 | 2.088957 | -1.170518 |
| H | -3.675707 | 2.283121 | 0.228630 |
| C | -2.306557 | 0.661482 | 1.982100 |
| H | -1.644756 | 1.392643 | 2.444556 |
| H | -3.324240 | 0.880269 | 2.313162 |
| H | -2.028207 | -0.333344 | 2.333435 |
| H | 0.413995 | 0.698858 | -2.298946 |
| H | -0.146510 | 2.352653 | 1.477671 |

**17H** radical cation

Imaginary frequency: None

Electronic energies: -924.073835

Free energies: -923.701538

Corrected Free energies: -923.698860

| | | | |
|---|---|---|---|
| C | -2.470634 | -1.224201 | -0.780694 |
| C | -0.971699 | -1.015225 | -0.727121 |
| C | -2.127880 | 0.759969 | 0.493251 |
| H | -0.536569 | -1.082656 | -1.722624 |
| N | -0.843570 | 0.339301 | -0.180214 |
| N | -3.046601 | -0.239202 | -0.062851 |
| O | -3.019367 | -2.158477 | -1.324151 |
| C | -4.483127 | -0.180880 | 0.150240 |
| H | -4.891347 | -1.135481 | -0.174797 |
| H | -4.708372 | -0.036849 | 1.207052 |
| H | -4.937187 | 0.620432 | -0.434640 |
| C | -0.367653 | -2.106948 | 0.199177 |
| H | -0.907685 | -2.101235 | 1.148589 |
| H | -0.583692 | -3.055818 | -0.296386 |
| C | 0.249709 | 1.090094 | -0.347325 |

| | | | |
|---|---|---|---|
| C | 0.503621 | 2.193252 | 0.488512 |
| C | 1.234651 | 0.749434 | -1.443906 |
| C | 1.700583 | 3.061291 | 0.374494 |
| C | 2.118111 | 1.944224 | -1.807102 |
| C | 2.776724 | 2.510731 | -0.557284 |
| H | 2.080200 | 3.254494 | 1.382153 |
| H | 1.344278 | 4.037685 | 0.010491 |
| H | 2.865213 | 1.607533 | -2.526751 |
| H | 1.518078 | 2.717969 | -2.295922 |
| H | 3.483620 | 3.301865 | -0.807432 |
| H | 3.332521 | 1.717076 | -0.047939 |
| H | 1.867550 | -0.081912 | -1.122916 |
| C | 1.107635 | -1.936048 | 0.424912 |
| C | 2.028862 | -2.535726 | -0.435688 |
| C | 1.572873 | -1.104147 | 1.445283 |
| C | 3.388482 | -2.275651 | -0.304707 |
| H | 1.675695 | -3.193746 | -1.222741 |
| C | 2.932689 | -0.835454 | 1.573433 |
| H | 0.867317 | -0.659058 | 2.140565 |
| C | 3.841523 | -1.412441 | 0.690727 |
| H | 4.094653 | -2.740458 | -0.982194 |
| H | 3.281302 | -0.178689 | 2.361711 |
| H | 4.899720 | -1.201219 | 0.786135 |
| C | -2.572183 | 2.148058 | 0.037259 |
| H | -1.949013 | 2.945447 | 0.433334 |
| H | -2.580235 | 2.197539 | -1.052210 |
| H | -3.583639 | 2.317943 | 0.407936 |
| C | -2.057676 | 0.622485 | 2.015502 |
| H | -1.354075 | 1.322003 | 2.463098 |
| H | -3.042336 | 0.840460 | 2.431240 |
| H | -1.780593 | -0.392124 | 2.299579 |
| H | 0.678365 | 0.416870 | -2.322202 |
| H | -0.175312 | 2.412167 | 1.297744 |

**18H**

Imaginary frequency: None

Electronic energies: -367.305226

Free energies: -367.140101

Corrected Free energies: -367.139837

| | | | |
|---|---|---|---|
| C | -2.422709 | 0.072938 | 0.537681 |
| C | -1.772693 | 1.355206 | 0.015604 |
| C | -0.293060 | 1.181584 | -0.213587 |
| C | 0.305147 | -0.012337 | -0.264509 |

| | | | |
|---|---|---|---|
| C | -0.441136 | -1.315802 | -0.123609 |
| C | -1.950247 | -1.129446 | -0.278161 |
| H | -2.258620 | 1.660059 | -0.920221 |
| H | -1.938024 | 2.175245 | 0.720763 |
| H | -2.140459 | -0.075554 | 1.586154 |
| H | -3.511041 | 0.161421 | 0.503629 |
| H | -0.054464 | -2.015201 | -0.870638 |
| H | -0.212172 | -1.753488 | 0.856125 |
| H | -2.186052 | -0.958439 | -1.334339 |
| H | -2.472625 | -2.038688 | 0.027428 |
| H | 0.303164 | 2.077430 | -0.361942 |
| C | 2.639369 | 0.752017 | 0.040211 |
| C | 2.534216 | -0.641898 | 0.557054 |
| H | 2.247923 | 1.537644 | 0.678168 |
| H | 3.468358 | 1.032425 | -0.597606 |
| H | 3.281413 | -1.381342 | 0.296927 |
| H | 2.066216 | -0.761536 | 1.529562 |
| N | 1.687579 | -0.176220 | -0.534016 |

**18H** radical cation

Imaginary frequency: None

Electronic energies: -367.105555

Free energies: -366.942871

Corrected Free energies: -366.942237

| | | | |
|---|---|---|---|
| C | -2.561792 | 0.002609 | 0.356091 |
| C | -1.893942 | 1.315043 | -0.059664 |
| C | -0.413188 | 1.237045 | -0.081974 |
| C | 0.275520 | 0.012487 | -0.018063 |
| C | -0.437064 | -1.305319 | 0.088177 |
| C | -1.899148 | -1.182480 | -0.343961 |
| H | -2.214707 | 1.600437 | -1.073201 |
| H | -2.195725 | 2.149319 | 0.580347 |
| H | -2.475882 | -0.122430 | 1.439881 |
| H | -3.624753 | 0.046189 | 0.117566 |
| H | 0.105082 | -2.047499 | -0.501107 |
| H | -0.378271 | -1.621917 | 1.136077 |
| H | -1.950438 | -1.046006 | -1.428565 |
| H | -2.418894 | -2.111199 | -0.107509 |
| H | 0.171842 | 2.145191 | -0.178883 |
| C | 2.786345 | 0.781033 | 0.001169 |
| C | 2.783523 | -0.731566 | 0.087343 |
| H | 2.936455 | 1.353090 | 0.909259 |
| H | 3.097504 | 1.241148 | -0.929223 |

| | | | |
|---|---|---|---|
| H | 3.093512 | -1.296739 | -0.784033 |
| H | 2.933297 | -1.197170 | 1.054587 |
| N | 1.582779 | 0.019211 | -0.058558 |

**19H**

Imaginary frequency: None

Electronic energies: -406.614128

Free energies: -406.420850

Corrected Free energies: -406.420479

| | | | |
|---|---|---|---|
| C | -2.832433 | 0.008786 | 0.515320 |
| C | -2.210012 | 1.329920 | 0.061995 |
| C | -0.716805 | 1.214178 | -0.117043 |
| C | -0.073758 | 0.039604 | -0.202150 |
| C | -0.784933 | -1.291180 | -0.125399 |
| C | -2.292829 | -1.145605 | -0.327175 |
| H | -2.679479 | 1.650365 | -0.877771 |
| H | -2.431345 | 2.116369 | 0.790185 |
| H | -2.579373 | -0.170176 | 1.566591 |
| H | -3.921783 | 0.060999 | 0.447417 |
| H | -0.355529 | -1.959785 | -0.877900 |
| H | -0.580504 | -1.751303 | 0.849540 |
| H | -2.497628 | -0.942096 | -1.384078 |
| H | -2.794617 | -2.082383 | -0.074508 |
| H | -0.148925 | 2.136054 | -0.205005 |
| C | 2.225615 | 1.045427 | -0.134224 |
| C | 2.147897 | -1.008340 | 0.331742 |
| C | 3.307417 | 0.001076 | 0.205549 |
| H | 1.911465 | 1.621100 | 0.747587 |
| H | 2.407377 | 1.727986 | -0.966510 |
| H | 1.816815 | -1.125481 | 1.371420 |
| H | 2.269565 | -1.990237 | -0.128297 |
| H | 3.904507 | 0.180157 | 1.096095 |
| H | 3.952318 | -0.218138 | -0.643893 |
| N | 1.300884 | -0.059518 | -0.423225 |

**19H** radical cation

Imaginary frequency: None

Electronic energies: -406.434718

Free energies: -406.243092

Corrected Free energies: -406.242355

| | | | |
|---|---|---|---|
| C | -2.914242 | 0.000372 | 0.357078 |
| C | -2.247506 | 1.314272 | -0.053320 |

| | | | |
|---|---|---|---|
| C | -0.765216 | 1.237139 | -0.067219 |
| C | -0.072626 | 0.016870 | -0.007006 |
| C | -0.786621 | -1.303377 | 0.079455 |
| C | -2.249480 | -1.178402 | -0.350220 |
| H | -2.565490 | 1.600646 | -1.067190 |
| H | -2.553068 | 2.145885 | 0.588221 |
| H | -2.827481 | -0.130164 | 1.440205 |
| H | -3.977422 | 0.043136 | 0.118967 |
| H | -0.254660 | -2.040323 | -0.526553 |
| H | -0.726687 | -1.643423 | 1.120164 |
| H | -2.300639 | -1.033624 | -1.433772 |
| H | -2.767402 | -2.110095 | -0.121379 |
| H | -0.192857 | 2.154513 | -0.151455 |
| C | 2.253087 | 1.094194 | -0.051283 |
| C | 2.236140 | -1.060642 | 0.048546 |
| C | 3.351349 | 0.010319 | 0.051767 |
| H | 2.162003 | 1.771271 | 0.798206 |
| H | 2.218813 | 1.651633 | -0.987791 |
| H | 2.132438 | -1.659596 | 0.953934 |
| H | 2.194833 | -1.701601 | -0.833292 |
| H | 3.922964 | 0.049041 | 0.974236 |
| H | 4.017927 | -0.034243 | -0.804039 |
| N | 1.241060 | 0.021781 | -0.016464 |

**20H**

Imaginary frequency: None

Electronic energies: -524.553737

Free energies: -524.274754

Corrected Free energies: -524.273753

| | | | |
|---|---|---|---|
| C | 3.548274 | 0.059536 | 0.112908 |
| C | 2.728723 | 1.321880 | 0.365003 |
| C | 1.299074 | 1.167676 | -0.094324 |
| C | 0.722430 | -0.015207 | -0.395878 |
| C | 1.468164 | -1.319845 | -0.189690 |
| C | 2.763038 | -1.150122 | 0.605103 |
| H | 2.763391 | 1.564798 | 1.436042 |
| H | 3.185106 | 2.174574 | -0.148171 |
| H | 3.737458 | -0.046540 | -0.961530 |
| H | 4.518314 | 0.125562 | 0.611911 |
| H | 0.827564 | -2.035410 | 0.331071 |
| H | 1.682078 | -1.758748 | -1.172205 |
| H | 2.520269 | -1.005966 | 1.664000 |
| H | 3.354335 | -2.065977 | 0.532775 |

| | | | |
|---|---|---|---|
| H | 0.737658 | 2.085981 | -0.212722 |
| C | -1.306767 | -1.362175 | -0.931104 |
| C | -1.319727 | 1.078890 | -1.221092 |
| C | -2.018772 | -1.623812 | 0.398121 |
| H | -2.055120 | -1.300815 | -1.727089 |
| H | -0.664115 | -2.206556 | -1.183816 |
| C | -1.929005 | 1.759395 | 0.027322 |
| H | -2.129013 | 0.788963 | -1.894482 |
| H | -0.701206 | 1.797450 | -1.768352 |
| C | -2.930544 | -0.478776 | 0.849855 |
| H | -1.273504 | -1.804939 | 1.181625 |
| H | -2.600940 | -2.545802 | 0.295353 |
| C | -2.170086 | 0.809813 | 1.203225 |
| H | -2.880428 | 2.210364 | -0.273156 |
| H | -1.294370 | 2.581250 | 0.367921 |
| H | -3.677660 | -0.270451 | 0.073140 |
| H | -3.487314 | -0.815220 | 1.728630 |
| H | -2.721554 | 1.359867 | 1.970789 |
| H | -1.205760 | 0.539440 | 1.647970 |
| N | -0.537714 | -0.122193 | -0.982341 |

**20H** radical cation

Imaginary frequency: None

Electronic energies: -524.375144

Free energies: -524.096372

Corrected Free energies: -524.095347

| | | | |
|---|---|---|---|
| C | -3.584887 | -0.050185 | -0.136242 |
| C | -2.838735 | 1.279304 | -0.201427 |
| C | -1.418010 | 1.180826 | 0.217185 |
| C | -0.742250 | -0.041201 | 0.391504 |
| C | -1.442115 | -1.343545 | 0.082025 |
| C | -2.716997 | -1.147190 | -0.739563 |
| H | -2.845817 | 1.669644 | -1.230332 |
| H | -3.322123 | 2.054413 | 0.400847 |
| H | -3.812911 | -0.293486 | 0.906177 |
| H | -4.533305 | 0.034294 | -0.667340 |
| H | -0.757532 | -2.005506 | -0.449742 |
| H | -1.683595 | -1.829043 | 1.034831 |
| H | -2.451312 | -0.880206 | -1.767222 |
| H | -3.253125 | -2.095816 | -0.779370 |
| H | -0.894463 | 2.110830 | 0.390371 |
| C | 1.272043 | -1.308102 | 1.008851 |
| C | 1.289248 | 1.168307 | 1.093401 |

| | | | |
|---|---|---|---|
| C | 2.138884 | -1.610228 | -0.216897 |
| H | 1.898186 | -1.170541 | 1.890487 |
| H | 0.586385 | -2.125079 | 1.216624 |
| C | 1.844208 | 1.779984 | -0.200580 |
| H | 2.108010 | 0.871009 | 1.744529 |
| H | 0.681225 | 1.876545 | 1.654056 |
| C | 3.055662 | -0.466033 | -0.665046 |
| H | 1.494585 | -1.893831 | -1.055012 |
| H | 2.735427 | -2.489086 | 0.039134 |
| C | 2.296571 | 0.742687 | -1.236876 |
| H | 2.689968 | 2.405805 | 0.094323 |
| H | 1.103740 | 2.442543 | -0.655016 |
| H | 3.707579 | -0.154767 | 0.159279 |
| H | 3.713452 | -0.864271 | -1.440094 |
| H | 2.923787 | 1.257629 | -1.966780 |
| H | 1.425017 | 0.376563 | -1.791126 |
| N | 0.509299 | -0.057911 | 0.841910 |

**21H**

Imaginary frequency: None

Electronic energies: -563.847963

Free energies: -563.542348

Corrected Free energies: -563.541049

| | | | |
|---|---|---|---|
| C | 3.869744 | 0.195000 | 0.801140 |
| C | 3.564214 | -1.039306 | -0.045998 |
| C | 2.100425 | -1.140141 | -0.399182 |
| C | 1.215364 | -0.140802 | -0.238665 |
| C | 1.647691 | 1.218571 | 0.273447 |
| C | 3.161666 | 1.412825 | 0.215012 |
| H | 4.164948 | -1.008387 | -0.964644 |
| H | 3.877380 | -1.944760 | 0.484062 |
| H | 3.508034 | 0.033912 | 1.823148 |
| H | 4.948543 | 0.358042 | 0.859278 |
| H | 1.148850 | 2.015459 | -0.283461 |
| H | 1.295290 | 1.312520 | 1.308609 |
| H | 3.473552 | 1.542802 | -0.827505 |
| H | 3.437079 | 2.323849 | 0.751486 |
| H | 1.762161 | -2.093317 | -0.791036 |
| C | -0.874753 | 0.729507 | -1.194038 |
| C | -0.710585 | -1.639603 | -0.500619 |
| C | -1.799364 | 1.668898 | -0.394600 |
| H | -1.455431 | 0.231233 | -1.979664 |
| H | -0.134853 | 1.332894 | -1.722902 |

| | | | |
|---|---|---|---|
| H | -0.167651 | -2.249050 | 0.226742 |
| H | -0.545188 | -2.090224 | -1.492926 |
| C | -2.202330 | -1.682715 | -0.153149 |
| C | -3.243654 | 1.184116 | -0.193633 |
| H | -1.328394 | 1.890797 | 0.569398 |
| H | -1.841604 | 2.613414 | -0.946522 |
| C | -2.513633 | -0.923829 | 1.150529 |
| H | -2.788821 | -1.278285 | -0.981855 |
| H | -2.489104 | -2.733948 | -0.073531 |
| C | -3.500356 | 0.238747 | 0.989964 |
| H | -3.888452 | 2.057183 | -0.056089 |
| H | -3.580748 | 0.718894 | -1.126623 |
| H | -1.575286 | -0.529217 | 1.549031 |
| H | -2.908179 | -1.611025 | 1.903246 |
| H | -3.491642 | 0.824409 | 1.915410 |
| H | -4.516867 | -0.156831 | 0.887413 |
| N | -0.170026 | -0.292568 | -0.413189 |

**21H** radical cation

Imaginary frequency: None

Electronic energies: -563.668298

Free energies: -563.362388

Corrected Free energies: -563.361059

| | | | |
|---|---|---|---|
| C | -3.484220 | -0.042999 | 1.042184 |
| C | -2.964703 | 1.314192 | 0.578750 |
| C | -1.630366 | 1.250321 | -0.070863 |
| C | -1.022170 | 0.054026 | -0.488617 |
| C | -1.762317 | -1.256192 | -0.327882 |
| C | -3.256171 | -1.066882 | -0.061262 |
| H | -3.657966 | 1.754291 | -0.154083 |
| H | -2.913057 | 2.038266 | 1.396648 |
| H | -2.952297 | -0.350873 | 1.947677 |
| H | -4.542414 | 0.033696 | 1.293098 |
| H | -1.627795 | -1.846973 | -1.235374 |
| H | -1.309487 | -1.825721 | 0.489281 |
| H | -3.751639 | -0.732144 | -0.977952 |
| H | -3.683976 | -2.034456 | 0.203272 |
| H | -1.111441 | 2.191085 | -0.181440 |
| C | 0.961937 | -1.217873 | -1.130278 |
| C | 0.949802 | 1.247564 | -1.418527 |
| C | 1.521400 | -1.756188 | 0.204842 |
| H | 1.773467 | -1.036173 | -1.834769 |
| H | 0.305057 | -1.958771 | -1.580915 |

| | | | |
|---|---|---|---|
| H | 0.287128 | 2.103582 | -1.380978 |
| H | 1.205141 | 1.089395 | -2.469106 |
| C | 2.217793 | 1.491334 | -0.588612 |
| C | 2.887769 | -1.202069 | 0.632450 |
| H | 0.789179 | -1.611817 | 1.004713 |
| H | 1.614820 | -2.835345 | 0.064382 |
| C | 2.029252 | 1.246565 | 0.919421 |
| H | 3.026841 | 0.868917 | -0.974796 |
| H | 2.513921 | 2.522636 | -0.786366 |
| C | 2.876595 | 0.087758 | 1.464839 |
| H | 3.385913 | -1.968190 | 1.231813 |
| H | 3.512749 | -1.080248 | -0.257738 |
| H | 0.975365 | 1.051051 | 1.140495 |
| H | 2.279814 | 2.149618 | 1.478282 |
| H | 2.525810 | -0.146359 | 2.474432 |
| H | 3.913012 | 0.423834 | 1.567747 |
| N | 0.213464 | 0.043337 | -0.999570 |

**22H**

Imaginary frequency: None

Electronic energies: -521.154530

Free energies: -520.927788

Corrected Free energies: -520.926718

| | | | |
|---|---|---|---|
| C | -2.861235 | -1.244972 | -0.422485 |
| C | -1.358661 | -1.115819 | -0.385593 |
| C | -0.709130 | -0.011714 | 0.011969 |
| C | -1.453892 | 1.241634 | 0.420933 |
| C | -2.925918 | 1.211242 | 0.009366 |
| C | -3.551781 | -0.133341 | 0.364861 |
| H | -0.795752 | -1.993670 | -0.681626 |
| H | -3.206411 | -1.225505 | -1.464221 |
| H | -3.151191 | -2.224318 | -0.029456 |
| H | -1.366254 | 1.343220 | 1.509457 |
| H | -0.981454 | 2.128765 | -0.004326 |
| H | -3.457700 | 2.033717 | 0.493283 |
| H | -3.003917 | 1.366869 | -1.072474 |
| H | -3.423813 | -0.313980 | 1.438164 |
| H | -4.624828 | -0.132725 | 0.159838 |
| C | 1.407937 | -1.229002 | 0.104029 |
| C | 1.405945 | 1.059625 | -0.584300 |
| C | 2.843638 | -1.049488 | 0.570104 |
| H | 1.412357 | -1.611828 | -0.930159 |
| H | 0.911741 | -1.965402 | 0.739393 |

| | | | |
|---|---|---|---|
| C | 2.844583 | 1.171094 | -0.107203 |
| H | 1.397163 | 0.792786 | -1.653759 |
| H | 0.928197 | 2.031089 | -0.469802 |
| H | 3.397189 | -1.981928 | 0.457485 |
| H | 2.849380 | -0.754267 | 1.628340 |
| H | 3.395587 | 1.879535 | -0.725973 |
| H | 2.855057 | 1.519101 | 0.934959 |
| N | 0.697011 | 0.040880 | 0.199921 |
| O | 3.517082 | -0.071647 | -0.202333 |

**22H** radical cation

Imaginary frequency: None

Electronic energies: -520.969051

Free energies: -520.742879

Corrected Free energies: -520.741521

| | | | |
|---|---|---|---|
| C | -2.750902 | -1.326620 | 0.181893 |
| C | -1.319672 | -1.231584 | -0.202268 |
| C | -0.622705 | -0.014944 | -0.306229 |
| C | -1.364597 | 1.291669 | -0.135501 |
| C | -2.883986 | 1.126529 | -0.172549 |
| C | -3.324970 | -0.022240 | 0.724471 |
| H | -0.818393 | -2.165389 | -0.408147 |
| H | -3.305410 | -1.642914 | -0.714381 |
| H | -2.859571 | -2.152740 | 0.891191 |
| H | -1.059722 | 1.734942 | 0.819290 |
| H | -1.054495 | 1.978926 | -0.924260 |
| H | -3.340303 | 2.067299 | 0.136732 |
| H | -3.205432 | 0.931203 | -1.200338 |
| H | -2.962439 | 0.145440 | 1.743274 |
| H | -4.412186 | -0.089079 | 0.769653 |
| C | 1.558561 | -1.161483 | -0.713519 |
| C | 1.493844 | 1.243168 | -0.520251 |
| C | 2.566084 | -1.189482 | 0.437170 |
| H | 2.085389 | -1.034191 | -1.661183 |
| H | 0.992942 | -2.083824 | -0.749309 |
| C | 2.509671 | 1.129858 | 0.620722 |
| H | 2.015113 | 1.316915 | -1.477073 |
| H | 0.871648 | 2.118700 | -0.379949 |
| H | 3.254302 | -2.020357 | 0.292654 |
| H | 2.033409 | -1.319382 | 1.387889 |
| H | 3.155041 | 2.006434 | 0.611843 |
| H | 1.976965 | 1.082129 | 1.578991 |
| N | 0.688700 | 0.012971 | -0.548602 |

| | | | |
|---|---|---|---|
| O | 3.330534 | -0.004267 | 0.454963 |

## Calculated Cartesian coordinates for α-branched aldehyde derived enamines

**1I-*Z***

Imaginary frequency: None

Electronic energies: -852.609574

Free energies: -852.182909

Corrected Free energies: -852.177840

| | | | |
|---|---|---|---|
| C | -1.887676 | 2.490386 | 0.110671 |
| C | -3.404785 | 2.640908 | -0.065448 |
| H | -3.945505 | 2.129625 | 0.737521 |
| H | -3.675260 | 3.699643 | -0.032322 |
| H | -3.751760 | 2.242140 | -1.020601 |
| C | -1.459844 | 3.313650 | 1.331778 |
| H | -1.996390 | 2.983666 | 2.226851 |
| H | -0.389389 | 3.210390 | 1.515856 |
| H | -1.686577 | 4.371187 | 1.171759 |
| C | -1.176564 | 3.036285 | -1.134084 |
| H | -0.089345 | 3.022823 | -1.014374 |
| H | -1.435805 | 2.472063 | -2.033697 |
| H | -1.472015 | 4.075725 | -1.300880 |
| C | -1.524542 | 1.003986 | 0.366477 |
| H | -1.979507 | 0.735078 | 1.326728 |
| C | -2.041775 | 0.025064 | -0.703919 |
| H | -1.511560 | 0.228734 | -1.639744 |
| H | -3.111065 | 0.193986 | -0.897232 |
| N | -0.081772 | 0.856561 | 0.542804 |
| N | -1.784420 | -1.356667 | -0.313302 |
| C | -1.419690 | -2.220867 | -1.433596 |
| H | -0.576353 | -1.743919 | -1.941602 |
| H | -1.038222 | -3.163648 | -1.033092 |
| C | -2.850425 | -1.881664 | 0.534672 |
| H | -3.010141 | -1.160379 | 1.341193 |
| H | -3.808216 | -1.949486 | -0.009416 |
| C | -2.507240 | -3.232049 | 1.150114 |
| H | -2.491671 | -4.029409 | 0.404394 |
| H | -1.524487 | -3.187586 | 1.626571 |

| | | | |
|---|---|---|---|
| H | -3.248698 | -3.499023 | 1.905145 |
| C | -2.537519 | -2.503465 | -2.441295 |
| H | -2.944492 | -1.573336 | -2.847002 |
| H | -2.155432 | -3.096796 | -3.274525 |
| H | -3.357335 | -3.061293 | -1.982188 |
| H | 0.440987 | 1.015482 | -0.311138 |
| C | 0.405428 | -0.180560 | 1.313708 |
| C | 1.641714 | -0.724747 | 1.305090 |
| C | 1.928483 | -1.905681 | 2.203294 |
| H | 2.868258 | -1.775073 | 2.748710 |
| H | 2.011920 | -2.842392 | 1.641700 |
| H | -0.325365 | -0.575241 | 2.014001 |
| H | 1.127205 | -2.036791 | 2.932772 |
| C | 2.723840 | -0.263845 | 0.410373 |
| C | 2.892439 | 1.092603 | 0.082763 |
| C | 3.660328 | -1.173253 | -0.108930 |
| C | 3.924022 | 1.512671 | -0.749441 |
| H | 2.225863 | 1.831470 | 0.513494 |
| C | 4.689645 | -0.753573 | -0.943164 |
| H | 3.575749 | -2.225395 | 0.137027 |
| C | 4.825536 | 0.591610 | -1.274867 |
| H | 4.030224 | 2.567180 | -0.977634 |
| H | 5.390514 | -1.481712 | -1.335928 |
| H | 5.628971 | 0.918272 | -1.924033 |

**1I-*E***

Imaginary frequency: -6.1757

Electronic energies: -852.610791

Free energies: -852.183717

Corrected Free energies: -852.179312

| | | | |
|---|---|---|---|
| C | -3.305517 | -1.402953 | -0.390814 |
| C | -4.403042 | -0.650423 | -1.157074 |
| H | -4.035251 | -0.304146 | -2.128041 |
| H | -5.249637 | -1.318051 | -1.336911 |
| H | -4.777709 | 0.212977 | -0.604770 |
| C | -3.013765 | -2.711848 | -1.134678 |
| H | -2.660051 | -2.508046 | -2.150228 |
| H | -2.250093 | -3.296148 | -0.620284 |
| H | -3.924251 | -3.312933 | -1.205717 |
| C | -3.807044 | -1.725632 | 1.022682 |
| H | -3.067931 | -2.292317 | 1.596584 |
| H | -4.058804 | -0.820211 | 1.580337 |
| H | -4.709958 | -2.339287 | 0.963697 |

| | | | |
|---|---|---|---|
| C | -2.015498 | -0.545705 | -0.353105 |
| H | -1.737263 | -0.352637 | -1.395673 |
| C | -2.170928 | 0.808738 | 0.362583 |
| H | -2.246692 | 0.617661 | 1.437559 |
| H | -3.102216 | 1.309451 | 0.061316 |
| N | -0.902905 | -1.292554 | 0.228022 |
| N | -1.007862 | 1.654460 | 0.115740 |
| C | -0.580404 | 2.414714 | 1.288244 |
| H | -0.436844 | 1.693644 | 2.098413 |
| H | 0.405196 | 2.840612 | 1.083331 |
| C | -1.176842 | 2.452364 | -1.095313 |
| H | -1.473230 | 1.768960 | -1.896805 |
| H | -2.001483 | 3.178617 | -0.991628 |
| C | 0.097396 | 3.175015 | -1.512666 |
| H | 0.349722 | 3.986225 | -0.826753 |
| H | 0.936364 | 2.475127 | -1.540351 |
| H | -0.026944 | 3.609046 | -2.506324 |
| C | -1.537570 | 3.519716 | 1.742651 |
| H | -2.536681 | 3.118245 | 1.932848 |
| H | -1.175796 | 3.978105 | 2.665288 |
| H | -1.625751 | 4.306945 | 0.990181 |
| H | -1.044479 | -1.549461 | 1.196204 |
| C | 0.391773 | -0.967824 | -0.105560 |
| C | 1.500690 | -1.286112 | 0.596880 |
| H | 0.470679 | -0.415721 | -1.035203 |
| C | 2.829027 | -0.860563 | 0.118733 |
| C | 3.112610 | -0.654658 | -1.243898 |
| C | 3.875135 | -0.641995 | 1.029988 |
| C | 4.363030 | -0.222089 | -1.664405 |
| H | 2.350280 | -0.858029 | -1.987398 |
| C | 5.130971 | -0.218045 | 0.606980 |
| H | 3.699077 | -0.788526 | 2.089556 |
| C | 5.384726 | 0.000325 | -0.742772 |
| H | 4.547595 | -0.075412 | -2.722801 |
| H | 5.912810 | -0.054319 | 1.340285 |
| H | 6.362223 | 0.329020 | -1.074266 |
| C | 1.391063 | -1.997611 | 1.924472 |
| H | 1.240938 | -1.307185 | 2.762983 |
| H | 0.554813 | -2.701445 | 1.924534 |
| H | 2.291865 | -2.576582 | 2.136111 |

**1I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -852.432710

Free energies: -852.004511

Corrected Free energies: -852.000283

| | | | |
|---|---|---|---|
| C | -3.586428 | -0.954476 | -0.331405 |
| C | -4.618348 | -0.004806 | -0.953165 |
| H | -4.321799 | 0.293863 | -1.962794 |
| H | -5.582632 | -0.513075 | -1.021113 |
| H | -4.759987 | 0.895679 | -0.352221 |
| C | -3.596531 | -2.277203 | -1.108980 |
| H | -3.371118 | -2.109094 | -2.165707 |
| H | -2.862992 | -2.982203 | -0.710062 |
| H | -4.583453 | -2.740585 | -1.040327 |
| C | -3.964729 | -1.222910 | 1.131511 |
| H | -3.320055 | -1.970275 | 1.603585 |
| H | -3.947648 | -0.314978 | 1.737431 |
| H | -4.980567 | -1.622840 | 1.166562 |
| C | -2.185904 | -0.321860 | -0.467700 |
| H | -1.954231 | -0.237819 | -1.534817 |
| C | -2.018789 | 1.094003 | 0.171484 |
| H | -2.308380 | 1.041483 | 1.223049 |
| H | -2.715296 | 1.771593 | -0.335086 |
| N | -1.149771 | -1.160188 | 0.116361 |
| N | -0.650736 | 1.548993 | 0.063309 |
| C | -0.077722 | 2.085068 | 1.297894 |
| H | -0.301676 | 1.369339 | 2.093826 |
| H | 1.010100 | 2.098919 | 1.193492 |
| C | -0.394259 | 2.326712 | -1.149247 |
| H | -0.786206 | 1.749751 | -1.993205 |
| H | -0.952163 | 3.275111 | -1.136803 |
| C | 1.087719 | 2.595696 | -1.372657 |
| H | 1.485392 | 3.307738 | -0.647039 |
| H | 1.664958 | 1.670312 | -1.294704 |
| H | 1.240302 | 3.015147 | -2.367969 |
| C | -0.587420 | 3.473257 | 1.685228 |
| H | -1.676892 | 3.479084 | 1.774285 |
| H | -0.165563 | 3.776017 | 2.645255 |
| H | -0.301284 | 4.220938 | 0.942032 |
| H | -1.356003 | -1.586803 | 1.013963 |
| C | 0.112588 | -0.971704 | -0.217268 |
| C | 1.209471 | -1.370915 | 0.572897 |
| H | 0.274586 | -0.491222 | -1.172119 |
| C | 2.548267 | -1.048615 | 0.120852 |
| C | 2.853826 | -0.876863 | -1.245758 |
| C | 3.582710 | -0.879275 | 1.062949 |

| | | | |
|---|---|---|---|
| C | 4.135602 | -0.539456 | -1.645370 |
| H | 2.096905 | -1.044949 | -2.002269 |
| C | 4.858360 | -0.524349 | 0.656662 |
| H | 3.374695 | -0.992774 | 2.119404 |
| C | 5.140888 | -0.354149 | -0.697051 |
| H | 4.355322 | -0.426035 | -2.699562 |
| H | 5.635328 | -0.378939 | 1.396837 |
| H | 6.140847 | -0.083440 | -1.012918 |
| C | 0.974577 | -2.006373 | 1.907134 |
| H | 0.739801 | -1.250923 | 2.665890 |
| H | 0.140419 | -2.709993 | 1.869295 |
| H | 1.849556 | -2.561360 | 2.238063 |

**1I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -852.429871

Free energies: -852.003753

Corrected Free energies: -851.998592

| | | | |
|---|---|---|---|
| C | -1.381840 | 2.701077 | 0.068069 |
| C | -2.834358 | 3.186955 | -0.019125 |
| H | -3.409861 | 2.872058 | 0.856194 |
| H | -2.848457 | 4.278357 | -0.057425 |
| H | -3.336018 | 2.818563 | -0.915785 |
| C | -0.684024 | 3.431758 | 1.222604 |
| H | -1.195059 | 3.241343 | 2.170271 |
| H | 0.357806 | 3.118463 | 1.328378 |
| H | -0.693649 | 4.508587 | 1.040446 |
| C | -0.661908 | 3.020192 | -1.249043 |
| H | 0.404343 | 2.772903 | -1.220747 |
| H | -1.115645 | 2.507734 | -2.099813 |
| H | -0.726014 | 4.094011 | -1.438328 |
| C | -1.382460 | 1.187675 | 0.377273 |
| H | -1.845258 | 1.038492 | 1.357617 |
| C | -2.119301 | 0.281586 | -0.647530 |
| H | -1.641736 | 0.391307 | -1.623901 |
| H | -3.149737 | 0.642950 | -0.742813 |
| N | -0.021680 | 0.672876 | 0.481024 |
| N | -2.068975 | -1.103938 | -0.224069 |
| C | -1.700988 | -2.042445 | -1.286292 |
| H | -0.780160 | -1.665766 | -1.741026 |
| H | -1.444824 | -2.998061 | -0.823153 |
| C | -3.238684 | -1.483513 | 0.570461 |
| H | -3.349860 | -0.735020 | 1.361319 |

| | | | |
|---|---|---|---|
| H | -4.160153 | -1.437807 | -0.030477 |
| C | -3.102456 | -2.860500 | 1.204491 |
| H | -3.151879 | -3.657201 | 0.459852 |
| H | -2.152303 | -2.946663 | 1.737385 |
| H | -3.912994 | -3.021079 | 1.916640 |
| C | -2.768712 | -2.250951 | -2.360768 |
| H | -3.051873 | -1.301491 | -2.822782 |
| H | -2.390684 | -2.910078 | -3.144397 |
| H | -3.668267 | -2.708594 | -1.943103 |
| H | 0.634928 | 0.961263 | -0.240444 |
| C | 0.265709 | -0.409004 | 1.174155 |
| C | 1.471811 | -1.131543 | 1.072830 |
| C | 1.500802 | -2.511894 | 1.643465 |
| H | 2.463357 | -2.719758 | 2.112787 |
| H | 1.355688 | -3.249725 | 0.845549 |
| H | -0.503809 | -0.757959 | 1.851236 |
| H | 0.702186 | -2.654947 | 2.370551 |
| C | 2.636957 | -0.607669 | 0.371144 |
| C | 2.974329 | 0.758010 | 0.426753 |
| C | 3.479131 | -1.482765 | -0.336654 |
| C | 4.097780 | 1.233727 | -0.232574 |
| H | 2.388265 | 1.436443 | 1.036571 |
| C | 4.590757 | -0.997582 | -1.006978 |
| H | 3.244463 | -2.539423 | -0.379107 |
| C | 4.901305 | 0.360139 | -0.960102 |
| H | 4.352857 | 2.284065 | -0.168156 |
| H | 5.219993 | -1.678528 | -1.566403 |
| H | 5.775843 | 0.733479 | -1.478682 |

**1I-*E*** α-iminio radicals

Imaginary frequency: None

Electronic energies: -852.439611

Free energies: -852.010130

Corrected Free energies: -852.005863

| | | | |
|---|---|---|---|
| C | -1.763870 | -2.499901 | -0.028030 |
| C | -2.991377 | -2.956845 | -0.826395 |
| H | -2.886606 | -2.711590 | -1.887557 |
| H | -3.101252 | -4.040323 | -0.740180 |
| H | -3.914423 | -2.504458 | -0.454967 |
| C | -0.544118 | -3.303908 | -0.492230 |
| H | -0.346622 | -3.144676 | -1.556343 |
| H | 0.352984 | -3.036213 | 0.071410 |
| H | -0.727330 | -4.369758 | -0.336747 |

| | | | |
|---|---|---|---|
| C | -1.983391 | -2.756178 | 1.466456 |
| H | -1.109807 | -2.453447 | 2.046187 |
| H | -2.856132 | -2.229378 | 1.859079 |
| H | -2.149199 | -3.824572 | 1.626441 |
| C | -1.500136 | -0.990765 | -0.324866 |
| H | -1.201526 | -0.933014 | -1.381966 |
| C | -2.770215 | -0.147526 | -0.118344 |
| H | -3.288051 | -0.443021 | 0.793894 |
| H | -3.451989 | -0.231503 | -0.962832 |
| N | -0.476032 | -0.440784 | 0.543339 |
| N | -2.414950 | 1.299895 | 0.054047 |
| C | -3.507285 | 2.088569 | 0.726142 |
| H | -3.743247 | 1.546431 | 1.641172 |
| H | -3.073537 | 3.047048 | 1.007096 |
| C | -1.922978 | 1.905080 | -1.231678 |
| H | -1.084250 | 1.288879 | -1.553462 |
| H | -2.725551 | 1.795483 | -1.960904 |
| C | -1.486878 | 3.348790 | -1.070304 |
| H | -2.326422 | 4.016158 | -0.875712 |
| H | -0.752827 | 3.453618 | -0.268075 |
| H | -1.015094 | 3.668061 | -1.999409 |
| C | -4.735771 | 2.267211 | -0.144426 |
| H | -5.167648 | 1.311910 | -0.445351 |
| H | -5.486233 | 2.802411 | 0.437265 |
| H | -4.522685 | 2.858826 | -1.035420 |
| C | 0.733691 | -0.386944 | 0.076242 |
| C | 1.817179 | 0.151924 | 0.825877 |
| H | 0.937184 | -0.733077 | -0.941222 |
| C | 3.157817 | 0.186083 | 0.266158 |
| C | 3.553750 | -0.655504 | -0.794456 |
| C | 4.118150 | 1.073216 | 0.792387 |
| C | 4.838044 | -0.594342 | -1.311068 |
| H | 2.865050 | -1.387308 | -1.198106 |
| C | 5.399497 | 1.135533 | 0.266087 |
| H | 3.850429 | 1.732902 | 1.608295 |
| C | 5.766964 | 0.304629 | -0.789163 |
| H | 5.120712 | -1.256828 | -2.120200 |
| H | 6.115113 | 1.835683 | 0.680326 |
| H | 6.769293 | 0.351505 | -1.197000 |
| C | 1.545105 | 0.754341 | 2.167564 |
| H | 1.501529 | 1.847893 | 2.097553 |
| H | 0.587742 | 0.406254 | 2.548985 |
| H | 2.334193 | 0.505058 | 2.879202 |
| H | -1.612008 | 1.276486 | 0.701116 |

**1I-*Z*** α-iminio radicals

Imaginary frequency: None

Electronic energies: -852.437212

Free energies: -852.007520

Corrected Free energies: -852.002978

| | | | |
|---|---|---|---|
| C | 2.051820 | 2.268019 | 0.342725 |
| C | 3.582308 | 2.371847 | 0.366398 |
| H | 4.004528 | 2.214048 | -0.630544 |
| H | 3.876054 | 3.368718 | 0.702804 |
| H | 4.032357 | 1.649642 | 1.052287 |
| C | 1.491533 | 3.415440 | -0.504239 |
| H | 1.870519 | 3.372054 | -1.529351 |
| H | 0.399693 | 3.396524 | -0.536398 |
| H | 1.794735 | 4.371744 | -0.071361 |
| C | 1.496243 | 2.389123 | 1.765396 |
| H | 0.405157 | 2.356778 | 1.764354 |
| H | 1.863496 | 1.603871 | 2.430068 |
| H | 1.807616 | 3.346891 | 2.189934 |
| C | 1.647558 | 0.916914 | -0.325112 |
| H | 1.944620 | 0.992198 | -1.381565 |
| C | 2.386506 | -0.271171 | 0.318930 |
| H | 2.420749 | -0.164763 | 1.403032 |
| H | 3.400017 | -0.371542 | -0.065167 |
| N | 0.227188 | 0.649893 | -0.198789 |
| N | 1.652805 | -1.551467 | 0.049456 |
| C | 2.020876 | -2.646259 | 1.014999 |
| H | 1.880275 | -2.224081 | 2.009516 |
| H | 1.287687 | -3.440222 | 0.882239 |
| C | 1.749919 | -1.953393 | -1.395956 |
| H | 1.389855 | -1.101648 | -1.971623 |
| H | 2.808356 | -2.089259 | -1.616787 |
| C | 0.932350 | -3.191456 | -1.711720 |
| H | 1.354977 | -4.092209 | -1.266399 |
| H | -0.101060 | -3.078632 | -1.375477 |
| H | 0.920854 | -3.327471 | -2.792880 |
| C | 3.436507 | -3.156685 | 0.825950 |
| H | 4.175831 | -2.362939 | 0.939120 |
| H | 3.629979 | -3.903880 | 1.595651 |
| H | 3.574198 | -3.636754 | -0.143658 |
| C | -0.532028 | 0.981967 | -1.196502 |
| C | -1.940642 | 0.770801 | -1.272801 |
| C | -2.591046 | 1.068737 | -2.591116 |

| | | | |
|---|---|---|---|
| H | -3.522209 | 1.623686 | -2.457408 |
| H | -2.840435 | 0.144292 | -3.124180 |
| H | -0.081467 | 1.432938 | -2.089388 |
| H | -1.928230 | 1.648586 | -3.232373 |
| C | -2.753695 | 0.240531 | -0.187439 |
| C | -2.350417 | 0.281477 | 1.163615 |
| C | -4.018172 | -0.313139 | -0.476819 |
| C | -3.169917 | -0.218567 | 2.164966 |
| H | -1.396875 | 0.719030 | 1.417709 |
| C | -4.826188 | -0.822577 | 0.527996 |
| H | -4.365917 | -0.360791 | -1.501047 |
| C | -4.406805 | -0.778654 | 1.855387 |
| H | -2.842770 | -0.165687 | 3.196649 |
| H | -5.787456 | -1.253689 | 0.275349 |
| H | -5.041310 | -1.171019 | 2.640882 |
| H | 0.665971 | -1.303114 | 0.223387 |

**2I-*Z***

Imaginary frequency: None

Electronic energies: -638.868984

Free energies: -638.580261

Corrected Free energies: -638.577624

| | | | |
|---|---|---|---|
| N | -0.611649 | 0.048054 | -0.749891 |
| C | 0.124966 | 1.224490 | -0.745927 |
| C | 1.432176 | 1.405032 | -0.472387 |
| C | 2.010768 | 2.800095 | -0.505889 |
| H | 2.912131 | 2.840868 | -1.124860 |
| H | 2.290995 | 3.151669 | 0.491847 |
| H | -0.189061 | -0.702609 | -0.212752 |
| C | -2.051107 | 0.158674 | -0.503495 |
| C | -2.721131 | -1.186549 | -0.774629 |
| C | -2.378518 | 0.650106 | 0.911424 |
| H | -2.440208 | 0.888874 | -1.224795 |
| C | -4.232455 | -1.113929 | -0.541778 |
| H | -2.286123 | -1.935245 | -0.099166 |
| H | -2.497136 | -1.502199 | -1.796771 |
| C | -3.889585 | 0.732959 | 1.137458 |
| H | -1.936036 | -0.053756 | 1.628464 |
| H | -1.906756 | 1.622774 | 1.080526 |
| C | -4.555081 | -0.618148 | 0.870017 |
| H | -4.682662 | -2.094595 | -0.714641 |
| H | -4.674575 | -0.426606 | -1.272855 |
| H | -4.099685 | 1.068988 | 2.155922 |

| | | | |
|---|---|---|---|
| H | -4.313892 | 1.483746 | 0.459821 |
| H | -5.637049 | -0.543974 | 1.006533 |
| H | -4.187892 | -1.349074 | 1.600481 |
| H | -0.465306 | 2.094926 | -1.024513 |
| H | 1.286038 | 3.509001 | -0.909297 |
| C | 2.345706 | 0.294854 | -0.118562 |
| C | 2.249830 | -0.962538 | -0.735150 |
| C | 3.375193 | 0.483728 | 0.816293 |
| C | 3.124722 | -1.993101 | -0.409687 |
| H | 1.497487 | -1.123750 | -1.498944 |
| C | 4.247870 | -0.546930 | 1.143932 |
| H | 3.489757 | 1.446939 | 1.299939 |
| C | 4.125998 | -1.793448 | 0.535670 |
| H | 3.029919 | -2.952064 | -0.906184 |
| H | 5.027682 | -0.375907 | 1.877315 |
| H | 4.807810 | -2.596151 | 0.789428 |

**2I-*E***

Imaginary frequency: None

Electronic energies: -638.869810

Free energies: -638.582302

Corrected Free energies: -638.579706

| | | | |
|---|---|---|---|
| N | -1.081072 | -0.873220 | -0.474250 |
| C | 0.172614 | -0.301568 | -0.400918 |
| C | 1.321103 | -0.941026 | -0.100087 |
| H | -1.188412 | -1.746861 | 0.025836 |
| C | -2.261309 | -0.016161 | -0.397857 |
| C | -3.495358 | -0.809089 | -0.825232 |
| C | -2.467216 | 0.596761 | 0.992515 |
| H | -2.108656 | 0.797983 | -1.117808 |
| C | -4.757569 | 0.055264 | -0.778775 |
| H | -3.613594 | -1.660836 | -0.142416 |
| H | -3.334848 | -1.215346 | -1.827002 |
| C | -3.723332 | 1.470477 | 1.032281 |
| H | -2.563360 | -0.221482 | 1.717600 |
| H | -1.581042 | 1.174604 | 1.272030 |
| C | -4.957652 | 0.671111 | 0.607878 |
| H | -5.627832 | -0.542253 | -1.061053 |
| H | -4.668323 | 0.858441 | -1.519750 |
| H | -3.860820 | 1.885926 | 2.033632 |
| H | -3.592553 | 2.318958 | 0.349949 |
| H | -5.844960 | 1.309302 | 0.613895 |
| H | -5.132655 | -0.130111 | 1.335725 |

| | | | |
|---|---|---|---|
| H | 0.182565 | 0.757762 | -0.643959 |
| C | 2.603541 | -0.209386 | -0.076647 |
| C | 2.851470 | 0.899228 | -0.902971 |
| C | 3.633574 | -0.615717 | 0.785493 |
| C | 4.058059 | 1.584426 | -0.845955 |
| H | 2.099330 | 1.212892 | -1.618003 |
| C | 4.845217 | 0.065469 | 0.836342 |
| H | 3.478072 | -1.467828 | 1.437667 |
| C | 5.065196 | 1.173163 | 0.024466 |
| H | 4.220643 | 2.433878 | -1.499729 |
| H | 5.618767 | -0.271139 | 1.517333 |
| H | 6.009265 | 1.703220 | 0.061061 |
| C | 1.306328 | -2.405569 | 0.268134 |
| H | 1.092845 | -2.571143 | 1.330167 |
| H | 0.548055 | -2.943310 | -0.307092 |
| H | 2.267021 | -2.874417 | 0.049682 |

**2I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -638.687838

Free energies: -638.397829

Corrected Free energies: -638.395822

| | | | |
|---|---|---|---|
| N | -0.995687 | -0.582930 | -0.176509 |
| C | 0.207929 | -0.071912 | -0.085928 |
| C | 1.393067 | -0.817069 | -0.253099 |
| H | -1.098400 | -1.570612 | -0.397622 |
| C | -2.242844 | 0.161774 | 0.029250 |
| C | -3.085334 | 0.119827 | -1.248162 |
| C | -3.001959 | -0.416643 | 1.226754 |
| H | -1.953203 | 1.194248 | 0.243651 |
| C | -4.404279 | 0.867195 | -1.034212 |
| H | -3.292707 | -0.926535 | -1.500634 |
| H | -2.518173 | 0.555670 | -2.073495 |
| C | -4.320935 | 0.334820 | 1.425955 |
| H | -3.209132 | -1.476243 | 1.035875 |
| H | -2.376214 | -0.355771 | 2.119964 |
| C | -5.175282 | 0.297783 | 0.157784 |
| H | -5.003605 | 0.809643 | -1.945051 |
| H | -4.191991 | 1.927539 | -0.856732 |
| H | -4.861143 | -0.103734 | 2.267415 |
| H | -4.105966 | 1.376415 | 1.689905 |
| H | -6.100325 | 0.857836 | 0.310972 |
| H | -5.457650 | -0.739379 | -0.057083 |

| | | | |
|---|---|---|---|
| H | 0.245722 | 0.980257 | 0.169968 |
| C | 2.669967 | -0.156713 | -0.085638 |
| C | 2.813951 | 1.237259 | -0.259684 |
| C | 3.813108 | -0.907635 | 0.259870 |
| C | 4.044321 | 1.846612 | -0.091565 |
| H | 1.972371 | 1.843219 | -0.570151 |
| C | 5.036726 | -0.287383 | 0.444712 |
| H | 3.732358 | -1.975101 | 0.419388 |
| C | 5.159213 | 1.089281 | 0.266236 |
| H | 4.139337 | 2.913832 | -0.247137 |
| H | 5.899384 | -0.877281 | 0.728043 |
| H | 6.120366 | 1.569918 | 0.401699 |
| C | 1.297976 | -2.283865 | -0.531821 |
| H | 1.014629 | -2.835987 | 0.370941 |
| H | 0.542186 | -2.484028 | -1.295632 |
| H | 2.238215 | -2.683385 | -0.901429 |

**2I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -638.685362

Free energies: -638.396723

Corrected Free energies: -638.394327

| | | | |
|---|---|---|---|
| N | -0.574967 | 0.475825 | -0.035176 |
| C | 0.193701 | 1.468896 | -0.417488 |
| C | 1.600966 | 1.477560 | -0.350810 |
| C | 2.291985 | 2.795044 | -0.482229 |
| H | 3.188193 | 2.703117 | -1.097358 |
| H | 2.606663 | 3.152942 | 0.504710 |
| H | -0.139555 | -0.340101 | 0.392109 |
| C | -2.038259 | 0.455959 | -0.120289 |
| C | -2.478810 | -0.709149 | -1.012601 |
| C | -2.631718 | 0.347153 | 1.286275 |
| H | -2.336221 | 1.403301 | -0.577430 |
| C | -4.006960 | -0.784322 | -1.071150 |
| H | -2.080459 | -1.641303 | -0.594843 |
| H | -2.053125 | -0.584298 | -2.010897 |
| C | -4.158684 | 0.267041 | 1.211850 |
| H | -2.239558 | -0.558512 | 1.763600 |
| H | -2.312717 | 1.203945 | 1.883920 |
| C | -4.609524 | -0.898260 | 0.329779 |
| H | -4.301200 | -1.635850 | -1.688085 |
| H | -4.393563 | 0.116212 | -1.561233 |
| H | -4.563620 | 0.165334 | 2.220684 |

| | | | |
|---|---|---|---|
| H | -4.549299 | 1.205624 | 0.802848 |
| H | -5.699679 | -0.924440 | 0.268796 |
| H | -4.288709 | -1.842025 | 0.785657 |
| H | -0.322752 | 2.355049 | -0.773122 |
| H | 1.630312 | 3.547491 | -0.908835 |
| C | 2.377951 | 0.268975 | -0.111172 |
| C | 1.988731 | -0.973780 | -0.646746 |
| C | 3.576419 | 0.343314 | 0.621121 |
| C | 2.755880 | -2.106923 | -0.424693 |
| H | 1.117611 | -1.040413 | -1.288718 |
| C | 4.328499 | -0.796470 | 0.852893 |
| H | 3.901111 | 1.292101 | 1.030178 |
| C | 3.919544 | -2.024088 | 0.334964 |
| H | 2.451486 | -3.052572 | -0.855190 |
| H | 5.237766 | -0.730347 | 1.437171 |
| H | 4.513764 | -2.911740 | 0.514059 |

**3I-*Z***

Imaginary frequency: None

Electronic energies: -522.151429

Free energies: -521.927963

Corrected Free energies: -521.925879

| | | | |
|---|---|---|---|
| C | 3.019262 | -0.309022 | -0.437817 |
| H | 3.141106 | 0.285251 | -1.354467 |
| N | 1.633870 | -0.208068 | 0.043716 |
| C | 1.054719 | 1.051325 | 0.092226 |
| C | -0.253130 | 1.378411 | 0.098573 |
| C | -0.645314 | 2.837534 | 0.098994 |
| H | -1.391755 | 3.046030 | 0.871262 |
| H | -1.077175 | 3.148616 | -0.857345 |
| H | 1.028988 | -0.917359 | -0.354374 |
| C | 3.306272 | -1.769030 | -0.761536 |
| H | 4.332182 | -1.886430 | -1.113025 |
| H | 3.173577 | -2.381818 | 0.134292 |
| H | 2.633868 | -2.139890 | -1.538976 |
| C | 3.987477 | 0.212140 | 0.619917 |
| H | 3.904304 | -0.393442 | 1.525939 |
| H | 5.013711 | 0.155043 | 0.250884 |
| H | 3.782915 | 1.251908 | 0.881943 |
| H | 1.779647 | 1.860177 | 0.133960 |
| H | 0.224325 | 3.469667 | 0.284464 |
| C | -1.343972 | 0.378148 | 0.074248 |
| C | -1.237815 | -0.857145 | 0.734060 |

| | | | |
|---|---|---|---|
| C | -2.552547 | 0.661655 | -0.580970 |
| C | -2.280935 | -1.776466 | 0.712832 |
| H | -0.338470 | -1.087832 | 1.293020 |
| C | -3.593038 | -0.258836 | -0.605614 |
| H | -2.678497 | 1.612775 | -1.084735 |
| C | -3.462436 | -1.486634 | 0.037529 |
| H | -2.172038 | -2.719826 | 1.235615 |
| H | -4.510713 | -0.015183 | -1.128568 |
| H | -4.274323 | -2.203686 | 0.019436 |

**3I-*E***

Imaginary frequency: None

Electronic energies: -522.152188

Free energies: -521.928443

Corrected Free energies: -521.926611

| | | | |
|---|---|---|---|
| C | 3.282883 | -0.414903 | 0.462588 |
| H | 3.016945 | -0.672997 | 1.497137 |
| N | 2.222890 | 0.405706 | -0.133805 |
| C | 0.907869 | -0.002280 | -0.027847 |
| C | -0.178370 | 0.763020 | -0.255523 |
| H | 2.369370 | 1.399632 | -0.021307 |
| C | 4.567949 | 0.401570 | 0.479514 |
| H | 5.382217 | -0.180019 | 0.913612 |
| H | 4.845021 | 0.680805 | -0.540644 |
| H | 4.447209 | 1.313407 | 1.069401 |
| C | 3.467871 | -1.703263 | -0.334133 |
| H | 3.762612 | -1.462976 | -1.358790 |
| H | 4.245312 | -2.319901 | 0.121817 |
| H | 2.550256 | -2.293586 | -0.370392 |
| H | 0.787493 | -1.043038 | 0.257842 |
| C | -1.535958 | 0.203876 | -0.094794 |
| C | -1.824181 | -1.149974 | -0.334307 |
| C | -2.597770 | 1.031087 | 0.301464 |
| C | -3.104740 | -1.655963 | -0.153589 |
| H | -1.040871 | -1.808903 | -0.691760 |
| C | -3.882104 | 0.525775 | 0.474922 |
| H | -2.412311 | 2.082206 | 0.492441 |
| C | -4.144225 | -0.822179 | 0.253433 |
| H | -3.296899 | -2.704731 | -0.350244 |
| H | -4.679969 | 1.189495 | 0.788255 |
| H | -5.144456 | -1.217126 | 0.384738 |
| C | -0.029555 | 2.220530 | -0.619542 |
| H | 0.023464 | 2.869989 | 0.261682 |

| | | | |
|---|---|---|---|
| H | 0.878377 | 2.384869 | -1.205043 |
| H | -0.872028 | 2.559157 | -1.225221 |

**3I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -521.970912

Free energies: -521.747117

Corrected Free energies: -521.745213

| | | | |
|---|---|---|---|
| C | 3.294707 | -0.627306 | 0.161374 |
| H | 2.894488 | -1.633278 | 0.296500 |
| N | 2.128718 | 0.241228 | -0.075053 |
| C | 0.879152 | -0.149115 | -0.027011 |
| C | -0.220241 | 0.713430 | -0.217077 |
| H | 2.334563 | 1.218194 | -0.271601 |
| C | 4.008065 | -0.174256 | 1.431004 |
| H | 4.853442 | -0.836811 | 1.620477 |
| H | 4.389541 | 0.842906 | 1.315238 |
| H | 3.337038 | -0.206682 | 2.289639 |
| C | 4.199697 | -0.585737 | -1.064897 |
| H | 4.580359 | 0.425651 | -1.225803 |
| H | 5.050300 | -1.248666 | -0.902758 |
| H | 3.665075 | -0.910887 | -1.957632 |
| H | 0.726644 | -1.195006 | 0.211494 |
| C | -1.560679 | 0.182694 | -0.093863 |
| C | -1.840348 | -1.187353 | -0.293296 |
| C | -2.629966 | 1.041365 | 0.236285 |
| C | -3.130133 | -1.669758 | -0.163403 |
| H | -1.056597 | -1.870372 | -0.595237 |
| C | -3.914391 | 0.547083 | 0.382959 |
| H | -2.444822 | 2.092677 | 0.414440 |
| C | -4.170731 | -0.807861 | 0.180909 |
| H | -3.329372 | -2.719554 | -0.337816 |
| H | -4.719628 | 1.217380 | 0.655635 |
| H | -5.178090 | -1.191326 | 0.286634 |
| C | 0.031354 | 2.165601 | -0.473213 |
| H | 0.355971 | 2.673713 | 0.441378 |
| H | 0.816549 | 2.294381 | -1.222669 |
| H | -0.855404 | 2.666368 | -0.851183 |

**3I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -521.968680

Free energies: -521.743930

Corrected Free energies: -521.742323

| | | | |
|---|---|---|---|
| C | 3.079296 | -0.129928 | -0.055278 |
| H | 3.524872 | 0.793638 | 0.317909 |
| N | 1.626913 | 0.109245 | -0.091311 |
| C | 1.035923 | 1.212198 | 0.303000 |
| C | -0.354774 | 1.437563 | 0.294370 |
| C | -0.829177 | 2.847453 | 0.427189 |
| H | -1.679649 | 2.904660 | 1.108491 |
| H | -1.164832 | 3.222910 | -0.546008 |
| H | 1.055139 | -0.637299 | -0.483869 |
| C | 3.572980 | -0.417335 | -1.468508 |
| H | 4.653642 | -0.561281 | -1.445792 |
| H | 3.115269 | -1.329964 | -1.858025 |
| H | 3.342901 | 0.410807 | -2.139054 |
| C | 3.366303 | -1.274541 | 0.912115 |
| H | 2.887674 | -2.194982 | 0.569254 |
| H | 4.442802 | -1.443699 | 0.955633 |
| H | 3.006252 | -1.038503 | 1.913971 |
| H | 1.695575 | 2.013413 | 0.620569 |
| H | -0.034064 | 3.504030 | 0.777111 |
| C | -1.320729 | 0.361754 | 0.116067 |
| C | -1.114688 | -0.915137 | 0.673026 |
| C | -2.520140 | 0.612482 | -0.573676 |
| C | -2.066649 | -1.911630 | 0.516758 |
| H | -0.237625 | -1.111393 | 1.279436 |
| C | -3.457222 | -0.393760 | -0.741728 |
| H | -2.702401 | 1.590946 | -1.000424 |
| C | -3.232960 | -1.657883 | -0.199528 |
| H | -1.903466 | -2.883566 | 0.965321 |
| H | -4.367157 | -0.192471 | -1.293000 |
| H | -3.972311 | -2.439368 | -0.325184 |

**4I-Z**

Imaginary frequency: None

Electronic energies: -674.553164

Free energies: -674.307540

Corrected Free energies: -674.304077

| | | | |
|---|---|---|---|
| C | -1.486864 | -1.246762 | 2.555784 |
| C | -1.238330 | -1.025710 | 1.083539 |
| C | -0.138340 | -1.539771 | 0.504745 |
| H | -1.437662 | -0.312593 | 3.123107 |
| H | -2.478568 | -1.675709 | 2.728256 |

| | | | |
|---|---|---|---|
| N | 0.263751 | -1.441843 | -0.822888 |
| C | 1.690104 | -1.515056 | -1.086676 |
| H | 2.066011 | -2.457298 | -0.676420 |
| H | 1.828362 | -1.573908 | -2.169317 |
| C | 2.530443 | -0.371230 | -0.539788 |
| C | 3.921580 | -0.496519 | -0.530010 |
| C | 1.958333 | 0.808735 | -0.068233 |
| C | 4.725889 | 0.536170 | -0.064575 |
| H | 4.375276 | -1.414531 | -0.891480 |
| C | 2.762999 | 1.845229 | 0.401631 |
| H | 0.879766 | 0.922028 | -0.056599 |
| C | 4.146718 | 1.713503 | 0.404714 |
| H | 5.803687 | 0.422303 | -0.063214 |
| H | 2.304595 | 2.756261 | 0.768598 |
| H | 4.771133 | 2.519241 | 0.771755 |
| H | -0.208803 | -0.719480 | -1.352901 |
| H | 0.548164 | -2.124095 | 1.113335 |
| H | -0.742927 | -1.925888 | 2.975010 |
| C | -2.231230 | -0.221327 | 0.331669 |
| C | -2.798645 | 0.929610 | 0.897328 |
| C | -2.662143 | -0.602183 | -0.947561 |
| C | -3.738237 | 1.681946 | 0.202352 |
| H | -2.494592 | 1.244863 | 1.888825 |
| C | -3.603495 | 0.149338 | -1.643008 |
| H | -2.271295 | -1.512150 | -1.389914 |
| C | -4.144033 | 1.297354 | -1.072943 |
| H | -4.156203 | 2.572003 | 0.658349 |
| H | -3.922988 | -0.170538 | -2.628049 |
| H | -4.878706 | 1.882429 | -1.612930 |

**4I-*E***

Imaginary frequency: None

Electronic energies: -674.553634

Free energies: -674.309441

Corrected Free energies: -674.305836

| | | | |
|---|---|---|---|
| C | -1.374884 | 1.073735 | 0.353872 |
| C | -0.278973 | 1.071920 | -0.430030 |
| N | 0.846623 | 1.848536 | -0.243770 |
| C | 2.074566 | 1.510084 | -0.930212 |
| H | 1.829159 | 1.294560 | -1.974815 |
| H | 2.716601 | 2.394253 | -0.942990 |
| C | 2.861186 | 0.340683 | -0.357719 |
| C | 4.092822 | 0.019664 | -0.933844 |

| | | | |
|---|---|---|---|
| C | 2.402887 | -0.415699 | 0.717659 |
| C | 4.851102 | -1.036580 | -0.447440 |
| H | 4.457626 | 0.607608 | -1.770763 |
| C | 3.162679 | -1.477906 | 1.207332 |
| H | 1.448475 | -0.181292 | 1.175927 |
| C | 4.386006 | -1.791579 | 0.628245 |
| H | 5.805154 | -1.271799 | -0.904639 |
| H | 2.794528 | -2.059131 | 2.044823 |
| H | 4.975675 | -2.616203 | 1.010522 |
| H | 0.971133 | 2.242170 | 0.678374 |
| H | -0.228685 | 0.436547 | -1.309891 |
| C | -2.526105 | 0.205272 | 0.036473 |
| C | -3.349064 | -0.282331 | 1.062777 |
| C | -2.849232 | -0.159895 | -1.280948 |
| C | -4.431025 | -1.112620 | 0.789190 |
| H | -3.130686 | -0.021261 | 2.092306 |
| C | -3.923508 | -0.996741 | -1.553054 |
| H | -2.268148 | 0.238345 | -2.104970 |
| C | -4.723736 | -1.479819 | -0.520004 |
| H | -5.045156 | -1.475796 | 1.605395 |
| H | -4.149337 | -1.257685 | -2.580944 |
| H | -5.567788 | -2.123865 | -0.735412 |
| C | -1.416018 | 1.927299 | 1.599219 |
| H | -0.927172 | 1.445628 | 2.454023 |
| H | -0.916396 | 2.885112 | 1.430925 |
| H | -2.443562 | 2.150145 | 1.889435 |

**4I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -674.368102

Free energies: -674.121586

Corrected Free energies: -674.118611

| | | | |
|---|---|---|---|
| C | -1.460549 | -0.863053 | -0.171917 |
| C | -0.399567 | -0.423902 | 0.645785 |
| N | 0.774160 | -1.008550 | 0.682442 |
| C | 1.906210 | -0.566660 | 1.504463 |
| H | 1.534569 | 0.197609 | 2.186828 |
| H | 2.245049 | -1.422640 | 2.088834 |
| C | 3.015062 | -0.037177 | 0.624361 |
| C | 4.169460 | -0.785191 | 0.409442 |
| C | 2.868474 | 1.203383 | 0.001604 |
| C | 5.174463 | -0.295034 | -0.420316 |
| H | 4.285183 | -1.749033 | 0.893370 |

| | | | |
|---|---|---|---|
| C | 3.870499 | 1.691781 | -0.826445 |
| H | 1.970615 | 1.789884 | 0.170114 |
| C | 5.025005 | 0.941490 | -1.038701 |
| H | 6.072289 | -0.878923 | -0.582535 |
| H | 3.753600 | 2.657411 | -1.303298 |
| H | 5.806906 | 1.322467 | -1.684447 |
| H | 0.951533 | -1.802222 | 0.072672 |
| C | -2.730293 | -0.172918 | -0.112496 |
| C | -2.825661 | 1.174366 | 0.300794 |
| C | -3.915409 | -0.845905 | -0.476351 |
| C | -4.051861 | 1.812399 | 0.345598 |
| H | -1.934884 | 1.739995 | 0.543388 |
| C | -5.140589 | -0.206299 | -0.408404 |
| H | -3.878055 | -1.884744 | -0.777738 |
| C | -5.214218 | 1.124940 | -0.002217 |
| H | -4.104208 | 2.851367 | 0.645631 |
| H | -6.041906 | -0.744789 | -0.672566 |
| H | -6.172965 | 1.627049 | 0.039920 |
| C | -1.257551 | -2.069586 | -1.032435 |
| H | -0.315551 | -1.993388 | -1.582416 |
| H | -1.216751 | -2.980353 | -0.425500 |
| H | -2.048176 | -2.178087 | -1.768923 |
| H | -0.527222 | 0.412433 | 1.322976 |

**4I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -674.365727

Free energies: -674.119607

Corrected Free energies: -674.116643

| | | | |
|---|---|---|---|
| C | -2.362177 | -2.777871 | 0.372400 |
| C | -1.757318 | -1.510518 | -0.136430 |
| C | -0.472692 | -1.586664 | -0.710285 |
| H | -2.254313 | -2.831321 | 1.461896 |
| H | -3.428276 | -2.817088 | 0.145586 |
| N | 0.319565 | -0.561616 | -0.928161 |
| C | 1.657682 | -0.647100 | -1.521433 |
| H | 1.832791 | -1.691332 | -1.780621 |
| H | 1.650311 | -0.056827 | -2.439350 |
| C | 2.698549 | -0.126155 | -0.558598 |
| C | 3.332919 | 1.090165 | -0.797154 |
| C | 3.020803 | -0.861998 | 0.583065 |
| C | 4.288190 | 1.567783 | 0.096021 |
| H | 3.083797 | 1.662578 | -1.684028 |

| | | | |
|---|---|---|---|
| C | 3.972755 | -0.384634 | 1.474701 |
| H | 2.531037 | -1.812403 | 0.770790 |
| C | 4.607652 | 0.831618 | 1.231361 |
| H | 4.780883 | 2.513084 | -0.096155 |
| H | 4.223315 | -0.961413 | 2.356731 |
| H | 5.351175 | 1.202664 | 1.926496 |
| H | 0.026764 | 0.360330 | -0.611303 |
| H | -0.066604 | -2.560315 | -0.966523 |
| H | -1.866023 | -3.650690 | -0.049505 |
| C | -2.468388 | -0.250222 | 0.019247 |
| C | -3.321658 | -0.062567 | 1.121379 |
| C | -2.369756 | 0.773998 | -0.942843 |
| C | -4.007566 | 1.129916 | 1.281866 |
| H | -3.423530 | -0.844172 | 1.864085 |
| C | -3.073203 | 1.957768 | -0.783689 |
| H | -1.790872 | 0.619112 | -1.846019 |
| C | -3.882265 | 2.144047 | 0.333431 |
| H | -4.644695 | 1.270669 | 2.145947 |
| H | -2.998566 | 2.730416 | -1.538438 |
| H | -4.425307 | 3.072621 | 0.459312 |

**5I-*Z***

Imaginary frequency: None

Electronic energies: -635.256270

Free energies: -635.037031

Corrected Free energies: -635.034578

| | | | |
|---|---|---|---|
| N | -0.762164 | 0.104953 | -0.276835 |
| C | -0.094732 | 1.305349 | -0.100881 |
| C | 1.237078 | 1.467481 | -0.006183 |
| C | 1.818218 | 2.859257 | 0.004931 |
| H | 2.347264 | 3.087041 | -0.925410 |
| H | 2.536909 | 2.975890 | 0.820699 |
| H | -0.220152 | -0.686320 | -0.594540 |
| C | -2.131866 | -0.083907 | -0.157659 |
| C | -2.705154 | -1.250330 | -0.687830 |
| C | -2.961942 | 0.841011 | 0.490380 |
| C | -4.068572 | -1.476520 | -0.580157 |
| H | -2.069272 | -1.971572 | -1.189938 |
| C | -4.329965 | 0.606358 | 0.577352 |
| H | -2.543141 | 1.727558 | 0.948488 |
| C | -4.896878 | -0.547454 | 0.047102 |
| H | -4.487899 | -2.385167 | -0.996597 |
| H | -4.954936 | 1.333752 | 1.082531 |

| | | | |
|---|---|---|---|
| H | -5.961990 | -0.724343 | 0.125808 |
| H | -0.735192 | 2.181043 | -0.105421 |
| H | 1.031949 | 3.605937 | 0.125899 |
| C | 2.184799 | 0.327320 | 0.046437 |
| C | 1.919087 | -0.809088 | 0.825254 |
| C | 3.403505 | 0.379153 | -0.643277 |
| C | 2.824702 | -1.861127 | 0.891356 |
| H | 1.001951 | -0.855410 | 1.401719 |
| C | 4.308460 | -0.674607 | -0.579531 |
| H | 3.644858 | 1.249376 | -1.242880 |
| C | 4.022764 | -1.801635 | 0.185019 |
| H | 2.597417 | -2.724998 | 1.505226 |
| H | 5.241013 | -0.613837 | -1.128521 |
| H | 4.729342 | -2.621188 | 0.236887 |

**5I-*E***

Imaginary frequency: None

Electronic energies: -635.257199

Free energies: -635.037735

Corrected Free energies: -635.035620

| | | | |
|---|---|---|---|
| N | -1.289228 | 0.914633 | 0.057746 |
| C | -0.052406 | 0.298974 | 0.014222 |
| C | 1.120905 | 0.918276 | 0.240287 |
| H | -1.314964 | 1.922332 | 0.015333 |
| C | -2.517266 | 0.264480 | -0.007682 |
| C | -3.664434 | 1.010534 | -0.315920 |
| C | -2.650778 | -1.107291 | 0.243078 |
| C | -4.906416 | 0.397460 | -0.379461 |
| H | -3.569342 | 2.073583 | -0.509813 |
| C | -3.901028 | -1.710722 | 0.161427 |
| H | -1.791325 | -1.701370 | 0.526116 |
| C | -5.036873 | -0.970627 | -0.148786 |
| H | -5.778815 | 0.993952 | -0.620198 |
| H | -3.983749 | -2.773408 | 0.358027 |
| H | -6.006913 | -1.448020 | -0.205331 |
| H | -0.078830 | -0.745000 | -0.273887 |
| C | 2.392826 | 0.181625 | 0.073235 |
| C | 2.495143 | -1.195209 | 0.326125 |
| C | 3.550711 | 0.856686 | -0.336892 |
| C | 3.694823 | -1.870514 | 0.146033 |
| H | 1.631471 | -1.739012 | 0.692277 |
| C | 4.754118 | 0.181159 | -0.511785 |
| H | 3.507298 | 1.921335 | -0.536856 |

| | | | |
|---|---|---|---|
| C | 4.833286 | -1.187047 | -0.275861 |
| H | 3.745545 | -2.933387 | 0.352585 |
| H | 5.632037 | 0.728363 | -0.835721 |
| H | 5.770775 | -1.713170 | -0.409188 |
| C | 1.171671 | 2.383175 | 0.597148 |
| H | 1.194544 | 3.025812 | -0.289838 |
| H | 0.301468 | 2.670439 | 1.192146 |
| H | 2.059700 | 2.609353 | 1.189130 |

**5I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -635.065181

Free energies: -634.846022

Corrected Free energies: -634.843725

| | | | |
|---|---|---|---|
| N | -1.245912 | 0.829253 | 0.163603 |
| C | -0.061990 | 0.234288 | 0.106346 |
| C | 1.146491 | 0.924741 | 0.235489 |
| H | -1.266740 | 1.839929 | 0.270191 |
| C | -2.508421 | 0.213907 | 0.044399 |
| C | -3.600381 | 1.036520 | -0.241085 |
| C | -2.672385 | -1.162187 | 0.216714 |
| C | -4.860037 | 0.473174 | -0.375685 |
| H | -3.455016 | 2.103279 | -0.367522 |
| C | -3.938398 | -1.709834 | 0.076203 |
| H | -1.839617 | -1.798364 | 0.485401 |
| C | -5.031818 | -0.899703 | -0.222475 |
| H | -5.706845 | 1.107857 | -0.603293 |
| H | -4.072914 | -2.775044 | 0.214363 |
| H | -6.016550 | -1.337441 | -0.327073 |
| H | -0.072512 | -0.825435 | -0.105475 |
| C | 2.389960 | 0.195162 | 0.079717 |
| C | 2.473784 | -1.192433 | 0.324593 |
| C | 3.554661 | 0.874716 | -0.331200 |
| C | 3.670385 | -1.865930 | 0.157898 |
| H | 1.614077 | -1.740398 | 0.689452 |
| C | 4.743177 | 0.189660 | -0.515573 |
| H | 3.517647 | 1.935772 | -0.542052 |
| C | 4.807126 | -1.180533 | -0.269064 |
| H | 3.721669 | -2.926787 | 0.367478 |
| H | 5.623486 | 0.723289 | -0.850984 |
| H | 5.741067 | -1.711962 | -0.404489 |
| C | 1.141658 | 2.405294 | 0.458809 |
| H | 0.930858 | 2.938839 | -0.474383 |

| | | | |
|---|---|---|---|
| H | 0.381983 | 2.690268 | 1.190101 |
| H | 2.097921 | 2.750367 | 0.842550 |

**5I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -635.063717

Free energies: -634.844846

Corrected Free energies: -634.842513

| | | | |
|---|---|---|---|
| N | -0.747231 | 0.164160 | -0.168862 |
| C | -0.119025 | 1.324365 | 0.013907 |
| C | 1.266785 | 1.471214 | 0.003408 |
| C | 1.823175 | 2.853595 | -0.101667 |
| H | 2.230563 | 3.015293 | -1.105531 |
| H | 2.641211 | 2.991735 | 0.607173 |
| H | -0.177995 | -0.636094 | -0.439469 |
| C | -2.131972 | -0.061729 | -0.105227 |
| C | -2.626932 | -1.224387 | -0.703603 |
| C | -2.987702 | 0.832101 | 0.545111 |
| C | -3.988692 | -1.478093 | -0.671310 |
| H | -1.947408 | -1.910734 | -1.195550 |
| C | -4.347163 | 0.563909 | 0.565661 |
| H | -2.602436 | 1.706152 | 1.053478 |
| C | -4.851737 | -0.583960 | -0.042483 |
| H | -4.376254 | -2.374783 | -1.137390 |
| H | -5.015065 | 1.248935 | 1.071907 |
| H | -5.915088 | -0.785608 | -0.016925 |
| H | -0.746394 | 2.200535 | 0.117386 |
| H | 1.055996 | 3.607045 | 0.069868 |
| C | 2.175932 | 0.331219 | 0.054803 |
| C | 1.894570 | -0.793540 | 0.853393 |
| C | 3.388254 | 0.371067 | -0.656300 |
| C | 2.784846 | -1.855350 | 0.910229 |
| H | 1.008020 | -0.809667 | 1.476989 |
| C | 4.263163 | -0.701419 | -0.608949 |
| H | 3.630384 | 1.232651 | -1.266064 |
| C | 3.963715 | -1.817224 | 0.171482 |
| H | 2.563342 | -2.706645 | 1.541356 |
| H | 5.183206 | -0.668842 | -1.178839 |
| H | 4.655229 | -2.649709 | 0.212905 |

**6I-*E***

Imaginary frequency: None

Electronic energies: -1814.671828

Free energies: -1814.212876

Corrected Free energies: -1814.204787

| | | | |
|---|---|---|---|
| S | -0.884774 | -2.557184 | 0.668520 |
| F | -0.534456 | -2.919110 | -1.903035 |
| F | -2.039854 | -4.196362 | -1.027706 |
| F | -2.465536 | -2.108712 | -1.376498 |
| O | -0.361621 | -1.193081 | 0.464363 |
| O | 0.157246 | -3.556641 | 0.904863 |
| O | -2.059398 | -2.637019 | 1.526242 |
| C | -1.521474 | -2.973089 | -1.010274 |
| N | 1.095062 | 1.632367 | 0.542110 |
| H | 1.353587 | 2.216484 | 1.327531 |
| N | 2.407942 | -0.926007 | 0.406073 |
| H | 1.392500 | -0.721953 | 0.488201 |
| C | 2.161166 | 1.388439 | -0.419437 |
| H | 1.687165 | 0.917257 | -1.289019 |
| C | 3.117974 | 0.379731 | 0.221585 |
| H | 4.009614 | 0.196641 | -0.374278 |
| H | 3.430416 | 0.736130 | 1.202869 |
| C | 2.534567 | -1.825008 | -0.795002 |
| H | 1.764462 | -2.585922 | -0.673222 |
| H | 2.284263 | -1.216647 | -1.665485 |
| C | 3.904874 | -2.461776 | -0.940149 |
| H | 4.127166 | -3.136954 | -0.113747 |
| H | 4.705979 | -1.726004 | -1.021023 |
| H | 3.904945 | -3.050035 | -1.858063 |
| C | 2.762617 | -1.633902 | 1.683083 |
| H | 2.384535 | -2.651201 | 1.576905 |
| H | 3.850226 | -1.656591 | 1.755839 |
| C | 2.118323 | -0.956991 | 2.879811 |
| H | 2.351593 | -1.534927 | 3.774221 |
| H | 1.033578 | -0.925255 | 2.761111 |
| H | 2.484077 | 0.059018 | 3.033075 |
| C | 2.874997 | 2.664847 | -0.939968 |
| C | 3.777643 | 2.296380 | -2.124767 |
| H | 4.609103 | 1.651185 | -1.832969 |
| H | 4.206483 | 3.204511 | -2.555062 |
| H | 3.206286 | 1.790555 | -2.908555 |
| C | 3.712796 | 3.322682 | 0.161993 |
| H | 3.110227 | 3.565794 | 1.042568 |
| H | 4.136160 | 4.259023 | -0.209638 |
| H | 4.545172 | 2.688188 | 0.477463 |
| C | 1.807237 | 3.651158 | -1.426936 |

| | | | |
|---|---|---|---|
| H | 1.158060 | 3.187284 | -2.175797 |
| H | 2.287241 | 4.520241 | -1.882996 |
| H | 1.178458 | 4.000511 | -0.605199 |
| C | -0.226547 | 1.714019 | 0.137626 |
| C | -1.194092 | 2.403395 | 0.766259 |
| C | -2.592732 | 2.243517 | 0.312699 |
| C | -3.495897 | 3.315652 | 0.322501 |
| C | -3.054223 | 1.001783 | -0.153428 |
| C | -4.798655 | 3.160224 | -0.138130 |
| H | -3.170510 | 4.289201 | 0.672187 |
| C | -4.353549 | 0.850223 | -0.623492 |
| H | -2.388306 | 0.146357 | -0.118826 |
| C | -5.234705 | 1.928125 | -0.618888 |
| H | -5.474146 | 4.008065 | -0.127581 |
| H | -4.682661 | -0.120846 | -0.976827 |
| H | -6.250278 | 1.808389 | -0.976742 |
| C | -0.861102 | 3.283624 | 1.947770 |
| H | -0.552975 | 2.684774 | 2.812405 |
| H | -0.040716 | 3.973833 | 1.720892 |
| H | -1.716344 | 3.880372 | 2.261837 |
| H | -0.456499 | 1.106345 | -0.731400 |

**6I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1814.484024

Free energies: -1814.024532

Corrected Free energies: -1814.016299

| | | | |
|---|---|---|---|
| S | -0.918901 | -2.203473 | 0.586691 |
| F | -0.273398 | -3.110070 | -1.783896 |
| F | -1.933124 | -4.137575 | -0.861862 |
| F | -2.211594 | -2.161770 | -1.688081 |
| O | -0.329294 | -0.906811 | 0.168455 |
| O | 0.080322 | -3.108712 | 1.149426 |
| O | -2.183837 | -2.090456 | 1.293417 |
| C | -1.362131 | -2.953734 | -1.037384 |
| N | 0.999825 | 1.824097 | 0.383112 |
| H | 1.216346 | 2.274720 | 1.268140 |
| N | 2.392425 | -0.896063 | 0.610241 |
| H | 1.357258 | -0.785575 | 0.595988 |
| C | 2.130805 | 1.364966 | -0.433460 |
| H | 1.688496 | 0.785627 | -1.249631 |
| C | 3.008041 | 0.456690 | 0.432175 |
| H | 3.989099 | 0.317246 | -0.014234 |

| | | | |
|---|---|---|---|
| H | 3.156314 | 0.896148 | 1.418503 |
| C | 2.671408 | -1.822733 | -0.548267 |
| H | 1.977323 | -2.652725 | -0.417959 |
| H | 2.391016 | -1.286177 | -1.455858 |
| C | 4.105920 | -2.311498 | -0.613892 |
| H | 4.374234 | -2.903357 | 0.261106 |
| H | 4.826276 | -1.500866 | -0.729896 |
| H | 4.195051 | -2.954798 | -1.489541 |
| C | 2.736140 | -1.525805 | 1.933462 |
| H | 2.473681 | -2.578918 | 1.839586 |
| H | 3.813884 | -1.431546 | 2.070380 |
| C | 1.951631 | -0.887651 | 3.064383 |
| H | 2.157503 | -1.437864 | 3.982440 |
| H | 0.878634 | -0.946259 | 2.869926 |
| H | 2.228660 | 0.152984 | 3.236982 |
| C | 2.902097 | 2.554951 | -1.071829 |
| C | 3.910948 | 1.994444 | -2.083674 |
| H | 4.713855 | 1.425866 | -1.610470 |
| H | 4.377410 | 2.824943 | -2.617035 |
| H | 3.418627 | 1.354911 | -2.821389 |
| C | 3.631382 | 3.382272 | -0.008456 |
| H | 2.943650 | 3.803509 | 0.730375 |
| H | 4.136518 | 4.221170 | -0.491974 |
| H | 4.393332 | 2.800105 | 0.515798 |
| C | 1.899588 | 3.439083 | -1.822226 |
| H | 1.331705 | 2.857610 | -2.554785 |
| H | 2.437736 | 4.221678 | -2.360194 |
| H | 1.195781 | 3.927828 | -1.145302 |
| C | -0.258318 | 1.741970 | 0.010188 |
| C | -1.333009 | 2.239392 | 0.774576 |
| C | -2.676717 | 2.031124 | 0.289274 |
| C | -3.725825 | 2.889439 | 0.681625 |
| C | -2.975151 | 0.954340 | -0.576459 |
| C | -5.009846 | 2.692305 | 0.205846 |
| H | -3.523768 | 3.733858 | 1.327757 |
| C | -4.266539 | 0.751114 | -1.026667 |
| H | -2.202283 | 0.245397 | -0.843763 |
| C | -5.286330 | 1.622147 | -0.645135 |
| H | -5.800750 | 3.371777 | 0.497149 |
| H | -4.483432 | -0.093414 | -1.668903 |
| H | -6.295471 | 1.465278 | -1.005954 |
| C | -1.037868 | 2.965935 | 2.047440 |
| H | -0.428703 | 2.333695 | 2.702918 |
| H | -0.477418 | 3.887259 | 1.858298 |

| | | | |
|---|---|---|---|
| H | -1.941226 | 3.213578 | 2.596129 |
| H | -0.434520 | 1.275697 | -0.950087 |

**6I-*Z***

Imaginary frequency: None

Electronic energies: -1814.673013

Free energies: -1814.212873

Corrected Free energies: -1814.204968

| | | | |
|---|---|---|---|
| S | 1.946899 | -1.231643 | -0.551383 |
| F | 4.360834 | -0.391172 | 0.090119 |
| F | 4.055488 | -2.510960 | 0.355721 |
| F | 4.297414 | -1.696184 | -1.628070 |
| O | 1.816788 | -0.040083 | -1.394018 |
| O | 1.557524 | -0.995605 | 0.850796 |
| O | 1.487226 | -2.488947 | -1.126870 |
| C | 3.774157 | -1.472553 | -0.425988 |
| N | -1.170648 | 0.660130 | -0.298898 |
| H | -1.886313 | 0.522734 | 0.407363 |
| N | 0.923355 | 1.753854 | 1.170063 |
| H | 0.766115 | 0.814870 | 0.761838 |
| C | -0.837253 | 2.055808 | -0.550323 |
| H | -0.052098 | 2.047148 | -1.317448 |
| C | -0.236260 | 2.601031 | 0.749243 |
| H | 0.115548 | 3.623845 | 0.644978 |
| H | -0.976805 | 2.575249 | 1.548347 |
| C | 2.229775 | 2.245216 | 0.610053 |
| H | 2.927492 | 1.416869 | 0.723359 |
| H | 2.066983 | 2.396155 | -0.456490 |
| C | 2.754399 | 3.497237 | 1.289291 |
| H | 3.014271 | 3.317853 | 2.332653 |
| H | 2.051801 | 4.330178 | 1.239227 |
| H | 3.662491 | 3.802423 | 0.768788 |
| C | 0.992366 | 1.527233 | 2.652534 |
| H | 1.976972 | 1.100379 | 2.846659 |
| H | 0.927534 | 2.502900 | 3.135210 |
| C | -0.093529 | 0.577289 | 3.124776 |
| H | 0.022627 | 0.424162 | 4.198096 |
| H | 0.007547 | -0.385112 | 2.623274 |
| H | -1.098394 | 0.967555 | 2.954693 |
| C | -1.998240 | 2.949464 | -1.077471 |
| C | -1.491136 | 4.385356 | -1.275649 |
| H | -1.311718 | 4.896979 | -0.327457 |
| H | -2.237947 | 4.966291 | -1.821752 |

| | | | |
|---|---|---|---|
| H | -0.563690 | 4.398878 | -1.856921 |
| C | -3.188394 | 2.949892 | -0.111575 |
| H | -3.590490 | 1.942309 | 0.028619 |
| H | -3.991384 | 3.565803 | -0.524292 |
| H | -2.932292 | 3.363294 | 0.867237 |
| C | -2.465743 | 2.410381 | -2.435059 |
| H | -1.636490 | 2.361823 | -3.147180 |
| H | -3.227831 | 3.075647 | -2.848545 |
| H | -2.901045 | 1.413400 | -2.345027 |
| C | -1.241296 | -0.243842 | -1.361229 |
| C | -1.890980 | -1.415688 | -1.360030 |
| H | -0.674279 | 0.062735 | -2.233652 |
| C | -1.882017 | -2.312898 | -2.569277 |
| H | -1.319901 | -1.857669 | -3.386726 |
| H | -1.424203 | -3.278748 | -2.334549 |
| H | -2.896447 | -2.513863 | -2.927785 |
| C | -2.597298 | -1.899716 | -0.145783 |
| C | -1.905708 | -2.002809 | 1.067708 |
| C | -3.941722 | -2.285602 | -0.183662 |
| C | -2.545628 | -2.457741 | 2.216200 |
| H | -0.852996 | -1.733684 | 1.086294 |
| C | -4.581621 | -2.742402 | 0.963995 |
| H | -4.491644 | -2.217519 | -1.116418 |
| C | -3.887420 | -2.826778 | 2.168044 |
| H | -1.994204 | -2.532072 | 3.146997 |
| H | -5.625550 | -3.031071 | 0.919678 |
| H | -4.387635 | -3.182698 | 3.060928 |

**6I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1814.482978

Free energies: -1814.020522

Corrected Free energies: -1814.013890

| | | | |
|---|---|---|---|
| S | 1.319841 | -1.611544 | -0.557998 |
| F | 3.869304 | -1.811120 | -0.017952 |
| F | 2.760208 | -3.646739 | 0.235816 |
| F | 3.234124 | -2.938281 | -1.747386 |
| O | 1.629585 | -0.433617 | -1.374959 |
| O | 1.106236 | -1.262057 | 0.864666 |
| O | 0.332556 | -2.528072 | -1.111772 |
| C | 2.897380 | -2.565780 | -0.519642 |
| N | -1.083113 | 1.037879 | -0.419446 |
| H | -1.727430 | 1.024350 | 0.369335 |

| | | | |
|---|---|---|---|
| N | 1.422136 | 1.444040 | 1.320362 |
| H | 1.123292 | 0.490027 | 1.035679 |
| C | -0.144139 | 2.163712 | -0.523213 |
| H | 0.653836 | 1.820524 | -1.187715 |
| C | 0.405933 | 2.446509 | 0.875267 |
| H | 0.877964 | 3.424463 | 0.918592 |
| H | -0.403595 | 2.444089 | 1.605586 |
| C | 2.770975 | 1.638197 | 0.670305 |
| H | 3.325213 | 0.724336 | 0.888525 |
| H | 2.601522 | 1.664801 | -0.404456 |
| C | 3.520536 | 2.864902 | 1.154414 |
| H | 3.752179 | 2.815938 | 2.218196 |
| H | 2.988116 | 3.793962 | 0.947658 |
| H | 4.464922 | 2.905764 | 0.611153 |
| C | 1.527593 | 1.378568 | 2.822695 |
| H | 2.463838 | 0.862635 | 3.036718 |
| H | 1.602292 | 2.402727 | 3.188702 |
| C | 0.358946 | 0.630495 | 3.439024 |
| H | 0.519564 | 0.573212 | 4.515620 |
| H | 0.304899 | -0.386273 | 3.046866 |
| H | -0.597448 | 1.130440 | 3.278440 |
| C | -0.807775 | 3.416479 | -1.175541 |
| C | 0.279333 | 4.477520 | -1.402013 |
| H | 0.634543 | 4.923198 | -0.471188 |
| H | -0.135884 | 5.286696 | -2.005835 |
| H | 1.135315 | 4.061428 | -1.940848 |
| C | -1.921425 | 3.981489 | -0.288782 |
| H | -2.713824 | 3.247676 | -0.117077 |
| H | -2.376352 | 4.841220 | -0.785251 |
| H | -1.544813 | 4.323662 | 0.678098 |
| C | -1.387354 | 3.024113 | -2.539276 |
| H | -0.622246 | 2.586106 | -3.187168 |
| H | -1.771086 | 3.918149 | -3.034058 |
| H | -2.218881 | 2.321452 | -2.449912 |
| C | -1.251503 | 0.133533 | -1.366249 |
| C | -2.192853 | -0.909426 | -1.318079 |
| H | -0.611724 | 0.229148 | -2.236284 |
| C | -2.414066 | -1.719782 | -2.546354 |
| H | -1.798012 | -1.377363 | -3.375570 |
| H | -2.175750 | -2.764270 | -2.326081 |
| H | -3.464409 | -1.682386 | -2.848720 |
| C | -2.939258 | -1.215086 | -0.099566 |
| C | -2.285870 | -1.261660 | 1.144515 |
| C | -4.309012 | -1.514342 | -0.165785 |

| | | | |
|---|---|---|---|
| C | -2.996257 | -1.576685 | 2.294468 |
| H | -1.210641 | -1.121502 | 1.192841 |
| C | -5.014221 | -1.806994 | 0.991403 |
| H | -4.826183 | -1.484835 | -1.116673 |
| C | -4.361638 | -1.837660 | 2.221903 |
| H | -2.480532 | -1.630224 | 3.245501 |
| H | -6.075397 | -2.014553 | 0.934667 |
| H | -4.915579 | -2.076707 | 3.121460 |

**7I-*Z***

Imaginary frequency: None

Electronic energies: -772.808084

Free energies: -772.450514

Corrected Free energies: -772.447393

| | | | |
|---|---|---|---|
| N | 0.286530 | -0.884970 | 0.451385 |
| C | -0.532695 | -1.880310 | -0.057968 |
| C | -1.864412 | -1.822592 | -0.250208 |
| C | -2.634478 | -3.064588 | -0.626427 |
| H | -3.269821 | -2.884882 | -1.498831 |
| H | -3.289795 | -3.402293 | 0.182834 |
| H | -0.147876 | 0.029511 | 0.512322 |
| C | 1.647036 | -0.751368 | -0.062337 |
| C | 2.170892 | 0.635484 | 0.343543 |
| C | 2.575815 | -1.836978 | 0.486726 |
| H | 1.655876 | -0.822147 | -1.162014 |
| C | 3.598886 | 0.836892 | -0.180835 |
| H | 2.205990 | 0.637165 | 1.441178 |
| C | 4.008445 | -1.643172 | -0.012215 |
| H | 2.547788 | -1.786512 | 1.581299 |
| H | 2.206306 | -2.825128 | 0.199518 |
| C | 4.532106 | -0.252898 | 0.353260 |
| H | 3.962934 | 1.827239 | 0.107276 |
| H | 3.595942 | 0.798878 | -1.276205 |
| H | 4.657504 | -2.416953 | 0.404706 |
| H | 4.031339 | -1.761139 | -1.102028 |
| H | 5.541071 | -0.109794 | -0.041490 |
| H | 4.599218 | -0.168154 | 1.444295 |
| N | 1.202684 | 1.679406 | -0.019470 |
| C | 1.364069 | 2.899497 | 0.756456 |
| H | 2.292763 | 3.443664 | 0.521480 |
| H | 0.524730 | 3.567989 | 0.550554 |
| H | 1.360175 | 2.663738 | 1.822147 |
| C | 1.148124 | 1.981584 | -1.442976 |

| | | | |
|---|---|---|---|
| H | 0.282173 | 2.619435 | -1.637910 |
| H | 2.043434 | 2.509690 | -1.805404 |
| H | 1.029572 | 1.066305 | -2.026723 |
| H | -1.953326 | -3.885134 | -0.858956 |
| H | -0.022707 | -2.821997 | -0.248233 |
| C | -2.638695 | -0.568700 | -0.064148 |
| C | -2.201455 | 0.644411 | -0.616933 |
| C | -3.854173 | -0.568458 | 0.632000 |
| C | -2.931408 | 1.815337 | -0.451798 |
| H | -1.285634 | 0.663700 | -1.198215 |
| C | -4.588539 | 0.601785 | 0.795076 |
| H | -4.225097 | -1.493257 | 1.059994 |
| C | -4.128649 | 1.800890 | 0.259286 |
| H | -2.570251 | 2.739041 | -0.890277 |
| H | -5.522190 | 0.576511 | 1.345206 |
| H | -4.699830 | 2.712580 | 0.387046 |

**7I-*E***

Imaginary frequency: None

Electronic energies: -772.808899

Free energies: -772.451900

Corrected Free energies: -772.448550

| | | | |
|---|---|---|---|
| N | -0.528367 | -0.185955 | 0.625874 |
| C | 0.769946 | 0.149233 | 0.308117 |
| C | 1.829442 | -0.686354 | 0.321644 |
| H | -0.750883 | -1.175978 | 0.601901 |
| C | -1.627935 | 0.599795 | 0.075954 |
| C | -2.920658 | -0.217737 | 0.220367 |
| C | -1.790701 | 1.946539 | 0.784735 |
| H | -1.457917 | 0.802279 | -0.993313 |
| C | -4.088628 | 0.553719 | -0.410094 |
| H | -3.113496 | -0.302232 | 1.298727 |
| C | -2.964273 | 2.731835 | 0.196147 |
| H | -1.959554 | 1.755457 | 1.850617 |
| H | -0.866058 | 2.524481 | 0.702389 |
| C | -4.257853 | 1.917338 | 0.266612 |
| H | -5.011113 | -0.026525 | -0.322651 |
| H | -3.897884 | 0.702113 | -1.479027 |
| H | -3.081996 | 3.681332 | 0.723612 |
| H | -2.747043 | 2.973386 | -0.851004 |
| H | -5.079669 | 2.467391 | -0.198417 |
| H | -4.528995 | 1.764159 | 1.317769 |
| N | -2.725403 | -1.596204 | -0.245523 |

| | | | |
|---|---|---|---|
| C | -3.793914 | -2.487194 | 0.181281 |
| H | -4.748074 | -2.297855 | -0.334515 |
| H | -3.504239 | -3.520494 | -0.021852 |
| H | -3.955295 | -2.380592 | 1.255802 |
| C | -2.486016 | -1.722978 | -1.677081 |
| H | -2.246910 | -2.764611 | -1.901587 |
| H | -3.354999 | -1.436777 | -2.288753 |
| H | -1.631395 | -1.113820 | -1.977279 |
| C | 3.189234 | -0.173451 | 0.054960 |
| C | 3.422862 | 0.911656 | -0.806043 |
| C | 4.306630 | -0.775218 | 0.653422 |
| C | 4.707054 | 1.388766 | -1.031815 |
| H | 2.589749 | 1.370932 | -1.326253 |
| C | 5.594158 | -0.302321 | 0.421008 |
| H | 4.165275 | -1.615053 | 1.324446 |
| C | 5.803926 | 0.785332 | -0.419920 |
| H | 4.854926 | 2.224636 | -1.706193 |
| H | 6.435881 | -0.785942 | 0.903823 |
| H | 6.806209 | 1.152957 | -0.604040 |
| C | 1.658576 | -2.141654 | 0.685214 |
| H | 1.671415 | -2.306014 | 1.768317 |
| H | 0.709772 | -2.535128 | 0.309514 |
| H | 2.452263 | -2.750288 | 0.248996 |
| H | 0.915317 | 1.203463 | 0.089465 |

**7I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -772.628993

Free energies: -772.271486

Corrected Free energies: -772.268387

| | | | |
|---|---|---|---|
| N | -0.490974 | 0.301433 | 0.341229 |
| C | 0.749910 | -0.098351 | 0.251938 |
| C | 1.833280 | 0.777838 | 0.026519 |
| H | -0.753877 | 1.285292 | 0.213142 |
| C | -1.683402 | -0.523871 | 0.554316 |
| C | -2.782394 | 0.102412 | -0.327729 |
| C | -1.471594 | -1.999670 | 0.240491 |
| H | -1.960215 | -0.413564 | 1.610265 |
| C | -4.093581 | -0.669278 | -0.154468 |
| H | -2.446812 | -0.024992 | -1.364531 |
| C | -2.794847 | -2.759066 | 0.378300 |
| H | -1.090599 | -2.095952 | -0.782880 |
| H | -0.730403 | -2.432692 | 0.916549 |

| | | | |
|---|---|---|---|
| C | -3.889083 | -2.146626 | -0.496781 |
| H | -4.862486 | -0.226200 | -0.792750 |
| H | -4.440044 | -0.584684 | 0.881160 |
| H | -2.634021 | -3.806553 | 0.117059 |
| H | -3.114206 | -2.735623 | 1.426058 |
| H | -4.825190 | -2.692626 | -0.363153 |
| H | -3.609159 | -2.241846 | -1.551895 |
| N | -2.826224 | 1.550112 | -0.088565 |
| C | -3.321649 | 2.289945 | -1.245123 |
| H | -4.376437 | 2.070241 | -1.467201 |
| H | -3.232879 | 3.359755 | -1.048813 |
| H | -2.720465 | 2.049734 | -2.123329 |
| C | -3.555385 | 1.937853 | 1.117157 |
| H | -3.370365 | 2.994722 | 1.314755 |
| H | -4.640067 | 1.790817 | 1.018269 |
| H | -3.206618 | 1.369197 | 1.980685 |
| C | 3.174969 | 0.235381 | -0.032606 |
| C | 3.414223 | -1.112759 | -0.376548 |
| C | 4.283614 | 1.058188 | 0.253463 |
| C | 4.704109 | -1.610658 | -0.425340 |
| H | 2.594036 | -1.764362 | -0.650152 |
| C | 5.570272 | 0.547449 | 0.220415 |
| H | 4.130784 | 2.092001 | 0.535524 |
| C | 5.786377 | -0.785931 | -0.121718 |
| H | 4.869927 | -2.642618 | -0.707872 |
| H | 6.408494 | 1.188864 | 0.461980 |
| H | 6.794449 | -1.180357 | -0.156368 |
| C | 1.576284 | 2.247316 | -0.080048 |
| H | 0.687867 | 2.445996 | -0.684755 |
| H | 1.406756 | 2.684645 | 0.910118 |
| H | 2.408641 | 2.765370 | -0.549361 |
| H | 0.926658 | -1.156413 | 0.395429 |

**7I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -772.627869

Free energies: -772.269249

Corrected Free energies: -772.266495

| | | | |
|---|---|---|---|
| N | -0.262060 | 0.839057 | -0.418969 |
| C | 0.483317 | 1.885083 | -0.167487 |
| C | 1.886720 | 1.832389 | -0.039553 |
| C | 2.645809 | 3.116538 | -0.107969 |
| H | 3.090599 | 3.238363 | -1.102377 |

| | | | |
|---|---|---|---|
| H | 3.459916 | 3.125632 | 0.617990 |
| H | 0.161380 | -0.084597 | -0.574099 |
| C | -1.720477 | 0.744860 | -0.469504 |
| C | -2.057548 | -0.622946 | 0.164050 |
| C | -2.441040 | 1.886933 | 0.234649 |
| H | -2.004521 | 0.730645 | -1.529132 |
| C | -3.569415 | -0.857732 | 0.114268 |
| H | -1.759581 | -0.550808 | 1.218008 |
| C | -3.951970 | 1.631438 | 0.222020 |
| H | -2.080111 | 1.952611 | 1.267618 |
| H | -2.225797 | 2.838584 | -0.256716 |
| C | -4.301725 | 0.275441 | 0.837500 |
| H | -3.802354 | -1.823663 | 0.570076 |
| H | -3.902605 | -0.898074 | -0.928323 |
| H | -4.455555 | 2.437291 | 0.759039 |
| H | -4.311248 | 1.662563 | -0.812416 |
| H | -5.380256 | 0.111228 | 0.792598 |
| H | -4.020116 | 0.272089 | 1.896539 |
| N | -1.201483 | -1.655422 | -0.431818 |
| C | -0.973121 | -2.782044 | 0.467276 |
| H | -1.888658 | -3.360207 | 0.660520 |
| H | -0.235896 | -3.451626 | 0.020587 |
| H | -0.579838 | -2.423905 | 1.420505 |
| C | -1.651010 | -2.127414 | -1.740073 |
| H | -0.862167 | -2.736844 | -2.183430 |
| H | -2.562824 | -2.737368 | -1.676072 |
| H | -1.842898 | -1.287217 | -2.409433 |
| H | 1.991683 | 3.970229 | 0.065664 |
| H | -0.016922 | 2.844198 | -0.084838 |
| C | 2.601023 | 0.569171 | 0.107015 |
| C | 3.880528 | 0.420630 | -0.456795 |
| C | 2.065189 | -0.498080 | 0.853316 |
| C | 4.573222 | -0.772107 | -0.322885 |
| H | 4.318349 | 1.234961 | -1.021161 |
| C | 2.771224 | -1.682454 | 0.997647 |
| H | 1.119751 | -0.378988 | 1.370446 |
| C | 4.020273 | -1.827506 | 0.399616 |
| H | 5.548884 | -0.880203 | -0.780280 |
| H | 2.351840 | -2.487775 | 1.587972 |
| H | 4.567759 | -2.755749 | 0.507677 |

**8I-*Z***

Imaginary frequency: None

Electronic energies: -1078.812740

Free energies: -1078.394128

Corrected Free energies: -1078.388414

| | | | |
|---|---|---|---|
| N | 0.795702 | 0.919898 | 0.466129 |
| C | 1.536409 | 1.834447 | -0.282483 |
| C | 2.840177 | 1.756983 | -0.600938 |
| C | 3.501071 | 2.854824 | -1.396263 |
| H | 3.894727 | 2.483842 | -2.346859 |
| H | 4.343489 | 3.286968 | -0.847742 |
| H | 1.305508 | 0.077936 | 0.715768 |
| C | -0.499986 | 0.538586 | -0.088314 |
| C | -0.932568 | -0.774994 | 0.607824 |
| H | -0.419084 | 0.362254 | -1.170154 |
| H | -1.160560 | -0.505671 | 1.645432 |
| N | 0.197109 | -1.712987 | 0.698053 |
| C | -0.082040 | -2.827198 | 1.590957 |
| H | -0.832010 | -3.522694 | 1.182872 |
| H | 0.841409 | -3.382876 | 1.767012 |
| H | -0.446830 | -2.449942 | 2.548595 |
| C | 0.734749 | -2.183426 | -0.571407 |
| H | 1.665837 | -2.719895 | -0.372755 |
| H | 0.054118 | -2.862667 | -1.105722 |
| H | 0.973332 | -1.339126 | -1.223269 |
| C | -1.552251 | 1.611892 | 0.121966 |
| C | -1.605553 | 2.327666 | 1.318656 |
| C | -2.507356 | 1.865761 | -0.861436 |
| C | -2.602787 | 3.274155 | 1.530237 |
| H | -0.850637 | 2.143947 | 2.074980 |
| C | -3.508240 | 2.810053 | -0.651052 |
| H | -2.468783 | 1.316145 | -1.796328 |
| C | -3.558886 | 3.515708 | 0.546863 |
| H | -2.632777 | 3.826257 | 2.462424 |
| H | -4.244833 | 2.996139 | -1.423902 |
| H | -4.334674 | 4.254240 | 0.711298 |
| C | -2.198617 | -1.359241 | 0.000454 |
| C | -3.261206 | -1.705937 | 0.836354 |
| C | -2.329805 | -1.592469 | -1.372363 |
| C | -4.426985 | -2.265900 | 0.322055 |
| H | -3.174812 | -1.528710 | 1.903910 |
| C | -3.492158 | -2.154358 | -1.890553 |
| H | -1.527473 | -1.326719 | -2.051389 |
| C | -4.545171 | -2.491931 | -1.045081 |
| H | -5.242137 | -2.522495 | 0.988365 |
| H | -3.576784 | -2.324524 | -2.957452 |

| | | | |
|---|---|---|---|
| H | -5.451984 | -2.924865 | -1.450391 |
| H | 0.958266 | 2.691725 | -0.622490 |
| H | 2.791233 | 3.653340 | -1.617309 |
| C | 3.671843 | 0.588561 | -0.212986 |
| C | 3.664153 | 0.082640 | 1.093166 |
| C | 4.483571 | -0.050663 | -1.159826 |
| C | 4.410654 | -1.041714 | 1.433483 |
| H | 3.076742 | 0.585378 | 1.854342 |
| C | 5.231806 | -1.172091 | -0.821422 |
| H | 4.514619 | 0.321785 | -2.177518 |
| C | 5.194291 | -1.677115 | 0.476106 |
| H | 4.384791 | -1.414796 | 2.450738 |
| H | 5.842919 | -1.656070 | -1.574452 |
| H | 5.776008 | -2.552706 | 0.738743 |

**8I-*E***

Imaginary frequency: None

Electronic energies: -1078.813870

Free energies: -1078.398805

Corrected Free energies: -1078.392467

| | | | |
|---|---|---|---|
| N | -0.547864 | -0.716917 | -0.590051 |
| C | -1.798083 | -0.295633 | -0.189356 |
| C | -2.959602 | -0.932945 | -0.437746 |
| H | -0.427992 | -1.696580 | -0.819804 |
| C | 0.634707 | -0.162449 | 0.047736 |
| C | 1.856868 | -0.928522 | -0.508815 |
| H | 0.587010 | -0.287826 | 1.138197 |
| H | 1.916425 | -0.658360 | -1.569105 |
| N | 1.609195 | -2.378671 | -0.498281 |
| C | 2.567914 | -3.100573 | -1.323611 |
| H | 3.587282 | -3.078959 | -0.907653 |
| H | 2.253948 | -4.142901 | -1.405917 |
| H | 2.594358 | -2.666983 | -2.325477 |
| C | 1.510081 | -2.983656 | 0.823818 |
| H | 1.173223 | -4.015700 | 0.707878 |
| H | 2.467821 | -2.994639 | 1.364290 |
| H | 0.770040 | -2.458121 | 1.431265 |
| C | 0.780388 | 1.322270 | -0.237437 |
| C | 0.542947 | 1.817724 | -1.520436 |
| C | 1.183884 | 2.202914 | 0.764398 |
| C | 0.717291 | 3.168717 | -1.798102 |
| H | 0.206930 | 1.136872 | -2.294944 |
| C | 1.360666 | 3.556494 | 0.488664 |

| | | | |
|---|---|---|---|
| H | 1.361563 | 1.826187 | 1.766638 |
| C | 1.129035 | 4.041945 | -0.793816 |
| H | 0.529260 | 3.542785 | -2.797764 |
| H | 1.674196 | 4.230377 | 1.277236 |
| H | 1.262762 | 5.095401 | -1.009250 |
| C | 3.162336 | -0.501485 | 0.143391 |
| C | 4.254695 | -0.180029 | -0.663925 |
| C | 3.324149 | -0.450635 | 1.531486 |
| C | 5.477722 | 0.182046 | -0.107251 |
| H | 4.142079 | -0.209706 | -1.743226 |
| C | 4.545250 | -0.091151 | 2.092432 |
| H | 2.494407 | -0.686930 | 2.188098 |
| C | 5.626116 | 0.226314 | 1.274802 |
| H | 6.311737 | 0.432302 | -0.752325 |
| H | 4.651491 | -0.056162 | 3.170334 |
| H | 6.575901 | 0.509051 | 1.712946 |
| H | -1.793811 | 0.646258 | 0.352299 |
| C | -4.237999 | -0.367483 | 0.037847 |
| C | -4.440774 | 1.016157 | 0.171235 |
| C | -5.307522 | -1.213158 | 0.369317 |
| C | -5.642523 | 1.525182 | 0.645810 |
| H | -3.656068 | 1.702545 | -0.126323 |
| C | -6.514203 | -0.702682 | 0.836431 |
| H | -5.187841 | -2.286818 | 0.275544 |
| C | -6.688936 | 0.669441 | 0.983244 |
| H | -5.769935 | 2.598207 | 0.734683 |
| H | -7.319600 | -1.382470 | 1.090292 |
| H | -7.629142 | 1.067848 | 1.345383 |
| C | -2.967323 | -2.262461 | -1.153317 |
| H | -2.171410 | -2.307829 | -1.901019 |
| H | -2.824334 | -3.106236 | -0.468809 |
| H | -3.912108 | -2.420564 | -1.675939 |

**8I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1078.629890

Free energies: -1078.213410

Corrected Free energies: -1078.207243

| | | | |
|---|---|---|---|
| N | -0.527098 | -0.877049 | 0.024154 |
| C | -1.732875 | -0.379208 | 0.137240 |
| C | -2.903059 | -1.115260 | -0.138024 |
| H | -0.350923 | -1.843653 | -0.276356 |
| C | 0.721551 | -0.186569 | 0.373177 |

| | | | |
|---|---|---|---|
| C | 1.842186 | -0.923208 | -0.399321 |
| H | 0.861754 | -0.307987 | 1.451528 |
| H | 1.682619 | -0.688897 | -1.456904 |
| N | 1.640375 | -2.375809 | -0.290344 |
| C | 2.344868 | -3.100280 | -1.344818 |
| H | 3.437142 | -3.019919 | -1.245999 |
| H | 2.070388 | -4.154794 | -1.294161 |
| H | 2.050410 | -2.711471 | -2.320993 |
| C | 1.952717 | -2.945436 | 1.018826 |
| H | 1.634263 | -3.988699 | 1.024990 |
| H | 3.025516 | -2.907100 | 1.250870 |
| H | 1.406240 | -2.426010 | 1.808751 |
| C | 0.680245 | 1.288586 | 0.046914 |
| C | 0.341989 | 1.719856 | -1.238012 |
| C | 1.013540 | 2.226855 | 1.019785 |
| C | 0.339889 | 3.075306 | -1.541720 |
| H | 0.071105 | 0.998212 | -2.002264 |
| C | 1.018752 | 3.584801 | 0.712651 |
| H | 1.273643 | 1.896103 | 2.019477 |
| C | 0.681743 | 4.010055 | -0.567046 |
| H | 0.073400 | 3.402208 | -2.539382 |
| H | 1.281870 | 4.307486 | 1.475349 |
| H | 0.682021 | 5.066726 | -0.805884 |
| C | 3.222242 | -0.413646 | -0.024190 |
| C | 4.134784 | -0.121714 | -1.038716 |
| C | 3.621999 | -0.249037 | 1.304762 |
| C | 5.418737 | 0.322536 | -0.738002 |
| H | 3.833858 | -0.237443 | -2.075043 |
| C | 4.903520 | 0.197019 | 1.608460 |
| H | 2.938341 | -0.466610 | 2.117726 |
| C | 5.805330 | 0.483738 | 0.587868 |
| H | 6.112872 | 0.546242 | -1.539173 |
| H | 5.196655 | 0.322029 | 2.643854 |
| H | 6.802831 | 0.832858 | 0.826126 |
| H | -1.792195 | 0.643114 | 0.492756 |
| C | -4.189148 | -0.473424 | 0.029135 |
| C | -4.331908 | 0.928766 | -0.059397 |
| C | -5.338826 | -1.248004 | 0.287775 |
| C | -5.569149 | 1.523625 | 0.110535 |
| H | -3.482419 | 1.552931 | -0.308197 |
| C | -6.569597 | -0.643037 | 0.476302 |
| H | -5.258037 | -2.323720 | 0.378006 |
| C | -6.690933 | 0.742370 | 0.385709 |
| H | -5.663947 | 2.598526 | 0.021362 |

| | | | |
|---|---|---|---|
| H | -7.438352 | -1.250821 | 0.695870 |
| H | -7.657235 | 1.211772 | 0.524248 |
| C | -2.780587 | -2.553665 | -0.527855 |
| H | -2.009854 | -2.679699 | -1.292998 |
| H | -2.493609 | -3.165907 | 0.334263 |
| H | -3.709351 | -2.941618 | -0.936720 |

**8I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1078.628252

Free energies: -1078.210402

Corrected Free energies: -1078.205101

| | | | |
|---|---|---|---|
| N | 0.860669 | 0.446083 | -0.523078 |
| C | 1.616561 | 1.513432 | -0.605022 |
| C | 3.021087 | 1.498480 | -0.500624 |
| C | 3.759688 | 2.720389 | -0.939857 |
| H | 4.182322 | 2.565021 | -1.939119 |
| H | 4.588139 | 2.936909 | -0.264085 |
| H | 1.260669 | -0.496654 | -0.428598 |
| C | -0.601471 | 0.393226 | -0.625940 |
| C | -1.017045 | -0.888564 | 0.139928 |
| H | -0.841978 | 0.294644 | -1.688874 |
| H | -0.808220 | -0.686450 | 1.195479 |
| N | -0.116128 | -1.990534 | -0.230822 |
| C | -0.084218 | -3.034606 | 0.789371 |
| H | -1.048791 | -3.554503 | 0.883321 |
| H | 0.679009 | -3.767194 | 0.522850 |
| H | 0.176790 | -2.598165 | 1.755293 |
| C | -0.357735 | -2.565421 | -1.552314 |
| H | 0.450011 | -3.263083 | -1.776807 |
| H | -1.312629 | -3.104877 | -1.608705 |
| H | -0.350212 | -1.788422 | -2.319788 |
| C | -1.268650 | 1.632748 | -0.080265 |
| C | -1.010982 | 2.054269 | 1.226270 |
| C | -2.162134 | 2.350974 | -0.870193 |
| C | -1.642893 | 3.182144 | 1.733359 |
| H | -0.307019 | 1.507828 | 1.846728 |
| C | -2.800150 | 3.477927 | -0.359086 |
| H | -2.361285 | 2.028706 | -1.886614 |
| C | -2.540775 | 3.894421 | 0.941310 |
| H | -1.435496 | 3.505617 | 2.746060 |
| H | -3.494555 | 4.030914 | -0.979690 |
| H | -3.033058 | 4.773830 | 1.338376 |

| | | | |
|---|---|---|---|
| C | -2.502954 | -1.172861 | 0.017998 |
| C | -3.222788 | -1.510005 | 1.165097 |
| C | -3.173045 | -1.133142 | -1.207752 |
| C | -4.580773 | -1.805847 | 1.093612 |
| H | -2.715203 | -1.533536 | 2.124177 |
| C | -4.530206 | -1.426877 | -1.281897 |
| H | -2.645084 | -0.872864 | -2.118605 |
| C | -5.237057 | -1.764891 | -0.131416 |
| H | -5.124829 | -2.062532 | 1.994646 |
| H | -5.035886 | -1.389668 | -2.239281 |
| H | -6.294898 | -1.991149 | -0.190184 |
| H | 1.109226 | 2.454998 | -0.792910 |
| H | 3.097274 | 3.583131 | -0.994724 |
| C | 3.758577 | 0.326025 | -0.048232 |
| C | 3.257583 | -0.535980 | 0.947382 |
| C | 5.031917 | 0.066044 | -0.585572 |
| C | 3.993471 | -1.636972 | 1.358942 |
| H | 2.319163 | -0.313131 | 1.442868 |
| C | 5.752994 | -1.045665 | -0.182325 |
| H | 5.441973 | 0.724246 | -1.341330 |
| C | 5.234949 | -1.902339 | 0.786997 |
| H | 3.602346 | -2.282389 | 2.135429 |
| H | 6.722438 | -1.244228 | -0.622004 |
| H | 5.804283 | -2.767305 | 1.104759 |

**9I-*Z***

Imaginary frequency: None

Electronic energies: -560.241615

Free energies: -560.008094

Corrected Free energies: -560.006700

| | | | |
|---|---|---|---|
| C | -3.779075 | -0.497212 | 0.491469 |
| C | -2.772984 | -1.621801 | 0.741469 |
| C | -1.413030 | -0.950906 | 0.500934 |
| C | -3.143301 | 0.228936 | -0.691534 |
| H | -4.786242 | -0.856559 | 0.279695 |
| H | -3.818172 | 0.172665 | 1.354918 |
| H | -2.927004 | -2.422476 | 0.013344 |
| H | -2.841943 | -2.053560 | 1.739726 |
| H | -0.985869 | -0.542130 | 1.425147 |
| H | -0.687494 | -1.654632 | 0.088733 |
| H | -3.458651 | 1.269300 | -0.786349 |
| H | -3.382615 | -0.283075 | -1.630161 |
| N | -1.701538 | 0.157825 | -0.420406 |

| | | | |
|---|---|---|---|
| C | -0.975509 | 1.328025 | -0.376443 |
| C | 0.338366 | 1.512853 | -0.116719 |
| H | -1.577045 | 2.217503 | -0.557185 |
| C | 0.842782 | 2.925036 | 0.080834 |
| H | 1.735608 | 3.116046 | -0.522264 |
| H | 0.076132 | 3.651119 | -0.195845 |
| H | 1.112438 | 3.123141 | 1.123253 |
| C | 1.350616 | 0.434999 | -0.067162 |
| C | 1.305140 | -0.646355 | -0.960608 |
| C | 2.447081 | 0.513512 | 0.803724 |
| C | 2.296932 | -1.619200 | -0.964413 |
| H | 0.481395 | -0.709607 | -1.663643 |
| C | 3.436657 | -0.463397 | 0.806059 |
| H | 2.521145 | 1.345442 | 1.494975 |
| C | 3.367009 | -1.537289 | -0.076449 |
| H | 2.238319 | -2.440975 | -1.669188 |
| H | 4.266711 | -0.383599 | 1.498836 |
| H | 4.139949 | -2.296590 | -0.078112 |

**9I-*E***

Imaginary frequency: None

Electronic energies: -560.240939

Free energies: -560.007524

Corrected Free energies: -560.005848

| | | | |
|---|---|---|---|
| C | 3.945740 | -1.000563 | 0.724316 |
| C | 4.104534 | 0.507544 | 0.529260 |
| C | 2.679292 | 0.973314 | 0.215365 |
| C | 2.944899 | -1.352398 | -0.373103 |
| H | 4.883079 | -1.549923 | 0.636570 |
| H | 3.507797 | -1.207660 | 1.704849 |
| H | 4.757874 | 0.703757 | -0.325072 |
| H | 4.516967 | 1.018932 | 1.398747 |
| H | 2.126762 | 1.212303 | 1.132385 |
| H | 2.678660 | 1.860278 | -0.418648 |
| H | 2.374249 | -2.259455 | -0.164738 |
| H | 3.457340 | -1.491394 | -1.331134 |
| N | 2.046460 | -0.188947 | -0.441460 |
| C | 0.687256 | -0.404338 | -0.310588 |
| C | -0.294595 | 0.516254 | -0.405372 |
| H | 0.421027 | -1.437322 | -0.098023 |
| C | -1.697363 | 0.126184 | -0.129197 |
| C | -2.187077 | -1.161688 | -0.399267 |
| C | -2.598450 | 1.062801 | 0.398251 |

| | | | |
|---|---|---|---|
| C | -3.505679 | -1.502703 | -0.128575 |
| H | -1.534440 | -1.899953 | -0.851202 |
| C | -3.921002 | 0.722913 | 0.666522 |
| H | -2.255449 | 2.068519 | 0.614830 |
| C | -4.383076 | -0.562882 | 0.408697 |
| H | -3.855347 | -2.503707 | -0.354396 |
| H | -4.591308 | 1.467547 | 1.080802 |
| H | -5.413351 | -0.827639 | 0.614323 |
| C | -0.027546 | 1.945426 | -0.817989 |
| H | 0.212474 | 2.606796 | 0.020699 |
| H | 0.809008 | 1.981039 | -1.517717 |
| H | -0.902173 | 2.361330 | -1.321981 |

**9I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -560.062765

Free energies: -559.829143

Corrected Free energies: -559.827469

| | | | |
|---|---|---|---|
| C | 4.134325 | -0.838076 | 0.657392 |
| C | 4.227135 | 0.386691 | -0.254362 |
| C | 2.795183 | 0.925047 | -0.285142 |
| C | 2.808214 | -1.453648 | 0.238661 |
| H | 4.960821 | -1.533302 | 0.524603 |
| H | 4.091375 | -0.536044 | 1.705871 |
| H | 4.531003 | 0.084702 | -1.258265 |
| H | 4.924279 | 1.140326 | 0.106315 |
| H | 2.614358 | 1.647641 | 0.512221 |
| H | 2.532803 | 1.366705 | -1.243989 |
| H | 2.332527 | -2.076915 | 0.993085 |
| H | 2.906317 | -2.017734 | -0.693233 |
| N | 1.956397 | -0.270739 | -0.034847 |
| C | 0.644920 | -0.375301 | -0.012502 |
| C | -0.340100 | 0.621133 | -0.157236 |
| H | 0.299782 | -1.381326 | 0.197414 |
| C | -1.728924 | 0.181079 | -0.076153 |
| C | -2.124205 | -1.101446 | -0.505804 |
| C | -2.712698 | 1.043642 | 0.443892 |
| C | -3.446256 | -1.502441 | -0.409835 |
| H | -1.404700 | -1.771968 | -0.959614 |
| C | -4.029604 | 0.628306 | 0.556614 |
| H | -2.437421 | 2.028505 | 0.798863 |
| C | -4.402541 | -0.643471 | 0.127885 |
| H | -3.734973 | -2.484701 | -0.762195 |

| | | | |
|---|---|---|---|
| H | -4.767537 | 1.298143 | 0.980103 |
| H | -5.434402 | -0.962888 | 0.207406 |
| C | -0.034030 | 2.080215 | -0.298396 |
| H | 0.381916 | 2.488733 | 0.627698 |
| H | 0.690589 | 2.254332 | -1.092099 |
| H | -0.930016 | 2.640579 | -0.550337 |

**9I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -560.061208

Free energies: -559.828890

Corrected Free energies: -559.827077

| | | | |
|---|---|---|---|
| C | -3.769460 | -0.536085 | 0.479996 |
| C | -2.730637 | -1.622984 | 0.773932 |
| C | -1.374500 | -0.954227 | 0.501027 |
| C | -3.139216 | 0.206201 | -0.689953 |
| H | -4.747226 | -0.941225 | 0.226736 |
| H | -3.875553 | 0.142086 | 1.328985 |
| H | -2.868357 | -2.461999 | 0.090694 |
| H | -2.786172 | -1.999319 | 1.793348 |
| H | -0.869910 | -0.606536 | 1.404342 |
| H | -0.698632 | -1.607950 | -0.044780 |
| H | -3.502820 | 1.218138 | -0.852881 |
| H | -3.224548 | -0.366649 | -1.617753 |
| N | -1.711318 | 0.240580 | -0.312915 |
| C | -0.983148 | 1.321518 | -0.475347 |
| C | 0.374253 | 1.514517 | -0.136223 |
| H | -1.524303 | 2.178091 | -0.867204 |
| C | 0.806662 | 2.918470 | 0.147290 |
| H | 1.779990 | 3.123490 | -0.300674 |
| H | 0.075939 | 3.641065 | -0.214116 |
| H | 0.904473 | 3.064873 | 1.229275 |
| C | 1.357705 | 0.444782 | -0.085637 |
| C | 1.307923 | -0.616821 | -1.006319 |
| C | 2.433494 | 0.511463 | 0.816941 |
| C | 2.287167 | -1.596908 | -1.001581 |
| H | 0.517017 | -0.645709 | -1.748099 |
| C | 3.397058 | -0.484242 | 0.831891 |
| H | 2.494566 | 1.331267 | 1.522309 |
| C | 3.326652 | -1.539711 | -0.075245 |
| H | 2.245288 | -2.402438 | -1.724003 |
| H | 4.208566 | -0.436081 | 1.547213 |
| H | 4.087189 | -2.311007 | -0.067631 |

**10I-*Z***

Imaginary frequency: None

Electronic energies: -599.550131

Free energies: -599.288364

Corrected Free energies: -599.286367

| | | | |
|---|---|---|---|
| C | 1.515172 | 2.936329 | -0.171959 |
| C | 0.794016 | 1.616250 | -0.013854 |
| C | -0.551269 | 1.617096 | 0.094134 |
| H | 1.959562 | 3.041823 | -1.167096 |
| H | 2.329423 | 3.029017 | 0.552862 |
| C | -1.149474 | -0.741285 | -0.467329 |
| C | -2.642950 | 0.670287 | 0.884204 |
| C | -2.358442 | -1.370929 | -1.158294 |
| H | -0.825877 | -1.394267 | 0.358730 |
| H | -0.313960 | -0.662258 | -1.163404 |
| C | -3.874034 | 0.055269 | 0.225541 |
| H | -2.436074 | 0.149263 | 1.833446 |
| H | -2.820556 | 1.720983 | 1.122871 |
| C | -3.575993 | -1.370394 | -0.235263 |
| H | -2.100787 | -2.388875 | -1.461664 |
| H | -2.587002 | -0.801297 | -2.065003 |
| H | -4.707607 | 0.073279 | 0.931944 |
| H | -4.155523 | 0.667375 | -0.637687 |
| H | -4.443356 | -1.802259 | -0.739680 |
| H | -3.365392 | -1.996630 | 0.640392 |
| N | -1.476539 | 0.592295 | 0.010430 |
| H | -1.036429 | 2.586879 | 0.202480 |
| H | 0.828736 | 3.773638 | -0.033404 |
| C | 1.658443 | 0.413545 | 0.053354 |
| C | 2.700991 | 0.222305 | -0.863028 |
| C | 1.513512 | -0.521105 | 1.087262 |
| C | 3.544675 | -0.878831 | -0.771310 |
| H | 2.842032 | 0.937061 | -1.666381 |
| C | 2.356902 | -1.622962 | 1.181879 |
| H | 0.734637 | -0.367829 | 1.827207 |
| C | 3.374991 | -1.809060 | 0.250714 |
| H | 4.335913 | -1.012075 | -1.500188 |
| H | 2.224870 | -2.333020 | 1.990296 |
| H | 4.033933 | -2.665952 | 0.324967 |

**10I-*E***

Imaginary frequency: None
Electronic energies: -599.548887
Free energies: -599.286974
Corrected Free energies: -599.285159

| | | | |
|---|---|---|---|
| C | -0.666414 | 0.694090 | 0.067305 |
| C | 0.303808 | -0.236748 | 0.223691 |
| C | 2.382175 | 1.004279 | -0.395550 |
| C | 2.455784 | -0.963628 | 1.078082 |
| C | 3.690172 | 0.566790 | -1.054239 |
| H | 2.607837 | 1.739819 | 0.392765 |
| H | 1.738338 | 1.482981 | -1.132155 |
| C | 3.767393 | -1.426716 | 0.451664 |
| H | 2.670945 | -0.385923 | 1.991420 |
| H | 1.846779 | -1.820687 | 1.371923 |
| C | 4.554790 | -0.230149 | -0.079092 |
| H | 4.220430 | 1.453656 | -1.410181 |
| H | 3.454986 | -0.053145 | -1.925616 |
| H | 4.346435 | -1.978192 | 1.196451 |
| H | 3.543265 | -2.112448 | -0.372015 |
| H | 5.477078 | -0.559057 | -0.563178 |
| H | 4.842066 | 0.414173 | 0.760862 |
| N | 1.678571 | -0.149241 | 0.148176 |
| H | -0.019974 | -1.256511 | 0.426462 |
| C | -2.064285 | 0.199693 | -0.019695 |
| C | -2.370011 | -0.985549 | -0.708123 |
| C | -3.130138 | 0.880918 | 0.590322 |
| C | -3.666695 | -1.486397 | -0.752605 |
| H | -1.579504 | -1.507064 | -1.235823 |
| C | -4.427824 | 0.386655 | 0.538517 |
| H | -2.944803 | 1.795954 | 1.139498 |
| C | -4.705830 | -0.802927 | -0.129806 |
| H | -3.867467 | -2.404560 | -1.292965 |
| H | -5.226083 | 0.930844 | 1.030636 |
| H | -5.718515 | -1.185553 | -0.171622 |
| C | -0.446061 | 2.188079 | -0.007081 |
| H | 0.495455 | 2.485783 | 0.448235 |
| H | -0.462151 | 2.556631 | -1.038465 |
| H | -1.236297 | 2.717640 | 0.526203 |

**10I-*E*** radical cation
Imaginary frequency: None
Electronic energies: -599.370748
Free energies: -599.108242

Corrected Free energies: -599.106352

| | | | |
|---|---|---|---|
| C | -0.663307 | 0.763914 | 0.354165 |
| C | 0.412174 | -0.094605 | 0.703772 |
| C | 2.280901 | 1.130595 | -0.351289 |
| C | 2.682847 | -0.748219 | 1.221552 |
| C | 3.180503 | 0.440738 | -1.379358 |
| H | 2.853616 | 1.833771 | 0.260167 |
| H | 1.482289 | 1.659128 | -0.859766 |
| C | 3.578498 | -1.447295 | 0.203718 |
| H | 3.278101 | -0.096420 | 1.868316 |
| H | 2.141023 | -1.453495 | 1.848449 |
| C | 4.244652 | -0.423341 | -0.711239 |
| H | 3.630977 | 1.220608 | -1.995612 |
| H | 2.553992 | -0.175729 | -2.030943 |
| H | 4.319092 | -2.031840 | 0.752060 |
| H | 2.973461 | -2.143484 | -0.384728 |
| H | 4.848076 | -0.927687 | -1.467456 |
| H | 4.918084 | 0.209899 | -0.123807 |
| N | 1.696265 | 0.122450 | 0.552219 |
| H | 0.171461 | -1.027781 | 1.204210 |
| C | -1.963306 | 0.173222 | 0.115549 |
| C | -2.116242 | -1.218119 | -0.080517 |
| C | -3.115341 | 0.983162 | 0.020234 |
| C | -3.361587 | -1.769405 | -0.322175 |
| H | -1.253061 | -1.871729 | -0.074649 |
| C | -4.357573 | 0.425056 | -0.227539 |
| H | -3.041402 | 2.055107 | 0.143357 |
| C | -4.489013 | -0.952255 | -0.392612 |
| H | -3.454812 | -2.838033 | -0.469532 |
| H | -5.228565 | 1.065266 | -0.290823 |
| H | -5.462808 | -1.386409 | -0.583612 |
| C | -0.505082 | 2.255453 | 0.373584 |
| H | 0.457444 | 2.561869 | 0.774243 |
| H | -0.636716 | 2.690880 | -0.621860 |
| H | -1.272855 | 2.685523 | 1.019391 |

**10I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -599.370946

Free energies: -599.109217

Corrected Free energies: -599.107466

| | | | |
|---|---|---|---|
| C | 1.122951 | 2.881527 | -0.347418 |
| C | 0.696724 | 1.503702 | 0.052191 |

| | | | |
|---|---|---|---|
| C | -0.640691 | 1.354030 | 0.487197 |
| H | 1.174451 | 2.950680 | -1.439884 |
| H | 2.113952 | 3.113564 | 0.044862 |
| C | -1.164383 | -0.913302 | -0.377296 |
| C | -2.703026 | 0.285322 | 1.154884 |
| C | -2.317756 | -1.094579 | -1.366974 |
| H | -1.091729 | -1.770162 | 0.298839 |
| H | -0.223037 | -0.800035 | -0.903900 |
| C | -3.862150 | 0.116031 | 0.177659 |
| H | -2.668113 | -0.555939 | 1.853870 |
| H | -2.778013 | 1.207360 | 1.727757 |
| C | -3.669108 | -1.144761 | -0.660540 |
| H | -2.127272 | -2.013012 | -1.924883 |
| H | -2.298750 | -0.264381 | -2.079214 |
| H | -4.787393 | 0.072763 | 0.754601 |
| H | -3.913476 | 0.997102 | -0.468940 |
| H | -4.472161 | -1.241386 | -1.392785 |
| H | -3.711146 | -2.025727 | -0.011191 |
| N | -1.408018 | 0.285984 | 0.446693 |
| H | -1.117265 | 2.234723 | 0.910520 |
| H | 0.410031 | 3.632141 | -0.007828 |
| C | 1.672212 | 0.427073 | 0.060422 |
| C | 2.785726 | 0.468591 | -0.797936 |
| C | 1.570620 | -0.628220 | 0.987308 |
| C | 3.739194 | -0.536787 | -0.757881 |
| H | 2.886368 | 1.276340 | -1.512709 |
| C | 2.536158 | -1.618484 | 1.034631 |
| H | 0.747997 | -0.648215 | 1.693111 |
| C | 3.618131 | -1.581160 | 0.156280 |
| H | 4.581651 | -0.505387 | -1.437426 |
| H | 2.451973 | -2.416554 | 1.761537 |
| H | 4.370443 | -2.359661 | 0.191648 |

**11I-*Z***

Imaginary frequency: None

Electronic energies: -748.816208

Free energies: -748.572690

Corrected Free energies: -748.569852

| | | | |
|---|---|---|---|
| C | -2.855599 | -1.309091 | -0.905648 |
| C | -1.738332 | -1.659155 | -1.889775 |
| C | -0.495189 | -1.105323 | -1.193643 |
| C | -2.436156 | 0.090128 | -0.409874 |
| H | -3.851527 | -1.301097 | -1.344485 |

| | | | |
|---|---|---|---|
| H | -2.850617 | -2.013518 | -0.068819 |
| H | -1.898166 | -1.136149 | -2.835862 |
| H | -1.670317 | -2.728669 | -2.087207 |
| H | -0.093238 | -1.828022 | -0.474010 |
| H | 0.309384 | -0.835661 | -1.881443 |
| H | -2.897272 | 0.872644 | -1.028796 |
| N | -0.995805 | 0.097273 | -0.527960 |
| C | -0.324143 | 1.301304 | -0.497106 |
| C | 1.002532 | 1.510150 | -0.375984 |
| H | -0.977596 | 2.166889 | -0.612056 |
| C | 1.550905 | 2.901259 | -0.586975 |
| H | 2.131395 | 2.976164 | -1.511941 |
| H | 0.740418 | 3.629205 | -0.654355 |
| H | 2.213998 | 3.191653 | 0.233100 |
| C | -2.896181 | 0.311032 | 1.018337 |
| O | -2.194431 | 0.330085 | 1.992876 |
| O | -4.227033 | 0.459604 | 1.067044 |
| H | -4.487454 | 0.564868 | 1.993308 |
| C | 1.965893 | 0.452629 | 0.006707 |
| C | 3.276172 | 0.450198 | -0.490246 |
| C | 1.621267 | -0.523555 | 0.954394 |
| C | 4.196576 | -0.510334 | -0.083191 |
| H | 3.578041 | 1.203107 | -1.209699 |
| C | 2.542696 | -1.477960 | 1.366309 |
| H | 0.619337 | -0.515902 | 1.371324 |
| C | 3.834506 | -1.481488 | 0.844832 |
| H | 5.201018 | -0.496920 | -0.490650 |
| H | 2.253367 | -2.218219 | 2.103695 |
| H | 4.551890 | -2.227565 | 1.165430 |

**11I-*E***

Imaginary frequency: None

Electronic energies: -748.813966

Free energies: -748.570961

Corrected Free energies: -748.567766

| | | | |
|---|---|---|---|
| C | -3.680394 | 0.507218 | 0.707852 |
| C | -3.035132 | 1.821119 | 1.145922 |
| C | -1.824253 | 1.921740 | 0.217122 |
| C | -2.453692 | -0.390820 | 0.468048 |
| H | -4.361395 | 0.076690 | 1.439540 |
| H | -4.222196 | 0.650130 | -0.231614 |
| H | -2.701393 | 1.743066 | 2.183624 |
| H | -3.706120 | 2.674937 | 1.056363 |

| | | | |
|---|---|---|---|
| H | -2.108390 | 2.386451 | -0.732861 |
| H | -0.997109 | 2.491161 | 0.646071 |
| H | -2.173393 | -0.901527 | 1.400718 |
| N | -1.416074 | 0.521143 | 0.028715 |
| C | -0.103204 | 0.101566 | 0.108888 |
| C | 0.988790 | 0.710941 | -0.400149 |
| H | 0.019525 | -0.842912 | 0.638248 |
| C | -2.752247 | -1.467228 | -0.556500 |
| O | -2.278989 | -1.551849 | -1.656086 |
| O | -3.652578 | -2.334756 | -0.072331 |
| H | -3.837131 | -2.993907 | -0.756855 |
| C | 0.902341 | 1.871499 | -1.359670 |
| H | -0.129677 | 2.109962 | -1.606179 |
| H | 1.383505 | 2.770921 | -0.963549 |
| H | 1.401652 | 1.627813 | -2.300912 |
| C | 2.329895 | 0.179570 | -0.064619 |
| C | 2.576994 | -0.475429 | 1.154070 |
| C | 3.412084 | 0.323342 | -0.947022 |
| C | 3.826671 | -1.003551 | 1.452068 |
| H | 1.786049 | -0.545745 | 1.891539 |
| C | 4.666106 | -0.195618 | -0.644021 |
| H | 3.276631 | 0.835213 | -1.891369 |
| C | 4.881784 | -0.869563 | 0.553587 |
| H | 3.982300 | -1.502511 | 2.401864 |
| H | 5.477808 | -0.072980 | -1.352019 |
| H | 5.859934 | -1.270639 | 0.790258 |

**11I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -748.629056

Free energies: -748.385199

Corrected Free energies: -748.382232

| | | | |
|---|---|---|---|
| C | -3.694995 | 0.501918 | 0.714014 |
| C | -3.052237 | 1.822627 | 1.135428 |
| C | -1.824456 | 1.898838 | 0.233104 |
| C | -2.484044 | -0.421973 | 0.517391 |
| H | -4.385173 | 0.094759 | 1.448857 |
| H | -4.226764 | 0.624057 | -0.232147 |
| H | -2.743867 | 1.784924 | 2.181895 |
| H | -3.709376 | 2.677537 | 0.989977 |
| H | -2.106575 | 2.213179 | -0.774656 |
| H | -1.022798 | 2.529609 | 0.610621 |
| H | -2.242629 | -0.955809 | 1.441802 |

| | | | |
|---|---|---|---|
| N | -1.372658 | 0.491076 | 0.192492 |
| C | -0.151030 | 0.030086 | 0.051599 |
| C | 0.997744 | 0.730686 | -0.382176 |
| H | -0.047770 | -1.025093 | 0.280071 |
| C | -2.673499 | -1.457365 | -0.581788 |
| O | -1.927367 | -1.631160 | -1.502851 |
| O | -3.786335 | -2.148518 | -0.359622 |
| H | -3.889597 | -2.812024 | -1.058403 |
| C | 0.902948 | 1.962016 | -1.228020 |
| H | -0.116731 | 2.204477 | -1.504755 |
| H | 1.356003 | 2.821672 | -0.725941 |
| H | 1.453225 | 1.800528 | -2.157576 |
| C | 2.297280 | 0.166320 | -0.073607 |
| C | 2.456705 | -0.833565 | 0.912998 |
| C | 3.455449 | 0.640606 | -0.725706 |
| C | 3.705607 | -1.351417 | 1.204172 |
| H | 1.606887 | -1.185807 | 1.483456 |
| C | 4.701881 | 0.117120 | -0.429788 |
| H | 3.380174 | 1.416054 | -1.475697 |
| C | 4.832947 | -0.884299 | 0.530459 |
| H | 3.805521 | -2.113632 | 1.966633 |
| H | 5.576149 | 0.488548 | -0.949342 |
| H | 5.809746 | -1.292672 | 0.759060 |

**11I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -748.630319

Free energies: -748.385862

Corrected Free energies: -748.383250

| | | | |
|---|---|---|---|
| C | -2.889654 | -1.095228 | -1.134790 |
| C | -1.725762 | -1.342074 | -2.097249 |
| C | -0.513527 | -0.934939 | -1.266188 |
| C | -2.476974 | 0.197131 | -0.405166 |
| H | -3.850223 | -0.975772 | -1.629992 |
| H | -2.968840 | -1.917473 | -0.420583 |
| H | -1.806783 | -0.699832 | -2.975996 |
| H | -1.661300 | -2.379223 | -2.420249 |
| H | -0.267496 | -1.705762 | -0.531919 |
| H | 0.377645 | -0.679432 | -1.835568 |
| H | -2.930401 | 1.080614 | -0.862607 |
| N | -1.016262 | 0.265075 | -0.566743 |
| C | -0.356507 | 1.355181 | -0.242795 |
| C | 1.043559 | 1.525416 | -0.212572 |

| | | | |
|---|---|---|---|
| H | -0.978097 | 2.215584 | -0.006787 |
| C | 1.573989 | 2.906674 | -0.423677 |
| H | 1.982736 | 2.994362 | -1.436767 |
| H | 0.787688 | 3.653933 | -0.324080 |
| H | 2.381330 | 3.124939 | 0.276640 |
| C | -2.827976 | 0.185400 | 1.075313 |
| O | -2.034675 | 0.277565 | 1.969838 |
| O | -4.139928 | 0.050038 | 1.228159 |
| H | -4.348498 | 0.033943 | 2.174417 |
| C | 1.955348 | 0.431977 | 0.064482 |
| C | 3.264800 | 0.447558 | -0.449122 |
| C | 1.573256 | -0.609983 | 0.931364 |
| C | 4.144521 | -0.579057 | -0.147736 |
| H | 3.577414 | 1.251025 | -1.104960 |
| C | 2.466191 | -1.621060 | 1.244769 |
| H | 0.588340 | -0.592070 | 1.387233 |
| C | 3.747703 | -1.614882 | 0.696659 |
| H | 5.143195 | -0.572332 | -0.565923 |
| H | 2.168452 | -2.410632 | 1.923163 |
| H | 4.441702 | -2.410901 | 0.937457 |

**12I-*Z***

Imaginary frequency: None

Electronic energies: -1136.797735

Free energies: -1136.382460

Corrected Free energies: -1136.377839

| | | | |
|---|---|---|---|
| C | -0.894892 | -1.081602 | -0.898730 |
| C | -1.233130 | -2.584617 | -0.896506 |
| C | 0.010458 | -3.255294 | -0.301771 |
| C | 1.149507 | -2.380412 | -0.809964 |
| H | -1.377228 | -2.920397 | -1.926102 |
| H | -2.149130 | -2.814140 | -0.349389 |
| H | 0.117889 | -4.293303 | -0.615804 |
| H | -0.016438 | -3.227259 | 0.788972 |
| H | 1.460666 | -2.677515 | -1.820919 |
| H | 2.025555 | -2.422814 | -0.161148 |
| C | -1.525725 | -0.306386 | 0.298063 |
| O | -1.094271 | -0.893951 | 1.518770 |
| C | -3.057794 | -0.292633 | 0.253712 |
| C | -3.738124 | 0.062945 | 1.422660 |
| C | -3.802780 | -0.583766 | -0.889753 |
| C | -5.125134 | 0.121977 | 1.450963 |
| H | -3.165348 | 0.295766 | 2.313248 |

| | | | |
|---|---|---|---|
| C | -5.195006 | -0.521902 | -0.863184 |
| H | -3.315009 | -0.869942 | -1.813675 |
| C | -5.860394 | -0.170549 | 0.304542 |
| H | -5.633859 | 0.398675 | 2.366901 |
| H | -5.756353 | -0.754692 | -1.760344 |
| H | -6.942653 | -0.125083 | 0.323387 |
| C | -1.012508 | 1.129930 | 0.287086 |
| C | -1.391162 | 1.990037 | -0.746776 |
| C | -0.126573 | 1.589593 | 1.257837 |
| C | -0.873333 | 3.276459 | -0.823182 |
| H | -2.094500 | 1.651487 | -1.501448 |
| C | 0.389470 | 2.881967 | 1.184751 |
| H | 0.162262 | 0.932237 | 2.066720 |
| C | 0.025178 | 3.726218 | 0.142243 |
| H | -1.172868 | 3.929654 | -1.634327 |
| H | 1.082552 | 3.225524 | 1.944197 |
| H | 0.430761 | 4.729291 | 0.083449 |
| N | 0.564251 | -1.036313 | -0.839284 |
| H | -1.234417 | -0.600387 | -1.823382 |
| C | 1.216194 | -0.003104 | -1.498989 |
| C | 2.493590 | 0.402973 | -1.350354 |
| C | 3.029988 | 1.440553 | -2.309490 |
| H | 3.766521 | 1.020769 | -3.001820 |
| H | 3.521869 | 2.256319 | -1.771561 |
| H | 0.600382 | 0.522236 | -2.230448 |
| H | 2.221369 | 1.859725 | -2.910695 |
| H | -1.575569 | -1.719196 | 1.639058 |
| C | 3.398788 | -0.043842 | -0.267017 |
| C | 4.790066 | 0.015051 | -0.430929 |
| C | 2.906494 | -0.449141 | 0.985781 |
| C | 5.654924 | -0.338736 | 0.600369 |
| H | 5.205882 | 0.337691 | -1.378405 |
| C | 3.770439 | -0.788990 | 2.018320 |
| H | 1.833422 | -0.493322 | 1.137666 |
| C | 5.150819 | -0.742269 | 1.831576 |
| H | 6.725994 | -0.294403 | 0.439520 |
| H | 3.364250 | -1.092826 | 2.976648 |
| H | 5.822255 | -1.015053 | 2.636980 |

**12I-*E***

Imaginary frequency: None

Electronic energies: -1136.797269

Free energies: -1136.382700

Corrected Free energies: -1136.377998

| | | | |
|---|---|---|---|
| C | -1.163159 | 1.280090 | 0.502928 |
| C | -1.953160 | 2.589881 | 0.684033 |
| C | -1.290867 | 3.566401 | -0.294965 |
| C | 0.175248 | 3.153202 | -0.243423 |
| H | -1.823963 | 2.948531 | 1.708021 |
| H | -3.025260 | 2.469496 | 0.516170 |
| H | -1.435518 | 4.609191 | -0.013488 |
| H | -1.678608 | 3.420782 | -1.304178 |
| H | 0.684163 | 3.617573 | 0.612902 |
| H | 0.717572 | 3.428948 | -1.148665 |
| C | -1.881812 | 0.249152 | -0.419079 |
| O | -2.210107 | 0.863823 | -1.660419 |
| C | -3.157636 | -0.317787 | 0.211902 |
| C | -4.013045 | -1.055232 | -0.613631 |
| C | -3.502255 | -0.156077 | 1.553564 |
| C | -5.179193 | -1.617344 | -0.112865 |
| H | -3.749967 | -1.184477 | -1.657535 |
| C | -4.672193 | -0.722168 | 2.058874 |
| H | -2.873612 | 0.416656 | 2.224099 |
| C | -5.512971 | -1.453120 | 1.230076 |
| H | -5.827345 | -2.187422 | -0.768141 |
| H | -4.922848 | -0.584318 | 3.103977 |
| H | -6.422259 | -1.890842 | 1.624437 |
| C | -0.904078 | -0.878501 | -0.726476 |
| C | -0.610879 | -1.830056 | 0.251065 |
| C | -0.217259 | -0.918090 | -1.937950 |
| C | 0.362320 | -2.797950 | 0.027747 |
| H | -1.144405 | -1.813774 | 1.196363 |
| C | 0.756770 | -1.887215 | -2.162488 |
| H | -0.437621 | -0.178180 | -2.695791 |
| C | 1.052194 | -2.827851 | -1.181365 |
| H | 0.579407 | -3.529782 | 0.797073 |
| H | 1.289242 | -1.903509 | -3.106790 |
| H | 1.812983 | -3.579778 | -1.355808 |
| N | 0.115495 | 1.695345 | -0.073330 |
| H | -0.981475 | 0.788307 | 1.465364 |
| C | 1.257366 | 1.010115 | 0.336485 |
| C | 2.424699 | 0.983716 | -0.332369 |
| H | 1.154958 | 0.429929 | 1.254583 |
| H | -2.962546 | 1.445832 | -1.512872 |
| C | 3.581814 | 0.281861 | 0.271443 |
| C | 3.839336 | 0.363782 | 1.647733 |
| C | 4.440816 | -0.511126 | -0.504638 |

| | | | |
|---|---|---|---|
| C | 4.891638 | -0.337114 | 2.227787 |
| H | 3.218618 | 1.004878 | 2.263342 |
| C | 5.496648 | -1.205721 | 0.072898 |
| H | 4.267997 | -0.610940 | -1.569793 |
| C | 5.728245 | -1.124709 | 1.443739 |
| H | 5.067814 | -0.252735 | 3.294065 |
| H | 6.137800 | -1.818657 | -0.550483 |
| H | 6.554280 | -1.662709 | 1.893305 |
| C | 2.544526 | 1.592423 | -1.705026 |
| H | 1.572370 | 1.568935 | -2.203539 |
| H | 2.879972 | 2.634194 | -1.662724 |
| H | 3.261960 | 1.052490 | -2.323229 |

**12I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1136.617360

Free energies: -1136.199754

Corrected Free energies: -1136.195703

| | | | |
|---|---|---|---|
| C | -1.270850 | 1.205378 | 0.779536 |
| C | -2.175197 | 2.423293 | 0.990633 |
| C | -1.634113 | 3.501311 | 0.038722 |
| C | -0.143640 | 3.187798 | -0.119576 |
| H | -2.084062 | 2.751983 | 2.027009 |
| H | -3.223211 | 2.193123 | 0.804088 |
| H | -1.776339 | 4.500349 | 0.446382 |
| H | -2.128421 | 3.461069 | -0.929131 |
| H | 0.474006 | 3.854334 | 0.482681 |
| H | 0.184080 | 3.224609 | -1.157656 |
| C | -1.742341 | 0.238214 | -0.362608 |
| O | -1.841348 | 0.984619 | -1.565424 |
| C | -3.081600 | -0.418295 | -0.027889 |
| C | -3.773596 | -1.030786 | -1.077028 |
| C | -3.619658 | -0.471606 | 1.257313 |
| C | -4.983803 | -1.671635 | -0.847526 |
| H | -3.352409 | -1.006858 | -2.075956 |
| C | -4.832512 | -1.117461 | 1.487042 |
| H | -3.114026 | -0.009292 | 2.096630 |
| C | -5.518366 | -1.715452 | 0.437425 |
| H | -5.507355 | -2.141496 | -1.671474 |
| H | -5.238949 | -1.146591 | 2.490651 |
| H | -6.462827 | -2.214219 | 0.617966 |
| C | -0.675445 | -0.832403 | -0.574641 |
| C | -0.508045 | -1.844497 | 0.374013 |

| | | | |
|---|---|---|---|
| C | 0.217054 | -0.745187 | -1.641805 |
| C | 0.554083 | -2.734989 | 0.272815 |
| H | -1.203423 | -1.932267 | 1.202654 |
| C | 1.275993 | -1.645334 | -1.746592 |
| H | 0.091159 | 0.037595 | -2.378921 |
| C | 1.454019 | -2.633987 | -0.786299 |
| H | 0.679432 | -3.508441 | 1.021144 |
| H | 1.969932 | -1.561399 | -2.574764 |
| H | 2.287251 | -3.322698 | -0.859502 |
| N | 0.023507 | 1.817209 | 0.409075 |
| H | -1.116249 | 0.628858 | 1.691919 |
| C | 1.145435 | 1.144408 | 0.572997 |
| C | 2.442209 | 1.426074 | 0.101067 |
| H | 1.012399 | 0.198582 | 1.083496 |
| H | -2.726150 | 1.360722 | -1.623950 |
| C | 3.443681 | 0.394781 | 0.344199 |
| C | 3.411395 | -0.425700 | 1.489143 |
| C | 4.450531 | 0.168568 | -0.613424 |
| C | 4.344561 | -1.434862 | 1.660375 |
| H | 2.678296 | -0.249538 | 2.267332 |
| C | 5.365625 | -0.858406 | -0.447697 |
| H | 4.488164 | 0.770012 | -1.512990 |
| C | 5.318566 | -1.661770 | 0.689521 |
| H | 4.316987 | -2.044384 | 2.555054 |
| H | 6.117887 | -1.033116 | -1.206824 |
| H | 6.041854 | -2.456989 | 0.822246 |
| C | 2.789322 | 2.604924 | -0.753502 |
| H | 2.365186 | 2.494197 | -1.757699 |
| H | 2.405687 | 3.531860 | -0.332199 |
| H | 3.867481 | 2.708323 | -0.845618 |

**12I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1136.615058

Free energies: -1136.201154

Corrected Free energies: -1136.196045

| | | | |
|---|---|---|---|
| C | -0.888745 | -1.035850 | -0.948676 |
| C | -1.139389 | -2.546926 | -0.972913 |
| C | 0.047012 | -3.190483 | -0.227367 |
| C | 1.144973 | -2.119201 | -0.144801 |
| H | -1.164869 | -2.881259 | -2.010059 |
| H | -2.097180 | -2.801752 | -0.520501 |
| H | 0.404832 | -4.071215 | -0.756955 |

| | | | |
|---|---|---|---|
| H | -0.237464 | -3.500821 | 0.776505 |
| H | 2.073104 | -2.394967 | -0.645413 |
| H | 1.361808 | -1.860659 | 0.889311 |
| C | -1.534566 | -0.286774 | 0.257297 |
| O | -1.021909 | -0.853859 | 1.452525 |
| C | -3.060822 | -0.366463 | 0.234213 |
| C | -3.737960 | -0.087870 | 1.424701 |
| C | -3.800082 | -0.655417 | -0.912753 |
| C | -5.125705 | -0.107050 | 1.469916 |
| H | -3.169754 | 0.151525 | 2.316654 |
| C | -5.192106 | -0.671004 | -0.866472 |
| H | -3.311519 | -0.880287 | -1.853673 |
| C | -5.857957 | -0.399304 | 0.322341 |
| H | -5.635744 | 0.110276 | 2.400623 |
| H | -5.752578 | -0.901715 | -1.764275 |
| H | -6.940476 | -0.414413 | 0.355580 |
| C | -1.102115 | 1.177701 | 0.217904 |
| C | -1.476654 | 1.979529 | -0.863950 |
| C | -0.304769 | 1.720991 | 1.221234 |
| C | -1.030755 | 3.291381 | -0.956754 |
| H | -2.124748 | 1.582193 | -1.639016 |
| C | 0.142073 | 3.038309 | 1.127170 |
| H | -0.039072 | 1.114495 | 2.077371 |
| C | -0.210865 | 3.822924 | 0.036675 |
| H | -1.325287 | 3.899780 | -1.803382 |
| H | 0.768363 | 3.446938 | 1.911284 |
| H | 0.141116 | 4.844646 | -0.037190 |
| N | 0.580994 | -0.941101 | -0.836353 |
| H | -1.182278 | -0.548107 | -1.877245 |
| C | 1.248857 | 0.016046 | -1.444355 |
| C | 2.637098 | 0.275926 | -1.400937 |
| C | 3.225616 | 0.975627 | -2.585274 |
| H | 3.748246 | 0.251319 | -3.220649 |
| H | 3.953392 | 1.725723 | -2.273188 |
| H | 0.649403 | 0.642817 | -2.098571 |
| H | 2.453216 | 1.443752 | -3.194373 |
| H | -1.555994 | -1.620489 | 1.689216 |
| C | 3.489908 | -0.059411 | -0.275063 |
| C | 4.852585 | -0.347797 | -0.473263 |
| C | 2.993750 | 0.002815 | 1.039390 |
| C | 5.674540 | -0.617932 | 0.608893 |
| H | 5.255374 | -0.385466 | -1.478192 |
| C | 3.826268 | -0.244044 | 2.118273 |
| H | 1.960286 | 0.284583 | 1.205848 |

| | | | |
|---|---|---|---|
| C | 5.165044 | -0.567102 | 1.905502 |
| H | 6.716252 | -0.863118 | 0.444017 |
| H | 3.434876 | -0.177945 | 3.125708 |
| H | 5.813601 | -0.768997 | 2.749240 |

**13I-*Z***

Imaginary frequency: None

Electronic energies: -1545.466805

Free energies: -1544.959590

Corrected Free energies: -1544.953409

| | | | |
|---|---|---|---|
| Si | 1.449918 | 2.314380 | -1.057460 |
| O | 0.974795 | 0.721613 | -0.829714 |
| N | -0.951624 | -0.004415 | 1.050295 |
| C | 0.473028 | -0.100190 | 1.371089 |
| C | 0.551618 | -1.237982 | 2.402916 |
| C | -0.685985 | -2.101641 | 2.133873 |
| C | -1.728856 | -1.119153 | 1.598266 |
| C | 1.345186 | -0.296124 | 0.088777 |
| C | -0.038014 | 3.112052 | -1.858976 |
| C | 1.906308 | 3.190596 | 0.537023 |
| C | 2.907311 | 2.429951 | -2.230158 |
| C | 2.846999 | -0.208008 | 0.380986 |
| C | 3.387506 | 0.065903 | 1.636871 |
| C | 4.767352 | 0.173683 | 1.807598 |
| C | 5.623465 | 0.006979 | 0.726919 |
| C | 5.094252 | -0.269115 | -0.532164 |
| C | 3.720486 | -0.374904 | -0.698239 |
| C | 0.987857 | -1.635546 | -0.549619 |
| C | -0.124058 | -1.710655 | -1.389191 |
| C | -0.564081 | -2.936842 | -1.876547 |
| C | 0.112179 | -4.106529 | -1.539860 |
| C | 1.240262 | -4.036870 | -0.728098 |
| C | 1.676738 | -2.809077 | -0.238224 |
| C | -1.499937 | 1.250466 | 0.901683 |
| C | -2.772162 | 1.634402 | 0.652867 |
| H | 0.794949 | 0.850761 | 1.809285 |
| H | 0.495738 | -0.804172 | 3.404362 |
| H | 1.477636 | -1.809520 | 2.336798 |
| H | -0.469100 | -2.860896 | 1.380753 |
| H | -1.036699 | -2.608087 | 3.033030 |
| H | -2.355970 | -1.590395 | 0.839296 |
| H | -2.391619 | -0.739624 | 2.387031 |
| H | -0.262011 | 2.625476 | -2.812106 |

| | | | |
|---|---|---|---|
| H | 0.154926 | 4.169669 | -2.058388 |
| H | -0.924150 | 3.034038 | -1.224613 |
| H | 1.077205 | 3.281943 | 1.241982 |
| H | 2.231177 | 4.204364 | 0.281730 |
| H | 2.737767 | 2.694489 | 1.043491 |
| H | 3.852883 | 2.191935 | -1.739483 |
| H | 2.973366 | 3.450568 | -2.618894 |
| H | 2.782397 | 1.754017 | -3.080123 |
| H | 2.748843 | 0.207114 | 2.500019 |
| H | 5.168285 | 0.388542 | 2.791076 |
| H | 6.695292 | 0.089871 | 0.862442 |
| H | 5.752833 | -0.398938 | -1.382903 |
| H | 3.307474 | -0.582449 | -1.680237 |
| H | -0.631743 | -0.793041 | -1.653972 |
| H | -1.434400 | -2.977411 | -2.522157 |
| H | -0.229764 | -5.063010 | -1.917459 |
| H | 1.784400 | -4.939193 | -0.474688 |
| H | 2.557244 | -2.770666 | 0.393671 |
| H | -0.775530 | 2.046426 | 1.054868 |
| C | -3.104255 | 3.107706 | 0.753922 |
| H | -3.616676 | 3.460093 | -0.146879 |
| H | -3.761077 | 3.324024 | 1.602235 |
| H | -2.197752 | 3.701548 | 0.890732 |
| C | -3.874559 | 0.743857 | 0.225888 |
| C | -5.185218 | 0.950997 | 0.679262 |
| C | -3.665468 | -0.272722 | -0.716696 |
| C | -6.234051 | 0.152500 | 0.236895 |
| H | -5.383912 | 1.738745 | 1.397192 |
| C | -4.712557 | -1.069816 | -1.163880 |
| H | -2.664950 | -0.426568 | -1.103971 |
| C | -6.003785 | -0.864928 | -0.685085 |
| H | -7.235547 | 0.325638 | 0.614037 |
| H | -4.520973 | -1.847486 | -1.894836 |
| H | -6.821746 | -1.485075 | -1.031854 |

**13I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1545.284589

Free energies: -1544.774351

Corrected Free energies: -1544.769249

| | | | |
|---|---|---|---|
| Si | 1.960408 | 2.238769 | -1.012541 |
| O | 1.084448 | 0.816058 | -0.758917 |
| N | -0.919049 | 0.242809 | 1.168965 |

| | | | |
|---|---|---|---|
| C | 0.526964 | 0.081158 | 1.432421 |
| C | 0.578658 | -0.929698 | 2.586067 |
| C | -0.792695 | -1.637066 | 2.632633 |
| C | -1.678165 | -0.953932 | 1.583163 |
| C | 1.267332 | -0.289440 | 0.102410 |
| C | 0.872282 | 3.154236 | -2.218553 |
| C | 2.150318 | 3.231748 | 0.567063 |
| C | 3.651024 | 1.919983 | -1.737849 |
| C | 2.759478 | -0.539571 | 0.341550 |
| C | 3.438701 | -0.041710 | 1.453674 |
| C | 4.819817 | -0.186033 | 1.563602 |
| C | 5.537208 | -0.833249 | 0.564856 |
| C | 4.866657 | -1.340683 | -0.544904 |
| C | 3.490496 | -1.193428 | -0.654252 |
| C | 0.590835 | -1.500086 | -0.543151 |
| C | -0.264952 | -1.326613 | -1.628480 |
| C | -0.960248 | -2.410028 | -2.162303 |
| C | -0.805899 | -3.679049 | -1.616608 |
| C | 0.073380 | -3.865021 | -0.552469 |
| C | 0.774643 | -2.786446 | -0.027191 |
| C | -1.400256 | 1.405134 | 0.779651 |
| C | -2.736036 | 1.783057 | 0.519521 |
| H | 0.905683 | 1.057710 | 1.736712 |
| H | 0.755905 | -0.388179 | 3.514837 |
| H | 1.398777 | -1.633514 | 2.464824 |
| H | -0.702326 | -2.697916 | 2.405480 |
| H | -1.237183 | -1.540737 | 3.621551 |
| H | -1.833106 | -1.594293 | 0.712519 |
| H | -2.647359 | -0.639122 | 1.965950 |
| H | 0.764842 | 2.592717 | -3.149651 |
| H | 1.303880 | 4.129465 | -2.457979 |
| H | -0.126117 | 3.319614 | -1.804643 |
| H | 1.198463 | 3.508748 | 1.027810 |
| H | 2.662524 | 4.164832 | 0.311449 |
| H | 2.763835 | 2.723260 | 1.314167 |
| H | 4.351994 | 1.534890 | -0.993158 |
| H | 4.047953 | 2.863399 | -2.124880 |
| H | 3.602585 | 1.207469 | -2.564612 |
| H | 2.909467 | 0.459433 | 2.255815 |
| H | 5.329640 | 0.205858 | 2.435281 |
| H | 6.611107 | -0.946597 | 0.652360 |
| H | 5.416101 | -1.848205 | -1.328732 |
| H | 2.976866 | -1.581681 | -1.526704 |
| H | -0.380929 | -0.337018 | -2.052848 |

| | | | |
|---|---|---|---|
| H | -1.624066 | -2.257278 | -3.005799 |
| H | -1.350192 | -4.520700 | -2.027505 |
| H | 0.222002 | -4.854093 | -0.135834 |
| H | 1.482328 | -2.957363 | 0.775859 |
| H | -0.657925 | 2.194186 | 0.731454 |
| C | -3.043388 | 3.243365 | 0.644247 |
| H | -3.710562 | 3.569646 | -0.154610 |
| H | -3.550602 | 3.435327 | 1.596718 |
| H | -2.135410 | 3.845192 | 0.632689 |
| C | -3.804953 | 0.871547 | 0.147353 |
| C | -5.127132 | 1.126627 | 0.553450 |
| C | -3.553537 | -0.226359 | -0.692040 |
| C | -6.150604 | 0.272020 | 0.176081 |
| H | -5.343923 | 1.976901 | 1.188561 |
| C | -4.583576 | -1.065460 | -1.083674 |
| H | -2.550463 | -0.393895 | -1.063778 |
| C | -5.882695 | -0.825550 | -0.640516 |
| H | -7.161261 | 0.462122 | 0.515076 |
| H | -4.374626 | -1.902254 | -1.739203 |
| H | -6.687780 | -1.485545 | -0.939540 |

**13I-*E***

Imaginary frequency: None

Electronic energies: -1545.467463

Free energies: -1544.958350

Corrected Free energies: -1544.952758

| | | | |
|---|---|---|---|
| Si | 0.219476 | -2.098680 | -0.889233 |
| O | -0.453614 | -0.561415 | -0.796990 |
| N | 0.416102 | 1.359252 | 1.060701 |
| C | -0.707764 | 0.477883 | 1.356805 |
| C | -1.563744 | 1.294114 | 2.337806 |
| C | -1.229523 | 2.763131 | 2.037626 |
| C | 0.198854 | 2.741056 | 1.480443 |
| C | -1.438558 | 0.015957 | 0.050655 |
| C | 1.809335 | -1.821950 | -1.828206 |
| C | 0.578582 | -2.869068 | 0.786386 |
| C | -0.884209 | -3.281933 | -1.831906 |
| C | -2.541018 | -1.013327 | 0.318415 |
| C | -2.749559 | -1.621692 | 1.555523 |
| C | -3.724992 | -2.607011 | 1.708932 |
| C | -4.510546 | -2.990162 | 0.629749 |
| C | -4.315613 | -2.384288 | -0.610226 |
| C | -3.338463 | -1.410835 | -0.760551 |

| | | | |
|---|---|---|---|
| C | -1.984933 | 1.252326 | -0.658961 |
| C | -1.125461 | 2.020336 | -1.447429 |
| C | -1.558081 | 3.221394 | -2.000233 |
| C | -2.857691 | 3.668819 | -1.778018 |
| C | -3.725793 | 2.900068 | -1.009412 |
| C | -3.291593 | 1.699815 | -0.454754 |
| C | 1.644560 | 0.818769 | 0.798389 |
| C | 2.811127 | 1.379536 | 0.394719 |
| H | -0.319633 | -0.430745 | 1.828656 |
| H | -1.265587 | 1.038067 | 3.356979 |
| H | -2.630172 | 1.087804 | 2.240701 |
| H | -1.912570 | 3.166554 | 1.289501 |
| H | -1.300099 | 3.386051 | 2.929035 |
| H | 0.291617 | 3.436430 | 0.642466 |
| H | 0.946112 | 3.010502 | 2.236837 |
| H | 1.608217 | -1.385362 | -2.810080 |
| H | 2.331058 | -2.770764 | -1.981335 |
| H | 2.478013 | -1.147956 | -1.285973 |
| H | 1.350001 | -2.345972 | 1.355681 |
| H | 0.942154 | -3.886485 | 0.608151 |
| H | -0.318809 | -2.946703 | 1.405088 |
| H | -1.718913 | -3.632163 | -1.220842 |
| H | -0.294765 | -4.152718 | -2.134985 |
| H | -1.292135 | -2.818809 | -2.733748 |
| H | -2.157890 | -1.343174 | 2.419294 |
| H | -3.868393 | -3.069351 | 2.678454 |
| H | -5.270480 | -3.752843 | 0.751890 |
| H | -4.921217 | -2.675578 | -1.460468 |
| H | -3.181665 | -0.949920 | -1.730322 |
| H | -0.114032 | 1.668815 | -1.611003 |
| H | -0.878425 | 3.810541 | -2.605333 |
| H | -3.193920 | 4.605496 | -2.207034 |
| H | -4.742686 | 3.233582 | -0.838729 |
| H | -3.977360 | 1.113760 | 0.146502 |
| H | 1.648309 | -0.257636 | 0.930832 |
| C | 3.000006 | 2.799926 | -0.084907 |
| H | 4.007043 | 3.152755 | 0.150608 |
| H | 2.879868 | 2.871596 | -1.171974 |
| H | 2.296383 | 3.495937 | 0.363039 |
| C | 3.970652 | 0.467873 | 0.265790 |
| C | 4.931648 | 0.655887 | -0.741203 |
| C | 4.145399 | -0.631353 | 1.123995 |
| C | 5.983621 | -0.238384 | -0.910934 |
| H | 4.842330 | 1.498534 | -1.417413 |

| | | | |
|---|---|---|---|
| C | 5.189572 | -1.530291 | 0.947912 |
| H | 3.467104 | -0.768451 | 1.958501 |
| C | 6.115095 | -1.343684 | -0.075539 |
| H | 6.701944 | -0.072661 | -1.706026 |
| H | 5.292475 | -2.368694 | 1.627541 |
| H | 6.934185 | -2.039846 | -0.209411 |

**13I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1545.287178

Free energies: -1544.777924

Corrected Free energies: -1544.772096

| | | | |
|---|---|---|---|
| Si | -0.334346 | -2.397638 | -0.730846 |
| O | -0.532984 | -0.720764 | -0.660314 |
| N | 0.531427 | 1.097782 | 1.244995 |
| C | -0.747931 | 0.382883 | 1.453894 |
| C | -1.523869 | 1.273738 | 2.439590 |
| C | -0.519302 | 2.337575 | 2.907267 |
| C | 0.434453 | 2.487386 | 1.726224 |
| C | -1.412539 | 0.127153 | 0.050932 |
| C | 1.226562 | -2.544167 | -1.742454 |
| C | -0.078554 | -3.132510 | 0.975901 |
| C | -1.776230 | -3.249439 | -1.554437 |
| C | -2.781597 | -0.539584 | 0.188359 |
| C | -3.161874 | -1.248728 | 1.327337 |
| C | -4.360222 | -1.959467 | 1.353063 |
| C | -5.193100 | -1.966117 | 0.241287 |
| C | -4.823754 | -1.257107 | -0.899539 |
| C | -3.627426 | -0.553919 | -0.925131 |
| C | -1.475346 | 1.454277 | -0.711675 |
| C | -0.424450 | 1.806305 | -1.560749 |
| C | -0.391705 | 3.057653 | -2.168258 |
| C | -1.414759 | 3.973043 | -1.943429 |
| C | -2.482787 | 3.618404 | -1.125482 |
| C | -2.515735 | 2.366812 | -0.518542 |
| C | 1.592802 | 0.466576 | 0.798080 |
| C | 2.793828 | 1.019306 | 0.300619 |
| H | -0.504952 | -0.590248 | 1.885693 |
| H | -1.907994 | 0.689685 | 3.273564 |
| H | -2.373274 | 1.743343 | 1.947342 |
| H | -0.997282 | 3.282929 | 3.157193 |
| H | 0.035550 | 1.985601 | 3.778197 |
| H | -0.000023 | 3.110839 | 0.937953 |

| | | | |
|---|---|---|---|
| H | 1.420763 | 2.855376 | 1.996831 |
| H | 1.086648 | -2.099946 | -2.731013 |
| H | 1.504560 | -3.592524 | -1.876904 |
| H | 2.065747 | -2.034003 | -1.259209 |
| H | 0.760345 | -2.692282 | 1.521624 |
| H | 0.142637 | -4.197281 | 0.853399 |
| H | -0.974964 | -3.056080 | 1.596004 |
| H | -2.658352 | -3.270501 | -0.909363 |
| H | -1.494241 | -4.282125 | -1.780483 |
| H | -2.047749 | -2.759170 | -2.492251 |
| H | -2.535478 | -1.267084 | 2.210919 |
| H | -4.637928 | -2.506264 | 2.246002 |
| H | -6.124411 | -2.519051 | 0.262157 |
| H | -5.464969 | -1.258212 | -1.772829 |
| H | -3.339055 | -0.017645 | -1.822259 |
| H | 0.368032 | 1.091262 | -1.745367 |
| H | 0.436203 | 3.314854 | -2.818745 |
| H | -1.388065 | 4.948644 | -2.413486 |
| H | -3.297444 | 4.313514 | -0.962161 |
| H | -3.371130 | 2.098346 | 0.090687 |
| H | 1.483452 | -0.609584 | 0.776494 |
| C | 2.874649 | 2.430778 | -0.189920 |
| H | 3.567330 | 3.018202 | 0.420581 |
| H | 3.255475 | 2.441370 | -1.213162 |
| H | 1.906741 | 2.922027 | -0.208715 |
| C | 3.935224 | 0.131793 | 0.167528 |
| C | 5.026351 | 0.474420 | -0.658007 |
| C | 4.001287 | -1.088557 | 0.876958 |
| C | 6.107379 | -0.380157 | -0.795819 |
| H | 5.025283 | 1.405307 | -1.208218 |
| C | 5.084834 | -1.936712 | 0.735928 |
| H | 3.221113 | -1.360524 | 1.576586 |
| C | 6.139248 | -1.590939 | -0.107605 |
| H | 6.929165 | -0.102853 | -1.443958 |
| H | 5.114833 | -2.864031 | 1.293850 |
| H | 6.985530 | -2.257527 | -0.219071 |

**14I-*Z***

Imaginary frequency: None

Electronic energies: -2893.647457

Free energies: -2893.139787

Corrected Free energies: -2893.128118

| | | | |
|---|---|---|---|
| Si | 0.559170 | -2.516023 | 1.916639 |

| | | | |
|---|---|---|---|
| O | -0.009287 | -1.134965 | 1.131108 |
| N | -1.744621 | -1.290442 | -1.032574 |
| C | -0.315363 | -1.115180 | -1.263284 |
| C | -0.234211 | -0.326420 | -2.581803 |
| C | -1.571249 | 0.421725 | -2.678080 |
| C | -2.566762 | -0.468859 | -1.927567 |
| C | 0.379331 | -0.438523 | -0.033597 |
| C | -0.962002 | -3.231803 | 2.724455 |
| C | 1.360505 | -3.739220 | 0.743177 |
| C | 1.800689 | -2.049663 | 3.241153 |
| C | 1.905311 | -0.440424 | -0.140379 |
| C | 2.616135 | -1.003986 | -1.190418 |
| C | 4.011365 | -1.031584 | -1.157002 |
| C | 4.715612 | -0.495961 | -0.095253 |
| C | 3.997688 | 0.081449 | 0.950058 |
| C | 2.615480 | 0.111585 | 0.931087 |
| C | -0.153379 | 0.984057 | 0.091599 |
| C | -1.397340 | 1.176645 | 0.690780 |
| C | -1.994196 | 2.428646 | 0.663781 |
| C | -1.363236 | 3.514843 | 0.068409 |
| C | -0.108776 | 3.323405 | -0.491507 |
| C | 0.497677 | 2.071836 | -0.483167 |
| C | -2.182261 | -2.528835 | -0.596717 |
| C | -3.432690 | -2.980154 | -0.379909 |
| H | 0.148842 | -2.101541 | -1.364500 |
| H | -0.142450 | -1.038238 | -3.405024 |
| H | 0.621342 | 0.349024 | -2.629751 |
| H | -1.505289 | 1.402214 | -2.202754 |
| H | -1.875861 | 0.577251 | -3.712445 |
| H | -3.292149 | 0.130171 | -1.371102 |
| H | -3.127060 | -1.126576 | -2.603230 |
| H | -1.393860 | -2.509950 | 3.422896 |
| H | -0.704708 | -4.132559 | 3.287926 |
| H | -1.726244 | -3.488065 | 1.987436 |
| H | 0.703527 | -4.070029 | -0.063914 |
| H | 1.634116 | -4.625661 | 1.324248 |
| H | 2.278064 | -3.342902 | 0.301016 |
| H | 2.801850 | -1.876546 | 2.840784 |
| H | 1.869180 | -2.868174 | 3.963852 |
| H | 1.485371 | -1.153279 | 3.781695 |
| H | 2.110663 | -1.441810 | -2.042828 |
| H | 5.797738 | -0.530008 | -0.072726 |
| H | 2.071526 | 0.550561 | 1.760418 |
| H | 1.471123 | 1.952743 | -0.944639 |

| | | | |
|---|---|---|---|
| H | -1.372367 | -3.238966 | -0.450476 |
| C | -3.636790 | -4.440831 | -0.047323 |
| H | -4.159312 | -4.555140 | 0.907856 |
| H | -4.240830 | -4.948079 | -0.805624 |
| H | -2.681451 | -4.966143 | 0.015950 |
| C | 4.731426 | -1.725482 | -2.276114 |
| C | 4.756800 | 0.678349 | 2.099631 |
| F | 4.271530 | -1.343168 | -3.475799 |
| F | 4.563939 | -3.056665 | -2.208444 |
| F | 6.047361 | -1.492582 | -2.257119 |
| F | 5.341894 | 1.836458 | 1.761249 |
| F | 5.734826 | -0.139466 | 2.516306 |
| F | 3.969182 | 0.926069 | 3.152143 |
| H | -1.837720 | 4.488730 | 0.046932 |
| H | -1.887411 | 0.334004 | 1.159102 |
| C | 0.610607 | 4.498992 | -1.085195 |
| C | -3.378813 | 2.610704 | 1.210626 |
| F | -0.233797 | 5.339009 | -1.699132 |
| F | 1.252202 | 5.215192 | -0.148229 |
| F | 1.529060 | 4.125992 | -1.984993 |
| F | -3.707604 | 1.658360 | 2.094027 |
| F | -4.298599 | 2.563933 | 0.230927 |
| F | -3.528881 | 3.792866 | 1.821241 |
| C | -4.652932 | -2.135595 | -0.364451 |
| C | -4.717439 | -0.988318 | 0.434283 |
| C | -5.797593 | -2.505111 | -1.081629 |
| C | -5.877248 | -0.223037 | 0.501148 |
| H | -3.848543 | -0.708975 | 1.020929 |
| C | -6.956044 | -1.738512 | -1.023033 |
| H | -5.774657 | -3.393397 | -1.703801 |
| C | -7.000870 | -0.593508 | -0.231710 |
| H | -5.899909 | 0.661143 | 1.126722 |
| H | -7.826506 | -2.035103 | -1.597095 |
| H | -7.905392 | 0.001105 | -0.183513 |

**14I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -2893.458880

Free energies: -2892.950413

Corrected Free energies: -2892.938973

| | | | |
|---|---|---|---|
| Si | 1.080343 | -2.416587 | 2.018510 |
| O | 0.193006 | -1.273916 | 1.124286 |
| N | -1.503850 | -1.652841 | -1.121476 |

| | | | |
|---|---|---|---|
| C | -0.046472 | -1.443974 | -1.238999 |
| C | 0.127202 | -0.915509 | -2.668712 |
| C | -1.239202 | -0.344354 | -3.104879 |
| C | -2.252062 | -0.752951 | -2.025089 |
| C | 0.461101 | -0.555938 | -0.054537 |
| C | -0.153034 | -2.922233 | 3.315934 |
| C | 1.575737 | -3.877875 | 0.953866 |
| C | 2.616606 | -1.671299 | 2.775916 |
| C | 1.961831 | -0.267404 | -0.163037 |
| C | 2.831150 | -1.067802 | -0.898134 |
| C | 4.204958 | -0.860107 | -0.827328 |
| C | 4.740592 | 0.146082 | -0.038127 |
| C | 3.868097 | 0.949915 | 0.682919 |
| C | 2.496497 | 0.751654 | 0.624611 |
| C | -0.337974 | 0.746586 | 0.004156 |
| C | -1.315660 | 0.917889 | 0.981230 |
| C | -2.105191 | 2.061915 | 0.983254 |
| C | -1.940440 | 3.053201 | 0.024090 |
| C | -0.941656 | 2.889869 | -0.924018 |
| C | -0.133825 | 1.758377 | -0.930990 |
| C | -1.976650 | -2.683561 | -0.448510 |
| C | -3.315821 | -3.093093 | -0.273635 |
| H | 0.426379 | -2.418332 | -1.111145 |
| H | 0.404049 | -1.753432 | -3.308166 |
| H | 0.928341 | -0.182430 | -2.741490 |
| H | -1.213738 | 0.739956 | -3.200501 |
| H | -1.530050 | -0.753851 | -4.070004 |
| H | -2.609750 | 0.109354 | -1.459025 |
| H | -3.114600 | -1.290638 | -2.415094 |
| H | -0.445611 | -2.063358 | 3.924581 |
| H | 0.277954 | -3.677281 | 3.977918 |
| H | -1.055050 | -3.343009 | 2.864337 |
| H | 0.731697 | -4.378907 | 0.473663 |
| H | 2.048581 | -4.614053 | 1.611781 |
| H | 2.310917 | -3.620607 | 0.187200 |
| H | 3.421197 | -1.554184 | 2.045321 |
| H | 2.975421 | -2.346397 | 3.558452 |
| H | 2.420960 | -0.699045 | 3.234329 |
| H | 2.464863 | -1.866558 | -1.532018 |
| H | 5.810544 | 0.296392 | 0.018870 |
| H | 1.840851 | 1.381101 | 1.217582 |
| H | 0.660911 | 1.682584 | -1.665734 |
| H | -1.211878 | -3.340204 | -0.049126 |
| C | -3.531634 | -4.545511 | 0.015497 |

| | | | |
|---|---|---|---|
| H | -4.312511 | -4.680681 | 0.764590 |
| H | -3.855655 | -5.058682 | -0.897325 |
| H | -2.613374 | -5.026864 | 0.350681 |
| C | 5.097887 | -1.746644 | -1.647867 |
| C | 4.387657 | 2.030268 | 1.588226 |
| F | 5.025895 | -1.444840 | -2.952142 |
| F | 4.742805 | -3.035560 | -1.532175 |
| F | 6.379452 | -1.647362 | -1.286640 |
| F | 3.877476 | 3.227407 | 1.268836 |
| F | 5.718168 | 2.135107 | 1.542860 |
| F | 4.046661 | 1.796868 | 2.865246 |
| H | -2.566584 | 3.936280 | 0.022535 |
| H | -1.447654 | 0.152416 | 1.735786 |
| C | -0.724202 | 3.920121 | -1.995238 |
| C | -3.124817 | 2.253142 | 2.070272 |
| F | -1.450903 | 5.021966 | -1.797369 |
| F | 0.560819 | 4.288962 | -2.072106 |
| F | -1.056182 | 3.436021 | -3.204247 |
| F | -3.574251 | 1.079645 | 2.540020 |
| F | -4.190349 | 2.940458 | 1.635246 |
| F | -2.624116 | 2.925854 | 3.112596 |
| C | -4.464989 | -2.209603 | -0.349557 |
| C | -4.390291 | -0.898206 | 0.148547 |
| C | -5.697702 | -2.683953 | -0.834007 |
| C | -5.502729 | -0.073354 | 0.134961 |
| H | -3.463731 | -0.551084 | 0.589183 |
| C | -6.800538 | -1.846178 | -0.870220 |
| H | -5.778272 | -3.697304 | -1.207936 |
| C | -6.706664 | -0.541556 | -0.388180 |
| H | -5.437769 | 0.929700 | 0.538161 |
| H | -7.739072 | -2.210977 | -1.268543 |
| H | -7.575129 | 0.105308 | -0.407564 |

**14I-*E***

Imaginary frequency: None

Electronic energies: -2893.648223

Free energies: -2893.140304

Corrected Free energies: -2893.128936

| | | | |
|---|---|---|---|
| Si | -0.577846 | -2.414110 | 1.296352 |
| O | -0.551672 | -0.821395 | 0.731696 |
| N | -1.831935 | 0.017207 | -1.652782 |
| C | -0.443433 | -0.416995 | -1.646861 |
| C | 0.189045 | 0.340668 | -2.825877 |

| | | | |
|---|---|---|---|
| C | -0.702201 | 1.572923 | -3.041783 |
| C | -2.086799 | 1.156453 | -2.533503 |
| C | 0.221940 | -0.157836 | -0.248693 |
| C | -2.220419 | -2.519340 | 2.169112 |
| C | -0.464049 | -3.684519 | -0.079868 |
| C | 0.829953 | -2.736578 | 2.488257 |
| C | 1.662307 | -0.665245 | -0.167026 |
| C | 2.235854 | -1.492312 | -1.123880 |
| C | 3.509296 | -2.024144 | -0.922489 |
| C | 4.236440 | -1.734663 | 0.217868 |
| C | 3.664731 | -0.893106 | 1.168139 |
| C | 2.396771 | -0.368603 | 0.985575 |
| C | 0.126077 | 1.334887 | 0.035194 |
| C | -1.093562 | 1.841686 | 0.490479 |
| C | -1.283365 | 3.211363 | 0.585315 |
| C | -0.268610 | 4.106709 | 0.259748 |
| C | 0.948785 | 3.594639 | -0.154974 |
| C | 1.151019 | 2.220553 | -0.272165 |
| C | -2.807570 | -0.815864 | -1.163287 |
| C | -4.110800 | -0.581340 | -0.886840 |
| H | -0.410066 | -1.500808 | -1.801680 |
| H | 0.163111 | -0.303217 | -3.707130 |
| H | 1.230773 | 0.613906 | -2.648447 |
| H | -0.333536 | 2.424294 | -2.468447 |
| H | -0.733788 | 1.870622 | -4.089134 |
| H | -2.564987 | 1.980621 | -1.998369 |
| H | -2.751073 | 0.845664 | -3.348240 |
| H | -2.278231 | -1.781411 | 2.973215 |
| H | -2.355692 | -3.511210 | 2.608957 |
| H | -3.046980 | -2.336408 | 1.477150 |
| H | -1.297797 | -3.652478 | -0.784152 |
| H | -0.476482 | -4.673018 | 0.391001 |
| H | 0.470906 | -3.608726 | -0.641238 |
| H | 1.775024 | -2.928501 | 1.974570 |
| H | 0.587426 | -3.625122 | 3.079147 |
| H | 0.977819 | -1.904209 | 3.180530 |
| H | 1.709003 | -1.742534 | -2.037504 |
| H | 5.226145 | -2.147382 | 0.366086 |
| H | 1.963790 | 0.271070 | 1.747517 |
| H | 2.110376 | 1.854675 | -0.622847 |
| H | -2.428581 | -1.807766 | -0.940998 |
| C | -4.789108 | 0.771009 | -0.917158 |
| H | -5.872999 | 0.648079 | -0.943166 |
| H | -4.549655 | 1.366979 | -0.029790 |

| | | | |
|---|---|---|---|
| H | -4.514086 | 1.360494 | -1.789616 |
| C | 4.060245 | -2.937768 | -1.978029 |
| C | 4.396782 | -0.621343 | 2.449857 |
| F | 4.094680 | -2.340096 | -3.178239 |
| F | 3.295851 | -4.032705 | -2.120876 |
| F | 5.299565 | -3.351521 | -1.700787 |
| F | 5.724393 | -0.679185 | 2.291140 |
| F | 4.078740 | -1.522884 | 3.393885 |
| F | 4.101237 | 0.583616 | 2.951188 |
| H | -0.425529 | 5.174826 | 0.337282 |
| H | -1.886819 | 1.151812 | 0.751924 |
| C | 2.078658 | 4.506670 | -0.529714 |
| C | -2.634975 | 3.736897 | 0.967494 |
| F | 1.763311 | 5.797889 | -0.386594 |
| F | 3.170802 | 4.277259 | 0.214648 |
| F | 2.446378 | 4.326750 | -1.809341 |
| F | -3.290648 | 2.900021 | 1.782383 |
| F | -3.416192 | 3.907941 | -0.115443 |
| F | -2.564402 | 4.924179 | 1.580781 |
| C | -4.887705 | -1.723251 | -0.350455 |
| C | -4.681711 | -3.037620 | -0.798166 |
| C | -5.827715 | -1.526384 | 0.673153 |
| C | -5.344819 | -4.110780 | -0.213688 |
| H | -4.007076 | -3.217174 | -1.628043 |
| C | -6.496636 | -2.598497 | 1.252290 |
| H | -6.012490 | -0.524034 | 1.043136 |
| C | -6.253142 | -3.899184 | 0.819620 |
| H | -5.163341 | -5.114919 | -0.579943 |
| H | -7.206029 | -2.417403 | 2.051833 |
| H | -6.773534 | -4.734371 | 1.272800 |

**14I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -2893.460104

Free energies: -2892.953170

Corrected Free energies: -2892.940963

| | | | |
|---|---|---|---|
| Si | 0.567885 | -2.365377 | -1.408057 |
| O | 0.613407 | -0.836297 | -0.665345 |
| N | 1.836833 | -0.101641 | 1.768024 |
| C | 0.415186 | -0.502178 | 1.709655 |
| C | -0.213680 | 0.246694 | 2.890379 |
| C | 0.665456 | 1.487079 | 3.114381 |
| C | 2.056785 | 1.091700 | 2.616002 |

| | | | |
|---|---|---|---|
| C | -0.189908 | -0.192281 | 0.292790 |
| C | 2.201136 | -2.403261 | -2.302010 |
| C | 0.450838 | -3.727148 | -0.126752 |
| C | -0.851631 | -2.538427 | -2.608633 |
| C | -1.634106 | -0.692524 | 0.188673 |
| C | -2.203781 | -1.584496 | 1.088152 |
| C | -3.482882 | -2.090492 | 0.861582 |
| C | -4.218327 | -1.713825 | -0.247276 |
| C | -3.648615 | -0.810343 | -1.139999 |
| C | -2.376372 | -0.306995 | -0.932035 |
| C | -0.095413 | 1.310662 | 0.031622 |
| C | 1.080741 | 1.823784 | -0.510925 |
| C | 1.251339 | 3.196265 | -0.631588 |
| C | 0.251904 | 4.082777 | -0.252246 |
| C | -0.931640 | 3.561919 | 0.248406 |
| C | -1.110812 | 2.190596 | 0.395157 |
| C | 2.762213 | -0.862674 | 1.214907 |
| C | 4.141318 | -0.628628 | 1.051231 |
| H | 0.385956 | -1.585803 | 1.836367 |
| H | -0.186083 | -0.400439 | 3.767814 |
| H | -1.255214 | 0.509664 | 2.705832 |
| H | 0.293294 | 2.344676 | 2.557298 |
| H | 0.699170 | 1.764361 | 4.165965 |
| H | 2.536380 | 1.880605 | 2.037398 |
| H | 2.711889 | 0.794188 | 3.436082 |
| H | 2.238896 | -1.617883 | -3.060840 |
| H | 2.334436 | -3.366091 | -2.802112 |
| H | 3.044817 | -2.259320 | -1.622100 |
| H | 1.281649 | -3.745662 | 0.582824 |
| H | 0.468565 | -4.683074 | -0.659540 |
| H | -0.485308 | -3.692572 | 0.436803 |
| H | -1.794997 | -2.773709 | -2.111678 |
| H | -0.618706 | -3.365390 | -3.286371 |
| H | -0.990159 | -1.639530 | -3.214077 |
| H | -1.678648 | -1.908966 | 1.979195 |
| H | -5.213106 | -2.106887 | -0.414244 |
| H | -1.950642 | 0.386819 | -1.648976 |
| H | -2.045114 | 1.818877 | 0.802891 |
| H | 2.374228 | -1.779254 | 0.793035 |
| C | 4.835822 | 0.651084 | 1.397041 |
| H | 5.908159 | 0.554516 | 1.250229 |
| H | 4.475781 | 1.486417 | 0.789295 |
| H | 4.673008 | 0.909811 | 2.443620 |
| C | -4.032961 | -3.066987 | 1.861241 |

| | | | |
|---|---|---|---|
| C | -4.390896 | -0.441754 | -2.392541 |
| F | -4.092755 | -2.529693 | 3.088171 |
| F | -3.249925 | -4.153045 | 1.958180 |
| F | -5.260245 | -3.485065 | 1.544773 |
| F | -5.716268 | -0.479963 | -2.217211 |
| F | -4.104617 | -1.290949 | -3.392905 |
| F | -4.072708 | 0.784773 | -2.820875 |
| H | 0.389936 | 5.151333 | -0.352395 |
| H | 1.857464 | 1.144083 | -0.842121 |
| C | -2.053073 | 4.468524 | 0.667133 |
| C | 2.574740 | 3.712565 | -1.116661 |
| F | -1.738043 | 5.759970 | 0.536352 |
| F | -3.159678 | 4.249818 | -0.056791 |
| F | -2.388580 | 4.265412 | 1.950661 |
| F | 3.069246 | 2.967289 | -2.111327 |
| F | 3.490366 | 3.688180 | -0.127749 |
| F | 2.502752 | 4.973818 | -1.548417 |
| C | 4.885644 | -1.702608 | 0.403647 |
| C | 4.556402 | -3.055373 | 0.619546 |
| C | 5.929993 | -1.396408 | -0.487835 |
| C | 5.238076 | -4.060798 | -0.045599 |
| H | 3.797327 | -3.320390 | 1.346510 |
| C | 6.588718 | -2.406583 | -1.170730 |
| H | 6.191765 | -0.363632 | -0.681930 |
| C | 6.246889 | -3.739192 | -0.951889 |
| H | 4.987521 | -5.096740 | 0.145558 |
| H | 7.371265 | -2.155227 | -1.875497 |
| H | 6.770499 | -4.526588 | -1.480172 |

**15I-*Z***

Imaginary frequency: None

Electronic energies: -886.160684

Free energies: -885.796096

Corrected Free energies: -885.793581

| | | | |
|---|---|---|---|
| C | 1.633437 | -1.919724 | -0.089465 |
| C | 0.236644 | -1.321755 | -0.177336 |
| C | 1.938389 | 0.373515 | -0.490574 |
| H | -0.241879 | -1.417245 | 0.806583 |
| H | 2.247986 | 0.805990 | -1.454355 |
| N | 0.508386 | 0.071807 | -0.517487 |
| C | -0.310895 | 0.847988 | -1.325376 |
| C | -1.651894 | 0.971132 | -1.285636 |
| H | 0.231041 | 1.414617 | -2.082661 |

| | | | |
|---|---|---|---|
| C | -2.339883 | 1.733059 | -2.393454 |
| H | -3.062535 | 2.447090 | -1.988839 |
| H | -1.611631 | 2.277766 | -2.996334 |
| H | -2.887395 | 1.066679 | -3.067424 |
| N | 2.533611 | -0.946529 | -0.332996 |
| O | 1.886811 | -3.093600 | 0.117229 |
| C | 3.944577 | -1.248090 | -0.478195 |
| H | 4.471324 | -1.213964 | 0.478501 |
| H | 4.033211 | -2.254748 | -0.886216 |
| H | 4.399337 | -0.534559 | -1.165015 |
| C | -0.571965 | -2.106027 | -1.206883 |
| H | -1.613537 | -1.790752 | -1.227655 |
| H | -0.140407 | -1.977940 | -2.202525 |
| H | -0.527684 | -3.161355 | -0.934481 |
| C | 2.322884 | 1.372945 | 0.636832 |
| C | 2.065822 | 0.738446 | 2.004330 |
| H | 2.728320 | -0.112964 | 2.180523 |
| H | 2.239305 | 1.470888 | 2.796524 |
| H | 1.031904 | 0.390776 | 2.087029 |
| C | 3.797188 | 1.780374 | 0.511831 |
| H | 4.022309 | 2.142796 | -0.496003 |
| H | 4.010237 | 2.591061 | 1.212855 |
| H | 4.477877 | 0.961806 | 0.744794 |
| C | 1.468262 | 2.636336 | 0.478965 |
| H | 1.792165 | 3.386450 | 1.204368 |
| H | 1.579396 | 3.067493 | -0.521285 |
| H | 0.408963 | 2.433937 | 0.646850 |
| C | -2.510931 | 0.408497 | -0.219263 |
| C | -3.815553 | -0.021143 | -0.502465 |
| C | -2.078886 | 0.349942 | 1.113936 |
| C | -4.641519 | -0.518664 | 0.499459 |
| H | -4.186925 | 0.025856 | -1.519668 |
| C | -2.907289 | -0.138143 | 2.117403 |
| H | -1.086522 | 0.708731 | 1.361504 |
| C | -4.191053 | -0.583456 | 1.814484 |
| H | -5.641871 | -0.854012 | 0.251203 |
| H | -2.549797 | -0.165286 | 3.140382 |
| H | -4.835658 | -0.968641 | 2.595343 |

**15I-*E***

Imaginary frequency: None

Electronic energies: -886.158873

Free energies: -885.797634

Corrected Free energies: -885.793935

| | | | |
|---|---|---|---|
| C | 2.566242 | -1.660174 | 0.043887 |
| C | 1.224807 | -1.476376 | 0.741150 |
| C | 1.789421 | 0.465275 | -0.582652 |
| H | 1.416476 | -1.419461 | 1.820505 |
| H | 1.397687 | 0.715901 | -1.580326 |
| N | 0.753844 | -0.196128 | 0.206025 |
| C | -0.574483 | 0.022970 | -0.151290 |
| C | -1.634772 | -0.106976 | 0.666966 |
| H | -0.727284 | 0.347679 | -1.181062 |
| N | 2.809840 | -0.568497 | -0.707104 |
| O | 3.276018 | -2.647683 | 0.125575 |
| C | 3.946561 | -0.513746 | -1.606246 |
| H | 4.844530 | -0.141870 | -1.106984 |
| H | 4.143465 | -1.523726 | -1.965702 |
| H | 3.710392 | 0.134357 | -2.449754 |
| C | 0.333576 | -2.677897 | 0.451151 |
| H | -0.605146 | -2.627465 | 1.000911 |
| H | 0.111967 | -2.738056 | -0.616972 |
| H | 0.872406 | -3.576945 | 0.752581 |
| C | 2.287920 | 1.775758 | 0.084780 |
| C | 2.940509 | 1.460420 | 1.430866 |
| H | 3.823194 | 0.827076 | 1.306601 |
| H | 3.255062 | 2.385591 | 1.920329 |
| H | 2.233826 | 0.951343 | 2.092626 |
| C | 3.281735 | 2.503184 | -0.829417 |
| H | 2.869547 | 2.637650 | -1.834412 |
| H | 3.492927 | 3.494472 | -0.420634 |
| H | 4.232442 | 1.975997 | -0.913160 |
| C | 1.073036 | 2.686248 | 0.299350 |
| H | 1.403682 | 3.652549 | 0.687863 |
| H | 0.542114 | 2.865323 | -0.641593 |
| H | 0.369585 | 2.250063 | 1.011239 |
| C | -3.000393 | -0.000735 | 0.103931 |
| C | -4.055990 | 0.547610 | 0.846958 |
| C | -3.284312 | -0.457422 | -1.191988 |
| C | -5.330426 | 0.665471 | 0.304008 |
| H | -3.882122 | 0.902125 | 1.855623 |
| C | -4.556953 | -0.333039 | -1.737564 |
| H | -2.503345 | -0.943095 | -1.765863 |
| C | -5.588073 | 0.230958 | -0.992844 |
| H | -6.125597 | 1.101365 | 0.897798 |
| H | -4.746727 | -0.696559 | -2.740945 |
| H | -6.582800 | 0.320067 | -1.412847 |

| | | | |
|---|---|---|---|
| C | -1.479724 | -0.333609 | 2.147525 |
| H | -1.919987 | -1.284050 | 2.465043 |
| H | -0.429512 | -0.319419 | 2.438140 |
| H | -1.982805 | 0.455402 | 2.712519 |

**15I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -885.966743

Free energies: -885.602003

Corrected Free energies: -885.599390

| | | | |
|---|---|---|---|
| C | 2.596831 | -1.603120 | -0.197729 |
| C | 1.235836 | -1.544781 | 0.498752 |
| C | 1.809714 | 0.580597 | -0.554783 |
| H | 1.408020 | -1.520039 | 1.578394 |
| H | 1.465502 | 0.998704 | -1.506725 |
| N | 0.720984 | -0.245673 | 0.022951 |
| C | -0.534629 | 0.136014 | -0.102051 |
| C | -1.659315 | -0.317360 | 0.621803 |
| H | -0.683427 | 0.944542 | -0.811429 |
| N | 2.841311 | -0.411178 | -0.780587 |
| O | 3.299906 | -2.587252 | -0.244906 |
| C | 3.949651 | -0.253718 | -1.713880 |
| H | 4.888303 | -0.070464 | -1.190055 |
| H | 4.042081 | -1.172809 | -2.292455 |
| H | 3.740115 | 0.578872 | -2.382658 |
| C | 0.393629 | -2.742219 | 0.082939 |
| H | -0.534400 | -2.820843 | 0.643100 |
| H | 0.170656 | -2.692274 | -0.984145 |
| H | 0.989664 | -3.634311 | 0.274746 |
| C | 2.212007 | 1.734204 | 0.405664 |
| C | 2.594188 | 1.184924 | 1.781722 |
| H | 3.396180 | 0.445286 | 1.711713 |
| H | 2.952571 | 2.002972 | 2.409832 |
| H | 1.736917 | 0.735373 | 2.290614 |
| C | 3.408291 | 2.472452 | -0.209661 |
| H | 3.201622 | 2.787970 | -1.236350 |
| H | 3.614372 | 3.367689 | 0.380165 |
| H | 4.310054 | 1.859519 | -0.202461 |
| C | 1.047342 | 2.720891 | 0.542913 |
| H | 1.380046 | 3.580851 | 1.127518 |
| H | 0.713899 | 3.090532 | -0.431286 |
| H | 0.193066 | 2.289105 | 1.070046 |
| C | -2.971902 | -0.041970 | 0.079675 |

| | | | |
|---|---|---|---|
| C | -4.112464 | -0.093557 | 0.909310 |
| C | -3.153735 | 0.249279 | -1.290538 |
| C | -5.370489 | 0.164526 | 0.395244 |
| H | -4.010553 | -0.318613 | 1.962727 |
| C | -4.415487 | 0.499377 | -1.798323 |
| H | -2.309335 | 0.242162 | -1.968685 |
| C | -5.527228 | 0.463728 | -0.957541 |
| H | -6.233888 | 0.134349 | 1.047685 |
| H | -4.537867 | 0.712226 | -2.852616 |
| H | -6.514230 | 0.661299 | -1.357581 |
| C | -1.530393 | -0.907224 | 1.990842 |
| H | -2.117740 | -1.822765 | 2.088029 |
| H | -0.502146 | -1.108021 | 2.273834 |
| H | -1.925888 | -0.187583 | 2.714590 |

**15I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -885.966481

Free energies: -885.603738

Corrected Free energies: -885.600817

| | | | |
|---|---|---|---|
| C | -1.649257 | 1.901176 | 0.024273 |
| C | -0.248178 | 1.286104 | -0.013950 |
| C | -1.984701 | -0.356741 | -0.525593 |
| H | 0.117805 | 1.192472 | 1.012323 |
| H | -2.292196 | -0.753680 | -1.499004 |
| N | -0.531912 | -0.047440 | -0.585238 |
| C | 0.263223 | -0.823036 | -1.298737 |
| C | 1.672618 | -0.835052 | -1.359017 |
| H | -0.259162 | -1.537185 | -1.930749 |
| C | 2.283503 | -1.370280 | -2.614618 |
| H | 3.148104 | -1.996282 | -2.392057 |
| H | 1.559173 | -1.935805 | -3.198955 |
| H | 2.626766 | -0.536834 | -3.238431 |
| N | -2.552364 | 0.957792 | -0.313097 |
| O | -1.880181 | 3.063040 | 0.273989 |
| C | -3.946514 | 1.303751 | -0.549219 |
| H | -4.521393 | 1.310645 | 0.378011 |
| H | -3.976215 | 2.300258 | -0.988611 |
| H | -4.381423 | 0.585646 | -1.242671 |
| C | 0.675855 | 2.164998 | -0.846830 |
| H | 1.724176 | 1.912761 | -0.714018 |
| H | 0.411287 | 2.102222 | -1.904086 |
| H | 0.520774 | 3.189324 | -0.507721 |

| | | | |
|---|---|---|---|
| C | -2.316099 | -1.395493 | 0.583296 |
| C | -1.974415 | -0.841340 | 1.967516 |
| H | -2.524348 | 0.078346 | 2.180274 |
| H | -2.246171 | -1.576608 | 2.727554 |
| H | -0.905799 | -0.640242 | 2.081166 |
| C | -3.817994 | -1.707971 | 0.510106 |
| H | -4.112064 | -2.024504 | -0.494348 |
| H | -4.042570 | -2.525114 | 1.198265 |
| H | -4.429547 | -0.855100 | 0.803706 |
| C | -1.544566 | -2.694767 | 0.326529 |
| H | -1.871537 | -3.447267 | 1.046496 |
| H | -1.740799 | -3.088495 | -0.675076 |
| H | -0.465168 | -2.578485 | 0.452566 |
| C | 2.525056 | -0.404391 | -0.271252 |
| C | 3.830797 | 0.051317 | -0.537995 |
| C | 2.097219 | -0.490142 | 1.066519 |
| C | 4.650644 | 0.466706 | 0.497019 |
| H | 4.183588 | 0.110717 | -1.560299 |
| C | 2.929901 | -0.093053 | 2.099212 |
| H | 1.128835 | -0.919686 | 1.294613 |
| C | 4.201805 | 0.400587 | 1.815923 |
| H | 5.643309 | 0.840452 | 0.280099 |
| H | 2.593347 | -0.177630 | 3.124675 |
| H | 4.849237 | 0.719060 | 2.623620 |

**16I-*Z***

Imaginary frequency: None

Electronic energies: -1117.169356

Free energies: -1116.729980

Corrected Free energies: -1116.725745

| | | | |
|---|---|---|---|
| C | 1.333722 | -1.655086 | 0.955801 |
| C | 0.473810 | -0.504192 | 0.458697 |
| C | 2.820405 | 0.061360 | 0.344017 |
| H | -0.203753 | -0.210040 | 1.264958 |
| N | 1.444479 | 0.564610 | 0.228319 |
| C | 1.212778 | 1.842677 | 0.744859 |
| C | 0.062667 | 2.517406 | 0.880404 |
| H | 2.124289 | 2.342106 | 1.064245 |
| C | 0.071875 | 3.887171 | 1.518044 |
| H | -0.565051 | 3.904966 | 2.408258 |
| H | 1.079398 | 4.185908 | 1.812791 |
| H | -0.326763 | 4.636124 | 0.826176 |
| N | 2.627779 | -1.291671 | 0.851712 |

| | | | |
|---|---|---|---|
| O | 0.926689 | -2.728134 | 1.369532 |
| C | 3.684044 | -2.137914 | 1.376403 |
| H | 4.499490 | -1.516846 | 1.746303 |
| H | 3.269848 | -2.723482 | 2.196887 |
| H | 4.069683 | -2.824480 | 0.619717 |
| C | -0.338145 | -0.913622 | -0.786014 |
| H | -0.401030 | -0.040579 | -1.438451 |
| H | 0.219320 | -1.677418 | -1.340324 |
| C | -1.738577 | -1.423500 | -0.524844 |
| C | -2.138621 | -1.959221 | 0.700098 |
| C | -2.670306 | -1.373762 | -1.563839 |
| C | -3.443731 | -2.407811 | 0.886217 |
| H | -1.422862 | -2.047972 | 1.508710 |
| C | -3.969882 | -1.832031 | -1.386333 |
| H | -2.373902 | -0.951414 | -2.519094 |
| C | -4.365070 | -2.343898 | -0.153513 |
| H | -3.738474 | -2.814206 | 1.847151 |
| H | -4.677939 | -1.776434 | -2.205424 |
| H | -5.379828 | -2.695209 | -0.007278 |
| C | 3.608537 | 0.157371 | -0.988513 |
| C | -1.281892 | 2.083166 | 0.397839 |
| C | -1.650943 | 2.307890 | -0.932316 |
| C | -2.237175 | 1.567089 | 1.276712 |
| C | -2.939788 | 2.021684 | -1.370354 |
| H | -0.918323 | 2.716540 | -1.621392 |
| C | -3.525474 | 1.274087 | 0.839747 |
| H | -1.963631 | 1.392045 | 2.312772 |
| C | -3.882015 | 1.508355 | -0.483129 |
| H | -3.208225 | 2.199511 | -2.405635 |
| H | -4.247694 | 0.858066 | 1.532729 |
| H | -4.883068 | 1.275706 | -0.826430 |
| H | 3.368825 | 0.644758 | 1.097250 |
| C | 2.950738 | -0.700559 | -2.067468 |
| H | 1.939311 | -0.346564 | -2.278502 |
| H | 3.530119 | -0.644008 | -2.992433 |
| H | 2.898748 | -1.750752 | -1.765200 |
| C | 5.063849 | -0.280590 | -0.782189 |
| H | 5.154562 | -1.356270 | -0.628662 |
| H | 5.647052 | -0.027069 | -1.670854 |
| H | 5.517750 | 0.232296 | 0.071567 |
| C | 3.605342 | 1.627448 | -1.424733 |
| H | 2.590229 | 1.982996 | -1.612075 |
| H | 4.062062 | 2.267457 | -0.662671 |
| H | 4.183663 | 1.737668 | -2.345134 |

**16I-*E***

Imaginary frequency: None

Electronic energies: -1117.168160

Free energies: -1116.729291

Corrected Free energies: -1116.724420

| | | | |
|---|---|---|---|
| C | 1.989724 | -1.040946 | -1.232814 |
| C | 1.127208 | -0.101592 | -0.401011 |
| C | 0.335763 | -2.377844 | -0.234476 |
| H | 0.721285 | 0.665247 | -1.068660 |
| H | -0.490920 | -2.814194 | -0.812600 |
| N | 0.040107 | -0.969316 | 0.060669 |
| C | -1.289574 | -0.577409 | -0.113523 |
| C | -1.839733 | 0.605683 | 0.215671 |
| H | -1.931668 | -1.353142 | -0.524884 |
| N | 1.512252 | -2.291646 | -1.090546 |
| O | 2.960254 | -0.718559 | -1.897962 |
| C | 2.062459 | -3.393929 | -1.858332 |
| H | 1.276168 | -4.118190 | -2.069435 |
| H | 2.450566 | -2.992721 | -2.794160 |
| H | 2.877709 | -3.890932 | -1.328040 |
| C | 1.973525 | 0.566756 | 0.713224 |
| H | 1.392892 | 0.546598 | 1.635410 |
| H | 2.867377 | -0.039687 | 0.895439 |
| C | 0.512767 | -3.231591 | 1.046917 |
| C | 1.712267 | -2.748021 | 1.860054 |
| H | 1.565453 | -1.719780 | 2.196837 |
| H | 1.837728 | -3.377194 | 2.744798 |
| H | 2.636713 | -2.797705 | 1.277214 |
| C | -0.769528 | -3.087449 | 1.875586 |
| H | -1.647368 | -3.401867 | 1.301449 |
| H | -0.706404 | -3.719732 | 2.764358 |
| H | -0.920563 | -2.055130 | 2.197333 |
| C | 0.688932 | -4.712458 | 0.684869 |
| H | 0.626183 | -5.315502 | 1.593936 |
| H | -0.096942 | -5.053207 | 0.003676 |
| H | 1.657457 | -4.915299 | 0.226699 |
| C | 2.391244 | 1.989091 | 0.415908 |
| C | 2.876170 | 2.359629 | -0.840965 |
| C | 2.298418 | 2.964170 | 1.411722 |
| C | 3.253647 | 3.675492 | -1.093347 |
| H | 2.966374 | 1.606678 | -1.617069 |
| C | 2.679598 | 4.278507 | 1.162301 |

| | | | |
|---|---|---|---|
| H | 1.915659 | 2.690497 | 2.389899 |
| C | 3.157379 | 4.639132 | -0.094056 |
| H | 3.625607 | 3.948104 | -2.074255 |
| H | 2.595680 | 5.021565 | 1.946897 |
| H | 3.449770 | 5.663372 | -0.293063 |
| C | -1.088150 | 1.677820 | 0.968502 |
| H | -0.670927 | 1.282249 | 1.900161 |
| H | -0.258986 | 2.088641 | 0.389030 |
| H | -1.740130 | 2.513519 | 1.218490 |
| C | -3.272067 | 0.820892 | -0.106801 |
| C | -3.825146 | 0.365671 | -1.311752 |
| C | -4.123426 | 1.468638 | 0.800099 |
| C | -5.179019 | 0.526380 | -1.587818 |
| H | -3.179057 | -0.095234 | -2.050210 |
| C | -5.474541 | 1.635231 | 0.521870 |
| H | -3.731067 | 1.825596 | 1.745709 |
| C | -6.011456 | 1.162696 | -0.672979 |
| H | -5.579159 | 0.167452 | -2.529208 |
| H | -6.112497 | 2.130957 | 1.244409 |
| H | -7.064229 | 1.296946 | -0.890420 |

**16I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1116.973426

Free energies: -1116.535743

Corrected Free energies: -1116.530229

| | | | |
|---|---|---|---|
| C | -2.086842 | -1.386358 | 1.019025 |
| C | -1.223422 | -0.248060 | 0.484361 |
| C | -0.085318 | -2.410990 | 0.319150 |
| H | -1.103725 | 0.470012 | 1.297345 |
| H | 0.682703 | -2.803844 | 0.993586 |
| N | 0.064595 | -0.927594 | 0.273381 |
| C | 1.280498 | -0.409179 | 0.288378 |
| C | 1.714559 | 0.929549 | 0.228327 |
| N | -1.393607 | -2.539653 | 0.930289 |
| O | -3.206957 | -1.254220 | 1.462913 |
| C | -1.891561 | -3.753510 | 1.564306 |
| H | -1.049864 | -4.391799 | 1.827416 |
| H | -2.428220 | -3.465296 | 2.467458 |
| H | -2.572089 | -4.297748 | 0.908508 |
| C | -1.836358 | 0.428068 | -0.766827 |
| H | -1.045241 | 0.599289 | -1.499552 |
| H | -2.544875 | -0.264714 | -1.228910 |

| | | | |
|---|---|---|---|
| C | 0.062942 | -3.092418 | -1.069845 |
| C | -1.001981 | -2.596910 | -2.047309 |
| H | -0.846281 | -1.549219 | -2.311758 |
| H | -0.940845 | -3.177677 | -2.969888 |
| H | -2.010407 | -2.719550 | -1.643269 |
| C | 1.458022 | -2.817381 | -1.644882 |
| H | 2.249689 | -3.137439 | -0.960420 |
| H | 1.572591 | -3.387019 | -2.568971 |
| H | 1.606529 | -1.764744 | -1.896667 |
| C | -0.081876 | -4.609129 | -0.873046 |
| H | 0.176256 | -5.109130 | -1.808396 |
| H | 0.592458 | -4.982467 | -0.097236 |
| H | -1.102899 | -4.894487 | -0.621293 |
| C | -2.535532 | 1.737980 | -0.471024 |
| C | -3.340837 | 1.899546 | 0.657754 |
| C | -2.390346 | 2.807484 | -1.356665 |
| C | -3.981675 | 3.111977 | 0.896815 |
| H | -3.478498 | 1.070611 | 1.343821 |
| C | -3.034509 | 4.017013 | -1.119921 |
| H | -1.765866 | 2.693845 | -2.236987 |
| C | -3.830451 | 4.173419 | 0.010461 |
| H | -4.603240 | 3.223757 | 1.777353 |
| H | -2.908866 | 4.837498 | -1.816236 |
| H | -4.328935 | 5.116635 | 0.199015 |
| C | 0.829031 | 2.112681 | -0.002752 |
| H | 0.689509 | 2.273630 | -1.078634 |
| H | -0.155973 | 2.009479 | 0.439982 |
| H | 1.283585 | 3.009815 | 0.412544 |
| C | 3.152599 | 1.142345 | 0.293105 |
| C | 4.013124 | 0.252880 | 0.971330 |
| C | 3.717761 | 2.274825 | -0.329193 |
| C | 5.376455 | 0.485526 | 1.014697 |
| H | 3.613315 | -0.596063 | 1.511555 |
| C | 5.084737 | 2.488085 | -0.300957 |
| H | 3.086098 | 2.969516 | -0.867490 |
| C | 5.918664 | 1.597329 | 0.372517 |
| H | 6.018778 | -0.195896 | 1.557808 |
| H | 5.503861 | 3.350816 | -0.803025 |
| H | 6.987051 | 1.772217 | 0.402015 |
| H | 2.056040 | -1.164173 | 0.314520 |

**16I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1116.973669

Free energies: -1116.532983

Corrected Free energies: -1116.528953

| | | | |
|---|---|---|---|
| C | 1.360456 | -1.703675 | 0.740494 |
| C | 0.474627 | -0.558223 | 0.278433 |
| C | 2.807634 | 0.145395 | 0.554823 |
| H | -0.294021 | -0.447034 | 1.041168 |
| N | 1.395362 | 0.588643 | 0.359429 |
| C | 1.088720 | 1.867823 | 0.295376 |
| C | -0.181796 | 2.466665 | 0.127503 |
| H | 1.941671 | 2.535872 | 0.323048 |
| C | -0.210491 | 3.801174 | -0.544844 |
| H | -0.856229 | 4.491173 | 0.001232 |
| H | 0.786573 | 4.226722 | -0.649479 |
| H | -0.629985 | 3.690705 | -1.551540 |
| N | 2.601233 | -1.227040 | 0.977549 |
| O | 0.980597 | -2.840678 | 0.920366 |
| C | 3.576677 | -2.030930 | 1.702913 |
| H | 4.325945 | -1.374145 | 2.140550 |
| H | 3.053373 | -2.566206 | 2.494830 |
| H | 4.062985 | -2.756143 | 1.049521 |
| C | -0.194487 | -0.756922 | -1.097627 |
| H | -0.136370 | 0.180754 | -1.656561 |
| H | 0.375838 | -1.496595 | -1.666476 |
| C | -1.642880 | -1.192903 | -1.022771 |
| C | -2.117133 | -2.026447 | -0.010483 |
| C | -2.525054 | -0.778684 | -2.023235 |
| C | -3.453531 | -2.419003 | 0.011197 |
| H | -1.439170 | -2.388690 | 0.755540 |
| C | -3.855346 | -1.178355 | -2.008562 |
| H | -2.166871 | -0.126693 | -2.813525 |
| C | -4.326135 | -1.995891 | -0.984983 |
| H | -3.808714 | -3.062576 | 0.807508 |
| H | -4.526746 | -0.842479 | -2.790150 |
| H | -5.365032 | -2.303470 | -0.966615 |
| C | 3.694485 | 0.292954 | -0.718467 |
| C | -1.432403 | 1.887063 | 0.596665 |
| C | -2.601964 | 1.999732 | -0.169396 |
| C | -1.500977 | 1.292168 | 1.868938 |
| C | -3.793607 | 1.463440 | 0.295899 |
| H | -2.565482 | 2.463905 | -1.148020 |
| C | -2.701433 | 0.789079 | 2.341691 |
| H | -0.613561 | 1.259059 | 2.492981 |
| C | -3.845914 | 0.858685 | 1.547649 |

| | | | |
|---|---|---|---|
| H | -4.681610 | 1.511451 | -0.321818 |
| H | -2.747972 | 0.342361 | 3.326962 |
| H | -4.779590 | 0.445170 | 1.909551 |
| H | 3.238121 | 0.734370 | 1.370602 |
| C | 3.108250 | -0.489953 | -1.892714 |
| H | 2.167426 | -0.053447 | -2.235642 |
| H | 3.806702 | -0.454511 | -2.731330 |
| H | 2.946058 | -1.541433 | -1.640661 |
| C | 5.089245 | -0.254277 | -0.377623 |
| H | 5.084380 | -1.336293 | -0.252225 |
| H | 5.766853 | -0.023957 | -1.201547 |
| H | 5.495076 | 0.206172 | 0.527587 |
| C | 3.851129 | 1.766545 | -1.116143 |
| H | 2.937147 | 2.185934 | -1.542061 |
| H | 4.176043 | 2.384677 | -0.273680 |
| H | 4.617786 | 1.836767 | -1.889925 |

**17I-*Z***

Imaginary frequency: None

Electronic energies: -1038.572827

Free energies: -1038.187471

Corrected Free energies: -1038.183887

| | | | |
|---|---|---|---|
| C | 1.010404 | -1.679172 | -1.130803 |
| C | -0.089011 | -0.711361 | -0.734837 |
| C | 1.199807 | -1.414046 | 1.211993 |
| H | -1.040222 | -1.152074 | -1.053925 |
| N | 0.042771 | -0.652418 | 0.708689 |
| C | -0.570443 | 0.286108 | 1.516056 |
| C | -1.780875 | 0.862050 | 1.367710 |
| H | 0.040651 | 0.618654 | 2.351749 |
| C | -2.134474 | 2.046813 | 2.235400 |
| H | -2.139141 | 2.981082 | 1.663927 |
| H | -3.129753 | 1.932755 | 2.673764 |
| H | -1.408472 | 2.166154 | 3.041738 |
| N | 1.674909 | -2.046094 | -0.020589 |
| O | 1.244266 | -2.040372 | -2.272999 |
| C | 2.822236 | -2.929244 | -0.055607 |
| H | 2.729784 | -3.705193 | 0.705397 |
| H | 2.849412 | -3.392496 | -1.039979 |
| H | 3.751281 | -2.376122 | 0.103208 |
| C | 0.073220 | 0.637962 | -1.467768 |
| H | 0.077887 | 0.406164 | -2.536107 |
| H | -0.802936 | 1.256337 | -1.263554 |

| | | | |
|---|---|---|---|
| C | 1.333951 | 1.364862 | -1.073754 |
| C | 1.294182 | 2.415085 | -0.155175 |
| C | 2.574811 | 0.964998 | -1.579622 |
| C | 2.465185 | 3.039248 | 0.265791 |
| H | 0.335755 | 2.738480 | 0.238484 |
| C | 3.747178 | 1.584959 | -1.159337 |
| H | 2.618286 | 0.156847 | -2.302768 |
| C | 3.696417 | 2.620814 | -0.229975 |
| H | 2.415343 | 3.852033 | 0.981133 |
| H | 4.700868 | 1.260292 | -1.559287 |
| H | 4.609240 | 3.103339 | 0.098832 |
| C | 0.734634 | -2.464085 | 2.221593 |
| H | 1.575436 | -3.036735 | 2.618146 |
| H | 0.242583 | -1.962772 | 3.058016 |
| H | 0.022867 | -3.142206 | 1.747595 |
| C | 2.305289 | -0.537891 | 1.810761 |
| H | 2.598429 | 0.243756 | 1.107964 |
| H | 1.980963 | -0.082220 | 2.747246 |
| H | 3.173692 | -1.158118 | 2.042485 |
| C | -2.809697 | 0.407392 | 0.406060 |
| C | -3.620868 | 1.326035 | -0.274291 |
| C | -3.061067 | -0.958822 | 0.213898 |
| C | -4.625118 | 0.895927 | -1.134849 |
| H | -3.458330 | 2.389150 | -0.134905 |
| C | -4.069122 | -1.389775 | -0.640407 |
| H | -2.458104 | -1.683273 | 0.752307 |
| C | -4.854113 | -0.463900 | -1.322609 |
| H | -5.232204 | 1.625694 | -1.657908 |
| H | -4.246715 | -2.451368 | -0.768562 |
| H | -5.639653 | -0.799324 | -1.989069 |

**17I-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1038.571175

Free energies: -1038.185975

Corrected Free energies: -1038.182559

| | | | |
|---|---|---|---|
| C | 2.605177 | -1.309629 | -0.812024 |
| C | 1.151825 | -1.088307 | -1.191685 |
| C | 1.412910 | -1.235125 | 1.230542 |
| H | 0.856749 | -1.907780 | -1.854507 |
| N | 0.477938 | -1.134816 | 0.095004 |
| C | -0.832178 | -0.759188 | 0.309159 |
| C | -1.885319 | -0.997532 | -0.502250 |

| | | | |
|---|---|---|---|
| H | -1.005247 | -0.235749 | 1.245669 |
| N | 2.688505 | -1.385063 | 0.527881 |
| O | 3.530521 | -1.376746 | -1.604531 |
| C | 3.955839 | -1.498605 | 1.219821 |
| H | 4.697747 | -1.829519 | 0.495690 |
| H | 4.265993 | -0.535380 | 1.633370 |
| H | 3.885835 | -2.231209 | 2.024446 |
| C | 0.998334 | 0.235403 | -1.972145 |
| H | 1.655952 | 0.156613 | -2.842060 |
| H | -0.027824 | 0.317641 | -2.334553 |
| C | 1.341906 | 1.448735 | -1.146497 |
| C | 0.328128 | 2.233448 | -0.596051 |
| C | 2.671686 | 1.783911 | -0.873654 |
| C | 0.627698 | 3.311544 | 0.232083 |
| H | -0.705766 | 1.992087 | -0.821863 |
| C | 2.975431 | 2.861415 | -0.047187 |
| H | 3.470776 | 1.192230 | -1.308537 |
| C | 1.954307 | 3.623554 | 0.514914 |
| H | -0.173651 | 3.907346 | 0.653848 |
| H | 4.011215 | 3.107564 | 0.156630 |
| H | 2.192254 | 4.460860 | 1.160194 |
| C | 1.091687 | -2.481775 | 2.056248 |
| H | 1.154659 | -3.369293 | 1.424779 |
| H | 1.772808 | -2.586050 | 2.903061 |
| H | 0.075829 | -2.397714 | 2.448586 |
| C | 1.446135 | 0.009050 | 2.124093 |
| H | 0.505723 | 0.128544 | 2.663471 |
| H | 2.231376 | -0.106004 | 2.874637 |
| H | 1.643188 | 0.904629 | 1.533412 |
| C | -1.772255 | -1.912818 | -1.697094 |
| H | -1.158767 | -2.783786 | -1.455167 |
| H | -2.747826 | -2.271956 | -2.019225 |
| H | -1.321533 | -1.419981 | -2.565555 |
| C | -3.190300 | -0.385546 | -0.156616 |
| C | -3.260402 | 0.874479 | 0.460389 |
| C | -4.402605 | -1.048806 | -0.404478 |
| C | -4.478008 | 1.431828 | 0.833974 |
| H | -2.348848 | 1.434055 | 0.635796 |
| C | -5.620368 | -0.487681 | -0.039873 |
| H | -4.399859 | -2.029863 | -0.863192 |
| C | -5.667658 | 0.755833 | 0.583981 |
| H | -4.496256 | 2.406896 | 1.307200 |
| H | -6.537694 | -1.029815 | -0.238847 |
| H | -6.617924 | 1.193614 | 0.864872 |

**17I-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1038.380655

Free energies: -1037.995921

Corrected Free energies: -1037.992305

| | | | |
|---|---|---|---|
| C | 2.770099 | -1.074411 | -0.804259 |
| C | 1.299032 | -1.107639 | -1.189482 |
| C | 1.602831 | -1.159259 | 1.258846 |
| H | 1.131702 | -2.022529 | -1.758816 |
| N | 0.624834 | -1.164832 | 0.113798 |
| C | -0.661986 | -1.062434 | 0.362510 |
| C | -1.763224 | -1.164143 | -0.520032 |
| H | -0.895517 | -0.896921 | 1.408572 |
| N | 2.867698 | -1.106483 | 0.536523 |
| O | 3.675785 | -1.004559 | -1.608389 |
| C | 4.145061 | -1.005038 | 1.221375 |
| H | 4.922448 | -1.169350 | 0.478578 |
| H | 4.271776 | -0.013356 | 1.660356 |
| H | 4.223474 | -1.764594 | 1.999104 |
| C | 0.928038 | 0.138151 | -2.021162 |
| H | 1.626568 | 0.141340 | -2.861004 |
| H | -0.076480 | 0.027454 | -2.430230 |
| C | 1.037388 | 1.410869 | -1.217537 |
| C | -0.105963 | 2.015287 | -0.691962 |
| C | 2.286239 | 1.972554 | -0.936262 |
| C | -0.006139 | 3.137093 | 0.126229 |
| H | -1.085196 | 1.613587 | -0.934139 |
| C | 2.387944 | 3.095521 | -0.121594 |
| H | 3.181401 | 1.527998 | -1.358808 |
| C | 1.243015 | 3.674067 | 0.420614 |
| H | -0.904496 | 3.590777 | 0.528159 |
| H | 3.362415 | 3.520887 | 0.086846 |
| H | 1.323033 | 4.546121 | 1.058269 |
| C | 1.460696 | -2.461364 | 2.042342 |
| H | 1.618496 | -3.316442 | 1.384166 |
| H | 2.194472 | -2.486727 | 2.848640 |
| H | 0.469174 | -2.528132 | 2.492543 |
| C | 1.426183 | 0.074644 | 2.140942 |
| H | 0.496748 | 0.028686 | 2.708778 |
| H | 2.241462 | 0.100597 | 2.865430 |
| H | 1.451390 | 0.986651 | 1.541761 |
| C | -1.723623 | -1.934395 | -1.801444 |

| | | | |
|---|---|---|---|
| H | -0.741584 | -2.318780 | -2.047370 |
| H | -2.383893 | -2.801260 | -1.704568 |
| H | -2.098104 | -1.334156 | -2.634068 |
| C | -3.017756 | -0.581557 | -0.084667 |
| C | -3.061011 | 0.407791 | 0.924012 |
| C | -4.230646 | -0.954450 | -0.701822 |
| C | -4.263189 | 0.969576 | 1.314011 |
| H | -2.147580 | 0.773312 | 1.378175 |
| C | -5.430019 | -0.392443 | -0.301645 |
| H | -4.237427 | -1.699157 | -1.486449 |
| C | -5.452776 | 0.567046 | 0.708955 |
| H | -4.274612 | 1.731828 | 2.082739 |
| H | -6.351808 | -0.701952 | -0.777699 |
| H | -6.393030 | 1.006999 | 1.018087 |

**17I-*E***

Imaginary frequency: None

Electronic energies: -1038.380379

Free energies: -1037.996194

Corrected Free energies: -1037.992173

| | | | |
|---|---|---|---|
| C | 1.026679 | -1.678105 | -1.141434 |
| C | -0.093429 | -0.733888 | -0.737511 |
| C | 1.278396 | -1.407159 | 1.202947 |
| H | -1.044622 | -1.199515 | -0.993349 |
| N | 0.078670 | -0.636854 | 0.719686 |
| C | -0.585052 | 0.137117 | 1.553190 |
| C | -1.795070 | 0.831309 | 1.331755 |
| H | -0.116688 | 0.272186 | 2.524276 |
| C | -2.038083 | 2.053952 | 2.157214 |
| H | -2.012376 | 2.945546 | 1.520667 |
| H | -3.030514 | 2.015276 | 2.611000 |
| H | -1.281574 | 2.179272 | 2.930236 |
| N | 1.737693 | -2.002380 | -0.045713 |
| O | 1.231050 | -2.033358 | -2.283566 |
| C | 2.923272 | -2.839314 | -0.108343 |
| H | 2.856421 | -3.651189 | 0.616035 |
| H | 2.969775 | -3.255331 | -1.112238 |
| H | 3.823514 | -2.250834 | 0.078902 |
| C | 0.042473 | 0.620939 | -1.465930 |
| H | 0.052106 | 0.371316 | -2.529413 |
| H | -0.845592 | 1.225770 | -1.277535 |
| C | 1.293457 | 1.365551 | -1.072448 |
| C | 1.236704 | 2.406037 | -0.144090 |

| | | | |
|---|---|---|---|
| C | 2.537551 | 0.988515 | -1.587247 |
| C | 2.398557 | 3.043304 | 0.282543 |
| H | 0.275439 | 2.730994 | 0.241311 |
| C | 3.699500 | 1.623089 | -1.161763 |
| H | 2.593676 | 0.192334 | -2.322582 |
| C | 3.633561 | 2.647082 | -0.219899 |
| H | 2.336508 | 3.849154 | 1.003975 |
| H | 4.656896 | 1.319307 | -1.568011 |
| H | 4.539427 | 3.139909 | 0.111834 |
| C | 0.817930 | -2.472864 | 2.194095 |
| H | 1.676111 | -3.059296 | 2.523954 |
| H | 0.375112 | -2.005923 | 3.075128 |
| H | 0.088199 | -3.135258 | 1.727059 |
| C | 2.340454 | -0.486726 | 1.799029 |
| H | 2.640525 | 0.277910 | 1.082016 |
| H | 1.984412 | -0.014834 | 2.715077 |
| H | 3.210005 | -1.089745 | 2.064857 |
| C | -2.826027 | 0.383355 | 0.410009 |
| C | -3.657987 | 1.317649 | -0.232729 |
| C | -3.074745 | -0.988950 | 0.225829 |
| C | -4.669659 | 0.888570 | -1.076201 |
| H | -3.489380 | 2.378395 | -0.092809 |
| C | -4.103551 | -1.410892 | -0.600564 |
| H | -2.484718 | -1.721910 | 0.765100 |
| C | -4.894801 | -0.474052 | -1.262032 |
| H | -5.288150 | 1.616028 | -1.586349 |
| H | -4.294482 | -2.469440 | -0.723293 |
| H | -5.693765 | -0.805741 | -1.913660 |

## Calculated Cartesian coordinates for α-branched ketone derived enamines

**1J-*Z***

Imaginary frequency: None

Electronic energies: -891.913391

Free energies: -891.462013

Corrected Free energies: -891.456335

| | | | |
|---|---|---|---|
| C | -1.809889 | 2.479810 | -0.219061 |
| C | -3.260554 | 2.534149 | -0.719378 |
| H | -3.934457 | 2.024704 | -0.022869 |
| H | -3.584751 | 3.575156 | -0.799047 |

| | | | |
|---|---|---|---|
| H | -3.378800 | 2.078638 | -1.704203 |
| C | -1.695191 | 3.382053 | 1.015316 |
| H | -2.378005 | 3.045710 | 1.802429 |
| H | -0.680713 | 3.366877 | 1.414577 |
| H | -1.957230 | 4.411799 | 0.756457 |
| C | -0.875142 | 3.003746 | -1.316458 |
| H | 0.163079 | 3.044209 | -0.973713 |
| H | -0.920277 | 2.384353 | -2.216420 |
| H | -1.165953 | 4.019515 | -1.598215 |
| C | -1.446005 | 1.028900 | 0.190255 |
| H | -2.136235 | 0.756763 | 0.993663 |
| C | -1.594555 | -0.007978 | -0.936977 |
| H | -0.757472 | 0.120333 | -1.631496 |
| H | -2.513767 | 0.163255 | -1.515237 |
| N | -0.083485 | 0.985130 | 0.733877 |
| N | -1.559535 | -1.365720 | -0.397785 |
| C | -0.763665 | -2.292006 | -1.199150 |
| H | 0.225818 | -1.839329 | -1.314756 |
| H | -0.611239 | -3.207016 | -0.619911 |
| C | -2.904706 | -1.834001 | -0.077940 |
| H | -3.356458 | -1.089673 | 0.587233 |
| H | -3.546345 | -1.870322 | -0.975709 |
| C | -2.920553 | -3.190397 | 0.614530 |
| H | -2.632679 | -3.995582 | -0.064451 |
| H | -2.231864 | -3.197737 | 1.463121 |
| H | -3.924552 | -3.409355 | 0.982020 |
| C | -1.342915 | -2.640757 | -2.572958 |
| H | -1.522400 | -1.737590 | -3.162594 |
| H | -0.649784 | -3.275300 | -3.129192 |
| H | -2.289659 | -3.179124 | -2.482232 |
| H | 0.587546 | 1.117431 | -0.013925 |
| C | 0.317478 | -0.048758 | 1.596601 |
| C | 1.539768 | -0.621054 | 1.513743 |
| C | 2.045053 | -1.706508 | 2.435193 |
| H | 2.901387 | -1.360162 | 3.024815 |
| H | 2.393886 | -2.567199 | 1.856111 |
| H | 1.286120 | -2.073756 | 3.122795 |
| C | 2.515394 | -0.199849 | 0.466695 |
| C | 2.963174 | 1.125076 | 0.381923 |
| C | 3.039641 | -1.126634 | -0.444219 |
| C | 3.882677 | 1.515389 | -0.587013 |
| H | 2.579980 | 1.854570 | 1.088487 |
| C | 3.961454 | -0.741328 | -1.411735 |
| H | 2.710237 | -2.159537 | -0.399516 |

| | | | |
|---|---|---|---|
| C | 4.385975 | 0.582574 | -1.488682 |
| H | 4.211647 | 2.547336 | -0.632107 |
| H | 4.346898 | -1.475254 | -2.110386 |
| H | 5.102948 | 0.883654 | -2.243225 |
| C | -0.695290 | -0.390993 | 2.657801 |
| H | -1.466458 | -1.049217 | 2.249922 |
| H | -0.239578 | -0.875459 | 3.516586 |
| H | -1.182609 | 0.522836 | 3.007422 |

**1J-*E***

Imaginary frequency: None

Electronic energies: -891.913813

Free energies: -891.460901

Corrected Free energies: -891.455697

| | | | |
|---|---|---|---|
| C | -3.245745 | -1.599216 | -0.056249 |
| C | -4.463442 | -0.993511 | -0.768803 |
| H | -4.242110 | -0.806161 | -1.824070 |
| H | -5.304150 | -1.690636 | -0.720865 |
| H | -4.789451 | -0.055393 | -0.316234 |
| C | -2.952299 | -2.962186 | -0.694813 |
| H | -2.663235 | -2.841794 | -1.743771 |
| H | -2.140554 | -3.475635 | -0.179075 |
| H | -3.844594 | -3.593245 | -0.657754 |
| C | -3.575137 | -1.795314 | 1.429153 |
| H | -2.737126 | -2.234929 | 1.978632 |
| H | -3.846642 | -0.852670 | 1.911194 |
| H | -4.423018 | -2.477913 | 1.532964 |
| C | -2.020255 | -0.668873 | -0.251325 |
| H | -1.928533 | -0.512083 | -1.329523 |
| C | -2.159521 | 0.703086 | 0.437297 |
| H | -1.960775 | 0.561835 | 1.504659 |
| H | -3.185984 | 1.090191 | 0.356359 |
| N | -0.792825 | -1.329892 | 0.200504 |
| N | -1.193269 | 1.657551 | -0.100048 |
| C | -0.605940 | 2.527987 | 0.916218 |
| H | -0.179125 | 1.873981 | 1.682532 |
| H | 0.238155 | 3.057938 | 0.467085 |
| C | -1.747208 | 2.361516 | -1.253788 |
| H | -2.104401 | 1.601281 | -1.957142 |
| H | -2.633507 | 2.957928 | -0.976729 |
| C | -0.730986 | 3.249763 | -1.959737 |
| H | -0.465726 | 4.122129 | -1.358779 |
| H | 0.183571 | 2.690648 | -2.172691 |

| | | | |
|---|---|---|---|
| H | -1.143479 | 3.611413 | -2.903259 |
| C | -1.565002 | 3.532568 | 1.559943 |
| H | -2.421701 | 3.024448 | 2.010712 |
| H | -1.054697 | 4.094834 | 2.344705 |
| H | -1.943289 | 4.248816 | 0.826416 |
| H | -0.832367 | -1.523267 | 1.192393 |
| C | 0.477702 | -0.918218 | -0.211767 |
| C | 1.504251 | -0.869336 | 0.671382 |
| C | 2.911632 | -0.624442 | 0.269093 |
| C | 3.553795 | -1.384127 | -0.717302 |
| C | 3.661789 | 0.369933 | 0.914442 |
| C | 4.880223 | -1.143667 | -1.063559 |
| H | 3.004025 | -2.179170 | -1.209879 |
| C | 4.987899 | 0.609291 | 0.575527 |
| H | 3.189346 | 0.971451 | 1.684561 |
| C | 5.604913 | -0.145781 | -0.418762 |
| H | 5.351917 | -1.747024 | -1.830894 |
| H | 5.539767 | 1.390783 | 1.085578 |
| H | 6.639384 | 0.038409 | -0.683309 |
| C | 1.251338 | -1.086559 | 2.151265 |
| H | 0.430924 | -0.464136 | 2.525652 |
| H | 0.997257 | -2.130295 | 2.374087 |
| H | 2.138050 | -0.846379 | 2.737271 |
| C | 0.596449 | -0.603733 | -1.678374 |
| H | 1.615262 | -0.339783 | -1.948091 |
| H | 0.278407 | -1.458826 | -2.282700 |
| H | -0.045677 | 0.244554 | -1.922274 |

**1J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -891.737108

Free energies: -891.282144

Corrected Free energies: -891.277714

| | | | |
|---|---|---|---|
| C | -2.264328 | -2.379157 | -0.109173 |
| C | -3.511960 | -2.502271 | -0.994723 |
| H | -3.296921 | -2.193929 | -2.021883 |
| H | -3.836351 | -3.545156 | -1.017285 |
| H | -4.346554 | -1.906850 | -0.621555 |
| C | -1.208461 | -3.368307 | -0.619318 |
| H | -0.923453 | -3.137893 | -1.650176 |
| H | -0.306593 | -3.358602 | -0.002895 |
| H | -1.614192 | -4.382130 | -0.600319 |
| C | -2.634583 | -2.719230 | 1.339577 |

| | | | |
|---|---|---|---|
| H | -1.774246 | -2.682294 | 2.014997 |
| H | -3.409645 | -2.055161 | 1.728117 |
| H | -3.021760 | -3.739927 | 1.380275 |
| C | -1.710648 | -0.937261 | -0.245502 |
| H | -1.543374 | -0.754447 | -1.307069 |
| C | -2.604926 | 0.175973 | 0.326526 |
| H | -2.606230 | 0.094638 | 1.417104 |
| H | -3.638531 | 0.018583 | -0.008274 |
| N | -0.409794 | -0.821040 | 0.425684 |
| N | -2.093366 | 1.486168 | -0.057149 |
| C | -2.210710 | 2.480249 | 1.014434 |
| H | -1.724544 | 2.054484 | 1.896427 |
| H | -1.620975 | 3.355497 | 0.733797 |
| C | -2.661587 | 1.914480 | -1.338144 |
| H | -2.469182 | 1.118479 | -2.065711 |
| H | -3.757093 | 2.012449 | -1.276623 |
| C | -2.055823 | 3.212651 | -1.853424 |
| H | -2.359828 | 4.069700 | -1.249543 |
| H | -0.964223 | 3.160455 | -1.846507 |
| H | -2.386520 | 3.394033 | -2.877073 |
| C | -3.638859 | 2.903458 | 1.363743 |
| H | -4.252648 | 2.038301 | 1.628456 |
| H | -3.630097 | 3.583421 | 2.217621 |
| H | -4.119967 | 3.419898 | 0.529945 |
| H | -0.402716 | -1.140346 | 1.389976 |
| C | 0.706388 | -0.306510 | -0.049491 |
| C | 1.826619 | -0.196929 | 0.834289 |
| C | 3.175126 | 0.008676 | 0.322454 |
| C | 3.610131 | -0.641613 | -0.846862 |
| C | 4.088027 | 0.818254 | 1.020828 |
| C | 4.909970 | -0.483445 | -1.300260 |
| H | 2.936279 | -1.304052 | -1.377379 |
| C | 5.379424 | 0.993429 | 0.547802 |
| H | 3.773342 | 1.340723 | 1.915853 |
| C | 5.795886 | 0.340292 | -0.609564 |
| H | 5.234184 | -1.007406 | -2.190727 |
| H | 6.063721 | 1.638324 | 1.084820 |
| H | 6.808928 | 0.468738 | -0.970602 |
| C | 1.606540 | -0.348786 | 2.307192 |
| H | 0.759767 | 0.246569 | 2.658042 |
| H | 1.405821 | -1.401212 | 2.547318 |
| H | 2.491554 | -0.070160 | 2.872457 |
| C | 0.722945 | 0.202721 | -1.459001 |
| H | 1.635112 | 0.754011 | -1.662600 |

| | | | |
|---|---|---|---|
| H | 0.632768 | -0.617154 | -2.176372 |
| H | -0.128742 | 0.872474 | -1.580654 |

**1J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -891.737832

Free energies: -891.284348

Corrected Free energies: -891.279325

| | | | |
|---|---|---|---|
| C | -0.933580 | 2.717556 | 0.058263 |
| C | -2.284915 | 3.424229 | -0.111118 |
| H | -2.973777 | 3.158229 | 0.695970 |
| H | -2.132253 | 4.505338 | -0.081356 |
| H | -2.758309 | 3.183755 | -1.064399 |
| C | -0.232418 | 3.291708 | 1.295821 |
| H | -0.848179 | 3.160075 | 2.190223 |
| H | 0.735063 | 2.815066 | 1.472012 |
| H | -0.056930 | 4.361240 | 1.160258 |
| C | -0.068266 | 2.968937 | -1.182916 |
| H | 0.940661 | 2.555993 | -1.080951 |
| H | -0.522205 | 2.562392 | -2.089405 |
| H | 0.047164 | 4.045772 | -1.326512 |
| C | -1.188556 | 1.207669 | 0.293933 |
| H | -1.755432 | 1.107718 | 1.220477 |
| C | -1.942073 | 0.465727 | -0.828449 |
| H | -1.324735 | 0.472375 | -1.731117 |
| H | -2.861959 | 1.014139 | -1.064349 |
| N | 0.079369 | 0.494867 | 0.470730 |
| N | -2.212413 | -0.910536 | -0.431840 |
| C | -1.946950 | -1.881568 | -1.497205 |
| H | -0.921527 | -1.708820 | -1.836640 |
| H | -1.957572 | -2.881301 | -1.057121 |
| C | -3.535413 | -1.031922 | 0.185395 |
| H | -3.577428 | -0.312248 | 1.010428 |
| H | -4.333943 | -0.740258 | -0.515476 |
| C | -3.814714 | -2.426737 | 0.728382 |
| H | -3.953350 | -3.154007 | -0.073841 |
| H | -2.992146 | -2.771144 | 1.360354 |
| H | -4.726897 | -2.414615 | 1.326619 |
| C | -2.907254 | -1.826727 | -2.686561 |
| H | -2.935562 | -0.825826 | -3.125626 |
| H | -2.587489 | -2.526201 | -3.461214 |
| H | -3.923664 | -2.096516 | -2.390618 |
| H | 0.727806 | 0.582100 | -0.308871 |

| | | | |
|---|---|---|---|
| C | 0.362971 | -0.431488 | 1.368097 |
| C | 1.564951 | -1.184740 | 1.227978 |
| C | 1.743355 | -2.441926 | 2.016229 |
| H | 1.991795 | -2.190807 | 3.054587 |
| H | 2.566996 | -3.033550 | 1.623361 |
| H | 0.836741 | -3.049469 | 2.032334 |
| C | 2.622287 | -0.754423 | 0.307122 |
| C | 3.066764 | 0.578848 | 0.291521 |
| C | 3.229234 | -1.680914 | -0.554614 |
| C | 4.082120 | 0.972708 | -0.568893 |
| H | 2.644913 | 1.294241 | 0.989047 |
| C | 4.228224 | -1.275994 | -1.427548 |
| H | 2.894218 | -2.711328 | -0.560608 |
| C | 4.658801 | 0.048599 | -1.435379 |
| H | 4.427349 | 1.999000 | -0.556166 |
| H | 4.673278 | -1.996025 | -2.102985 |
| H | 5.446906 | 0.358377 | -2.110562 |
| C | -0.594124 | -0.681283 | 2.490601 |
| H | -1.522801 | -1.091648 | 2.089644 |
| H | -0.177892 | -1.370377 | 3.218188 |
| H | -0.820201 | 0.258457 | 2.998133 |

**2J-*Z***

Imaginary frequency: None

Electronic energies: -678.172207

Free energies: -677.858634

Corrected Free energies: -677.855521

| | | | |
|---|---|---|---|
| N | -0.498006 | 0.488985 | -0.925741 |
| C | 0.219826 | 1.587846 | -0.405199 |
| C | 1.486936 | 1.476778 | 0.041748 |
| C | 2.335989 | 2.617109 | 0.549011 |
| H | 3.178646 | 2.806255 | -0.124995 |
| H | 2.766052 | 2.359566 | 1.521643 |
| H | 0.020216 | -0.375542 | -0.805621 |
| C | -1.878885 | 0.290743 | -0.467012 |
| C | -2.491773 | -0.882443 | -1.230061 |
| C | -1.977891 | 0.056527 | 1.045096 |
| H | -2.452789 | 1.189321 | -0.719685 |
| C | -3.939062 | -1.132859 | -0.800355 |
| H | -1.893289 | -1.781398 | -1.029382 |
| H | -2.429466 | -0.684669 | -2.303239 |
| C | -3.425881 | -0.183458 | 1.478005 |
| H | -1.367281 | -0.821593 | 1.295225 |

| | | | |
|---|---|---|---|
| H | -1.547479 | 0.907007 | 1.583200 |
| C | -4.037673 | -1.357383 | 0.710269 |
| H | -4.345825 | -1.991122 | -1.341058 |
| H | -4.549711 | -0.264486 | -1.075167 |
| H | -3.472899 | -0.364366 | 2.554855 |
| H | -4.013968 | 0.721338 | 1.280893 |
| H | -5.080411 | -1.502813 | 1.004296 |
| H | -3.498872 | -2.275959 | 0.972268 |
| H | 1.783099 | 3.545721 | 0.674024 |
| C | 2.181834 | 0.154515 | 0.037961 |
| C | 2.507772 | -0.488357 | -1.160998 |
| C | 2.545737 | -0.460628 | 1.240861 |
| C | 3.166171 | -1.715008 | -1.159266 |
| H | 2.235946 | -0.018622 | -2.100758 |
| C | 3.203062 | -1.686233 | 1.246185 |
| H | 2.299788 | 0.024730 | 2.179804 |
| C | 3.515338 | -2.317646 | 0.044939 |
| H | 3.408553 | -2.197809 | -2.098886 |
| H | 3.469612 | -2.151044 | 2.188347 |
| H | 4.028785 | -3.271777 | 0.048415 |
| C | -0.543943 | 2.886277 | -0.464075 |
| H | -1.087988 | 2.943088 | -1.409666 |
| H | -1.280615 | 2.956025 | 0.341964 |
| H | 0.110586 | 3.750572 | -0.398943 |

**2J-*E***

Imaginary frequency: None

Electronic energies: -678.173465

Free energies: -677.858395

Corrected Free energies: -677.855776

| | | | |
|---|---|---|---|
| N | -1.084569 | -0.970656 | -0.445875 |
| C | 0.163701 | -0.334621 | -0.504021 |
| C | 1.217851 | -0.802470 | 0.203478 |
| H | -1.132193 | -1.669211 | 0.286022 |
| C | -2.307470 | -0.161050 | -0.449100 |
| C | -3.519834 | -1.085078 | -0.551001 |
| C | -2.423710 | 0.742365 | 0.784984 |
| H | -2.293240 | 0.471157 | -1.343152 |
| C | -4.825845 | -0.287054 | -0.566998 |
| H | -3.518236 | -1.761538 | 0.314200 |
| H | -3.427682 | -1.703588 | -1.447438 |
| C | -3.724184 | 1.548846 | 0.764060 |
| H | -2.400350 | 0.104043 | 1.678078 |

| | | | |
|---|---|---|---|
| H | -1.554495 | 1.405238 | 0.841496 |
| C | -4.937282 | 0.621548 | 0.659562 |
| H | -5.678661 | -0.968581 | -0.615548 |
| H | -4.857600 | 0.328780 | -1.473707 |
| H | -3.794217 | 2.173573 | 1.658123 |
| H | -3.713382 | 2.226117 | -0.098576 |
| H | -5.860241 | 1.205524 | 0.615900 |
| H | -4.991696 | 0.001328 | 1.562396 |
| C | 2.574883 | -0.209943 | 0.117658 |
| C | 3.698849 | -1.031829 | -0.048362 |
| C | 2.790614 | 1.167906 | 0.252544 |
| C | 4.980814 | -0.497277 | -0.103547 |
| H | 3.561602 | -2.103808 | -0.146872 |
| C | 4.071983 | 1.706377 | 0.194698 |
| H | 1.941344 | 1.820182 | 0.423987 |
| C | 5.174199 | 0.876651 | 0.014230 |
| H | 5.830909 | -1.155498 | -0.241913 |
| H | 4.209943 | 2.776008 | 0.304784 |
| H | 6.173244 | 1.293876 | -0.026893 |
| C | 1.051267 | -2.011041 | 1.103475 |
| H | 0.262846 | -1.848509 | 1.846958 |
| H | 0.787459 | -2.914882 | 0.542776 |
| H | 1.969121 | -2.218562 | 1.652232 |
| C | 0.237075 | 0.780980 | -1.515259 |
| H | -0.228052 | 1.701070 | -1.149062 |
| H | 1.266765 | 1.005618 | -1.782229 |
| H | -0.298675 | 0.480394 | -2.418855 |

**2J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -677.993578

Free energies: -677.677174

Corrected Free energies: -677.674997

| | | | |
|---|---|---|---|
| N | -0.997326 | -0.453980 | -0.270804 |
| C | 0.182427 | 0.022136 | 0.076645 |
| C | 1.334156 | -0.797991 | -0.135637 |
| H | -1.030803 | -1.369914 | -0.709164 |
| C | -2.306766 | 0.186661 | -0.095358 |
| C | -3.174216 | -0.110207 | -1.319438 |
| C | -2.971561 | -0.311627 | 1.194263 |
| H | -2.143289 | 1.264108 | -0.032726 |
| C | -4.556659 | 0.524620 | -1.152676 |
| H | -3.281787 | -1.197125 | -1.423206 |

| | | | |
|---|---|---|---|
| H | -2.679891 | 0.263453 | -2.218984 |
| C | -4.353549 | 0.326730 | 1.352112 |
| H | -3.068750 | -1.401513 | 1.135757 |
| H | -2.336468 | -0.083816 | 2.053989 |
| C | -5.234164 | 0.046783 | 0.132988 |
| H | -5.170967 | 0.285046 | -2.022924 |
| H | -4.450772 | 1.614956 | -1.125170 |
| H | -4.823939 | -0.052214 | 2.261710 |
| H | -4.237724 | 1.409318 | 1.477685 |
| H | -6.204962 | 0.533408 | 0.250311 |
| H | -5.420487 | -1.031087 | 0.063278 |
| C | 2.680962 | -0.247255 | -0.060825 |
| C | 2.974133 | 1.027551 | -0.578134 |
| C | 3.729024 | -1.007671 | 0.487675 |
| C | 4.267268 | 1.524289 | -0.540548 |
| H | 2.192470 | 1.611608 | -1.048615 |
| C | 5.015437 | -0.494491 | 0.546181 |
| H | 3.527426 | -1.987338 | 0.903410 |
| C | 5.289667 | 0.769332 | 0.029401 |
| H | 4.478765 | 2.499437 | -0.961164 |
| H | 5.807076 | -1.082387 | 0.993620 |
| H | 6.298078 | 1.162787 | 0.066361 |
| C | 1.141823 | -2.243610 | -0.473762 |
| H | 0.454319 | -2.737011 | 0.218175 |
| H | 0.729687 | -2.337754 | -1.486377 |
| H | 2.086263 | -2.779973 | -0.475315 |
| C | 0.237558 | 1.364675 | 0.742716 |
| H | 1.205296 | 1.527402 | 1.206216 |
| H | 0.049512 | 2.164058 | 0.021013 |
| H | -0.531020 | 1.422858 | 1.514148 |

**2J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -677.993703

Free energies: -677.678969

Corrected Free energies: -677.676594

| | | | |
|---|---|---|---|
| N | -0.492161 | 0.293091 | -0.152007 |
| C | 0.190339 | 1.405575 | -0.348663 |
| C | 1.598373 | 1.414487 | -0.128547 |
| C | 2.305107 | 2.727709 | -0.044169 |
| H | 2.438010 | 3.132569 | -1.055211 |
| H | 3.297337 | 2.613146 | 0.386123 |
| H | 0.027049 | -0.501801 | 0.214329 |

| | | | |
|---|---|---|---|
| C | -1.937871 | 0.074989 | -0.303403 |
| C | -2.187654 | -1.426097 | -0.447297 |
| C | -2.701745 | 0.655718 | 0.892135 |
| H | -2.255880 | 0.574133 | -1.222603 |
| C | -3.685887 | -1.703554 | -0.587254 |
| H | -1.804948 | -1.934181 | 0.446609 |
| H | -1.637935 | -1.809613 | -1.310689 |
| C | -4.198771 | 0.377115 | 0.740756 |
| H | -2.322645 | 0.184318 | 1.805498 |
| H | -2.515064 | 1.728875 | 0.974290 |
| C | -4.468138 | -1.121395 | 0.591658 |
| H | -3.848738 | -2.780472 | -0.662419 |
| H | -4.048633 | -1.259216 | -1.520915 |
| H | -4.730823 | 0.779326 | 1.605227 |
| H | -4.575511 | 0.905563 | -0.142473 |
| H | -5.537123 | -1.301236 | 0.458317 |
| H | -4.166496 | -1.633893 | 1.512340 |
| H | 1.743474 | 3.465315 | 0.531251 |
| C | 2.359556 | 0.169306 | -0.010365 |
| C | 2.137348 | -0.900439 | -0.896788 |
| C | 3.358966 | 0.039626 | 0.968183 |
| C | 2.886633 | -2.063698 | -0.797879 |
| H | 1.404717 | -0.800877 | -1.690020 |
| C | 4.087725 | -1.134864 | 1.075597 |
| H | 3.539371 | 0.848756 | 1.665471 |
| C | 3.856926 | -2.187102 | 0.192266 |
| H | 2.717664 | -2.870406 | -1.500004 |
| H | 4.840302 | -1.230441 | 1.848438 |
| H | 4.436588 | -3.098582 | 0.271578 |
| C | -0.516195 | 2.664443 | -0.740983 |
| H | -1.489272 | 2.469529 | -1.183530 |
| H | -0.663020 | 3.285423 | 0.147908 |
| H | 0.088436 | 3.231215 | -1.446955 |

**3J-*E***

Imaginary frequency: None

Electronic energies: -561.453769

Free energies: -561.203054

Corrected Free energies: -561.201052

| | | | |
|---|---|---|---|
| C | 3.311783 | -0.157156 | 0.399683 |
| H | 3.044711 | -0.317669 | 1.450528 |
| N | 2.117373 | 0.241968 | -0.358819 |
| C | 0.821704 | -0.152073 | -0.030297 |

| | | | |
|---|---|---|---|
| C | -0.227514 | 0.674254 | -0.265424 |
| H | 2.176681 | 1.191642 | -0.694714 |
| C | 4.316106 | 0.989534 | 0.341620 |
| H | 5.229355 | 0.724727 | 0.876114 |
| H | 4.579734 | 1.204384 | -0.698443 |
| H | 3.902160 | 1.895517 | 0.789725 |
| C | 3.929414 | -1.436975 | -0.162135 |
| H | 4.227662 | -1.271799 | -1.200757 |
| H | 4.813893 | -1.718465 | 0.414846 |
| H | 3.225836 | -2.269456 | -0.137441 |
| C | -1.639675 | 0.250603 | -0.105274 |
| C | -2.131292 | -0.933815 | -0.670412 |
| C | -2.545638 | 1.060554 | 0.595424 |
| C | -3.463214 | -1.306890 | -0.519779 |
| H | -1.459851 | -1.560983 | -1.246817 |
| C | -3.877337 | 0.693156 | 0.744483 |
| H | -2.193321 | 1.985354 | 1.040660 |
| C | -4.343963 | -0.495913 | 0.189143 |
| H | -3.816073 | -2.228654 | -0.968455 |
| H | -4.552119 | 1.334506 | 1.299979 |
| H | -5.382357 | -0.783241 | 0.303025 |
| C | 0.016255 | 2.085739 | -0.760243 |
| H | 0.719998 | 2.631248 | -0.121930 |
| H | 0.426817 | 2.092190 | -1.777372 |
| H | -0.911194 | 2.656186 | -0.789973 |
| C | 0.691801 | -1.534369 | 0.553104 |
| H | 0.863684 | -2.299984 | -0.209094 |
| H | 1.428511 | -1.692079 | 1.343075 |
| H | -0.296324 | -1.687102 | 0.979437 |

**3J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -561.276175

Free energies: -561.025369

Corrected Free energies: -561.023692

| | | | |
|---|---|---|---|
| C | 3.333637 | -0.329856 | 0.232846 |
| H | 3.200562 | -0.864868 | 1.172163 |
| N | 2.060142 | 0.347787 | -0.068229 |
| C | 0.846509 | -0.032965 | 0.280399 |
| C | -0.259383 | 0.780949 | -0.116757 |
| H | 2.146534 | 1.155435 | -0.678896 |
| C | 4.412886 | 0.731556 | 0.401419 |
| H | 5.356340 | 0.246468 | 0.652004 |

| | | | |
|---|---|---|---|
| H | 4.553821 | 1.287671 | -0.529214 |
| H | 4.155755 | 1.429441 | 1.198760 |
| C | 3.662007 | -1.318967 | -0.885001 |
| H | 3.784956 | -0.791725 | -1.833274 |
| H | 4.596601 | -1.828954 | -0.647788 |
| H | 2.877689 | -2.068218 | -0.999569 |
| C | -1.627569 | 0.279474 | -0.063586 |
| C | -1.932724 | -1.033227 | -0.465618 |
| C | -2.676900 | 1.123158 | 0.339517 |
| C | -3.243059 | -1.484852 | -0.459187 |
| H | -1.143313 | -1.685741 | -0.820605 |
| C | -3.982015 | 0.656327 | 0.370573 |
| H | -2.463064 | 2.134059 | 0.664655 |
| C | -4.269613 | -0.644891 | -0.033347 |
| H | -3.465111 | -2.491547 | -0.790438 |
| H | -4.777357 | 1.309800 | 0.706529 |
| H | -5.291743 | -1.002927 | -0.020347 |
| C | 0.001067 | 2.157205 | -0.643450 |
| H | 0.717594 | 2.706202 | -0.028355 |
| H | 0.405423 | 2.091848 | -1.661989 |
| H | -0.917602 | 2.733281 | -0.714828 |
| C | 0.702759 | -1.243689 | 1.151956 |
| H | 1.075597 | -2.138583 | 0.648694 |
| H | 1.291390 | -1.098810 | 2.060283 |
| H | -0.330685 | -1.398670 | 1.441235 |

**3J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -561.277121

Free energies: -561.027413

Corrected Free energies: -561.025250

| | | | |
|---|---|---|---|
| C | 2.757440 | -0.710607 | -0.289540 |
| H | 3.447026 | 0.119435 | -0.440232 |
| N | 1.394433 | -0.153071 | -0.277158 |
| C | 1.026945 | 1.068808 | 0.057399 |
| C | -0.355942 | 1.412422 | 0.049249 |
| C | -0.749918 | 2.853669 | 0.053862 |
| H | -0.681408 | 3.245536 | 1.076285 |
| H | -1.782854 | 2.977490 | -0.263338 |
| H | 0.658467 | -0.800930 | -0.549825 |
| C | 2.867423 | -1.678165 | -1.460594 |
| H | 3.879090 | -2.082207 | -1.498821 |
| H | 2.171972 | -2.512332 | -1.336132 |

| | | | |
|---|---|---|---|
| H | 2.656251 | -1.176056 | -2.405248 |
| C | 3.032280 | -1.388875 | 1.052511 |
| H | 2.329918 | -2.210866 | 1.208206 |
| H | 4.045809 | -1.791934 | 1.052018 |
| H | 2.936633 | -0.685040 | 1.880847 |
| H | -0.102703 | 3.462863 | -0.578559 |
| C | -1.391637 | 0.376624 | 0.053004 |
| C | -1.289454 | -0.740549 | 0.902507 |
| C | -2.528825 | 0.504739 | -0.760947 |
| C | -2.291709 | -1.699125 | 0.927969 |
| H | -0.442709 | -0.831614 | 1.574024 |
| C | -3.515605 | -0.468875 | -0.746461 |
| H | -2.620593 | 1.351255 | -1.430370 |
| C | -3.402321 | -1.569863 | 0.099181 |
| H | -2.209052 | -2.542944 | 1.601457 |
| H | -4.376782 | -0.368899 | -1.395301 |
| H | -4.181385 | -2.322192 | 0.116313 |
| C | 2.081986 | 2.079581 | 0.385078 |
| H | 1.652413 | 2.946949 | 0.876566 |
| H | 2.834242 | 1.647426 | 1.044772 |
| H | 2.580662 | 2.406865 | -0.531865 |

**3J-*Z***

Imaginary frequency: None

Electronic energies: -561.455864

Free energies: -561.205202

Corrected Free energies: -561.203249

| | | | |
|---|---|---|---|
| C | -2.682641 | -0.768794 | 0.202850 |
| H | -3.491513 | -0.053912 | 0.375249 |
| N | -1.442281 | -0.153895 | 0.694048 |
| C | -1.041295 | 1.088945 | 0.179056 |
| C | 0.238329 | 1.387467 | -0.133917 |
| C | 0.682116 | 2.799112 | -0.475388 |
| H | 0.025009 | 3.266223 | -1.210742 |
| H | 1.685050 | 2.781884 | -0.903482 |
| H | -0.685998 | -0.828384 | 0.706986 |
| C | -2.963267 | -2.016539 | 1.030524 |
| H | -3.898400 | -2.483065 | 0.715723 |
| H | -2.160006 | -2.748249 | 0.897370 |
| H | -3.031429 | -1.768621 | 2.090815 |
| C | -2.624567 | -1.095853 | -1.290914 |
| H | -1.883233 | -1.879283 | -1.476111 |
| H | -3.592472 | -1.454234 | -1.649095 |

| | | | |
|---|---|---|---|
| H | -2.344419 | -0.214932 | -1.874747 |
| H | 0.713209 | 3.452662 | 0.403103 |
| C | 1.319917 | 0.366500 | -0.071957 |
| C | 1.248291 | -0.834577 | -0.790051 |
| C | 2.476066 | 0.612840 | 0.679644 |
| C | 2.282716 | -1.763547 | -0.740299 |
| H | 0.379019 | -1.026890 | -1.410362 |
| C | 3.512548 | -0.312365 | 0.729086 |
| H | 2.558199 | 1.542301 | 1.233798 |
| C | 3.418586 | -1.508204 | 0.022393 |
| H | 2.206092 | -2.683625 | -1.308304 |
| H | 4.395030 | -0.099378 | 1.321498 |
| H | 4.226018 | -2.229650 | 0.059419 |
| C | -2.147022 | 2.111705 | 0.127572 |
| H | -1.759462 | 3.121907 | 0.026729 |
| H | -2.823711 | 1.922744 | -0.711714 |
| H | -2.739677 | 2.059623 | 1.043947 |

**4J-*Z***

Imaginary frequency: None

Electronic energies: -713.858858

Free energies: -713.586481

Corrected Free energies: -713.583405

| | | | |
|---|---|---|---|
| C | 2.032343 | 2.012264 | 1.677081 |
| C | 1.330501 | 1.387098 | 0.497343 |
| C | 0.410824 | 1.997030 | -0.274178 |
| H | 1.834422 | 1.428190 | 2.581623 |
| H | 3.117193 | 2.003073 | 1.529026 |
| N | -0.082870 | 1.406214 | -1.461173 |
| C | -1.543276 | 1.282589 | -1.601820 |
| H | -1.999364 | 2.253520 | -1.400462 |
| H | -1.754504 | 1.030460 | -2.642926 |
| C | -2.113467 | 0.222764 | -0.686940 |
| C | -2.159044 | -1.108060 | -1.104847 |
| C | -2.483309 | 0.529375 | 0.623573 |
| C | -2.552208 | -2.115549 | -0.229894 |
| H | -1.872228 | -1.356831 | -2.122265 |
| C | -2.876420 | -0.475014 | 1.503432 |
| H | -2.460057 | 1.560971 | 0.959337 |
| C | -2.906425 | -1.801118 | 1.079610 |
| H | -2.580318 | -3.144939 | -0.568065 |
| H | -3.158265 | -0.223513 | 2.519333 |
| H | -3.210360 | -2.584262 | 1.763984 |

| | | | |
|---|---|---|---|
| H | 0.346609 | 0.500149 | -1.618304 |
| H | 1.725313 | 3.038341 | 1.869514 |
| C | 1.752540 | -0.019108 | 0.216434 |
| C | 0.897739 | -1.090664 | 0.496558 |
| C | 3.022683 | -0.296068 | -0.300007 |
| C | 1.296238 | -2.401483 | 0.251331 |
| H | -0.086489 | -0.890694 | 0.907974 |
| C | 3.423812 | -1.606041 | -0.542843 |
| H | 3.696101 | 0.525695 | -0.521716 |
| C | 2.560279 | -2.663412 | -0.268611 |
| H | 0.615654 | -3.217140 | 0.468797 |
| H | 4.409187 | -1.800649 | -0.950516 |
| H | 2.871251 | -3.683778 | -0.459571 |
| C | -0.116181 | 3.389258 | -0.029741 |
| H | -1.056511 | 3.375469 | 0.528776 |
| H | 0.588283 | 3.998722 | 0.530777 |
| H | -0.305599 | 3.880542 | -0.985984 |

**4J-*E***

Imaginary frequency: None

Electronic energies: -713.856967

Free energies: -713.584321

Corrected Free energies: -713.581162

| | | | |
|---|---|---|---|
| C | -0.890637 | -0.715889 | -0.585274 |
| C | -0.164884 | -1.355821 | 0.355647 |
| N | 1.005245 | -2.069013 | 0.022959 |
| C | 2.228122 | -1.731385 | 0.769485 |
| H | 2.009486 | -1.782523 | 1.837554 |
| H | 2.974088 | -2.497603 | 0.550172 |
| C | 2.764145 | -0.365179 | 0.400354 |
| C | 3.683112 | -0.230424 | -0.641850 |
| C | 2.285510 | 0.787170 | 1.027043 |
| C | 4.114704 | 1.027217 | -1.052199 |
| H | 4.064186 | -1.120171 | -1.133886 |
| C | 2.712672 | 2.046957 | 0.618393 |
| H | 1.577998 | 0.699116 | 1.845108 |
| C | 3.627252 | 2.169602 | -0.423823 |
| H | 4.832957 | 1.115992 | -1.858895 |
| H | 2.333991 | 2.932616 | 1.115013 |
| H | 3.961967 | 3.149890 | -0.741548 |
| H | 1.197844 | -2.036757 | -0.970552 |
| C | -2.196595 | -0.073247 | -0.288793 |
| C | -2.353362 | 0.836020 | 0.763568 |

| | | | |
|---|---|---|---|
| C | -3.305692 | -0.330948 | -1.105717 |
| C | -3.579935 | 1.446065 | 1.008172 |
| H | -1.496708 | 1.079335 | 1.382608 |
| C | -4.532686 | 0.274865 | -0.862519 |
| H | -3.204041 | -1.023832 | -1.934618 |
| C | -4.676123 | 1.165276 | 0.198444 |
| H | -3.675620 | 2.150333 | 1.826537 |
| H | -5.379066 | 0.050699 | -1.501553 |
| H | -5.631151 | 1.641338 | 0.386492 |
| C | -0.426940 | -0.665285 | -2.028208 |
| H | 0.626212 | -0.374484 | -2.092851 |
| H | -0.536514 | -1.628234 | -2.539700 |
| H | -1.001549 | 0.070332 | -2.590775 |
| C | -0.569062 | -1.501291 | 1.802360 |
| H | -0.083478 | -0.767214 | 2.451292 |
| H | -1.644426 | -1.384226 | 1.923780 |
| H | -0.280486 | -2.493732 | 2.154617 |

**4J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -713.672820

Free energies: -713.400022

Corrected Free energies: -713.396805

| | | | |
|---|---|---|---|
| C | 1.437601 | -1.001219 | 0.109351 |
| C | 0.358240 | -0.638055 | -0.755011 |
| N | -0.805693 | -1.235000 | -0.578869 |
| C | -2.055674 | -1.011573 | -1.318594 |
| H | -1.833753 | -0.484241 | -2.241609 |
| H | -2.452626 | -1.996169 | -1.569393 |
| C | -3.037409 | -0.234156 | -0.469634 |
| C | -3.828903 | -0.897780 | 0.467309 |
| C | -3.139900 | 1.150044 | -0.600321 |
| C | -4.709486 | -0.182691 | 1.271575 |
| H | -3.764331 | -1.976986 | 0.562791 |
| C | -4.023639 | 1.864788 | 0.201485 |
| H | -2.541584 | 1.670134 | -1.340539 |
| C | -4.806411 | 1.199467 | 1.139799 |
| H | -5.323540 | -0.704749 | 1.995122 |
| H | -4.103692 | 2.939275 | 0.089254 |
| H | -5.495634 | 1.756858 | 1.762536 |
| H | -0.896849 | -1.866625 | 0.210666 |
| C | 2.647921 | -0.194219 | 0.188431 |
| C | 2.585062 | 1.211194 | 0.171780 |

| | | | |
|---|---|---|---|
| C | 3.902821 | -0.811003 | 0.337905 |
| C | 3.738202 | 1.969574 | 0.293595 |
| H | 1.624017 | 1.707363 | 0.102920 |
| C | 5.055465 | -0.046881 | 0.431707 |
| H | 3.977157 | -1.891524 | 0.341010 |
| C | 4.976841 | 1.343506 | 0.414186 |
| H | 3.671419 | 3.050229 | 0.298585 |
| H | 6.017319 | -0.535991 | 0.522426 |
| H | 5.878377 | 1.937974 | 0.498390 |
| C | 1.299843 | -2.213489 | 0.976429 |
| H | 0.578971 | -2.016358 | 1.780326 |
| H | 0.950766 | -3.083320 | 0.414552 |
| H | 2.239018 | -2.460748 | 1.463004 |
| C | 0.512318 | 0.316412 | -1.900606 |
| H | -0.067054 | 1.227355 | -1.731858 |
| H | 1.553841 | 0.582122 | -2.046011 |
| H | 0.150674 | -0.153114 | -2.816396 |

**4J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -713.674636

Free energies: -713.403100

Corrected Free energies: -713.399481

| | | | |
|---|---|---|---|
| C | 3.382572 | 1.935176 | 0.437434 |
| C | 2.141637 | 1.151542 | 0.152550 |
| C | 0.907219 | 1.837229 | -0.037448 |
| H | 3.341952 | 2.323440 | 1.461874 |
| H | 4.266124 | 1.305805 | 0.368095 |
| N | -0.104593 | 1.195455 | -0.592725 |
| C | -1.468597 | 1.683799 | -0.818219 |
| H | -1.608292 | 2.608289 | -0.262379 |
| H | -1.581236 | 1.898825 | -1.883167 |
| C | -2.449374 | 0.625076 | -0.372368 |
| C | -3.154494 | -0.128735 | -1.306388 |
| C | -2.622300 | 0.375697 | 0.990559 |
| C | -4.031998 | -1.123480 | -0.882536 |
| H | -3.021069 | 0.063687 | -2.365340 |
| C | -3.495082 | -0.618798 | 1.413015 |
| H | -2.075130 | 0.965411 | 1.719785 |
| C | -4.200974 | -1.369831 | 0.475204 |
| H | -4.581015 | -1.704254 | -1.613631 |
| H | -3.628803 | -0.806158 | 2.471494 |
| H | -4.882706 | -2.144292 | 0.805389 |

| | | | |
|---|---|---|---|
| H | 0.065468 | 0.246599 | -0.917201 |
| H | 3.492485 | 2.788918 | -0.233872 |
| C | 2.210880 | -0.309034 | 0.076494 |
| C | 1.235081 | -1.115631 | 0.691283 |
| C | 3.285232 | -0.931259 | -0.581353 |
| C | 1.329883 | -2.498490 | 0.638502 |
| H | 0.423878 | -0.655228 | 1.244814 |
| C | 3.360467 | -2.313634 | -0.649848 |
| H | 4.042526 | -0.328200 | -1.067380 |
| C | 2.386882 | -3.100312 | -0.038502 |
| H | 0.581317 | -3.105356 | 1.132232 |
| H | 4.182324 | -2.780470 | -1.178330 |
| H | 2.455932 | -4.180238 | -0.084497 |
| C | 0.725596 | 3.272196 | 0.346029 |
| H | -0.042638 | 3.349241 | 1.119590 |
| H | 1.642458 | 3.696676 | 0.740310 |
| H | 0.402792 | 3.860055 | -0.515155 |

**5J-*Z***

Imaginary frequency: None

Electronic energies: -674.559056

Free energies: -674.313667

Corrected Free energies: -674.311213

| | | | |
|---|---|---|---|
| N | -0.655073 | 0.467001 | -0.945030 |
| C | 0.031165 | 1.539873 | -0.334016 |
| C | 1.305754 | 1.418150 | 0.082933 |
| C | 2.119219 | 2.619898 | 0.499488 |
| H | 2.772858 | 2.959082 | -0.311349 |
| H | 2.759739 | 2.370155 | 1.348099 |
| H | -0.056519 | -0.239444 | -1.352241 |
| C | -1.862470 | -0.033928 | -0.447904 |
| C | -2.513464 | -1.060815 | -1.147547 |
| C | -2.438866 | 0.448813 | 0.733192 |
| C | -3.712613 | -1.578301 | -0.680839 |
| H | -2.068617 | -1.441705 | -2.060628 |
| C | -3.653252 | -0.064291 | 1.179496 |
| H | -1.930445 | 1.211504 | 1.310477 |
| C | -4.299347 | -1.077371 | 0.480732 |
| H | -4.197557 | -2.374996 | -1.233312 |
| H | -4.085596 | 0.325436 | 2.093974 |
| H | -5.240517 | -1.477224 | 0.837109 |
| H | 1.489191 | 3.461281 | 0.784095 |
| C | 2.012688 | 0.109308 | 0.095701 |

| | | | |
|---|---|---|---|
| C | 1.408477 | -1.042755 | 0.619939 |
| C | 3.330782 | 0.009999 | -0.365723 |
| C | 2.091210 | -2.252070 | 0.661161 |
| H | 0.399638 | -0.979439 | 1.014945 |
| C | 4.014024 | -1.201171 | -0.327325 |
| H | 3.824771 | 0.888368 | -0.765831 |
| C | 3.396913 | -2.338039 | 0.183813 |
| H | 1.606300 | -3.127822 | 1.076391 |
| H | 5.031352 | -1.255151 | -0.697152 |
| H | 3.929971 | -3.280634 | 0.217183 |
| C | -0.717571 | 2.854280 | -0.335208 |
| H | -1.732380 | 2.711445 | -0.704104 |
| H | -0.772749 | 3.297494 | 0.661303 |
| H | -0.219826 | 3.573145 | -0.991119 |

**5J-*E***

Imaginary frequency: None

Electronic energies: -674.557655

Free energies: -674.311889

Corrected Free energies: -674.309507

| | | | |
|---|---|---|---|
| N | -1.260783 | 0.850320 | -0.025712 |
| C | -0.042760 | 0.158999 | -0.116639 |
| C | 1.081452 | 0.769439 | 0.321884 |
| H | -1.213193 | 1.856194 | -0.087649 |
| C | -2.542785 | 0.309033 | -0.016402 |
| C | -3.610418 | 1.069667 | -0.514932 |
| C | -2.811336 | -0.957622 | 0.518341 |
| C | -4.904286 | 0.569028 | -0.491288 |
| H | -3.412079 | 2.053214 | -0.927310 |
| C | -4.108345 | -1.457450 | 0.515354 |
| H | -2.010545 | -1.536156 | 0.960219 |
| C | -5.164064 | -0.703538 | 0.012222 |
| H | -5.714008 | 1.175525 | -0.880163 |
| H | -4.293845 | -2.441309 | 0.930954 |
| H | -6.173093 | -1.095956 | 0.020226 |
| C | 2.435367 | 0.198443 | 0.127015 |
| C | 2.739329 | -1.137575 | 0.418981 |
| C | 3.476843 | 1.023040 | -0.322893 |
| C | 4.025897 | -1.636227 | 0.241900 |
| H | 1.964790 | -1.785752 | 0.811536 |
| C | 4.762249 | 0.526466 | -0.502247 |
| H | 3.271086 | 2.064763 | -0.545486 |
| C | 5.042892 | -0.808693 | -0.223760 |

| | | | |
|---|---|---|---|
| H | 4.235557 | -2.672944 | 0.479466 |
| H | 5.546285 | 1.183119 | -0.861248 |
| H | 6.045017 | -1.197641 | -0.359228 |
| C | 1.002620 | 2.138567 | 0.961405 |
| H | 0.876027 | 2.938827 | 0.221447 |
| H | 0.155642 | 2.195136 | 1.649323 |
| H | 1.910207 | 2.357878 | 1.523812 |
| C | -0.071182 | -1.156991 | -0.858882 |
| H | -0.185890 | -2.020900 | -0.201765 |
| H | -0.904059 | -1.165489 | -1.563300 |
| H | 0.858737 | -1.288280 | -1.411207 |

**5J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -674.368664

Free energies: -674.121308

Corrected Free energies: -674.119207

| | | | |
|---|---|---|---|
| N | -1.216355 | 0.714906 | 0.306245 |
| C | -0.063439 | 0.136118 | -0.016787 |
| C | 1.132088 | 0.857776 | 0.263249 |
| H | -1.169613 | 1.644672 | 0.711184 |
| C | -2.541758 | 0.225803 | 0.125116 |
| C | -3.498052 | 1.123751 | -0.347058 |
| C | -2.888225 | -1.080083 | 0.465555 |
| C | -4.807827 | 0.696818 | -0.511564 |
| H | -3.210142 | 2.139129 | -0.593196 |
| C | -4.202759 | -1.494318 | 0.294527 |
| H | -2.152984 | -1.752861 | 0.886532 |
| C | -5.160812 | -0.612922 | -0.197358 |
| H | -5.551386 | 1.388201 | -0.887250 |
| H | -4.478585 | -2.507051 | 0.559937 |
| H | -6.183746 | -0.943846 | -0.325647 |
| C | 2.442027 | 0.244019 | 0.087518 |
| C | 2.688861 | -1.080908 | 0.488023 |
| C | 3.501967 | 0.996155 | -0.450247 |
| C | 3.952548 | -1.633386 | 0.350970 |
| H | 1.901533 | -1.660645 | 0.953288 |
| C | 4.754685 | 0.426608 | -0.615348 |
| H | 3.331364 | 2.015702 | -0.774354 |
| C | 4.985049 | -0.886012 | -0.210538 |
| H | 4.133624 | -2.646849 | 0.686266 |
| H | 5.554606 | 1.008344 | -1.055940 |
| H | 5.968971 | -1.323817 | -0.327269 |

| | | | |
|---|---|---|---|
| C | 1.046940 | 2.274126 | 0.743228 |
| H | 0.445162 | 2.899320 | 0.076988 |
| H | 0.592014 | 2.305193 | 1.740509 |
| H | 2.034105 | 2.716632 | 0.838118 |
| C | -0.080934 | -1.162806 | -0.763343 |
| H | -0.111015 | -2.021429 | -0.090812 |
| H | -0.964440 | -1.205510 | -1.400754 |
| H | 0.812859 | -1.243976 | -1.376972 |

**5J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -674.370345

Free energies: -674.124309

Corrected Free energies: -674.122067

| | | | |
|---|---|---|---|
| N | -0.638366 | 0.114511 | -0.217543 |
| C | -0.058525 | 1.303197 | -0.049175 |
| C | 1.356672 | 1.377485 | -0.021134 |
| C | 2.012612 | 2.717646 | -0.127166 |
| H | 1.842824 | 3.164539 | -1.112784 |
| H | 3.082860 | 2.642873 | 0.045471 |
| H | -0.023404 | -0.657947 | -0.464971 |
| C | -2.016252 | -0.217012 | -0.142875 |
| C | -2.518079 | -1.124748 | -1.075338 |
| C | -2.826802 | 0.298357 | 0.867804 |
| C | -3.853984 | -1.493341 | -1.011225 |
| H | -1.867089 | -1.522646 | -1.844749 |
| C | -4.161906 | -0.078342 | 0.918761 |
| H | -2.413906 | 0.962691 | 1.616252 |
| C | -4.678191 | -0.967576 | -0.019873 |
| H | -4.250890 | -2.191725 | -1.737043 |
| H | -4.796272 | 0.315689 | 1.702424 |
| H | -5.720180 | -1.258365 | 0.027399 |
| H | 1.593802 | 3.404802 | 0.612738 |
| C | 2.194108 | 0.182658 | 0.069967 |
| C | 1.896510 | -0.874371 | 0.949392 |
| C | 3.360333 | 0.106047 | -0.711870 |
| C | 2.734500 | -1.978167 | 1.027237 |
| H | 1.036878 | -0.808404 | 1.606668 |
| C | 4.176717 | -1.010740 | -0.647626 |
| H | 3.604978 | 0.914142 | -1.390813 |
| C | 3.867451 | -2.054306 | 0.223071 |
| H | 2.505970 | -2.775614 | 1.722973 |
| H | 5.058877 | -1.066791 | -1.273041 |

| | | | |
|---|---|---|---|
| H | 4.514797 | -2.920745 | 0.280378 |
| C | -0.890718 | 2.544523 | 0.020029 |
| H | -1.900109 | 2.370171 | -0.343360 |
| H | -0.940435 | 2.919139 | 1.045539 |
| H | -0.426811 | 3.318761 | -0.590164 |

**6J-*Z***

Imaginary frequency: None

Electronic energies: -1853.976773

Free energies: -1853.488073

Corrected Free energies: -1853.480859

| | | | |
|---|---|---|---|
| S | 2.972107 | -0.763038 | 0.706397 |
| F | 3.214889 | 0.292760 | -1.682294 |
| F | 4.679821 | -1.229669 | -1.239118 |
| F | 2.643394 | -1.789326 | -1.689814 |
| O | 1.533032 | -0.467722 | 0.649490 |
| O | 3.793512 | 0.350072 | 1.185363 |
| O | 3.306163 | -2.077015 | 1.243696 |
| C | 3.405627 | -0.883556 | -1.081539 |
| N | -1.212932 | 0.408817 | -0.369646 |
| H | -1.816401 | 0.005284 | 0.336839 |
| N | 0.448029 | 2.075208 | 0.912093 |
| H | 0.438717 | 1.081855 | 0.600443 |
| C | -1.493349 | 1.819026 | -0.600931 |
| H | -0.946310 | 2.131947 | -1.493889 |
| C | -0.915804 | 2.598042 | 0.598153 |
| H | -0.841394 | 3.664263 | 0.394538 |
| H | -1.537104 | 2.462080 | 1.482126 |
| C | 1.533673 | 2.741486 | 0.115022 |
| H | 2.393398 | 2.073681 | 0.172772 |
| H | 1.185757 | 2.771440 | -0.918576 |
| C | 1.890987 | 4.130481 | 0.612812 |
| H | 2.343707 | 4.098140 | 1.603813 |
| H | 1.029609 | 4.799595 | 0.638663 |
| H | 2.622007 | 4.557953 | -0.073804 |
| C | 0.768886 | 2.019389 | 2.376284 |
| H | 1.831699 | 1.776164 | 2.433413 |
| H | 0.604557 | 3.013984 | 2.792210 |
| C | -0.052360 | 0.957187 | 3.087579 |
| H | 0.276294 | 0.904092 | 4.125999 |
| H | 0.108169 | -0.016960 | 2.623444 |
| H | -1.120356 | 1.179997 | 3.092151 |
| C | -2.992194 | 2.141793 | -0.856261 |

| | | | |
|---|---|---|---|
| C | -3.189856 | 3.661746 | -0.916091 |
| H | -3.067151 | 4.129433 | 0.064181 |
| H | -4.200237 | 3.888463 | -1.264566 |
| H | -2.482231 | 4.123608 | -1.611650 |
| C | -3.894874 | 1.549637 | 0.233817 |
| H | -3.872477 | 0.455687 | 0.228713 |
| H | -4.928551 | 1.851169 | 0.047246 |
| H | -3.630347 | 1.898707 | 1.235479 |
| C | -3.386003 | 1.532611 | -2.206925 |
| H | -2.812664 | 1.984913 | -3.021700 |
| H | -4.446361 | 1.711887 | -2.402106 |
| H | -3.215922 | 0.452491 | -2.219072 |
| C | -0.886339 | -0.505244 | -1.394584 |
| C | -0.060337 | 0.069879 | -2.510779 |
| H | -0.658703 | 0.685665 | -3.188300 |
| H | 0.421465 | -0.710812 | -3.091653 |
| H | 0.730725 | 0.699410 | -2.094381 |
| C | -1.231215 | -1.802280 | -1.293816 |
| C | -0.885333 | -2.877705 | -2.292015 |
| H | -0.151156 | -3.575947 | -1.875138 |
| H | -0.491312 | -2.484678 | -3.227305 |
| H | -1.777171 | -3.464265 | -2.532799 |
| C | -1.964437 | -2.278524 | -0.083579 |
| C | -3.289822 | -2.716066 | -0.166134 |
| C | -1.327609 | -2.293524 | 1.163124 |
| C | -3.968416 | -3.145359 | 0.970646 |
| H | -3.793746 | -2.707286 | -1.127551 |
| C | -2.006377 | -2.721693 | 2.300697 |
| H | -0.297811 | -1.950925 | 1.223011 |
| C | -3.328930 | -3.147319 | 2.207126 |
| H | -4.998012 | -3.474894 | 0.892182 |
| H | -1.501553 | -2.723757 | 3.260220 |
| H | -3.858633 | -3.478561 | 3.092582 |

**6J-*E***

Imaginary frequency: None

Electronic energies: -1853.977355

Free energies: -1853.493005

Corrected Free energies: -1853.484442

| | | | |
|---|---|---|---|
| S | -1.184518 | -2.600269 | 0.692401 |
| F | -0.877890 | -2.586385 | -1.913538 |
| F | -2.531528 | -3.793000 | -1.225974 |
| F | -2.694845 | -1.640514 | -1.235100 |

| | | | |
|---|---|---|---|
| O | -0.503954 | -1.294670 | 0.707437 |
| O | -0.272900 | -3.744528 | 0.735854 |
| O | -2.363261 | -2.686112 | 1.544881 |
| C | -1.867023 | -2.660815 | -1.020726 |
| N | 1.254933 | 1.374367 | 0.391513 |
| H | 1.455702 | 1.793775 | 1.288767 |
| N | 2.290978 | -1.213542 | 0.383633 |
| H | 1.330103 | -0.843405 | 0.516938 |
| C | 2.441158 | 1.124943 | -0.411832 |
| H | 2.113060 | 0.785242 | -1.396490 |
| C | 3.196816 | -0.029621 | 0.258535 |
| H | 4.078748 | -0.334109 | -0.300598 |
| H | 3.507693 | 0.255374 | 1.263142 |
| C | 2.233747 | -2.047526 | -0.867895 |
| H | 1.368968 | -2.698109 | -0.744323 |
| H | 2.034516 | -1.362791 | -1.693220 |
| C | 3.488636 | -2.863705 | -1.119223 |
| H | 3.646310 | -3.612047 | -0.342434 |
| H | 4.384178 | -2.247222 | -1.205039 |
| H | 3.360400 | -3.389710 | -2.065511 |
| C | 2.559431 | -2.051466 | 1.602719 |
| H | 2.015273 | -2.984473 | 1.449104 |
| H | 3.629674 | -2.258838 | 1.628586 |
| C | 2.075976 | -1.363445 | 2.867035 |
| H | 2.225099 | -2.041490 | 3.707671 |
| H | 1.011152 | -1.136746 | 2.791393 |
| H | 2.621888 | -0.444262 | 3.083262 |
| C | 3.329658 | 2.376877 | -0.655648 |
| C | 4.532145 | 1.996243 | -1.528903 |
| H | 5.258941 | 1.388046 | -0.985591 |
| H | 5.047603 | 2.901221 | -1.859091 |
| H | 4.214945 | 1.445521 | -2.419836 |
| C | 3.827908 | 2.986621 | 0.659077 |
| H | 3.001775 | 3.311044 | 1.298153 |
| H | 4.432120 | 3.870885 | 0.441693 |
| H | 4.455271 | 2.293994 | 1.225803 |
| C | 2.482640 | 3.414419 | -1.402223 |
| H | 2.157598 | 3.028110 | -2.372874 |
| H | 3.071189 | 4.317510 | -1.581101 |
| H | 1.595070 | 3.694324 | -0.828496 |
| C | -0.026421 | 1.640904 | -0.106670 |
| C | -0.338841 | 1.031311 | -1.445125 |
| H | 0.291572 | 1.469651 | -2.223790 |
| H | -1.373710 | 1.210173 | -1.721667 |

| | | | |
|---|---|---|---|
| H | -0.167697 | -0.048558 | -1.431868 |
| C | -0.893812 | 2.375308 | 0.623886 |
| C | -2.340969 | 2.441935 | 0.300604 |
| C | -3.010490 | 3.668519 | 0.214561 |
| C | -3.086794 | 1.269208 | 0.126976 |
| C | -4.372083 | 3.722362 | -0.063433 |
| H | -2.454240 | 4.589903 | 0.354016 |
| C | -4.447007 | 1.320548 | -0.159255 |
| H | -2.580745 | 0.314463 | 0.222960 |
| C | -5.096009 | 2.548210 | -0.256601 |
| H | -4.868494 | 4.683373 | -0.136126 |
| H | -5.000328 | 0.397998 | -0.295335 |
| H | -6.156559 | 2.590424 | -0.474823 |
| C | -0.443472 | 3.063153 | 1.894955 |
| H | -0.280848 | 2.346252 | 2.709660 |
| H | 0.489386 | 3.619716 | 1.753261 |
| H | -1.196568 | 3.770968 | 2.240594 |

**6J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1853.791052

Free energies: -1853.300724

Corrected Free energies: -1853.294058

| | | | |
|---|---|---|---|
| S | -1.100164 | -2.318678 | 0.635392 |
| F | -0.465260 | -2.832989 | -1.855312 |
| F | -2.120289 | -3.999285 | -1.102213 |
| F | -2.402405 | -1.917682 | -1.605015 |
| O | -0.481231 | -0.986061 | 0.423424 |
| O | -0.129133 | -3.328274 | 1.048349 |
| O | -2.368867 | -2.284723 | 1.343523 |
| C | -1.551859 | -2.802432 | -1.086764 |
| N | 1.102971 | 1.640132 | 0.264108 |
| H | 1.239437 | 1.948544 | 1.222231 |
| N | 2.272370 | -1.129882 | 0.592025 |
| H | 1.248562 | -0.936383 | 0.621671 |
| C | 2.329477 | 1.187382 | -0.405764 |
| H | 2.040543 | 0.709073 | -1.341859 |
| C | 3.008953 | 0.168664 | 0.512670 |
| H | 4.016995 | -0.050690 | 0.171770 |
| H | 3.083440 | 0.565980 | 1.524942 |
| C | 2.459024 | -2.000932 | -0.626355 |
| H | 1.747763 | -2.816193 | -0.498112 |
| H | 2.147086 | -1.415840 | -1.491668 |

| | | | |
|---|---|---|---|
| C | 3.870989 | -2.528290 | -0.799698 |
| H | 4.189243 | -3.130683 | 0.051270 |
| H | 4.600967 | -1.737056 | -0.972604 |
| H | 3.875470 | -3.171138 | -1.680252 |
| C | 2.592592 | -1.876225 | 1.863269 |
| H | 2.280733 | -2.905935 | 1.693483 |
| H | 3.674422 | -1.842337 | 1.995424 |
| C | 1.848944 | -1.292911 | 3.050368 |
| H | 2.072465 | -1.898269 | 3.928804 |
| H | 0.771492 | -1.322884 | 2.881974 |
| H | 2.144776 | -0.267229 | 3.273187 |
| C | 3.259943 | 2.390568 | -0.752275 |
| C | 4.493174 | 1.866278 | -1.501904 |
| H | 5.189863 | 1.338098 | -0.848615 |
| H | 5.033360 | 2.713049 | -1.930112 |
| H | 4.208954 | 1.201368 | -2.322833 |
| C | 3.698319 | 3.138928 | 0.511252 |
| H | 2.850655 | 3.576760 | 1.046178 |
| H | 4.355231 | 3.963132 | 0.226226 |
| H | 4.257636 | 2.501000 | 1.199488 |
| C | 2.506466 | 3.352235 | -1.678259 |
| H | 2.267653 | 2.874149 | -2.631913 |
| H | 3.140644 | 4.214688 | -1.892160 |
| H | 1.584251 | 3.726759 | -1.226426 |
| C | -0.127219 | 1.723699 | -0.222663 |
| C | -0.385745 | 1.295463 | -1.633416 |
| H | 0.377636 | 1.701563 | -2.295628 |
| H | -1.353247 | 1.651972 | -1.971925 |
| H | -0.365875 | 0.205221 | -1.701623 |
| C | -1.131096 | 2.300561 | 0.616437 |
| C | -2.545186 | 2.188357 | 0.295137 |
| C | -3.422288 | 3.258608 | 0.550551 |
| C | -3.070903 | 0.992323 | -0.225993 |
| C | -4.771688 | 3.142718 | 0.257294 |
| H | -3.039222 | 4.193756 | 0.940906 |
| C | -4.425731 | 0.872843 | -0.487936 |
| H | -2.412777 | 0.147017 | -0.369903 |
| C | -5.278095 | 1.950602 | -0.257771 |
| H | -5.432922 | 3.981793 | 0.433814 |
| H | -4.815914 | -0.063967 | -0.867094 |
| H | -6.335986 | 1.860826 | -0.472544 |
| C | -0.712785 | 3.008777 | 1.866527 |
| H | -0.333634 | 2.279241 | 2.594123 |
| H | 0.073421 | 3.745985 | 1.681091 |

| | | | |
|---|---|---|---|
| H | -1.554135 | 3.504496 | 2.341735 |

**6J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1853.793112

Free energies: -1853.304217

Corrected Free energies: -1853.297121

| | | | |
|---|---|---|---|
| S | 2.703064 | -0.237477 | 0.397226 |
| F | 3.212342 | 1.957197 | -0.929311 |
| F | 4.946300 | 0.716362 | -0.580385 |
| F | 3.490577 | 0.146934 | -2.070912 |
| O | 1.318318 | -0.095001 | -0.110436 |
| O | 2.931358 | 0.496270 | 1.639215 |
| O | 3.224146 | -1.594520 | 0.324189 |
| C | 3.653579 | 0.702313 | -0.872891 |
| N | -1.654890 | 0.008980 | -0.659648 |
| H | -1.907068 | -0.653770 | 0.071154 |
| N | -0.290194 | 1.645493 | 1.295402 |
| H | 0.131394 | 0.888125 | 0.720855 |
| C | -2.111489 | 1.385411 | -0.436328 |
| H | -1.563212 | 2.038699 | -1.117382 |
| C | -1.757206 | 1.742205 | 1.011163 |
| H | -2.073783 | 2.756041 | 1.243664 |
| H | -2.267065 | 1.069121 | 1.699353 |
| C | 0.485862 | 2.874302 | 0.889682 |
| H | 1.533720 | 2.578659 | 0.951025 |
| H | 0.248357 | 3.063093 | -0.158044 |
| C | 0.210482 | 4.090595 | 1.752668 |
| H | 0.479128 | 3.916981 | 2.794808 |
| H | -0.827694 | 4.419827 | 1.701636 |
| H | 0.830407 | 4.906840 | 1.381412 |
| C | -0.018482 | 1.243083 | 2.723400 |
| H | 1.031648 | 1.469665 | 2.904628 |
| H | -0.642151 | 1.866563 | 3.364212 |
| C | -0.275865 | -0.239583 | 2.931213 |
| H | -0.001632 | -0.499556 | 3.953743 |
| H | 0.336696 | -0.838310 | 2.253651 |
| H | -1.323692 | -0.516188 | 2.795274 |
| C | -3.631753 | 1.537695 | -0.738810 |
| C | -4.052900 | 2.985896 | -0.457702 |
| H | -4.091699 | 3.204409 | 0.611082 |
| H | -5.054203 | 3.150984 | -0.860512 |
| H | -3.375466 | 3.697828 | -0.937867 |

| | | | |
|---|---|---|---|
| C | -4.474069 | 0.577522 | 0.109538 |
| H | -4.220712 | -0.469681 | -0.078981 |
| H | -5.526399 | 0.705735 | -0.151701 |
| H | -4.381715 | 0.774029 | 1.179728 |
| C | -3.862589 | 1.234209 | -2.223639 |
| H | -3.334507 | 1.948409 | -2.861048 |
| H | -4.928056 | 1.316246 | -2.447090 |
| H | -3.547181 | 0.221428 | -2.488826 |
| C | -0.872919 | -0.462700 | -1.621027 |
| C | -0.410474 | 0.427960 | -2.725324 |
| H | -1.148683 | 1.182504 | -2.982713 |
| H | -0.186610 | -0.156610 | -3.614495 |
| H | 0.511614 | 0.923490 | -2.400861 |
| C | -0.367977 | -1.788779 | -1.501281 |
| C | 0.738929 | -2.233513 | -2.394121 |
| H | 1.494335 | -1.455051 | -2.516450 |
| H | 0.340224 | -2.473610 | -3.387218 |
| H | 1.207119 | -3.133397 | -2.000882 |
| C | -0.825518 | -2.665350 | -0.417537 |
| C | -2.188248 | -2.933279 | -0.219513 |
| C | 0.122140 | -3.226409 | 0.450804 |
| C | -2.595563 | -3.741738 | 0.834385 |
| H | -2.920944 | -2.539419 | -0.917030 |
| C | -0.295799 | -4.016140 | 1.512986 |
| H | 1.175336 | -3.005582 | 0.309966 |
| C | -1.650964 | -4.275812 | 1.706138 |
| H | -3.648034 | -3.957056 | 0.970421 |
| H | 0.437892 | -4.429341 | 2.194315 |
| H | -1.969393 | -4.898552 | 2.533158 |

**7J-*Z***

Imaginary frequency: None

Electronic energies: -812.107467

Free energies: -811.724519

Corrected Free energies: -811.720914

| | | | |
|---|---|---|---|
| N | 0.097144 | -0.498014 | -0.589474 |
| C | -0.800392 | -1.577450 | -0.592887 |
| C | -2.126744 | -1.406529 | -0.406508 |
| C | -3.188087 | -2.462599 | -0.598819 |
| H | -3.942863 | -2.122090 | -1.314946 |
| H | -3.713751 | -2.652181 | 0.342860 |
| H | -0.347534 | 0.391400 | -0.397373 |
| C | 1.376637 | -0.616035 | 0.103804 |

| | | | |
|---|---|---|---|
| C | 2.192632 | 0.675723 | -0.065115 |
| C | 1.233173 | -0.928574 | 1.600453 |
| H | 1.939564 | -1.436630 | -0.357017 |
| C | 3.581405 | 0.478669 | 0.572656 |
| H | 1.674022 | 1.456425 | 0.511990 |
| C | 2.598290 | -1.119962 | 2.260916 |
| H | 0.705245 | -0.095151 | 2.080364 |
| H | 0.608549 | -1.818140 | 1.729103 |
| C | 3.467439 | 0.121571 | 2.057282 |
| H | 4.172218 | 1.390817 | 0.456653 |
| H | 4.114459 | -0.321701 | 0.046356 |
| H | 2.478637 | -1.333579 | 3.326006 |
| H | 3.095298 | -1.989070 | 1.813326 |
| H | 4.461694 | -0.030757 | 2.484935 |
| H | 3.015651 | 0.965156 | 2.592899 |
| N | 2.192054 | 1.151159 | -1.450228 |
| C | 2.808156 | 2.459005 | -1.597655 |
| H | 3.906226 | 2.444608 | -1.506367 |
| H | 2.563601 | 2.862926 | -2.583231 |
| H | 2.411713 | 3.140679 | -0.841384 |
| C | 2.731019 | 0.208024 | -2.415950 |
| H | 2.630807 | 0.636419 | -3.415963 |
| H | 3.796689 | -0.024405 | -2.257793 |
| H | 2.158182 | -0.720249 | -2.394782 |
| H | -2.797082 | -3.410951 | -0.961078 |
| C | -2.661587 | -0.075040 | 0.008498 |
| C | -3.517278 | 0.656129 | -0.821919 |
| C | -2.342630 | 0.458354 | 1.262937 |
| C | -4.028562 | 1.885862 | -0.416837 |
| H | -3.776540 | 0.260740 | -1.798647 |
| C | -2.850475 | 1.687329 | 1.670630 |
| H | -1.693152 | -0.109135 | 1.921250 |
| C | -3.695937 | 2.406310 | 0.830154 |
| H | -4.685065 | 2.440068 | -1.077782 |
| H | -2.591310 | 2.080500 | 2.646940 |
| H | -4.093850 | 3.363378 | 1.146059 |
| C | -0.147893 | -2.893159 | -0.929614 |
| H | 0.492140 | -3.232040 | -0.109743 |
| H | -0.871326 | -3.678391 | -1.125756 |
| H | 0.488378 | -2.776411 | -1.811123 |

**7J-*E***

Imaginary frequency: None

Electronic energies: -812.108530

Free energies: -811.724986

Corrected Free energies: -811.721601

| | | | |
|---|---|---|---|
| N | -0.557704 | -0.388525 | 0.231109 |
| C | 0.747437 | -0.111893 | -0.170955 |
| C | 1.775698 | -0.142995 | 0.710121 |
| H | -0.661805 | -0.647363 | 1.202267 |
| C | -1.694463 | 0.376144 | -0.266273 |
| C | -2.999743 | -0.178536 | 0.326014 |
| C | -1.596143 | 1.877049 | 0.045127 |
| H | -1.740190 | 0.259003 | -1.355532 |
| C | -4.191197 | 0.566617 | -0.303874 |
| H | -2.991063 | 0.065984 | 1.398946 |
| C | -2.776586 | 2.642924 | -0.551715 |
| H | -1.577224 | 2.002497 | 1.134907 |
| H | -0.648184 | 2.268364 | -0.335459 |
| C | -4.101487 | 2.072946 | -0.043917 |
| H | -5.127571 | 0.176741 | 0.103063 |
| H | -4.206469 | 0.383568 | -1.384498 |
| H | -2.699661 | 3.706317 | -0.311791 |
| H | -2.741530 | 2.558564 | -1.644693 |
| H | -4.944080 | 2.586009 | -0.514404 |
| H | -4.179290 | 2.253962 | 1.034737 |
| N | -3.054035 | -1.640919 | 0.260833 |
| C | -4.199467 | -2.192420 | 0.965387 |
| H | -5.156561 | -2.038700 | 0.441677 |
| H | -4.059998 | -3.268817 | 1.092317 |
| H | -4.276295 | -1.739116 | 1.956606 |
| C | -2.950189 | -2.191455 | -1.080898 |
| H | -2.936982 | -3.281516 | -1.011277 |
| H | -3.788193 | -1.908920 | -1.738575 |
| H | -2.013532 | -1.876177 | -1.542960 |
| C | 3.197252 | -0.097515 | 0.284432 |
| C | 3.702827 | -0.974324 | -0.684511 |
| C | 4.090558 | 0.808185 | 0.873693 |
| C | 5.038579 | -0.929688 | -1.071109 |
| H | 3.035572 | -1.703719 | -1.131310 |
| C | 5.426441 | 0.853295 | 0.492719 |
| H | 3.725386 | 1.497413 | 1.628155 |
| C | 5.907289 | -0.014569 | -0.485024 |
| H | 5.403621 | -1.619478 | -1.823599 |
| H | 6.093798 | 1.571130 | 0.955951 |
| H | 6.948827 | 0.019214 | -0.782085 |
| C | 1.510604 | -0.305709 | 2.192398 |

| | | | |
|---|---|---|---|
| H | 0.686864 | 0.330387 | 2.530821 |
| H | 1.253616 | -1.340710 | 2.449074 |
| H | 2.393190 | -0.044703 | 2.776461 |
| C | 0.898075 | 0.159455 | -1.646064 |
| H | 1.924890 | 0.404460 | -1.903224 |
| H | 0.584099 | -0.711247 | -2.229982 |
| H | 0.268028 | 0.997899 | -1.952500 |

**7J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -811.932312

Free energies: -811.547106

Corrected Free energies: -811.544235

| | | | |
|---|---|---|---|
| N | -0.539382 | 0.111205 | 0.447569 |
| C | 0.680586 | 0.429966 | 0.061935 |
| C | 1.776488 | -0.210658 | 0.716191 |
| H | -0.654022 | -0.686893 | 1.067556 |
| C | -1.807653 | 0.642748 | -0.057063 |
| C | -2.888855 | -0.420635 | 0.198473 |
| C | -2.210117 | 1.958266 | 0.626376 |
| H | -1.697157 | 0.814182 | -1.131939 |
| C | -4.206624 | 0.055450 | -0.427130 |
| H | -3.033981 | -0.458099 | 1.286984 |
| C | -3.541681 | 2.444873 | 0.047830 |
| H | -2.306663 | 1.775382 | 1.701563 |
| H | -1.436272 | 2.716712 | 0.495789 |
| C | -4.636593 | 1.386802 | 0.195838 |
| H | -4.979595 | -0.702093 | -0.276239 |
| H | -4.078778 | 0.181118 | -1.508170 |
| H | -3.835255 | 3.370655 | 0.546565 |
| H | -3.404228 | 2.681321 | -1.013263 |
| H | -5.561911 | 1.736509 | -0.266808 |
| H | -4.848101 | 1.232875 | 1.259937 |
| N | -2.407340 | -1.749382 | -0.176759 |
| C | -3.209644 | -2.816114 | 0.408740 |
| H | -4.221092 | -2.879533 | -0.020014 |
| H | -2.711954 | -3.772226 | 0.236907 |
| H | -3.297197 | -2.663011 | 1.485900 |
| C | -2.251854 | -1.949297 | -1.612779 |
| H | -1.765874 | -2.911581 | -1.782370 |
| H | -3.211705 | -1.952817 | -2.149665 |
| H | -1.615918 | -1.174429 | -2.045494 |
| C | 3.146038 | -0.075732 | 0.233419 |

| | | | |
|---|---|---|---|
| C | 3.455787 | -0.120460 | -1.137458 |
| C | 4.197945 | 0.057921 | 1.156965 |
| C | 4.771385 | -0.029639 | -1.565084 |
| H | 2.668288 | -0.270121 | -1.865561 |
| C | 5.508336 | 0.177105 | 0.721901 |
| H | 3.981165 | 0.105261 | 2.217150 |
| C | 5.799877 | 0.128364 | -0.639204 |
| H | 4.995414 | -0.087249 | -2.622937 |
| H | 6.303945 | 0.303811 | 1.445416 |
| H | 6.825611 | 0.207642 | -0.977928 |
| C | 1.505118 | -1.042666 | 1.931728 |
| H | 0.925918 | -0.495669 | 2.680204 |
| H | 0.932187 | -1.935639 | 1.651190 |
| H | 2.427206 | -1.396436 | 2.383939 |
| C | 0.843808 | 1.471958 | -1.003175 |
| H | 1.844207 | 1.893951 | -0.984961 |
| H | 0.666848 | 1.029893 | -1.988225 |
| H | 0.121877 | 2.274207 | -0.866214 |

**7J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -811.935572

Free energies: -811.550906

Corrected Free energies: -811.547830

| | | | |
|---|---|---|---|
| N | 0.265881 | -0.794334 | 0.036962 |
| C | -0.499018 | -1.786015 | -0.365506 |
| C | -1.913699 | -1.689449 | -0.177805 |
| C | -2.741894 | -2.932047 | -0.114853 |
| H | -3.714022 | -2.771597 | -0.582120 |
| H | -2.921525 | -3.197731 | 0.934123 |
| H | -0.188995 | 0.035106 | 0.421351 |
| C | 1.714715 | -0.623667 | -0.113161 |
| C | 2.032058 | 0.827181 | 0.292605 |
| C | 2.540340 | -1.586994 | 0.748100 |
| H | 1.963047 | -0.778769 | -1.169142 |
| C | 3.513009 | 1.107704 | 0.013803 |
| H | 1.881196 | 0.880591 | 1.379241 |
| C | 4.031931 | -1.311090 | 0.528929 |
| H | 2.274116 | -1.429422 | 1.798465 |
| H | 2.309428 | -2.624777 | 0.504536 |
| C | 4.388100 | 0.146993 | 0.824548 |
| H | 3.746193 | 2.144119 | 0.270460 |
| H | 3.718270 | 0.981051 | -1.054925 |

| | | | |
|---|---|---|---|
| H | 4.619582 | -1.981329 | 1.159370 |
| H | 4.287616 | -1.544446 | -0.510900 |
| H | 5.443116 | 0.326588 | 0.607508 |
| H | 4.241905 | 0.345577 | 1.892223 |
| N | 1.050405 | 1.747545 | -0.281879 |
| C | 1.020480 | 3.035472 | 0.399806 |
| H | 1.922434 | 3.637938 | 0.215788 |
| H | 0.156899 | 3.604298 | 0.049028 |
| H | 0.915814 | 2.881261 | 1.475170 |
| C | 1.163977 | 1.926840 | -1.724114 |
| H | 0.312911 | 2.516295 | -2.072726 |
| H | 2.084003 | 2.451908 | -2.018389 |
| H | 1.136792 | 0.963068 | -2.237883 |
| H | -2.256021 | -3.785637 | -0.581012 |
| C | -2.568053 | -0.400633 | 0.031586 |
| C | -2.156307 | 0.752907 | -0.663022 |
| C | -3.681694 | -0.308705 | 0.885557 |
| C | -2.819031 | 1.958184 | -0.485067 |
| H | -1.338018 | 0.696652 | -1.371080 |
| C | -4.329144 | 0.902489 | 1.070834 |
| H | -4.023005 | -1.185391 | 1.422411 |
| C | -3.899330 | 2.039461 | 0.388948 |
| H | -2.498638 | 2.831965 | -1.039621 |
| H | -5.172772 | 0.961268 | 1.747214 |
| H | -4.411869 | 2.983044 | 0.530739 |
| C | 0.118310 | -3.002329 | -0.982826 |
| H | 0.223478 | -3.789632 | -0.230966 |
| H | -0.516459 | -3.378411 | -1.782750 |
| H | 1.102013 | -2.783877 | -1.391868 |

**8J-*Z***

Imaginary frequency: None

Electronic energies: -1118.117646

Free energies: -1117.672990

Corrected Free energies: -1117.667261

| | | | |
|---|---|---|---|
| N | 0.765080 | 1.013369 | 0.369545 |
| C | 1.532621 | 1.877081 | -0.441653 |
| C | 2.843844 | 1.653747 | -0.677013 |
| C | 3.761584 | 2.576002 | -1.443395 |
| H | 4.263452 | 2.034144 | -2.250361 |
| H | 4.550398 | 2.958495 | -0.786891 |
| H | 1.288627 | 0.190744 | 0.654457 |
| C | -0.531140 | 0.554896 | -0.130829 |

| | | | |
|---|---|---|---|
| C | -0.814810 | -0.823935 | 0.522110 |
| H | -0.505787 | 0.434571 | -1.222676 |
| H | -1.001832 | -0.620386 | 1.582698 |
| N | 0.382533 | -1.674115 | 0.508764 |
| C | 0.241972 | -2.840101 | 1.367090 |
| H | -0.480350 | -3.573007 | 0.974507 |
| H | 1.213242 | -3.330503 | 1.462073 |
| H | -0.087585 | -2.530181 | 2.361134 |
| C | 0.880564 | -2.051160 | -0.806860 |
| H | 1.859082 | -2.520636 | -0.681735 |
| H | 0.220311 | -2.757203 | -1.332579 |
| H | 1.022677 | -1.164621 | -1.430631 |
| C | -1.675144 | 1.496922 | 0.204936 |
| C | -1.753841 | 2.090457 | 1.464534 |
| C | -2.683491 | 1.746401 | -0.723742 |
| C | -2.823984 | 2.917152 | 1.789974 |
| H | -0.957890 | 1.912798 | 2.179474 |
| C | -3.756743 | 2.572717 | -0.401535 |
| H | -2.625214 | 1.293722 | -1.708821 |
| C | -3.830031 | 3.159744 | 0.857526 |
| H | -2.873237 | 3.375184 | 2.771175 |
| H | -4.532092 | 2.759870 | -1.135367 |
| H | -4.663009 | 3.804974 | 1.110491 |
| C | -2.069414 | -1.476304 | -0.038349 |
| C | -3.052921 | -1.934250 | 0.839665 |
| C | -2.266615 | -1.659765 | -1.410720 |
| C | -4.205433 | -2.555568 | 0.367652 |
| H | -2.915359 | -1.794300 | 1.907477 |
| C | -3.415614 | -2.282631 | -1.887032 |
| H | -1.529085 | -1.303940 | -2.121329 |
| C | -4.389506 | -2.731829 | -0.999548 |
| H | -4.958915 | -2.898599 | 1.066998 |
| H | -3.553329 | -2.412156 | -2.954216 |
| H | -5.286512 | -3.211674 | -1.372478 |
| H | 3.252647 | 3.427000 | -1.889236 |
| C | 3.523247 | 0.434879 | -0.142957 |
| C | 3.598242 | 0.176874 | 1.229906 |
| C | 4.124265 | -0.477089 | -1.018957 |
| C | 4.222489 | -0.970236 | 1.711605 |
| H | 3.152969 | 0.881608 | 1.924936 |
| C | 4.753618 | -1.621031 | -0.541892 |
| H | 4.077890 | -0.296744 | -2.087966 |
| C | 4.799997 | -1.875460 | 0.826729 |
| H | 4.260783 | -1.153950 | 2.779091 |

| | | | |
|---|---|---|---|
| H | 5.200324 | -2.320222 | -1.239635 |
| H | 5.285597 | -2.769428 | 1.199668 |
| C | 0.762437 | 3.062525 | -0.959280 |
| H | -0.016586 | 2.743043 | -1.657999 |
| H | 0.255243 | 3.562078 | -0.129792 |
| H | 1.393089 | 3.784303 | -1.468433 |

**8J-*E***

Imaginary frequency: None

Electronic energies: -1118.117917

Free energies: -1117.672869

Corrected Free energies: -1117.667534

| | | | |
|---|---|---|---|
| N | -0.550040 | -0.218435 | -0.685387 |
| C | -1.788699 | 0.092951 | -0.118207 |
| C | -2.859104 | -0.701959 | -0.356693 |
| H | -0.508634 | -1.131289 | -1.124118 |
| C | 0.707601 | 0.048324 | -0.001637 |
| C | 1.773497 | -0.884027 | -0.633743 |
| H | 0.629041 | -0.172372 | 1.071295 |
| H | 1.918073 | -0.517892 | -1.656582 |
| N | 1.254791 | -2.250360 | -0.793316 |
| C | 2.107386 | -3.060744 | -1.651672 |
| H | 3.078159 | -3.293697 | -1.187080 |
| H | 1.598844 | -4.000904 | -1.873958 |
| H | 2.291443 | -2.535818 | -2.591354 |
| C | 0.944832 | -2.955610 | 0.443261 |
| H | 0.412697 | -3.875966 | 0.192779 |
| H | 1.840080 | -3.227547 | 1.020930 |
| H | 0.288323 | -2.351826 | 1.074537 |
| C | 1.169595 | 1.489588 | -0.148304 |
| C | 1.026910 | 2.151422 | -1.367471 |
| C | 1.775269 | 2.155326 | 0.915701 |
| C | 1.486340 | 3.454939 | -1.521710 |
| H | 0.535154 | 1.640935 | -2.188407 |
| C | 2.237311 | 3.459902 | 0.764591 |
| H | 1.884853 | 1.650277 | 1.870543 |
| C | 2.094290 | 4.113251 | -0.455360 |
| H | 1.366572 | 3.959296 | -2.473628 |
| H | 2.704692 | 3.966476 | 1.600990 |
| H | 2.450536 | 5.129654 | -0.573861 |
| C | 3.115606 | -0.784425 | 0.073501 |
| C | 4.264998 | -0.526172 | -0.674526 |
| C | 3.247547 | -0.967561 | 1.453466 |

| | | | |
|---|---|---|---|
| C | 5.515274 | -0.451002 | -0.067684 |
| H | 4.176586 | -0.375757 | -1.746030 |
| C | 4.495831 | -0.897980 | 2.063755 |
| H | 2.373232 | -1.155823 | 2.066356 |
| C | 5.633807 | -0.639090 | 1.305095 |
| H | 6.394114 | -0.241751 | -0.666254 |
| H | 4.578450 | -1.041124 | 3.134800 |
| H | 6.604888 | -0.579547 | 1.782090 |
| C | -4.241393 | -0.327887 | 0.030166 |
| C | -4.781361 | 0.923961 | -0.292348 |
| C | -5.070510 | -1.243204 | 0.693828 |
| C | -6.085741 | 1.259201 | 0.056664 |
| H | -4.169606 | 1.635838 | -0.835846 |
| C | -6.375660 | -0.913127 | 1.040704 |
| H | -4.679699 | -2.221835 | 0.952647 |
| C | -6.889969 | 0.342018 | 0.725918 |
| H | -6.477628 | 2.234847 | -0.207296 |
| H | -6.992015 | -1.636853 | 1.561617 |
| H | -7.907907 | 0.599216 | 0.993902 |
| C | -2.681289 | -2.002455 | -1.114761 |
| H | -2.433919 | -1.822399 | -2.168215 |
| H | -1.878089 | -2.618088 | -0.694960 |
| H | -3.595883 | -2.594230 | -1.097912 |
| C | -1.818987 | 1.342357 | 0.720250 |
| H | -1.050024 | 1.295198 | 1.495977 |
| H | -1.603219 | 2.227594 | 0.114982 |
| H | -2.782654 | 1.468983 | 1.206291 |

**8J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1117.937363

Free energies: -1117.492776

Corrected Free energies: -1117.487158

| | | | |
|---|---|---|---|
| N | -0.508243 | -0.564862 | -0.111357 |
| C | -1.704073 | -0.157196 | 0.266218 |
| C | -2.827629 | -0.924572 | -0.171141 |
| H | -0.396581 | -1.431694 | -0.649127 |
| C | 0.795943 | -0.025865 | 0.279349 |
| C | 1.846427 | -0.870798 | -0.487662 |
| H | 0.905422 | -0.165543 | 1.359397 |
| H | 1.792627 | -0.536964 | -1.529398 |
| N | 1.433651 | -2.281174 | -0.517852 |
| C | 2.138923 | -3.033384 | -1.551243 |

| | | | |
|---|---|---|---|
| H | 3.210067 | -3.143487 | -1.328846 |
| H | 1.697411 | -4.027963 | -1.627902 |
| H | 2.030571 | -2.529744 | -2.513388 |
| C | 1.506052 | -2.971837 | 0.767074 |
| H | 1.047809 | -3.955653 | 0.655442 |
| H | 2.538250 | -3.106266 | 1.117107 |
| H | 0.945542 | -2.427038 | 1.530423 |
| C | 0.955088 | 1.444105 | -0.049219 |
| C | 0.546845 | 1.939266 | -1.287537 |
| C | 1.548855 | 2.300906 | 0.873713 |
| C | 0.722822 | 3.283734 | -1.593820 |
| H | 0.080833 | 1.277000 | -2.010549 |
| C | 1.732168 | 3.644844 | 0.563529 |
| H | 1.865985 | 1.917334 | 1.837991 |
| C | 1.317220 | 4.138228 | -0.668873 |
| H | 0.396229 | 3.663509 | -2.554333 |
| H | 2.193500 | 4.306191 | 1.286848 |
| H | 1.454430 | 5.185813 | -0.907856 |
| C | 3.259468 | -0.605796 | -0.000369 |
| C | 4.264298 | -0.380099 | -0.942294 |
| C | 3.601916 | -0.620679 | 1.354772 |
| C | 5.582450 | -0.177646 | -0.546349 |
| H | 4.009909 | -0.360068 | -1.997343 |
| C | 4.918729 | -0.416956 | 1.753659 |
| H | 2.846952 | -0.791868 | 2.114539 |
| C | 5.912455 | -0.196442 | 0.804479 |
| H | 6.348554 | -0.003203 | -1.292367 |
| H | 5.167532 | -0.430070 | 2.808110 |
| H | 6.937287 | -0.037355 | 1.117603 |
| C | -4.193792 | -0.457691 | 0.020234 |
| C | -4.542907 | 0.892229 | -0.166093 |
| C | -5.205897 | -1.374900 | 0.355723 |
| C | -5.857125 | 1.306249 | -0.016809 |
| H | -3.789583 | 1.607845 | -0.472221 |
| C | -6.512850 | -0.949486 | 0.531447 |
| H | -4.958872 | -2.417286 | 0.515662 |
| C | -6.843429 | 0.390229 | 0.341321 |
| H | -6.113581 | 2.344689 | -0.185276 |
| H | -7.276450 | -1.663574 | 0.813363 |
| H | -7.867918 | 0.719049 | 0.465520 |
| C | -2.580779 | -2.239752 | -0.843604 |
| H | -2.084887 | -2.075520 | -1.808000 |
| H | -1.935725 | -2.889699 | -0.244420 |
| H | -3.510429 | -2.760606 | -1.052915 |

| | | | |
|---|---|---|---|
| C | -1.806854 | 1.015292 | 1.192394 |
| H | -1.005874 | 0.969041 | 1.931711 |
| H | -1.689071 | 1.954678 | 0.645093 |
| H | -2.763747 | 1.018813 | 1.706187 |

**8J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1117.938412

Free energies: -1117.492964

Corrected Free energies: -1117.487714

| | | | |
|---|---|---|---|
| N | 0.845817 | 0.486609 | -0.523763 |
| C | 1.649148 | 1.489003 | -0.821591 |
| C | 3.051087 | 1.329666 | -0.620559 |
| C | 3.984662 | 2.377399 | -1.138257 |
| H | 4.997778 | 2.205133 | -0.783957 |
| H | 3.667113 | 3.367758 | -0.801736 |
| H | 1.238433 | -0.435761 | -0.288040 |
| C | -0.615050 | 0.418428 | -0.587532 |
| C | -0.986141 | -0.918186 | 0.113862 |
| H | -0.909581 | 0.394612 | -1.641660 |
| H | -0.811253 | -0.747296 | 1.181815 |
| N | -0.030947 | -1.966408 | -0.266267 |
| C | -0.018604 | -3.070476 | 0.688006 |
| H | -0.957802 | -3.642168 | 0.676297 |
| H | 0.801741 | -3.744692 | 0.437369 |
| H | 0.145752 | -2.684452 | 1.695759 |
| C | -0.160651 | -2.457315 | -1.635213 |
| H | 0.687227 | -3.109341 | -1.849536 |
| H | -1.086785 | -3.025264 | -1.794901 |
| H | -0.131601 | -1.627599 | -2.345117 |
| C | -1.303874 | 1.581071 | 0.096224 |
| C | -0.874618 | 2.022612 | 1.347534 |
| C | -2.399471 | 2.191975 | -0.509081 |
| C | -1.527185 | 3.074827 | 1.979698 |
| H | -0.022634 | 1.553294 | 1.829448 |
| C | -3.057589 | 3.239539 | 0.127331 |
| H | -2.735385 | 1.852226 | -1.483318 |
| C | -2.620189 | 3.684784 | 1.370421 |
| H | -1.182243 | 3.417719 | 2.947533 |
| H | -3.907282 | 3.710708 | -0.351569 |
| H | -3.127673 | 4.505329 | 1.863092 |
| C | -2.455230 | -1.259353 | -0.055631 |
| C | -3.198455 | -1.623830 | 1.067874 |

| | | | |
|---|---|---|---|
| C | -3.087090 | -1.242955 | -1.302118 |
| C | -4.542599 | -1.965268 | 0.954112 |
| H | -2.720353 | -1.632417 | 2.042219 |
| C | -4.430278 | -1.584393 | -1.418773 |
| H | -2.540312 | -0.962363 | -2.195768 |
| C | -5.161278 | -1.945906 | -0.290882 |
| H | -5.105511 | -2.240986 | 1.837863 |
| H | -4.906196 | -1.564724 | -2.391796 |
| H | -6.208358 | -2.208126 | -0.383003 |
| H | 3.992519 | 2.397453 | -2.233549 |
| C | 3.606600 | 0.138049 | 0.025527 |
| C | 3.051131 | -0.420391 | 1.190483 |
| C | 4.754262 | -0.456752 | -0.525153 |
| C | 3.614377 | -1.550126 | 1.767469 |
| H | 2.205304 | 0.057011 | 1.671928 |
| C | 5.298531 | -1.597700 | 0.043054 |
| H | 5.199433 | -0.037188 | -1.419621 |
| C | 4.730376 | -2.148143 | 1.189757 |
| H | 3.184852 | -1.958375 | 2.673891 |
| H | 6.169315 | -2.057765 | -0.407032 |
| H | 5.163280 | -3.034173 | 1.637537 |
| C | 1.088915 | 2.754138 | -1.391260 |
| H | 0.131014 | 2.580803 | -1.875508 |
| H | 0.941605 | 3.487059 | -0.591943 |
| H | 1.778780 | 3.177996 | -2.118295 |

**9J-*Z***

Imaginary frequency: None

Electronic energies: -599.540369

Free energies: -599.282599

Corrected Free energies: -599.279956

| | | | |
|---|---|---|---|
| C | 3.368373 | -1.377985 | -0.331464 |
| C | 2.144753 | -2.165352 | -0.802943 |
| C | 0.991103 | -1.153105 | -0.707015 |
| C | 2.769275 | -0.513749 | 0.774484 |
| H | 4.182948 | -2.014183 | 0.016195 |
| H | 3.741526 | -0.734258 | -1.133397 |
| H | 1.963849 | -2.999902 | -0.120596 |
| H | 2.248290 | -2.569927 | -1.809780 |
| H | 0.785753 | -0.663971 | -1.666685 |
| H | 0.067472 | -1.641055 | -0.385833 |
| H | 3.376974 | 0.354570 | 1.014774 |
| H | 2.656261 | -1.104032 | 1.693692 |

| | | | |
|---|---|---|---|
| N | 1.455514 | -0.136833 | 0.249589 |
| C | 1.004453 | 1.179971 | 0.172077 |
| C | -0.290183 | 1.486918 | -0.095098 |
| C | -0.751066 | 2.900374 | -0.400577 |
| H | -0.942877 | 3.472011 | 0.514810 |
| H | -0.034098 | 3.461271 | -1.000836 |
| H | -1.688341 | 2.878822 | -0.958365 |
| C | -1.375723 | 0.474912 | 0.015788 |
| C | -1.494514 | -0.302357 | 1.175584 |
| C | -2.333941 | 0.298620 | -0.989329 |
| C | -2.519142 | -1.229712 | 1.319408 |
| H | -0.758006 | -0.178672 | 1.962084 |
| C | -3.359461 | -0.632198 | -0.851300 |
| H | -2.264555 | 0.883829 | -1.900614 |
| C | -3.457862 | -1.401433 | 0.303990 |
| H | -2.588085 | -1.818122 | 2.227461 |
| H | -4.082214 | -0.757973 | -1.649567 |
| H | -4.256707 | -2.125263 | 0.413704 |
| C | 2.045570 | 2.255165 | 0.372008 |
| H | 2.421808 | 2.240335 | 1.398429 |
| H | 2.900420 | 2.110105 | -0.294700 |
| H | 1.631159 | 3.243839 | 0.198424 |

**9J-*E***

Imaginary frequency: None

Electronic energies: -599.541389

Free energies: -599.281928

Corrected Free energies: -599.279830

| | | | |
|---|---|---|---|
| C | 4.177820 | -0.683217 | 0.361440 |
| C | 4.050590 | 0.836992 | 0.479557 |
| C | 2.538245 | 1.029155 | 0.545211 |
| C | 3.038254 | -1.031349 | -0.598727 |
| H | 5.150976 | -1.014848 | -0.001303 |
| H | 3.997760 | -1.143350 | 1.337785 |
| H | 4.450222 | 1.317417 | -0.417913 |
| H | 4.559047 | 1.251658 | 1.350110 |
| H | 2.175430 | 0.863895 | 1.570500 |
| H | 2.226738 | 2.029325 | 0.235895 |
| H | 2.654229 | -2.039526 | -0.439157 |
| H | 3.381947 | -0.974917 | -1.637611 |
| N | 2.007393 | -0.003233 | -0.364493 |
| C | 0.663568 | -0.393652 | -0.132391 |
| C | -0.332971 | 0.459049 | -0.449214 |

| | | | |
|---|---|---|---|
| C | -1.764020 | 0.179448 | -0.154792 |
| C | -2.380817 | -1.015401 | -0.543656 |
| C | -2.552928 | 1.152953 | 0.471135 |
| C | -3.730622 | -1.240610 | -0.293240 |
| H | -1.796799 | -1.768583 | -1.060836 |
| C | -3.901251 | 0.929000 | 0.726794 |
| H | -2.100549 | 2.092420 | 0.770307 |
| C | -4.496138 | -0.270924 | 0.347106 |
| H | -4.186232 | -2.172824 | -0.606907 |
| H | -4.488034 | 1.693195 | 1.223366 |
| H | -5.547523 | -0.445730 | 0.542182 |
| C | -0.056407 | 1.780538 | -1.126910 |
| H | -0.008564 | 2.609103 | -0.411722 |
| H | 0.898939 | 1.738994 | -1.650886 |
| H | -0.850365 | 2.015230 | -1.839488 |
| C | 0.449966 | -1.711184 | 0.579996 |
| H | -0.521860 | -1.743838 | 1.068407 |
| H | 0.508736 | -2.567988 | -0.097005 |
| H | 1.224401 | -1.841795 | 1.341872 |

**9J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -599.370698

Free energies: -599.110092

Corrected Free energies: -599.108509

| | | | |
|---|---|---|---|
| C | 4.202059 | -0.340213 | -0.325648 |
| C | 3.482277 | 0.384758 | -1.464738 |
| C | 2.278946 | 0.991772 | -0.753149 |
| C | 3.056402 | -0.976869 | 0.457304 |
| H | 4.910630 | -1.089916 | -0.672065 |
| H | 4.733574 | 0.377983 | 0.301679 |
| H | 3.148280 | -0.327247 | -2.222562 |
| H | 4.091913 | 1.149044 | -1.942675 |
| H | 2.569702 | 1.893315 | -0.210659 |
| H | 1.426763 | 1.208632 | -1.395061 |
| H | 3.241328 | -1.062400 | 1.527836 |
| H | 2.796873 | -1.961482 | 0.061778 |
| N | 1.909021 | -0.065172 | 0.219443 |
| C | 0.706520 | -0.289936 | 0.677606 |
| C | -0.355577 | 0.676639 | 0.491748 |
| C | -1.681043 | 0.234776 | 0.126287 |
| C | -1.892192 | -1.036148 | -0.454175 |
| C | -2.793403 | 1.091182 | 0.262809 |

| | | | |
|---|---|---|---|
| C | -3.157172 | -1.440023 | -0.842953 |
| H | -1.052202 | -1.697061 | -0.632525 |
| C | -4.056963 | 0.679842 | -0.128660 |
| H | -2.670954 | 2.079157 | 0.686655 |
| C | -4.247271 | -0.587182 | -0.676658 |
| H | -3.293951 | -2.417029 | -1.289866 |
| H | -4.898577 | 1.350249 | -0.006297 |
| H | -5.236555 | -0.904394 | -0.982636 |
| C | -0.079611 | 2.126999 | 0.754785 |
| H | 0.926536 | 2.289356 | 1.133064 |
| H | -0.232726 | 2.737636 | -0.140587 |
| H | -0.770403 | 2.492761 | 1.518688 |
| C | 0.477251 | -1.536409 | 1.481979 |
| H | -0.557874 | -1.605838 | 1.801826 |
| H | 0.749702 | -2.431846 | 0.917660 |
| H | 1.113466 | -1.499852 | 2.370412 |

**9J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -599.369047

Free energies: -599.109689

Corrected Free energies: -599.107815

| | | | |
|---|---|---|---|
| C | 3.535502 | -1.300500 | -0.351698 |
| C | 2.278128 | -2.089022 | -0.713938 |
| C | 1.245930 | -0.995782 | -0.956110 |
| C | 2.997579 | -0.186682 | 0.539712 |
| H | 4.286444 | -1.895557 | 0.164190 |
| H | 3.984862 | -0.872242 | -1.249983 |
| H | 1.965162 | -2.713645 | 0.126050 |
| H | 2.402197 | -2.721048 | -1.591190 |
| H | 1.337854 | -0.559773 | -1.954339 |
| H | 0.224091 | -1.323550 | -0.802052 |
| H | 3.587783 | 0.726337 | 0.501335 |
| H | 2.901275 | -0.507716 | 1.580610 |
| N | 1.630138 | 0.065556 | 0.014653 |
| C | 0.950902 | 1.149091 | 0.279551 |
| C | -0.399928 | 1.358350 | -0.194509 |
| C | -0.723007 | 2.698800 | -0.782696 |
| H | -1.578923 | 3.156033 | -0.279257 |
| H | 0.124345 | 3.380292 | -0.739921 |
| H | -0.988750 | 2.580571 | -1.838014 |
| C | -1.441467 | 0.371408 | -0.017459 |
| C | -1.318100 | -0.656530 | 0.942343 |

| | | | |
|---|---|---|---|
| C | -2.645543 | 0.462536 | -0.743324 |
| C | -2.341824 | -1.565273 | 1.143566 |
| H | -0.419200 | -0.726032 | 1.545480 |
| C | -3.663663 | -0.456618 | -0.541566 |
| H | -2.775528 | 1.243553 | -1.481710 |
| C | -3.517266 | -1.474016 | 0.398402 |
| H | -2.228909 | -2.342691 | 1.889036 |
| H | -4.575799 | -0.380771 | -1.120549 |
| H | -4.315680 | -2.188840 | 0.554768 |
| C | 1.600658 | 2.222528 | 1.104187 |
| H | 2.003399 | 1.783431 | 2.019150 |
| H | 2.428587 | 2.685552 | 0.559879 |
| H | 0.878427 | 2.987461 | 1.375177 |

**10J-*Z***

Imaginary frequency: None

Electronic energies: -638.852261

Free energies: -638.565690

Corrected Free energies: -638.563577

| | | | |
|---|---|---|---|
| C | 1.575966 | 2.857215 | -0.208385 |
| C | 0.794528 | 1.572504 | -0.057486 |
| C | -0.550818 | 1.552869 | 0.020442 |
| H | 2.333747 | 2.755676 | -0.990245 |
| H | 2.109884 | 3.098468 | 0.717043 |
| C | -0.952539 | -0.744939 | -0.905931 |
| C | -2.152730 | 0.011052 | 1.071571 |
| C | -2.202083 | -1.459752 | -1.421442 |
| H | -0.340659 | -1.466483 | -0.341111 |
| H | -0.343021 | -0.375761 | -1.732598 |
| C | -3.429455 | -0.700952 | 0.634546 |
| H | -1.565965 | -0.660451 | 1.722949 |
| H | -2.387107 | 0.901014 | 1.657434 |
| C | -3.089092 | -1.897046 | -0.254424 |
| H | -1.902669 | -2.323781 | -2.021033 |
| H | -2.759339 | -0.777741 | -2.071835 |
| H | -3.992926 | -1.019891 | 1.515406 |
| H | -4.051993 | 0.007353 | 0.077528 |
| H | -3.999986 | -2.376248 | -0.621343 |
| H | -2.550069 | -2.643204 | 0.342216 |
| N | -1.351342 | 0.393601 | -0.087970 |
| H | 0.943786 | 3.704599 | -0.469616 |
| C | 1.624322 | 0.343697 | 0.063130 |
| C | 2.558701 | -0.004141 | -0.918273 |

| | | | |
|---|---|---|---|
| C | 1.517627 | -0.473604 | 1.193722 |
| C | 3.341140 | -1.145866 | -0.788545 |
| H | 2.655829 | 0.613962 | -1.804713 |
| C | 2.303350 | -1.614004 | 1.329650 |
| H | 0.810965 | -0.203092 | 1.971278 |
| C | 3.216144 | -1.956656 | 0.336653 |
| H | 4.048473 | -1.404743 | -1.568009 |
| H | 2.205710 | -2.233048 | 2.214176 |
| H | 3.828435 | -2.844642 | 0.439977 |
| C | -1.362223 | 2.830362 | 0.109363 |
| H | -2.386678 | 2.609063 | 0.407362 |
| H | -0.939478 | 3.546441 | 0.815205 |
| H | -1.414568 | 3.312869 | -0.871819 |

**10J-*E***

Imaginary frequency: None

Electronic energies: -638.850248

Free energies: -638.563701

Corrected Free energies: -638.561147

| | | | |
|---|---|---|---|
| C | -0.615172 | 0.437779 | 0.661874 |
| C | 0.451302 | -0.314669 | 0.324344 |
| C | 2.285717 | 1.312353 | 0.087752 |
| C | 2.786798 | -0.892306 | 0.974270 |
| C | 3.062669 | 1.002833 | -1.194996 |
| H | 2.959088 | 1.803617 | 0.803458 |
| H | 1.465180 | 2.000005 | -0.114786 |
| C | 3.636193 | -1.256324 | -0.250176 |
| H | 3.455393 | -0.467871 | 1.734978 |
| H | 2.330401 | -1.776738 | 1.421164 |
| C | 4.190954 | 0.012358 | -0.902769 |
| H | 3.462468 | 1.930754 | -1.614007 |
| H | 2.375425 | 0.578070 | -1.935995 |
| H | 4.451842 | -1.914065 | 0.063470 |
| H | 3.034373 | -1.810132 | -0.975929 |
| H | 4.738073 | -0.233637 | -1.816008 |
| H | 4.906340 | 0.483897 | -0.217324 |
| N | 1.749276 | 0.105190 | 0.720894 |
| C | -2.000031 | 0.140580 | 0.193488 |
| C | -2.656076 | 1.040821 | -0.652574 |
| C | -2.700226 | -0.987952 | 0.631296 |
| C | -3.963705 | 0.810636 | -1.067439 |
| H | -2.129111 | 1.925491 | -0.995084 |
| C | -4.008884 | -1.220854 | 0.219244 |

| | | | |
|---|---|---|---|
| H | -2.209708 | -1.686018 | 1.301555 |
| C | -4.644789 | -0.322864 | -0.632956 |
| H | -4.450204 | 1.515992 | -1.731283 |
| H | -4.533725 | -2.102998 | 0.567594 |
| H | -5.663954 | -0.503516 | -0.953501 |
| C | -0.500010 | 1.671289 | 1.524520 |
| H | 0.447153 | 1.675515 | 2.064498 |
| H | -0.558801 | 2.593111 | 0.934613 |
| H | -1.324457 | 1.701051 | 2.241738 |
| C | 0.344405 | -1.564887 | -0.516759 |
| H | 0.816110 | -2.419912 | -0.026100 |
| H | -0.690864 | -1.824752 | -0.723504 |
| H | 0.859177 | -1.416946 | -1.470524 |

**10J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -638.676538

Free energies: -638.387353

Corrected Free energies: -638.385511

| | | | |
|---|---|---|---|
| C | -0.649633 | 0.931267 | 0.345318 |
| C | 0.481914 | 0.206405 | 0.893888 |
| C | 1.984410 | 1.024714 | -0.869444 |
| C | 2.906465 | -0.124215 | 1.096424 |
| C | 2.628295 | -0.020746 | -1.783909 |
| H | 2.659119 | 1.866149 | -0.692883 |
| H | 1.063449 | 1.391198 | -1.310986 |
| C | 3.555589 | -1.197708 | 0.225026 |
| H | 3.581022 | 0.729149 | 1.208961 |
| H | 2.659106 | -0.492255 | 2.086053 |
| C | 3.879173 | -0.629738 | -1.155454 |
| H | 2.860376 | 0.465701 | -2.732887 |
| H | 1.888708 | -0.802407 | -1.985010 |
| H | 4.457361 | -1.548007 | 0.729684 |
| H | 2.872435 | -2.048123 | 0.136141 |
| H | 4.280684 | -1.410781 | -1.802941 |
| H | 4.650922 | 0.141106 | -1.057426 |
| N | 1.693420 | 0.401755 | 0.439361 |
| C | -1.887213 | 0.246106 | 0.065086 |
| C | -1.915993 | -1.152698 | -0.127615 |
| C | -3.089503 | 0.964579 | -0.098533 |
| C | -3.097264 | -1.801893 | -0.440633 |
| H | -0.997661 | -1.725859 | -0.061520 |
| C | -4.268585 | 0.307069 | -0.409092 |

| | | | |
|---|---|---|---|
| H | -3.101346 | 2.039064 | 0.031449 |
| C | -4.279957 | -1.076260 | -0.577991 |
| H | -3.096931 | -2.874271 | -0.590710 |
| H | -5.184659 | 0.873864 | -0.520498 |
| H | -5.203524 | -1.585927 | -0.823390 |
| C | -0.551752 | 2.421866 | 0.194809 |
| H | 0.448578 | 2.790425 | 0.413207 |
| H | -0.846051 | 2.747240 | -0.806938 |
| H | -1.236696 | 2.896516 | 0.904690 |
| C | 0.263591 | -0.691826 | 2.080181 |
| H | 0.687789 | -0.212591 | 2.966940 |
| H | -0.798902 | -0.831379 | 2.254386 |
| H | 0.745056 | -1.662648 | 1.949781 |

**10J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -638.676783

Free energies: -638.388034

Corrected Free energies: -638.386116

| | | | |
|---|---|---|---|
| C | 0.936760 | 2.525087 | -1.103082 |
| C | 0.671370 | 1.309517 | -0.267717 |
| C | -0.626885 | 1.181784 | 0.359123 |
| H | 0.074460 | 3.186061 | -1.152820 |
| H | 1.166818 | 2.218930 | -2.128237 |
| C | -1.008332 | -1.085762 | -0.540591 |
| C | -2.529347 | -0.154353 | 1.147384 |
| C | -2.191005 | -1.296991 | -1.487981 |
| H | -0.842389 | -1.963502 | 0.090463 |
| H | -0.103631 | -0.884078 | -1.102900 |
| C | -3.735879 | -0.331958 | 0.228607 |
| H | -2.357473 | -1.068241 | 1.723927 |
| H | -2.662483 | 0.663358 | 1.846466 |
| C | -3.500172 | -1.496853 | -0.729956 |
| H | -1.961173 | -2.161604 | -2.113297 |
| H | -2.265981 | -0.425018 | -2.145200 |
| H | -4.614643 | -0.505764 | 0.851913 |
| H | -3.903034 | 0.594523 | -0.329436 |
| H | -4.331020 | -1.586241 | -1.431510 |
| H | -3.452667 | -2.430381 | -0.159217 |
| N | -1.300209 | 0.056299 | 0.353916 |
| H | 1.798918 | 3.084792 | -0.729347 |
| C | 1.719618 | 0.338044 | -0.043255 |
| C | 2.879887 | 0.342537 | -0.845239 |

| | | | |
|---|---|---|---|
| C | 1.648285 | -0.595739 | 1.014526 |
| C | 3.900724 | -0.567198 | -0.619772 |
| H | 2.975459 | 1.049345 | -1.659168 |
| C | 2.675281 | -1.495162 | 1.237495 |
| H | 0.793028 | -0.598415 | 1.680028 |
| C | 3.803454 | -1.491665 | 0.417446 |
| H | 4.776826 | -0.556385 | -1.256443 |
| H | 2.602314 | -2.197855 | 2.058204 |
| H | 4.603657 | -2.200395 | 0.591357 |
| C | -1.184809 | 2.378618 | 1.076894 |
| H | -2.212473 | 2.589256 | 0.776515 |
| H | -1.169903 | 2.185524 | 2.152739 |
| H | -0.566848 | 3.252566 | 0.895259 |

**11J-*Z***

Imaginary frequency: None

Electronic energies: -788.118044

Free energies: -787.848391

Corrected Free energies: -787.845484

| | | | |
|---|---|---|---|
| C | -2.465414 | -1.556540 | -1.064540 |
| C | -1.429726 | -1.517631 | -2.186990 |
| C | -0.243390 | -0.840072 | -1.504467 |
| C | -2.278678 | -0.177269 | -0.399531 |
| H | -3.489805 | -1.707204 | -1.400515 |
| H | -2.210480 | -2.346882 | -0.352381 |
| H | -1.793990 | -0.898347 | -3.010585 |
| H | -1.185979 | -2.507823 | -2.571580 |
| H | 0.353945 | -1.575085 | -0.951799 |
| H | 0.423758 | -0.319461 | -2.195395 |
| H | -2.954996 | 0.548218 | -0.867847 |
| N | -0.881578 | 0.131776 | -0.613954 |
| C | -0.333727 | 1.379751 | -0.308014 |
| C | 0.996154 | 1.555622 | -0.122013 |
| C | 1.653726 | 2.915236 | -0.031416 |
| H | 2.585381 | 2.927511 | -0.601682 |
| H | 1.033573 | 3.717726 | -0.425549 |
| H | 1.917236 | 3.159930 | 1.003593 |
| C | -2.643662 | -0.247129 | 1.070514 |
| O | -1.874897 | -0.238778 | 1.994343 |
| O | -3.971593 | -0.343015 | 1.223691 |
| H | -4.163467 | -0.418482 | 2.169460 |
| C | 1.909948 | 0.403327 | 0.115218 |
| C | 3.146475 | 0.289602 | -0.529775 |

| | | | |
|---|---|---|---|
| C | 1.568434 | -0.574323 | 1.060382 |
| C | 4.007062 | -0.769011 | -0.252536 |
| H | 3.435042 | 1.026016 | -1.272044 |
| C | 2.429255 | -1.627732 | 1.343421 |
| H | 0.603963 | -0.502476 | 1.553699 |
| C | 3.654531 | -1.731476 | 0.687665 |
| H | 4.954946 | -0.840877 | -0.773819 |
| H | 2.144433 | -2.370877 | 2.079907 |
| H | 4.325614 | -2.553401 | 0.907578 |
| C | -1.338648 | 2.502688 | -0.232481 |
| H | -1.874133 | 2.620001 | -1.178964 |
| H | -2.084376 | 2.295860 | 0.541094 |
| H | -0.871750 | 3.447311 | 0.027618 |

**11J-*E***

Imaginary frequency: None

Electronic energies: -788.117627

Free energies: -787.846725

Corrected Free energies: -787.843891

| | | | |
|---|---|---|---|
| C | -3.700711 | 0.887991 | 0.251329 |
| C | -2.973275 | 2.219209 | 0.434009 |
| C | -1.637367 | 1.961785 | -0.262171 |
| C | -2.568598 | -0.125235 | 0.499117 |
| H | -4.535774 | 0.735664 | 0.932749 |
| H | -4.062883 | 0.794668 | -0.776638 |
| H | -2.812280 | 2.409000 | 1.498215 |
| H | -3.514006 | 3.062561 | 0.005190 |
| H | -1.713379 | 2.189013 | -1.330801 |
| H | -0.816922 | 2.553684 | 0.150685 |
| H | -2.504351 | -0.333119 | 1.574831 |
| N | -1.388327 | 0.531344 | -0.025491 |
| C | -0.099231 | 0.048731 | 0.232637 |
| C | 0.933752 | 0.396013 | -0.570829 |
| C | -2.854694 | -1.440792 | -0.195896 |
| O | -2.287050 | -1.872305 | -1.162016 |
| O | -3.864616 | -2.083007 | 0.409608 |
| H | -4.034364 | -2.903536 | -0.074803 |
| C | 0.693090 | 1.078151 | -1.898290 |
| H | -0.265013 | 0.762982 | -2.316884 |
| H | 0.682753 | 2.170628 | -1.818651 |
| H | 1.480983 | 0.820151 | -2.607338 |
| C | 2.346227 | 0.118837 | -0.202531 |
| C | 2.860738 | 0.512709 | 1.039452 |

| | | | |
|---|---|---|---|
| C | 3.216403 | -0.518314 | -1.097214 |
| C | 4.184396 | 0.260962 | 1.385104 |
| H | 2.208696 | 1.028793 | 1.736281 |
| C | 4.540718 | -0.768977 | -0.756297 |
| H | 2.846690 | -0.840236 | -2.064699 |
| C | 5.031599 | -0.381767 | 0.487768 |
| H | 4.556022 | 0.577331 | 2.353018 |
| H | 5.190516 | -1.272641 | -1.462731 |
| H | 6.064503 | -0.575382 | 0.751844 |
| C | 0.028058 | -0.888869 | 1.407803 |
| H | -0.252424 | -0.399466 | 2.345292 |
| H | -0.635050 | -1.749472 | 1.278318 |
| H | 1.041257 | -1.270145 | 1.499876 |

**11J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -787.936349

Free energies: -787.664044

Corrected Free energies: -787.661709

| | | | |
|---|---|---|---|
| C | -3.367623 | 1.131122 | 0.916770 |
| C | -2.351306 | 2.273292 | 0.955917 |
| C | -1.346151 | 1.861665 | -0.111700 |
| C | -2.501069 | -0.120569 | 0.653981 |
| H | -3.937669 | 1.022725 | 1.836193 |
| H | -4.068936 | 1.278717 | 0.093279 |
| H | -1.859178 | 2.321738 | 1.928835 |
| H | -2.800053 | 3.240217 | 0.737141 |
| H | -1.744980 | 2.040077 | -1.113151 |
| H | -0.366315 | 2.323848 | -0.013849 |
| H | -2.317612 | -0.674749 | 1.576160 |
| N | -1.234299 | 0.403893 | 0.119528 |
| C | -0.140075 | -0.309516 | 0.000175 |
| C | 0.993448 | 0.212566 | -0.726310 |
| C | -3.150534 | -1.049760 | -0.361539 |
| O | -2.702871 | -1.306597 | -1.443676 |
| O | -4.297933 | -1.514300 | 0.120596 |
| H | -4.712692 | -2.082716 | -0.545770 |
| C | 0.752319 | 0.891922 | -2.041232 |
| H | -0.300052 | 0.879672 | -2.315264 |
| H | 1.119011 | 1.922768 | -2.039914 |
| H | 1.293352 | 0.355710 | -2.825313 |
| C | 2.335816 | 0.006895 | -0.236822 |
| C | 2.575626 | -0.281034 | 1.125056 |

| | | | |
|---|---|---|---|
| C | 3.448899 | 0.168056 | -1.087532 |
| C | 3.865325 | -0.432071 | 1.602351 |
| H | 1.745256 | -0.352048 | 1.817757 |
| C | 4.737135 | 0.012004 | -0.603251 |
| H | 3.304093 | 0.403126 | -2.133680 |
| C | 4.951541 | -0.292799 | 0.739548 |
| H | 4.028130 | -0.646201 | 2.651207 |
| H | 5.578657 | 0.128121 | -1.274703 |
| H | 5.960412 | -0.411596 | 1.115169 |
| C | -0.119883 | -1.707928 | 0.547124 |
| H | -0.368946 | -1.724640 | 1.611364 |
| H | -0.860967 | -2.304955 | 0.010627 |
| H | 0.854223 | -2.162960 | 0.396638 |

**11J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -787.939227

Free energies: -787.667558

Corrected Free energies: -787.665237

| | | | |
|---|---|---|---|
| C | -2.777643 | -0.820298 | -1.508385 |
| C | -1.637013 | -0.617443 | -2.505742 |
| C | -0.424197 | -0.475120 | -1.596590 |
| C | -2.400752 | 0.109012 | -0.333961 |
| H | -3.758208 | -0.567623 | -1.904194 |
| H | -2.799966 | -1.858083 | -1.169725 |
| H | -1.781641 | 0.300118 | -3.079000 |
| H | -1.529449 | -1.452980 | -3.194643 |
| H | -0.117530 | -1.442749 | -1.191603 |
| H | 0.433937 | 0.015864 | -2.049258 |
| H | -2.954314 | 1.048739 | -0.381089 |
| N | -0.959646 | 0.363634 | -0.499526 |
| C | -0.316846 | 1.315731 | 0.142167 |
| C | 1.111264 | 1.449361 | 0.051521 |
| C | 1.693661 | 2.825142 | -0.051656 |
| H | 2.210832 | 2.925703 | -1.011021 |
| H | 0.933532 | 3.601736 | -0.015081 |
| H | 2.431855 | 3.000260 | 0.735211 |
| C | -2.664282 | -0.553267 | 1.010345 |
| O | -1.821408 | -0.833910 | 1.817150 |
| O | -3.961970 | -0.793722 | 1.150590 |
| H | -4.111794 | -1.238936 | 1.998328 |
| C | 1.986201 | 0.298139 | 0.117479 |
| C | 3.318601 | 0.385373 | -0.333991 |

| | | | |
|---|---|---|---|
| C | 1.558715 | -0.904459 | 0.721056 |
| C | 4.172988 | -0.698986 | -0.222036 |
| H | 3.678512 | 1.298028 | -0.791493 |
| C | 2.423821 | -1.978584 | 0.839516 |
| H | 0.554587 | -0.977377 | 1.125820 |
| C | 3.730255 | -1.884344 | 0.361973 |
| H | 5.188634 | -0.621004 | -0.589401 |
| H | 2.083652 | -2.890339 | 1.314716 |
| H | 4.403599 | -2.727832 | 0.452800 |
| C | -1.102622 | 2.292652 | 0.968403 |
| H | -1.736430 | 1.758472 | 1.676358 |
| H | -0.438186 | 2.935157 | 1.538198 |
| H | -1.739989 | 2.911015 | 0.329235 |

**12J-*Z***

Imaginary frequency: None

Electronic energies: -1176.095244

Free energies: -1175.654830

Corrected Free energies: -1175.649437

| | | | |
|---|---|---|---|
| C | 0.797709 | -1.336356 | 0.187986 |
| C | 1.061949 | -2.651461 | -0.566925 |
| C | -0.087844 | -2.755725 | -1.586195 |
| C | -1.193552 | -1.814483 | -1.057849 |
| H | 1.006122 | -3.474290 | 0.149049 |
| H | 2.049325 | -2.690619 | -1.031807 |
| H | -0.449756 | -3.780961 | -1.665008 |
| H | 0.231261 | -2.446940 | -2.581719 |
| H | -2.107299 | -2.354298 | -0.800737 |
| H | -1.450951 | -1.058116 | -1.804119 |
| C | 1.505064 | -0.119869 | -0.474041 |
| O | 1.140215 | -0.054340 | -1.848758 |
| C | 3.034586 | -0.187927 | -0.358063 |
| C | 3.788228 | 0.620579 | -1.215598 |
| C | 3.706872 | -0.980103 | 0.573054 |
| C | 5.174902 | 0.635877 | -1.147250 |
| H | 3.273730 | 1.243717 | -1.938342 |
| C | 5.098931 | -0.964486 | 0.642955 |
| H | 3.163468 | -1.627986 | 1.249926 |
| C | 5.837136 | -0.158649 | -0.214718 |
| H | 5.740432 | 1.270035 | -1.819890 |
| H | 5.603051 | -1.589767 | 1.370224 |
| H | 6.919007 | -0.149161 | -0.158828 |
| C | 1.038454 | 1.184202 | 0.166951 |

| | | | |
|---|---|---|---|
| C | 1.138895 | 1.357940 | 1.549235 |
| C | 0.537336 | 2.228528 | -0.607108 |
| C | 0.707329 | 2.534116 | 2.149851 |
| H | 1.572382 | 0.576664 | 2.165075 |
| C | 0.115171 | 3.413362 | -0.006594 |
| H | 0.464093 | 2.104734 | -1.679503 |
| C | 0.187381 | 3.566834 | 1.372564 |
| H | 0.784415 | 2.648157 | 3.224876 |
| H | -0.277670 | 4.214154 | -0.622629 |
| H | -0.148561 | 4.484960 | 1.839606 |
| N | -0.652336 | -1.203551 | 0.162805 |
| H | 1.139031 | -1.397463 | 1.217580 |
| C | -1.426766 | -1.157571 | 1.331453 |
| C | -2.726580 | -0.776792 | 1.320559 |
| C | -3.615431 | -0.924982 | 2.545030 |
| H | -4.631071 | -0.605108 | 2.313115 |
| H | -3.266970 | -0.305158 | 3.376282 |
| H | -3.671214 | -1.955801 | 2.905173 |
| H | 1.649814 | -0.718220 | -2.324599 |
| C | -3.359159 | -0.144817 | 0.132077 |
| C | -4.603859 | -0.569209 | -0.347575 |
| C | -2.742300 | 0.936469 | -0.507812 |
| C | -5.200749 | 0.049977 | -1.441635 |
| H | -5.103811 | -1.404511 | 0.132615 |
| C | -3.338307 | 1.561653 | -1.596304 |
| H | -1.780361 | 1.275795 | -0.142720 |
| C | -4.571135 | 1.119258 | -2.072333 |
| H | -6.159926 | -0.304236 | -1.802190 |
| H | -2.840518 | 2.400585 | -2.071215 |
| H | -5.037104 | 1.604064 | -2.922068 |
| C | -0.769599 | -1.636249 | 2.604899 |
| H | -0.227731 | -2.570876 | 2.437133 |
| H | -0.058452 | -0.901368 | 2.992432 |
| H | -1.508086 | -1.809123 | 3.383046 |

**12J-*E***

Imaginary frequency: None

Electronic energies: -1176.100257

Free energies: -1175.657397

Corrected Free energies: -1175.653368

| | | | |
|---|---|---|---|
| C | 1.224614 | 1.334182 | -0.332189 |
| C | 1.972050 | 2.679819 | -0.222369 |
| C | 1.181302 | 3.471040 | 0.825237 |

| | | | |
|---|---|---|---|
| C | -0.247092 | 3.029109 | 0.543743 |
| H | 1.921384 | 3.196247 | -1.184409 |
| H | 3.029020 | 2.563188 | 0.025133 |
| H | 1.314638 | 4.548720 | 0.729830 |
| H | 1.466484 | 3.169626 | 1.834673 |
| H | -0.664184 | 3.591755 | -0.306844 |
| H | -0.916174 | 3.161976 | 1.397700 |
| C | 1.918785 | 0.186848 | 0.459091 |
| O | 2.093951 | 0.575228 | 1.816871 |
| C | 3.281841 | -0.202969 | -0.126011 |
| C | 4.105406 | -1.025114 | 0.651063 |
| C | 3.734485 | 0.193474 | -1.384716 |
| C | 5.345733 | -1.439259 | 0.185817 |
| H | 3.758680 | -1.338670 | 1.629312 |
| C | 4.979818 | -0.223060 | -1.854121 |
| H | 3.132366 | 0.836154 | -2.015513 |
| C | 5.788166 | -1.039091 | -1.073416 |
| H | 5.967584 | -2.076895 | 0.803417 |
| H | 5.315124 | 0.097794 | -2.833290 |
| H | 6.755246 | -1.361752 | -1.440194 |
| C | 1.001986 | -1.031612 | 0.456555 |
| C | 0.805004 | -1.746684 | -0.726515 |
| C | 0.312061 | -1.419339 | 1.602112 |
| C | -0.088838 | -2.810007 | -0.772954 |
| H | 1.355533 | -1.470237 | -1.620984 |
| C | -0.580140 | -2.487595 | 1.558886 |
| H | 0.468277 | -0.875378 | 2.523542 |
| C | -0.790522 | -3.180909 | 0.371792 |
| H | -0.235480 | -3.349897 | -1.701117 |
| H | -1.116941 | -2.774123 | 2.456652 |
| H | -1.489245 | -4.008740 | 0.338328 |
| N | -0.104594 | 1.605484 | 0.220215 |
| H | 1.160962 | 1.019906 | -1.377260 |
| C | -1.264258 | 1.001512 | -0.345840 |
| C | -2.280753 | 0.666699 | 0.470123 |
| H | 2.812750 | 1.214554 | 1.850643 |
| C | -3.596281 | 0.180412 | -0.033056 |
| C | -4.413636 | 0.980980 | -0.837845 |
| C | -4.065996 | -1.084097 | 0.338790 |
| C | -5.653537 | 0.524743 | -1.275349 |
| H | -4.068576 | 1.970292 | -1.119724 |
| C | -5.303882 | -1.543184 | -0.097834 |
| H | -3.443848 | -1.716298 | 0.964099 |
| C | -6.102696 | -0.739904 | -0.907805 |

| | | | |
|---|---|---|---|
| H | -6.271413 | 1.160369 | -1.899371 |
| H | -5.645053 | -2.529895 | 0.193421 |
| H | -7.068344 | -1.095825 | -1.246866 |
| C | -2.173760 | 0.785046 | 1.968727 |
| H | -1.137227 | 0.942427 | 2.264278 |
| H | -2.782347 | 1.618184 | 2.338557 |
| H | -2.548029 | -0.123284 | 2.449872 |
| C | -1.292987 | 0.838375 | -1.845806 |
| H | -2.268406 | 0.510661 | -2.197121 |
| H | -1.042502 | 1.785882 | -2.335106 |
| H | -0.560951 | 0.096561 | -2.174769 |

**12J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1175.919645

Free energies: -1175.476230

Corrected Free energies: -1175.472024

| | | | |
|---|---|---|---|
| C | -0.887962 | 1.135944 | 0.140231 |
| C | -1.122621 | 2.614674 | -0.193302 |
| C | -0.369964 | 2.877558 | -1.514352 |
| C | 0.598682 | 1.698695 | -1.695518 |
| H | -0.703730 | 3.222965 | 0.608690 |
| H | -2.184387 | 2.847372 | -0.264246 |
| H | 0.173549 | 3.819169 | -1.466822 |
| H | -1.050751 | 2.928665 | -2.361746 |
| H | 1.640187 | 2.004752 | -1.777826 |
| H | 0.321595 | 1.094150 | -2.557295 |
| C | -1.959985 | 0.175908 | -0.469253 |
| O | -2.017203 | 0.392448 | -1.874200 |
| C | -3.338102 | 0.407519 | 0.151460 |
| C | -4.438112 | -0.128122 | -0.524896 |
| C | -3.548575 | 1.074211 | 1.357925 |
| C | -5.720648 | 0.005030 | -0.009982 |
| H | -4.280372 | -0.657571 | -1.457706 |
| C | -4.835774 | 1.206160 | 1.874768 |
| H | -2.724450 | 1.503931 | 1.914439 |
| C | -5.923483 | 0.674167 | 1.194139 |
| H | -6.561434 | -0.417848 | -0.546537 |
| H | -4.982420 | 1.728229 | 2.812447 |
| H | -6.922948 | 0.778895 | 1.598601 |
| C | -1.517367 | -1.270374 | -0.259899 |
| C | -1.824629 | -1.956649 | 0.916389 |
| C | -0.725536 | -1.894882 | -1.223219 |

| | | | |
|---|---|---|---|
| C | -1.319431 | -3.234336 | 1.137028 |
| H | -2.454976 | -1.493378 | 1.667494 |
| C | -0.212803 | -3.168554 | -0.998338 |
| H | -0.525036 | -1.384016 | -2.156929 |
| C | -0.502592 | -3.838709 | 0.186222 |
| H | -1.564513 | -3.756517 | 2.053963 |
| H | 0.407221 | -3.638133 | -1.752878 |
| H | -0.104578 | -4.830906 | 0.361391 |
| N | 0.442724 | 0.888825 | -0.462550 |
| H | -0.822302 | 0.956940 | 1.210031 |
| C | 1.424474 | 0.232993 | 0.109788 |
| C | 2.659204 | -0.017847 | -0.605559 |
| H | -2.616080 | 1.126733 | -2.049646 |
| C | 3.929374 | 0.134561 | 0.069208 |
| C | 4.051017 | 0.954051 | 1.212283 |
| C | 5.096577 | -0.468783 | -0.441503 |
| C | 5.275316 | 1.133430 | 1.831955 |
| H | 3.183169 | 1.477696 | 1.596256 |
| C | 6.318214 | -0.288578 | 0.186766 |
| H | 5.046257 | -1.093351 | -1.323798 |
| C | 6.413662 | 0.507773 | 1.325931 |
| H | 5.346028 | 1.771459 | 2.704043 |
| H | 7.201653 | -0.770330 | -0.213407 |
| H | 7.371733 | 0.647857 | 1.811408 |
| C | 2.619932 | -0.530269 | -2.013592 |
| H | 1.608703 | -0.603730 | -2.401444 |
| H | 3.220688 | 0.091081 | -2.683859 |
| H | 3.043079 | -1.539415 | -2.036201 |
| C | 1.254761 | -0.326397 | 1.494097 |
| H | 0.982210 | 0.451754 | 2.211227 |
| H | 0.457958 | -1.073478 | 1.479307 |
| H | 2.170720 | -0.809368 | 1.819830 |

**12J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1175.918318

Free energies: -1175.476575

Corrected Free energies: -1175.471723

| | | | |
|---|---|---|---|
| C | -0.822356 | -1.075424 | -0.758215 |
| C | -1.040251 | -2.587602 | -0.615446 |
| C | 0.056423 | -3.077100 | 0.344881 |
| C | 1.168782 | -2.022959 | 0.278610 |
| H | -0.913375 | -3.045105 | -1.597671 |

| | | | |
|---|---|---|---|
| H | -2.041279 | -2.826313 | -0.261932 |
| H | 0.430459 | -4.053317 | 0.042111 |
| H | -0.313033 | -3.170056 | 1.364711 |
| H | 2.099679 | -2.413383 | -0.128116 |
| H | 1.361969 | -1.573606 | 1.250000 |
| C | -1.519654 | -0.216824 | 0.346156 |
| O | -0.948304 | -0.546329 | 1.601886 |
| C | -3.033466 | -0.448263 | 0.369159 |
| C | -3.718187 | -0.164810 | 1.553208 |
| C | -3.761877 | -0.865994 | -0.746166 |
| C | -5.098392 | -0.311317 | 1.626306 |
| H | -3.167164 | 0.181055 | 2.420261 |
| C | -5.144438 | -1.007664 | -0.673219 |
| H | -3.267900 | -1.095101 | -1.683335 |
| C | -5.816524 | -0.734325 | 0.512607 |
| H | -5.612318 | -0.089669 | 2.553821 |
| H | -5.693553 | -1.336416 | -1.547248 |
| H | -6.892267 | -0.848869 | 0.567726 |
| C | -1.253660 | 1.270401 | 0.103871 |
| C | -1.870329 | 1.928015 | -0.964804 |
| C | -0.394760 | 1.986606 | 0.932978 |
| C | -1.602077 | 3.266743 | -1.219230 |
| H | -2.565294 | 1.395272 | -1.605726 |
| C | -0.119773 | 3.328612 | 0.672542 |
| H | 0.041440 | 1.499407 | 1.794973 |
| C | -0.715535 | 3.969649 | -0.406019 |
| H | -2.086987 | 3.761781 | -2.051999 |
| H | 0.556586 | 3.871298 | 1.322319 |
| H | -0.503533 | 5.012922 | -0.606349 |
| N | 0.658437 | -0.977342 | -0.650497 |
| H | -1.125583 | -0.712663 | -1.737223 |
| C | 1.428497 | -0.303076 | -1.477091 |
| C | 2.868861 | -0.331056 | -1.364057 |
| C | 3.660290 | -0.471712 | -2.630333 |
| H | 4.248475 | -1.393227 | -2.588054 |
| H | 4.363522 | 0.357068 | -2.750774 |
| H | 3.027202 | -0.536909 | -3.511756 |
| H | -1.413465 | -1.307262 | 1.966115 |
| C | 3.560677 | -0.179247 | -0.103766 |
| C | 4.917516 | -0.541952 | 0.021934 |
| C | 2.926928 | 0.417688 | 1.005291 |
| C | 5.591941 | -0.348068 | 1.216428 |
| H | 5.439112 | -0.994948 | -0.811096 |
| C | 3.609328 | 0.619665 | 2.191686 |

| | | | |
|---|---|---|---|
| H | 1.900170 | 0.749432 | 0.915544 |
| C | 4.943305 | 0.230304 | 2.305891 |
| H | 6.629122 | -0.648239 | 1.299540 |
| H | 3.104928 | 1.089666 | 3.027159 |
| H | 5.475975 | 0.385175 | 3.236074 |
| C | 0.825749 | 0.484480 | -2.604495 |
| H | 0.097152 | 1.192143 | -2.210427 |
| H | 1.594127 | 1.047839 | -3.125578 |
| H | 0.321104 | -0.174562 | -3.316908 |

**13J-*Z***

Imaginary frequency: None

Electronic energies: -1584.765810

Free energies: -1584.227813

Corrected Free energies: -1584.223082

| | | | |
|---|---|---|---|
| Si | -1.166913 | -2.045603 | -1.418433 |
| O | -0.734746 | -0.519188 | -0.875465 |
| N | 0.977552 | -0.168550 | 1.274448 |
| C | -0.458418 | -0.015156 | 1.467865 |
| C | -0.570331 | 1.041073 | 2.580308 |
| C | 0.667526 | 1.931270 | 2.394899 |
| C | 1.715333 | 1.020222 | 1.733157 |
| C | -1.222100 | 0.340036 | 0.144373 |
| C | 0.435249 | -2.987002 | -1.645881 |
| C | -2.338926 | -2.958903 | -0.269742 |
| C | -1.986890 | -1.887038 | -3.095965 |
| C | -2.737611 | 0.148071 | 0.289885 |
| C | -3.375629 | -0.241213 | 1.465310 |
| C | -4.752719 | -0.464609 | 1.484438 |
| C | -5.508408 | -0.299062 | 0.331775 |
| C | -4.883147 | 0.112971 | -0.844417 |
| C | -3.514841 | 0.340968 | -0.857227 |
| C | -0.917582 | 1.778231 | -0.275851 |
| C | 0.240302 | 2.050003 | -1.001596 |
| C | 0.609330 | 3.359579 | -1.290686 |
| C | -0.185740 | 4.420132 | -0.865856 |
| C | -1.358869 | 4.157465 | -0.164272 |
| C | -1.723836 | 2.846365 | 0.125298 |
| C | 1.606846 | -1.421604 | 1.360128 |
| C | 2.872077 | -1.615566 | 0.920577 |
| H | -0.881207 | -0.966391 | 1.788497 |
| H | -0.523648 | 0.525864 | 3.543648 |
| H | -1.500344 | 1.610039 | 2.547302 |

| | | | |
|---|---|---|---|
| H | 0.439479 | 2.783068 | 1.752898 |
| H | 1.028707 | 2.319487 | 3.347687 |
| H | 2.221626 | 1.529936 | 0.907718 |
| H | 2.485423 | 0.696833 | 2.441408 |
| H | 1.021665 | -2.545100 | -2.456525 |
| H | 0.220614 | -4.024440 | -1.918551 |
| H | 1.055155 | -2.981048 | -0.745997 |
| H | -2.055652 | -2.918969 | 0.784240 |
| H | -2.360566 | -4.011268 | -0.570511 |
| H | -3.353351 | -2.559551 | -0.353648 |
| H | -2.991751 | -1.465829 | -3.023110 |
| H | -2.066706 | -2.873317 | -3.562757 |
| H | -1.392067 | -1.250806 | -3.756885 |
| H | -2.818399 | -0.389676 | 2.381898 |
| H | -5.229529 | -0.774588 | 2.406874 |
| H | -6.576420 | -0.480369 | 0.347714 |
| H | -5.462764 | 0.258365 | -1.748598 |
| H | -3.029259 | 0.667937 | -1.771241 |
| H | 0.857800 | 1.223711 | -1.320935 |
| H | 1.521798 | 3.549771 | -1.845215 |
| H | 0.099325 | 5.441750 | -1.088478 |
| H | -1.993882 | 4.974695 | 0.157460 |
| H | -2.642022 | 2.658310 | 0.670635 |
| C | 3.644111 | -2.896400 | 1.181579 |
| H | 3.286663 | -3.718223 | 0.550536 |
| H | 4.699192 | -2.752381 | 0.947086 |
| H | 3.583761 | -3.225906 | 2.220480 |
| C | 3.555630 | -0.620337 | 0.052163 |
| C | 4.836180 | -0.138857 | 0.343692 |
| C | 2.934023 | -0.179825 | -1.120618 |
| C | 5.465996 | 0.774275 | -0.496476 |
| H | 5.336378 | -0.470334 | 1.248205 |
| C | 3.560937 | 0.731314 | -1.963747 |
| H | 1.940786 | -0.555827 | -1.345647 |
| C | 4.829939 | 1.215468 | -1.653645 |
| H | 6.453779 | 1.143650 | -0.245442 |
| H | 3.060264 | 1.062316 | -2.867621 |
| H | 5.319188 | 1.926081 | -2.309295 |
| C | 0.843625 | -2.534341 | 2.037055 |
| H | 0.410595 | -2.199391 | 2.983806 |
| H | 0.026164 | -2.896154 | 1.407202 |
| H | 1.488752 | -3.385647 | 2.236665 |

**13J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1584.589190

Free energies: -1584.051803

Corrected Free energies: -1584.046572

| | | | |
|---|---|---|---|
| Si | -1.173093 | -1.536793 | -1.906278 |
| O | -0.626635 | -0.687330 | -0.550573 |
| N | 0.998103 | -0.244812 | 1.499933 |
| C | -0.456741 | -0.129633 | 1.730745 |
| C | -0.527715 | 0.915241 | 2.844998 |
| C | 0.669023 | 1.855056 | 2.605428 |
| C | 1.675801 | 1.049072 | 1.768156 |
| C | -1.220791 | 0.182073 | 0.394346 |
| C | 0.412091 | -2.315784 | -2.516335 |
| C | -2.407709 | -2.849636 | -1.409878 |
| C | -1.872376 | -0.414317 | -3.233098 |
| C | -2.720724 | -0.135497 | 0.537922 |
| C | -3.243606 | -0.998764 | 1.501463 |
| C | -4.591867 | -1.351711 | 1.485766 |
| C | -5.438764 | -0.855484 | 0.503915 |
| C | -4.932555 | 0.015746 | -0.457009 |
| C | -3.592348 | 0.376043 | -0.431181 |
| C | -1.015420 | 1.640258 | -0.036660 |
| C | -0.048269 | 1.970598 | -0.982313 |
| C | 0.196907 | 3.299699 | -1.321320 |
| C | -0.536918 | 4.318252 | -0.726832 |
| C | -1.534369 | 3.997181 | 0.191065 |
| C | -1.774578 | 2.671532 | 0.527923 |
| C | 1.617737 | -1.391735 | 1.340190 |
| C | 3.040807 | -1.446375 | 1.108971 |
| H | -0.797335 | -1.097049 | 2.077324 |
| H | -0.414061 | 0.399551 | 3.799481 |
| H | -1.481692 | 1.438943 | 2.863242 |
| H | 0.369952 | 2.749770 | 2.062303 |
| H | 1.115073 | 2.165843 | 3.548529 |
| H | 1.909329 | 1.542739 | 0.825677 |
| H | 2.606126 | 0.839812 | 2.294683 |
| H | 1.095987 | -1.561278 | -2.914728 |
| H | 0.198640 | -3.027935 | -3.317930 |
| H | 0.928239 | -2.854142 | -1.716227 |
| H | -2.030659 | -3.453020 | -0.579653 |
| H | -2.581368 | -3.519649 | -2.257058 |
| H | -3.368022 | -2.421372 | -1.112306 |
| H | -2.941098 | -0.231940 | -3.110973 |

| | | | |
|---|---|---|---|
| H | -1.724074 | -0.892575 | -4.205873 |
| H | -1.356139 | 0.549132 | -3.254641 |
| H | -2.628781 | -1.420594 | 2.285076 |
| H | -4.973753 | -2.022464 | 2.245856 |
| H | -6.484761 | -1.137328 | 0.490375 |
| H | -5.581985 | 0.419103 | -1.224731 |
| H | -3.215999 | 1.065672 | -1.177358 |
| H | 0.510511 | 1.184053 | -1.470286 |
| H | 0.959112 | 3.531329 | -2.056096 |
| H | -0.348085 | 5.352651 | -0.987658 |
| H | -2.131270 | 4.780558 | 0.642413 |
| H | -2.572094 | 2.440858 | 1.224580 |
| C | 3.847498 | -2.472383 | 1.843147 |
| H | 4.418783 | -3.094569 | 1.149013 |
| H | 4.568313 | -1.967142 | 2.494025 |
| H | 3.232344 | -3.107696 | 2.476727 |
| C | 3.674971 | -0.584186 | 0.135823 |
| C | 5.060291 | -0.336387 | 0.165694 |
| C | 2.918485 | -0.047702 | -0.924933 |
| C | 5.651084 | 0.454779 | -0.807541 |
| H | 5.668748 | -0.745201 | 0.962638 |
| C | 3.516012 | 0.733146 | -1.898941 |
| H | 1.861697 | -0.285624 | -0.984465 |
| C | 4.884784 | 0.994007 | -1.839221 |
| H | 6.714935 | 0.652402 | -0.763658 |
| H | 2.920855 | 1.129565 | -2.713524 |
| H | 5.353935 | 1.606607 | -2.599245 |
| C | 0.858398 | -2.685984 | 1.436118 |
| H | -0.015740 | -2.648588 | 0.787646 |
| H | 1.486810 | -3.517389 | 1.127757 |
| H | 0.522363 | -2.858247 | 2.463577 |

**13J-*E***

Imaginary frequency: None

Electronic energies: -1584.767457

Free energies: -1584.231499

Corrected Free energies: -1584.225968

| | | | |
|---|---|---|---|
| Si | 0.428755 | -2.280937 | 0.984800 |
| O | 0.608715 | -0.656298 | 0.632313 |
| N | -0.578070 | 1.236899 | -0.981479 |
| C | 0.685943 | 0.610041 | -1.380671 |
| C | 1.387553 | 1.665061 | -2.259117 |
| C | 0.693717 | 2.982452 | -1.903166 |

| | | | |
|---|---|---|---|
| C | -0.738115 | 2.529069 | -1.664512 |
| C | 1.500164 | 0.142524 | -0.132420 |
| C | -1.389844 | -2.449168 | 1.389569 |
| C | 0.930073 | -3.395935 | -0.438880 |
| C | 1.398059 | -2.761879 | 2.518725 |
| C | 2.734390 | -0.680202 | -0.521085 |
| C | 3.031879 | -1.073288 | -1.825234 |
| C | 4.121222 | -1.903757 | -2.086040 |
| C | 4.926605 | -2.354177 | -1.048109 |
| C | 4.649622 | -1.953184 | 0.257480 |
| C | 3.570208 | -1.118196 | 0.511289 |
| C | 1.896956 | 1.350584 | 0.712867 |
| C | 1.024130 | 1.824000 | 1.691980 |
| C | 1.315316 | 2.985206 | 2.402000 |
| C | 2.487740 | 3.689379 | 2.144039 |
| C | 3.375283 | 3.212266 | 1.184317 |
| C | 3.084425 | 2.048044 | 0.479717 |
| C | -1.763624 | 0.460636 | -0.875862 |
| C | -2.751722 | 0.861905 | -0.052043 |
| H | 0.503185 | -0.298514 | -1.959653 |
| H | 1.204077 | 1.429056 | -3.311107 |
| H | 2.466631 | 1.694808 | -2.111348 |
| H | 1.109593 | 3.400052 | -0.983117 |
| H | 0.771037 | 3.728383 | -2.694481 |
| H | -1.310837 | 3.227072 | -1.050851 |
| H | -1.268916 | 2.404585 | -2.621463 |
| H | -1.635943 | -1.824918 | 2.253606 |
| H | -1.629221 | -3.485442 | 1.645009 |
| H | -2.033242 | -2.136195 | 0.564767 |
| H | 0.549334 | -3.046231 | -1.402069 |
| H | 0.530633 | -4.399572 | -0.264383 |
| H | 2.018478 | -3.468839 | -0.516922 |
| H | 2.458744 | -2.919899 | 2.316697 |
| H | 0.990838 | -3.692261 | 2.925932 |
| H | 1.303797 | -1.992197 | 3.290003 |
| H | 2.420567 | -0.750024 | -2.658349 |
| H | 4.333332 | -2.200350 | -3.106534 |
| H | 5.768322 | -3.004916 | -1.253154 |
| H | 5.276936 | -2.287633 | 1.075628 |
| H | 3.362577 | -0.800756 | 1.528157 |
| H | 0.117425 | 1.268695 | 1.889499 |
| H | 0.624196 | 3.340221 | 3.158308 |
| H | 2.714894 | 4.594377 | 2.695157 |
| H | 4.300526 | 3.741217 | 0.987755 |

| | | | |
|---|---|---|---|
| H | 3.795885 | 1.679315 | -0.250988 |
| C | -2.603468 | 2.030316 | 0.890370 |
| H | -3.200405 | 2.885253 | 0.552550 |
| H | -2.970229 | 1.764710 | 1.885975 |
| H | -1.563356 | 2.342098 | 0.968020 |
| C | -4.089364 | 0.204022 | -0.023913 |
| C | -4.559964 | -0.390875 | 1.152071 |
| C | -4.926219 | 0.203169 | -1.145064 |
| C | -5.814065 | -0.989660 | 1.199076 |
| H | -3.927310 | -0.398336 | 2.033512 |
| C | -6.182450 | -0.393515 | -1.101423 |
| H | -4.580101 | 0.675062 | -2.058896 |
| C | -6.630829 | -0.993777 | 0.071226 |
| H | -6.154068 | -1.455523 | 2.116871 |
| H | -6.813082 | -0.384901 | -1.983094 |
| H | -7.609100 | -1.458179 | 0.108050 |
| C | -1.875024 | -0.749942 | -1.769209 |
| H | -1.706400 | -0.470365 | -2.814935 |
| H | -1.124816 | -1.500230 | -1.510707 |
| H | -2.851366 | -1.221133 | -1.686661 |

**13J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1584.589877

Free energies: -1584.053269

Corrected Free energies: -1584.047711

| | | | |
|---|---|---|---|
| Si | 1.881531 | -1.845979 | 1.745396 |
| O | 1.013845 | -0.948033 | 0.600936 |
| N | -0.983718 | 0.550370 | -0.850063 |
| C | 0.309320 | 0.078507 | -1.399487 |
| C | 0.555345 | 1.001954 | -2.599935 |
| C | -0.356740 | 2.234591 | -2.420761 |
| C | -1.173827 | 1.992704 | -1.145414 |
| C | 1.424391 | 0.068024 | -0.295417 |
| C | 0.514260 | -2.736890 | 2.653003 |
| C | 3.028237 | -3.070940 | 0.921962 |
| C | 2.840988 | -0.751887 | 2.921659 |
| C | 2.774566 | -0.316571 | -0.920029 |
| C | 2.834672 | -1.286841 | -1.925118 |
| C | 4.056298 | -1.738625 | -2.408879 |
| C | 5.245249 | -1.238276 | -1.886729 |
| C | 5.199790 | -0.278790 | -0.882804 |
| C | 3.974436 | 0.180136 | -0.406915 |

| | | | |
|---|---|---|---|
| C | 1.439455 | 1.421763 | 0.417179 |
| C | 0.754709 | 1.572008 | 1.622833 |
| C | 0.636789 | 2.821971 | 2.224742 |
| C | 1.199281 | 3.943178 | 1.624635 |
| C | 1.895543 | 3.802105 | 0.427617 |
| C | 2.017768 | 2.552027 | -0.169052 |
| C | -1.935128 | -0.235485 | -0.395228 |
| C | -3.108048 | 0.330263 | 0.233008 |
| H | 0.176072 | -0.953345 | -1.709229 |
| H | 0.294875 | 0.467187 | -3.512718 |
| H | 1.606408 | 1.272736 | -2.677991 |
| H | 0.220464 | 3.152650 | -2.323450 |
| H | -1.021084 | 2.342956 | -3.276358 |
| H | -0.803610 | 2.592772 | -0.313997 |
| H | -2.237062 | 2.182889 | -1.277865 |
| H | -0.217791 | -2.026125 | 3.045519 |
| H | 0.922099 | -3.302621 | 3.494764 |
| H | -0.007160 | -3.439535 | 1.998187 |
| H | 2.510492 | -3.620922 | 0.132049 |
| H | 3.371367 | -3.793187 | 1.668901 |
| H | 3.906177 | -2.589876 | 0.484728 |
| H | 3.545694 | -0.097907 | 2.404301 |
| H | 3.417712 | -1.393950 | 3.594626 |
| H | 2.182214 | -0.129673 | 3.531307 |
| H | 1.930262 | -1.716761 | -2.337812 |
| H | 4.078129 | -2.488532 | -3.190457 |
| H | 6.197867 | -1.594095 | -2.260499 |
| H | 6.117470 | 0.118857 | -0.466144 |
| H | 3.962241 | 0.929984 | 0.373794 |
| H | 0.292963 | 0.707281 | 2.082710 |
| H | 0.097699 | 2.916971 | 3.160130 |
| H | 1.103067 | 4.917468 | 2.088425 |
| H | 2.348537 | 4.665805 | -0.044024 |
| H | 2.574490 | 2.463714 | -1.094812 |
| C | -2.955103 | 1.456906 | 1.210019 |
| H | -3.572814 | 2.316072 | 0.932759 |
| H | -3.289233 | 1.121305 | 2.196242 |
| H | -1.921449 | 1.774216 | 1.315558 |
| C | -4.416806 | -0.240564 | -0.005021 |
| C | -5.481406 | 0.001412 | 0.886855 |
| C | -4.686876 | -0.983691 | -1.174124 |
| C | -6.745351 | -0.506683 | 0.635502 |
| H | -5.316367 | 0.574764 | 1.789492 |
| C | -5.953552 | -1.483033 | -1.422451 |

| | | | |
|---|---|---|---|
| H | -3.904982 | -1.138549 | -1.908175 |
| C | -6.987151 | -1.252643 | -0.515745 |
| H | -7.546320 | -0.321457 | 1.340373 |
| H | -6.141349 | -2.043038 | -2.330065 |
| H | -7.977507 | -1.645979 | -0.709964 |
| C | -1.780007 | -1.729226 | -0.474744 |
| H | -1.704973 | -2.058044 | -1.515157 |
| H | -0.862090 | -2.010681 | 0.039655 |
| H | -2.625270 | -2.222401 | -0.004360 |

**14J-*Z***

Imaginary frequency: None

Electronic energies: -2932.945472

Free energies: -2932.409866

Corrected Free energies: -2932.398872

| | | | |
|---|---|---|---|
| Si | -0.329981 | -2.382603 | -1.896693 |
| O | 0.205854 | -1.039074 | -1.024212 |
| N | 1.693634 | -1.409239 | 1.288750 |
| C | 0.277099 | -1.103802 | 1.397009 |
| C | 0.155992 | -0.303651 | 2.705189 |
| C | 1.506276 | 0.418991 | 2.843599 |
| C | 2.507640 | -0.457122 | 2.067663 |
| C | -0.276400 | -0.373504 | 0.123357 |
| C | 1.137611 | -3.510433 | -2.144783 |
| C | -1.729976 | -3.308727 | -1.050862 |
| C | -0.915123 | -1.777480 | -3.567178 |
| C | -1.810320 | -0.369805 | 0.088035 |
| C | -2.619508 | -0.912452 | 1.076518 |
| C | -4.002269 | -0.962995 | 0.901279 |
| C | -4.603023 | -0.464002 | -0.240028 |
| C | -3.790379 | 0.109228 | -1.215051 |
| C | -2.416272 | 0.161099 | -1.055094 |
| C | 0.237953 | 1.064492 | 0.081088 |
| C | 1.505430 | 1.330636 | -0.424138 |
| C | 2.032501 | 2.617194 | -0.341311 |
| C | 1.312295 | 3.657107 | 0.225090 |
| C | 0.035942 | 3.389498 | 0.703615 |
| C | -0.501604 | 2.112859 | 0.631879 |
| C | 2.140325 | -2.746838 | 1.219307 |
| C | 3.399318 | -3.047620 | 0.836216 |
| H | -0.287027 | -2.034208 | 1.448174 |
| H | 0.023799 | -1.014377 | 3.524751 |
| H | -0.689572 | 0.386417 | 2.724684 |

| | | | |
|---|---|---|---|
| H | 1.459709 | 1.423251 | 2.419865 |
| H | 1.798222 | 0.519181 | 3.888640 |
| H | 3.152268 | 0.147785 | 1.422848 |
| H | 3.157731 | -1.025525 | 2.739141 |
| H | 1.896926 | -3.036081 | -2.771534 |
| H | 0.803538 | -4.417235 | -2.657580 |
| H | 1.610607 | -3.798503 | -1.203041 |
| H | -1.573221 | -3.480858 | 0.016369 |
| H | -1.818344 | -4.288045 | -1.531295 |
| H | -2.687246 | -2.794066 | -1.169575 |
| H | -1.849295 | -1.215472 | -3.502996 |
| H | -1.081797 | -2.629818 | -4.232002 |
| H | -0.160093 | -1.135416 | -4.028385 |
| H | -2.201630 | -1.322540 | 1.987921 |
| H | -5.675965 | -0.518705 | -0.373564 |
| H | -1.796572 | 0.599475 | -1.830655 |
| H | -1.497511 | 1.940502 | 1.022137 |
| C | 3.962322 | -4.454509 | 0.938378 |
| H | 3.486361 | -5.130349 | 0.219762 |
| H | 5.029022 | -4.450601 | 0.715294 |
| H | 3.836343 | -4.888203 | 1.932801 |
| C | -4.823418 | -1.651575 | 1.951667 |
| C | -4.424259 | 0.716050 | -2.433357 |
| F | -4.446189 | -1.296546 | 3.187831 |
| F | -4.686426 | -2.985838 | 1.877021 |
| F | -6.127793 | -1.383279 | 1.836014 |
| F | -4.775067 | 1.993811 | -2.225093 |
| F | -5.535817 | 0.063151 | -2.793985 |
| F | -3.594430 | 0.708536 | -3.486017 |
| H | 1.732135 | 4.652581 | 0.292308 |
| H | 2.086565 | 0.524782 | -0.856927 |
| C | -0.782073 | 4.514531 | 1.265662 |
| C | 3.428211 | 2.856494 | -0.837971 |
| F | -0.025778 | 5.387846 | 1.944738 |
| F | -1.398697 | 5.212198 | 0.297994 |
| F | -1.736677 | 4.078732 | 2.097375 |
| F | 3.590716 | 2.421011 | -2.096589 |
| F | 4.334577 | 2.213831 | -0.085420 |
| F | 3.758637 | 4.153597 | -0.824825 |
| C | 4.288361 | -2.047524 | 0.185977 |
| C | 3.846701 | -1.352163 | -0.945839 |
| C | 5.602573 | -1.843905 | 0.616691 |
| C | 4.696644 | -0.494374 | -1.633079 |
| H | 2.824626 | -1.502570 | -1.277182 |

| | | | |
|---|---|---|---|
| C | 6.449879 | -0.969315 | -0.058334 |
| H | 5.963913 | -2.373854 | 1.492378 |
| C | 6.002456 | -0.296306 | -1.190202 |
| H | 4.339676 | 0.025551 | -2.514549 |
| H | 7.462239 | -0.819327 | 0.299104 |
| H | 6.661984 | 0.379344 | -1.721841 |
| C | 1.184905 | -3.826286 | 1.669069 |
| H | 0.682195 | -3.550159 | 2.599917 |
| H | 0.412300 | -4.020290 | 0.917862 |
| H | 1.707201 | -4.765185 | 1.831576 |

**14J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -2932.764041

Free energies: -2932.226890

Corrected Free energies: -2932.215904

| | | | |
|---|---|---|---|
| Si | 1.128313 | -1.251542 | 2.682587 |
| O | 0.322943 | -1.321826 | 1.183563 |
| N | -1.505037 | -1.840733 | -1.016622 |
| C | -0.041408 | -1.620119 | -1.132162 |
| C | 0.144730 | -1.175941 | -2.589063 |
| C | -1.208849 | -0.611342 | -3.061308 |
| C | -2.225907 | -0.950837 | -1.964979 |
| C | 0.495324 | -0.639643 | -0.034975 |
| C | 0.089645 | -2.404520 | 3.713084 |
| C | 2.883146 | -1.878335 | 2.535546 |
| C | 1.124648 | 0.478054 | 3.393858 |
| C | 1.991785 | -0.367587 | -0.256763 |
| C | 2.839194 | -1.379707 | -0.711746 |
| C | 4.211388 | -1.181851 | -0.758330 |
| C | 4.782108 | 0.016776 | -0.350858 |
| C | 3.939939 | 1.020198 | 0.098679 |
| C | 2.561659 | 0.838217 | 0.143376 |
| C | -0.328762 | 0.648902 | -0.027601 |
| C | -1.275379 | 0.852169 | 0.972233 |
| C | -2.065993 | 1.994322 | 0.971367 |
| C | -1.955487 | 2.944356 | -0.035194 |
| C | -1.010653 | 2.737131 | -1.029394 |
| C | -0.190559 | 1.614691 | -1.022502 |
| C | -2.037535 | -2.888673 | -0.398172 |
| C | -3.444304 | -3.162491 | -0.406229 |
| H | 0.447390 | -2.571741 | -0.952519 |
| H | 0.413527 | -2.051376 | -3.179424 |

| | | | |
|---|---|---|---|
| H | 0.959491 | -0.461226 | -2.695232 |
| H | -1.172961 | 0.465000 | -3.220346 |
| H | -1.503800 | -1.072036 | -4.002092 |
| H | -2.570723 | -0.063217 | -1.431023 |
| H | -3.093985 | -1.475356 | -2.352654 |
| H | -0.958553 | -2.094360 | 3.710227 |
| H | 0.439837 | -2.406918 | 4.748326 |
| H | 0.145112 | -3.428810 | 3.336788 |
| H | 2.931444 | -2.790712 | 1.935450 |
| H | 3.250588 | -2.116541 | 3.538076 |
| H | 3.562529 | -1.141157 | 2.100454 |
| H | 1.706241 | 1.183295 | 2.796484 |
| H | 1.593774 | 0.429323 | 4.381772 |
| H | 0.119426 | 0.883396 | 3.526990 |
| H | 2.451250 | -2.341339 | -1.025053 |
| H | 5.853825 | 0.161931 | -0.382090 |
| H | 1.939890 | 1.648838 | 0.505224 |
| H | 0.564902 | 1.511399 | -1.794239 |
| C | -3.875730 | -4.589800 | -0.260096 |
| H | -4.848865 | -4.747164 | -0.720805 |
| H | -3.161607 | -5.292428 | -0.686964 |
| H | -3.993432 | -4.825890 | 0.805098 |
| C | 5.085651 | -2.328141 | -1.180005 |
| C | 4.489150 | 2.343011 | 0.550986 |
| F | 4.572039 | -2.985358 | -2.227750 |
| F | 5.217590 | -3.224761 | -0.189397 |
| F | 6.315584 | -1.928242 | -1.515867 |
| F | 4.108188 | 3.337158 | -0.263777 |
| F | 5.823622 | 2.350779 | 0.594662 |
| F | 4.043308 | 2.659881 | 1.776649 |
| H | -2.580684 | 3.827986 | -0.039672 |
| H | -1.391387 | 0.112934 | 1.753892 |
| C | -0.847830 | 3.718952 | -2.154412 |
| C | -2.997231 | 2.234557 | 2.124327 |
| F | -1.603103 | 4.807373 | -1.994253 |
| F | 0.424371 | 4.121041 | -2.274889 |
| F | -1.187180 | 3.166254 | -3.331063 |
| F | -3.442829 | 1.082999 | 2.651104 |
| F | -4.070268 | 2.950118 | 1.763103 |
| F | -2.393814 | 2.904805 | 3.114226 |
| C | -4.476034 | -2.130324 | -0.447899 |
| C | -4.325552 | -0.942049 | 0.286216 |
| C | -5.657021 | -2.324236 | -1.185037 |
| C | -5.317652 | 0.026200 | 0.269403 |

| | | | |
|---|---|---|---|
| H | -3.440026 | -0.803027 | 0.895939 |
| C | -6.634352 | -1.341746 | -1.217607 |
| H | -5.789835 | -3.224326 | -1.771797 |
| C | -6.469085 | -0.166084 | -0.490637 |
| H | -5.207300 | 0.929949 | 0.854319 |
| H | -7.527652 | -1.494213 | -1.810379 |
| H | -7.238228 | 0.596235 | -0.509713 |
| C | -1.133998 | -3.897671 | 0.256888 |
| H | -0.693553 | -4.547506 | -0.506951 |
| H | -0.338603 | -3.399317 | 0.802315 |
| H | -1.694549 | -4.517347 | 0.950547 |

**14J-*E***

Imaginary frequency: None

Electronic energies: -2932.947989

Free energies: -2932.415087

Corrected Free energies: -2932.402968

| | | | |
|---|---|---|---|
| Si | -0.328847 | -2.022092 | 1.906230 |
| O | -0.489105 | -0.798480 | 0.765694 |
| N | -1.810861 | -0.207984 | -1.605082 |
| C | -0.408609 | -0.629051 | -1.609815 |
| C | 0.197677 | 0.019786 | -2.872661 |
| C | -0.816503 | 1.091763 | -3.281646 |
| C | -2.134253 | 0.448550 | -2.881247 |
| C | 0.288549 | -0.233051 | -0.268752 |
| C | -2.097306 | -2.413852 | 2.358720 |
| C | 0.581551 | -3.509842 | 1.215736 |
| C | 0.548364 | -1.401208 | 3.440930 |
| C | 1.725742 | -0.756401 | -0.183777 |
| C | 2.258567 | -1.674132 | -1.081299 |
| C | 3.523477 | -2.217395 | -0.865847 |
| C | 4.287452 | -1.852266 | 0.228304 |
| C | 3.763480 | -0.912805 | 1.111655 |
| C | 2.503951 | -0.370488 | 0.912037 |
| C | 0.241737 | 1.282620 | -0.108029 |
| C | -0.885692 | 1.851125 | 0.480412 |
| C | -1.026223 | 3.231134 | 0.531389 |
| C | -0.050673 | 4.072102 | 0.009427 |
| C | 1.081195 | 3.499847 | -0.552113 |
| C | 1.236117 | 2.118039 | -0.608307 |
| C | -2.821010 | -1.074551 | -1.095121 |
| C | -3.954981 | -0.548214 | -0.594852 |
| H | -0.325311 | -1.717786 | -1.668170 |

| | | | |
|---|---|---|---|
| H | 0.270991 | -0.734694 | -3.659842 |
| H | 1.199797 | 0.419006 | -2.711713 |
| H | -0.663336 | 2.010650 | -2.709576 |
| H | -0.769880 | 1.331070 | -4.343736 |
| H | -2.941993 | 1.170381 | -2.751393 |
| H | -2.452714 | -0.288060 | -3.634908 |
| H | -2.567123 | -1.531837 | 2.803179 |
| H | -2.133084 | -3.220743 | 3.095759 |
| H | -2.695194 | -2.707009 | 1.493658 |
| H | 0.272211 | -3.767569 | 0.199079 |
| H | 0.377940 | -4.374725 | 1.854063 |
| H | 1.663544 | -3.350064 | 1.207598 |
| H | 1.634347 | -1.377949 | 3.338636 |
| H | 0.307650 | -2.060108 | 4.280452 |
| H | 0.205042 | -0.395661 | 3.699671 |
| H | 1.702081 | -1.997274 | -1.952527 |
| H | 5.265444 | -2.286298 | 0.393867 |
| H | 2.112163 | 0.350684 | 1.622001 |
| H | 2.137419 | 1.705767 | -1.047248 |
| C | -4.174253 | 0.935759 | -0.434759 |
| H | -4.946768 | 1.289436 | -1.126612 |
| H | -4.525048 | 1.166610 | 0.575325 |
| H | -3.261859 | 1.497065 | -0.624220 |
| C | 4.004552 | -3.273841 | -1.816509 |
| C | 4.599629 | -0.450769 | 2.270092 |
| F | 3.849202 | -2.899662 | -3.094336 |
| F | 3.308128 | -4.412561 | -1.664137 |
| F | 5.294734 | -3.573845 | -1.639849 |
| F | 5.410691 | 0.559557 | 1.922335 |
| F | 5.380263 | -1.430254 | 2.742501 |
| F | 3.845908 | -0.011113 | 3.287335 |
| H | -0.166220 | 5.148607 | 0.048396 |
| H | -1.642711 | 1.197120 | 0.891776 |
| C | 2.175127 | 4.392834 | -1.058067 |
| C | -2.276795 | 3.833185 | 1.100965 |
| F | 1.688463 | 5.514689 | -1.606518 |
| F | 3.003159 | 4.775190 | -0.071984 |
| F | 2.930753 | 3.788926 | -1.984513 |
| F | -2.895250 | 3.008052 | 1.954407 |
| F | -3.166180 | 4.129811 | 0.136184 |
| F | -2.030167 | 4.976876 | 1.755008 |
| C | -5.117277 | -1.391186 | -0.192759 |
| C | -5.803603 | -2.176830 | -1.124112 |
| C | -5.579873 | -1.372418 | 1.127558 |

| | | | |
|---|---|---|---|
| C | -6.903513 | -2.939826 | -0.744316 |
| H | -5.465015 | -2.187258 | -2.155017 |
| C | -6.678446 | -2.134751 | 1.510803 |
| H | -5.062979 | -0.766150 | 1.864036 |
| C | -7.344238 | -2.922269 | 0.575534 |
| H | -7.419486 | -3.543777 | -1.481677 |
| H | -7.013961 | -2.115139 | 2.541287 |
| H | -8.201585 | -3.514924 | 0.872089 |
| C | -2.574054 | -2.556354 | -1.222704 |
| H | -2.359704 | -2.817400 | -2.264839 |
| H | -1.710260 | -2.862440 | -0.628899 |
| H | -3.428207 | -3.138967 | -0.886831 |

**14J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -2932.763953

Free energies: -2932.229729

Corrected Free energies: -2932.217774

| | | | |
|---|---|---|---|
| Si | 0.558553 | -1.120443 | 2.709523 |
| O | -0.151418 | -0.946591 | 1.169635 |
| N | -1.959239 | -0.669511 | -1.037672 |
| C | -0.554399 | -1.115321 | -1.147120 |
| C | -0.189747 | -0.817851 | -2.607337 |
| C | -1.186681 | 0.248846 | -3.111302 |
| C | -2.232866 | 0.427728 | -2.001255 |
| C | 0.328443 | -0.429990 | -0.048793 |
| C | -0.880519 | -1.734463 | 3.720266 |
| C | 1.942216 | -2.376170 | 2.684760 |
| C | 1.187448 | 0.517683 | 3.358203 |
| C | 1.802089 | -0.825305 | -0.222156 |
| C | 2.144503 | -2.121159 | -0.614054 |
| C | 3.469314 | -2.530698 | -0.609772 |
| C | 4.488499 | -1.673881 | -0.212346 |
| C | 4.146912 | -0.389168 | 0.174106 |
| C | 2.822570 | 0.037507 | 0.167040 |
| C | 0.118921 | 1.084862 | -0.091027 |
| C | -0.726714 | 1.687905 | 0.835732 |
| C | -0.982567 | 3.053138 | 0.770883 |
| C | -0.426322 | 3.841933 | -0.225484 |
| C | 0.413578 | 3.235080 | -1.149000 |
| C | 0.697673 | 1.876927 | -1.081523 |
| C | -2.901136 | -1.319800 | -0.382743 |
| C | -4.208900 | -0.729546 | -0.225981 |

| | | | |
|---|---|---|---|
| H | -0.524943 | -2.180196 | -0.936504 |
| H | -0.299891 | -1.736622 | -3.182117 |
| H | 0.848078 | -0.503268 | -2.709245 |
| H | -0.695891 | 1.198480 | -3.318716 |
| H | -1.664815 | -0.084420 | -4.030136 |
| H | -2.130394 | 1.395148 | -1.509368 |
| H | -3.255127 | 0.323320 | -2.359977 |
| H | -1.741330 | -1.067802 | 3.623227 |
| H | -0.604538 | -1.778764 | 4.776990 |
| H | -1.185657 | -2.737297 | 3.412029 |
| H | 1.660143 | -3.272941 | 2.127232 |
| H | 2.153197 | -2.674881 | 3.715985 |
| H | 2.868014 | -1.980481 | 2.259500 |
| H | 1.978018 | 0.944479 | 2.737202 |
| H | 1.615748 | 0.344878 | 4.350516 |
| H | 0.393785 | 1.260143 | 3.465170 |
| H | 1.388254 | -2.836726 | -0.912639 |
| H | 5.519472 | -2.002844 | -0.202774 |
| H | 2.598884 | 1.050992 | 0.479229 |
| H | 1.387207 | 1.448073 | -1.801177 |
| C | -4.319584 | 0.723978 | 0.121333 |
| H | -4.939443 | 1.267475 | -0.597782 |
| H | -4.793770 | 0.824312 | 1.101927 |
| H | -3.348934 | 1.204235 | 0.194316 |
| C | 3.784882 | -3.958425 | -0.953194 |
| C | 5.194440 | 0.581705 | 0.638688 |
| F | 2.999375 | -4.420854 | -1.933851 |
| F | 3.597427 | -4.762448 | 0.105541 |
| F | 5.053875 | -4.113772 | -1.342767 |
| F | 5.234236 | 1.672854 | -0.138445 |
| F | 6.417421 | 0.045929 | 0.642684 |
| F | 4.937774 | 1.007863 | 1.885421 |
| H | -0.630330 | 4.903245 | -0.273614 |
| H | -1.188823 | 1.086127 | 1.609159 |
| C | 1.040947 | 4.029853 | -2.258694 |
| C | -1.894612 | 3.656243 | 1.801740 |
| F | 0.771378 | 5.333701 | -2.166153 |
| F | 2.373346 | 3.890736 | -2.269968 |
| F | 0.602605 | 3.614851 | -3.459215 |
| F | -1.557573 | 3.267219 | 3.039604 |
| F | -3.170130 | 3.275312 | 1.616854 |
| F | -1.874302 | 4.990602 | 1.777994 |
| C | -5.402761 | -1.541681 | -0.311075 |
| C | -5.404084 | -2.764245 | -1.016836 |

| | | | |
|---|---|---|---|
| C | -6.620883 | -1.090468 | 0.237716 |
| C | -6.561592 | -3.512648 | -1.138960 |
| H | -4.499274 | -3.109398 | -1.502944 |
| C | -7.774206 | -1.847376 | 0.116634 |
| H | -6.662724 | -0.152436 | 0.775212 |
| C | -7.749878 | -3.061584 | -0.566386 |
| H | -6.542853 | -4.443475 | -1.691712 |
| H | -8.697360 | -1.490169 | 0.555881 |
| H | -8.655093 | -3.648898 | -0.660122 |
| C | -2.595456 | -2.647558 | 0.251872 |
| H | -2.291626 | -3.379103 | -0.502283 |
| H | -1.772785 | -2.518527 | 0.954371 |
| H | -3.464965 | -3.021397 | 0.783567 |

**15J-*Z***

Imaginary frequency: None

Electronic energies: -925.460432

Free energies: -925.071049

Corrected Free energies: -925.068309

| | | | |
|---|---|---|---|
| C | 1.457616 | -1.853115 | -0.734423 |
| C | 0.101345 | -1.169579 | -0.727488 |
| C | 1.873495 | 0.400120 | -0.216200 |
| H | -0.505085 | -1.598438 | 0.081419 |
| H | 2.320785 | 1.132587 | -0.899455 |
| N | 0.440341 | 0.231847 | -0.475338 |
| C | -0.342038 | 1.276954 | -1.012500 |
| C | -1.677305 | 1.332503 | -0.818499 |
| C | -2.551808 | 2.335336 | -1.551256 |
| H | -3.573208 | 2.289167 | -1.174185 |
| H | -2.199020 | 3.358660 | -1.408061 |
| H | -2.588512 | 2.146107 | -2.628694 |
| N | 2.406628 | -0.921164 | -0.527634 |
| O | 1.655833 | -3.036197 | -0.956063 |
| C | 3.812499 | -1.245888 | -0.675141 |
| H | 4.233027 | -1.669740 | 0.239951 |
| H | 3.908687 | -1.984565 | -1.471135 |
| H | 4.367061 | -0.347225 | -0.942574 |
| C | -0.571216 | -1.445987 | -2.071253 |
| H | -1.583567 | -1.049427 | -2.104894 |
| H | 0.012341 | -0.999395 | -2.881083 |
| H | -0.609658 | -2.526203 | -2.218282 |
| C | 2.174492 | 0.854226 | 1.240685 |
| C | 1.680132 | -0.207503 | 2.225157 |

| | | | |
|---|---|---|---|
| H | 2.253690 | -1.133059 | 2.124884 |
| H | 1.794204 | 0.148626 | 3.252108 |
| H | 0.625816 | -0.440565 | 2.057500 |
| C | 3.678214 | 1.087574 | 1.441947 |
| H | 4.087122 | 1.739575 | 0.663661 |
| H | 3.840514 | 1.578757 | 2.404958 |
| H | 4.247796 | 0.158610 | 1.451361 |
| C | 1.467242 | 2.193079 | 1.486435 |
| H | 1.627957 | 2.507341 | 2.520569 |
| H | 1.878148 | 2.972668 | 0.837489 |
| H | 0.392886 | 2.134178 | 1.308247 |
| C | -2.393393 | 0.385869 | 0.079826 |
| C | -3.508968 | -0.324159 | -0.380447 |
| C | -2.009446 | 0.211576 | 1.413374 |
| C | -4.194542 | -1.203512 | 0.451684 |
| H | -3.838078 | -0.191507 | -1.406452 |
| C | -2.694657 | -0.662135 | 2.249942 |
| H | -1.168572 | 0.775807 | 1.796167 |
| C | -3.787294 | -1.380150 | 1.770397 |
| H | -5.048857 | -1.749903 | 0.068975 |
| H | -2.377951 | -0.777054 | 3.280369 |
| H | -4.321151 | -2.063308 | 2.420137 |
| C | 0.376331 | 2.270391 | -1.893443 |
| H | -0.325163 | 2.875109 | -2.461689 |
| H | 1.006362 | 2.950997 | -1.314124 |
| H | 1.022800 | 1.743394 | -2.600641 |

**15J-*E***

Imaginary frequency: None

Electronic energies: -925.462555

Free energies: -925.073481

Corrected Free energies: -925.070448

| | | | |
|---|---|---|---|
| C | -2.512656 | 1.718633 | 0.298926 |
| C | -1.092292 | 1.434325 | 0.759217 |
| C | -1.942693 | -0.377195 | -0.598724 |
| H | -1.110994 | 1.315361 | 1.851278 |
| H | -1.742489 | -0.569268 | -1.659651 |
| N | -0.771358 | 0.182538 | 0.073075 |
| C | 0.544204 | -0.079265 | -0.360355 |
| C | 1.538957 | -0.101614 | 0.552798 |
| N | -2.912577 | 0.707496 | -0.495127 |
| O | -3.160282 | 2.715542 | 0.571671 |
| C | -4.180653 | 0.760961 | -1.195609 |

| | | | |
|---|---|---|---|
| H | -4.999112 | 0.361791 | -0.591037 |
| H | -4.397387 | 1.804683 | -1.422736 |
| H | -4.109562 | 0.192527 | -2.122732 |
| C | -0.201273 | 2.620515 | 0.402101 |
| H | 0.810783 | 2.492322 | 0.784438 |
| H | -0.152588 | 2.744777 | -0.682991 |
| H | -0.635366 | 3.519675 | 0.841062 |
| C | -2.421079 | -1.706968 | 0.053495 |
| C | -2.901760 | -1.446592 | 1.481320 |
| H | -3.776875 | -0.791348 | 1.495787 |
| H | -3.178133 | -2.388772 | 1.961384 |
| H | -2.111443 | -0.983123 | 2.078734 |
| C | -3.545109 | -2.341667 | -0.775526 |
| H | -3.253971 | -2.438580 | -1.826210 |
| H | -3.756059 | -3.344275 | -0.394842 |
| H | -4.473674 | -1.772880 | -0.725828 |
| C | -1.238590 | -2.683362 | 0.078944 |
| H | -1.566380 | -3.643458 | 0.485101 |
| H | -0.852362 | -2.865224 | -0.929109 |
| H | -0.422437 | -2.307787 | 0.698915 |
| C | 2.976037 | -0.091249 | 0.169704 |
| C | 3.859211 | -1.056394 | 0.668427 |
| C | 3.492504 | 0.909493 | -0.661563 |
| C | 5.207635 | -1.034168 | 0.331002 |
| H | 3.481994 | -1.841391 | 1.315271 |
| C | 4.841743 | 0.935071 | -0.999899 |
| H | 2.822320 | 1.674119 | -1.041047 |
| C | 5.704829 | -0.037974 | -0.505166 |
| H | 5.871993 | -1.797338 | 0.719471 |
| H | 5.219635 | 1.719389 | -1.645468 |
| H | 6.756489 | -0.018741 | -0.765594 |
| C | 1.244264 | -0.074513 | 2.032151 |
| H | 1.237087 | 0.946928 | 2.433115 |
| H | 0.270841 | -0.522560 | 2.241527 |
| H | 2.009494 | -0.622655 | 2.584224 |
| C | 0.750003 | -0.302170 | -1.837676 |
| H | 0.363233 | 0.543135 | -2.415684 |
| H | 1.802405 | -0.439660 | -2.071358 |
| H | 0.222690 | -1.197403 | -2.176434 |

**15J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -925.270027

Free energies: -924.878862

Corrected Free energies: -924.876233

| | | | |
|---|---|---|---|
| C | -2.167781 | 1.839092 | 0.300718 |
| C | -0.901516 | 1.228534 | 0.910584 |
| C | -1.979962 | -0.299154 | -0.642485 |
| H | -1.130951 | 0.925186 | 1.934958 |
| H | -1.786626 | -0.564226 | -1.683881 |
| N | -0.702801 | 0.043610 | 0.038131 |
| C | 0.474454 | -0.462995 | -0.298010 |
| C | 1.583829 | -0.382539 | 0.609011 |
| N | -2.687229 | 0.965825 | -0.584031 |
| O | -2.587568 | 2.946435 | 0.553400 |
| C | -3.770715 | 1.354678 | -1.476021 |
| H | -4.738078 | 1.307457 | -0.974414 |
| H | -3.593698 | 2.379099 | -1.803649 |
| H | -3.778458 | 0.692548 | -2.339838 |
| C | 0.218567 | 2.257758 | 0.879472 |
| H | 1.087774 | 1.965841 | 1.463936 |
| H | 0.520877 | 2.464212 | -0.149424 |
| H | -0.188348 | 3.173415 | 1.309062 |
| C | -2.719653 | -1.467928 | 0.074800 |
| C | -2.955516 | -1.150505 | 1.554054 |
| H | -3.448557 | -0.184666 | 1.691200 |
| H | -3.607295 | -1.914891 | 1.981618 |
| H | -2.024964 | -1.164421 | 2.126805 |
| C | -4.071976 | -1.674416 | -0.621960 |
| H | -3.956174 | -1.791237 | -1.703197 |
| H | -4.529851 | -2.587187 | -0.235391 |
| H | -4.760635 | -0.852206 | -0.425516 |
| C | -1.914387 | -2.765738 | -0.043174 |
| H | -2.439955 | -3.554819 | 0.498323 |
| H | -1.823648 | -3.088728 | -1.083528 |
| H | -0.917075 | -2.682317 | 0.397399 |
| C | 2.937868 | -0.214470 | 0.126524 |
| C | 4.033584 | -0.625910 | 0.911744 |
| C | 3.197403 | 0.440147 | -1.095727 |
| C | 5.330721 | -0.423393 | 0.471783 |
| H | 3.868169 | -1.123599 | 1.858492 |
| C | 4.496630 | 0.651151 | -1.522993 |
| H | 2.375520 | 0.814520 | -1.694870 |
| C | 5.567322 | 0.213337 | -0.744964 |
| H | 6.161909 | -0.759636 | 1.078762 |
| H | 4.677696 | 1.164444 | -2.458850 |
| H | 6.583500 | 0.375100 | -1.083162 |

| | | | |
|---|---|---|---|
| C | 1.349785 | -0.588162 | 2.075234 |
| H | 1.874306 | 0.155503 | 2.678700 |
| H | 0.295444 | -0.593340 | 2.337562 |
| H | 1.747316 | -1.570297 | 2.353196 |
| C | 0.623464 | -1.183069 | -1.610948 |
| H | 0.384006 | -0.511986 | -2.440566 |
| H | 1.636942 | -1.554022 | -1.724219 |
| H | -0.051118 | -2.035789 | -1.661264 |

**15J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -925.269901

Free energies: -924.877780

Corrected Free energies: -924.875475

| | | | |
|---|---|---|---|
| C | 1.618002 | -1.679488 | 0.955221 |
| C | 0.212809 | -1.196781 | 0.588843 |
| C | 1.949386 | 0.124830 | -0.503089 |
| H | -0.221273 | -0.666177 | 1.440118 |
| H | 2.343965 | 0.116239 | -1.520410 |
| N | 0.503448 | -0.250030 | -0.523044 |
| C | -0.302196 | 0.000208 | -1.543665 |
| C | -1.721092 | -0.202535 | -1.457421 |
| C | -2.430501 | -0.769123 | -2.648589 |
| H | -3.267220 | -0.133243 | -2.947827 |
| H | -1.769392 | -0.923225 | -3.496802 |
| H | -2.844789 | -1.747630 | -2.382652 |
| N | 2.520263 | -0.976235 | 0.245749 |
| O | 1.855152 | -2.594866 | 1.712437 |
| C | 3.922094 | -1.368556 | 0.215348 |
| H | 4.445968 | -1.051645 | 1.118346 |
| H | 3.971589 | -2.454954 | 0.143622 |
| H | 4.399346 | -0.923852 | -0.655899 |
| C | -0.624234 | -2.415200 | 0.212492 |
| H | -1.689665 | -2.208233 | 0.184171 |
| H | -0.297341 | -2.821518 | -0.747336 |
| H | -0.443763 | -3.163761 | 0.984177 |
| C | 2.200441 | 1.514489 | 0.156331 |
| C | 1.712654 | 1.530052 | 1.608923 |
| H | 2.171759 | 0.731085 | 2.196204 |
| H | 1.994784 | 2.479667 | 2.067720 |
| H | 0.627296 | 1.441593 | 1.690656 |
| C | 3.713348 | 1.782149 | 0.138842 |
| H | 4.134969 | 1.651021 | -0.861593 |

| | | | |
|---|---|---|---|
| H | 3.889883 | 2.815923 | 0.443009 |
| H | 4.250459 | 1.139487 | 0.836134 |
| C | 1.519476 | 2.634568 | -0.638816 |
| H | 1.650013 | 3.575104 | -0.100300 |
| H | 1.975588 | 2.759874 | -1.623864 |
| H | 0.445134 | 2.483314 | -0.768201 |
| C | -2.489071 | 0.149848 | -0.279121 |
| C | -3.771923 | -0.398451 | -0.072536 |
| C | -2.015616 | 1.097188 | 0.649396 |
| C | -4.518470 | -0.047077 | 1.039541 |
| H | -4.175350 | -1.121029 | -0.770272 |
| C | -2.770660 | 1.453920 | 1.753843 |
| H | -1.067609 | 1.588410 | 0.477121 |
| C | -4.020930 | 0.874714 | 1.959458 |
| H | -5.493417 | -0.493241 | 1.191388 |
| H | -2.388827 | 2.191604 | 2.448716 |
| H | -4.610290 | 1.148750 | 2.825822 |
| C | 0.269132 | 0.455805 | -2.858911 |
| H | 0.745555 | -0.395306 | -3.357038 |
| H | -0.516138 | 0.848233 | -3.498361 |
| H | 1.015675 | 1.232940 | -2.731620 |

**16J-*E***

Imaginary frequency: None

Electronic energies: -1156.470224

Free energies: -1156.006250

Corrected Free energies: -1156.000544

| | | | |
|---|---|---|---|
| C | 2.504208 | -0.200957 | -1.003099 |
| C | 1.258513 | 0.336029 | -0.321397 |
| C | 1.275121 | -2.073716 | -0.292447 |
| H | 0.698855 | 0.894687 | -1.083267 |
| H | 0.701866 | -2.708414 | -0.980737 |
| N | 0.510131 | -0.866722 | 0.069625 |
| C | -0.859805 | -0.844129 | -0.372101 |
| C | -1.820291 | -0.429693 | 0.469855 |
| N | 2.436466 | -1.544969 | -1.001548 |
| O | 3.405773 | 0.467788 | -1.484257 |
| C | 3.400525 | -2.336954 | -1.743747 |
| H | 2.934648 | -3.268027 | -2.064490 |
| H | 3.708688 | -1.763064 | -2.617618 |
| H | 4.287132 | -2.565031 | -1.148152 |
| C | 1.593654 | 1.295679 | 0.844795 |
| H | 0.942957 | 1.046418 | 1.682100 |

| | | | |
|---|---|---|---|
| H | 2.621421 | 1.111391 | 1.176314 |
| C | 1.608922 | -2.928504 | 0.956703 |
| C | 2.426133 | -2.111125 | 1.956220 |
| H | 1.865433 | -1.233056 | 2.285824 |
| H | 2.662546 | -2.717290 | 2.834510 |
| H | 3.370047 | -1.776034 | 1.515166 |
| C | 0.275896 | -3.353339 | 1.584203 |
| H | -0.321376 | -3.935864 | 0.874521 |
| H | 0.463838 | -3.980513 | 2.459293 |
| H | -0.311521 | -2.489433 | 1.897172 |
| C | 2.376018 | -4.198113 | 0.565101 |
| H | 2.416899 | -4.873961 | 1.423011 |
| H | 1.877911 | -4.728542 | -0.252686 |
| H | 3.403487 | -3.986772 | 0.267944 |
| C | 1.425108 | 2.758828 | 0.507409 |
| C | 2.002884 | 3.306397 | -0.642174 |
| C | 0.681628 | 3.592431 | 1.344151 |
| C | 1.840129 | 4.654802 | -0.942490 |
| H | 2.585059 | 2.663464 | -1.294963 |
| C | 0.519489 | 4.943037 | 1.046381 |
| H | 0.226465 | 3.180128 | 2.239036 |
| C | 1.098924 | 5.478613 | -0.098892 |
| H | 2.293858 | 5.064852 | -1.837487 |
| H | -0.063183 | 5.574280 | 1.707380 |
| H | 0.972092 | 6.528696 | -0.334066 |
| C | -1.559945 | -0.029995 | 1.900236 |
| H | -0.567938 | -0.343310 | 2.219605 |
| H | -1.632755 | 1.055534 | 2.024643 |
| H | -2.310076 | -0.477946 | 2.557141 |
| C | -3.243960 | -0.329271 | 0.040312 |
| C | -3.946050 | 0.868673 | 0.209352 |
| C | -3.921426 | -1.429713 | -0.492262 |
| C | -5.281227 | 0.969989 | -0.166110 |
| H | -3.438951 | 1.732909 | 0.624556 |
| C | -5.259074 | -1.332516 | -0.861815 |
| H | -3.394105 | -2.370281 | -0.608698 |
| C | -5.942668 | -0.131049 | -0.702467 |
| H | -5.805242 | 1.909975 | -0.038564 |
| H | -5.767883 | -2.197346 | -1.271253 |
| H | -6.984087 | -0.054004 | -0.991327 |
| C | -1.096484 | -1.192884 | -1.826528 |
| H | -1.225984 | -2.267966 | -1.979569 |
| H | -1.984712 | -0.698705 | -2.217021 |
| H | -0.235104 | -0.882364 | -2.425931 |

**16J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1156.272226

Free energies: -1155.808540

Corrected Free energies: -1155.802541

| | | | |
|---|---|---|---|
| C | -1.816128 | 0.346493 | 1.538288 |
| C | -0.785329 | 0.542182 | 0.428431 |
| C | -1.983652 | -1.561591 | 0.166772 |
| H | 0.180768 | 0.748739 | 0.890385 |
| H | -1.718833 | -2.576630 | 0.463018 |
| N | -0.727486 | -0.820660 | -0.154018 |
| C | 0.421607 | -1.453838 | -0.383512 |
| C | 1.631345 | -0.733289 | -0.654668 |
| N | -2.434429 | -0.834362 | 1.342190 |
| O | -2.040504 | 1.146154 | 2.421967 |
| C | -3.428076 | -1.336922 | 2.278338 |
| H | -3.392676 | -2.425486 | 2.292084 |
| H | -3.180329 | -0.950721 | 3.265925 |
| H | -4.433513 | -1.006127 | 2.011755 |
| C | -1.207433 | 1.720156 | -0.489706 |
| H | -1.162571 | 1.414445 | -1.534052 |
| H | -2.252340 | 1.965410 | -0.283094 |
| C | -3.021308 | -1.651786 | -0.993269 |
| C | -3.699172 | -0.310747 | -1.280743 |
| H | -3.032864 | 0.384163 | -1.791175 |
| H | -4.548397 | -0.485793 | -1.944621 |
| H | -4.081669 | 0.160186 | -0.371808 |
| C | -2.347784 | -2.160816 | -2.274802 |
| H | -2.044060 | -3.206197 | -2.187962 |
| H | -3.071070 | -2.106690 | -3.091092 |
| H | -1.483873 | -1.554905 | -2.561197 |
| C | -4.092840 | -2.674588 | -0.580352 |
| H | -4.719082 | -2.895750 | -1.447247 |
| H | -3.645042 | -3.613680 | -0.243645 |
| H | -4.746475 | -2.296655 | 0.206071 |
| C | -0.368195 | 2.962459 | -0.286169 |
| C | -0.061322 | 3.420161 | 0.997054 |
| C | 0.093401 | 3.681493 | -1.389334 |
| C | 0.703990 | 4.568909 | 1.170069 |
| H | -0.433409 | 2.880573 | 1.862407 |
| C | 0.854964 | 4.832639 | -1.216238 |
| H | -0.139088 | 3.334483 | -2.391013 |

| | | | |
|---|---|---|---|
| C | 1.165543 | 5.277404 | 0.064866 |
| H | 0.936477 | 4.912728 | 2.170987 |
| H | 1.209200 | 5.378018 | -2.082937 |
| H | 1.761899 | 6.171509 | 0.201212 |
| C | 1.610420 | 0.545046 | -1.425471 |
| H | 0.693261 | 0.660543 | -1.996954 |
| H | 1.734901 | 1.407976 | -0.760616 |
| H | 2.446612 | 0.574189 | -2.123451 |
| C | 2.901703 | -1.272112 | -0.190892 |
| C | 2.962405 | -1.968695 | 1.032846 |
| C | 4.097505 | -1.060454 | -0.900832 |
| C | 4.168944 | -2.438892 | 1.521965 |
| H | 2.061043 | -2.104626 | 1.619740 |
| C | 5.299710 | -1.550561 | -0.415053 |
| H | 4.087641 | -0.544993 | -1.851747 |
| C | 5.340978 | -2.236579 | 0.796188 |
| H | 4.198447 | -2.958050 | 2.471587 |
| H | 6.208644 | -1.396881 | -0.982948 |
| H | 6.284380 | -2.610202 | 1.175440 |
| C | 0.453067 | -2.957320 | -0.414015 |
| H | 1.428564 | -3.304618 | -0.737868 |
| H | 0.236851 | -3.376438 | 0.572714 |
| H | -0.292018 | -3.335108 | -1.111392 |

**16J-*Z***

Imaginary frequency: None

Electronic energies: -1156.472444

Free energies: -1156.007655

Corrected Free energies: -1156.003066

| | | | |
|---|---|---|---|
| C | -0.523144 | 1.048879 | 1.827671 |
| C | 0.617952 | 0.242677 | 1.226705 |
| C | -0.870079 | 1.026861 | -0.495893 |
| H | 0.615408 | -0.750750 | 1.686943 |
| N | 0.263350 | 0.140073 | -0.191557 |
| C | 0.271415 | -1.173211 | -0.776183 |
| C | -0.792668 | -1.996840 | -0.827153 |
| C | -0.701539 | -3.298099 | -1.599695 |
| H | 0.187774 | -3.865912 | -1.317204 |
| H | -1.574714 | -3.922002 | -1.410720 |
| H | -0.640412 | -3.119058 | -2.678587 |
| N | -1.285541 | 1.513657 | 0.815914 |
| O | -0.707022 | 1.240956 | 3.017999 |
| C | -2.586255 | 2.101384 | 1.081777 |

| | | | |
|---|---|---|---|
| H | -3.299498 | 1.749210 | 0.334249 |
| H | -2.909006 | 1.768379 | 2.068700 |
| H | -2.555677 | 3.192285 | 1.069708 |
| C | 1.955022 | 0.923955 | 1.574685 |
| H | 1.935783 | 1.962614 | 1.239069 |
| H | 2.015516 | 0.936565 | 2.667618 |
| C | 3.149427 | 0.214166 | 0.994436 |
| C | 3.938811 | 0.823381 | 0.019697 |
| C | 3.470532 | -1.083918 | 1.399624 |
| C | 5.008561 | 0.145336 | -0.559762 |
| H | 3.712168 | 1.837469 | -0.292566 |
| C | 4.537635 | -1.764444 | 0.825211 |
| H | 2.875883 | -1.568041 | 2.168557 |
| C | 5.305900 | -1.154054 | -0.163812 |
| H | 5.606667 | 0.632513 | -1.321056 |
| H | 4.770992 | -2.772627 | 1.147690 |
| H | 6.134797 | -1.685616 | -0.616029 |
| C | -0.500237 | 2.123215 | -1.526105 |
| C | -2.117596 | -1.704044 | -0.212391 |
| C | -3.266502 | -1.700586 | -1.015761 |
| C | -2.264953 | -1.453220 | 1.153586 |
| C | -4.514126 | -1.413441 | -0.476652 |
| H | -3.171404 | -1.906298 | -2.077304 |
| C | -3.515393 | -1.170027 | 1.697611 |
| H | -1.399027 | -1.495264 | 1.803454 |
| C | -4.642590 | -1.141440 | 0.884140 |
| H | -5.388085 | -1.402052 | -1.117528 |
| H | -3.604873 | -0.975854 | 2.760434 |
| H | -5.615192 | -0.918399 | 1.306411 |
| H | -1.702108 | 0.463905 | -0.930382 |
| C | -0.065573 | 1.402191 | -2.807364 |
| H | -0.857176 | 0.740124 | -3.174566 |
| H | 0.154587 | 2.132767 | -3.589925 |
| H | 0.831344 | 0.803761 | -2.632606 |
| C | 0.637137 | 3.007533 | -1.023251 |
| H | 0.383206 | 3.476885 | -0.068010 |
| H | 1.546566 | 2.417639 | -0.897138 |
| H | 0.842025 | 3.800644 | -1.747117 |
| C | -1.729325 | 2.984118 | -1.841143 |
| H | -2.594188 | 2.365339 | -2.101138 |
| H | -2.002039 | 3.626841 | -1.002942 |
| H | -1.512282 | 3.630966 | -2.695003 |
| C | 1.578365 | -1.586167 | -1.417207 |
| H | 2.285754 | -0.759836 | -1.398581 |

| | | | |
|---|---|---|---|
| H | 2.033762 | -2.435443 | -0.898574 |
| H | 1.420306 | -1.889737 | -2.456966 |

**16J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1156.277840

Free energies: -1155.811360

Corrected Free energies: -1155.806894

| | | | |
|---|---|---|---|
| C | 0.231965 | 2.312383 | 1.256908 |
| C | 1.075089 | 1.058120 | 1.068537 |
| C | -0.909236 | 1.029345 | -0.362590 |
| H | 1.225116 | 0.600320 | 2.046684 |
| N | 0.158539 | 0.194886 | 0.281757 |
| C | 0.124588 | -1.123420 | 0.362482 |
| C | -0.999216 | -1.919161 | -0.076298 |
| C | -0.706151 | -3.167351 | -0.852957 |
| H | -1.142245 | -4.041353 | -0.362382 |
| H | -1.157796 | -3.094046 | -1.847690 |
| H | 0.360514 | -3.327166 | -0.995689 |
| N | -0.844252 | 2.233380 | 0.446477 |
| O | 0.511742 | 3.218747 | 2.009771 |
| C | -1.916935 | 3.214784 | 0.524372 |
| H | -2.869566 | 2.724567 | 0.324104 |
| H | -1.920248 | 3.622240 | 1.534360 |
| H | -1.769003 | 4.030486 | -0.184783 |
| C | 2.434412 | 1.463662 | 0.465049 |
| H | 2.275490 | 2.028384 | -0.451505 |
| H | 2.846029 | 2.161876 | 1.199020 |
| C | 3.394470 | 0.327656 | 0.237071 |
| C | 3.539760 | -0.246420 | -1.025963 |
| C | 4.123355 | -0.195948 | 1.306263 |
| C | 4.368911 | -1.349743 | -1.210336 |
| H | 3.003036 | 0.165246 | -1.873859 |
| C | 4.948186 | -1.299831 | 1.126922 |
| H | 4.032423 | 0.257355 | 2.288873 |
| C | 5.064649 | -1.886141 | -0.131457 |
| H | 4.470619 | -1.788908 | -2.195626 |
| H | 5.501871 | -1.702062 | 1.966809 |
| H | 5.705900 | -2.747786 | -0.272306 |
| C | -0.766766 | 1.237259 | -1.899695 |
| C | -2.363592 | -1.633065 | 0.326262 |
| C | -3.446976 | -2.145094 | -0.410590 |
| C | -2.635214 | -0.892604 | 1.495944 |

| | | | |
|---|---|---|---|
| C | -4.751100 | -1.889302 | -0.013699 |
| H | -3.268763 | -2.724013 | -1.308201 |
| C | -3.939138 | -0.650399 | 1.890912 |
| H | -1.816985 | -0.524318 | 2.105975 |
| C | -5.002266 | -1.141212 | 1.133262 |
| H | -5.574528 | -2.274337 | -0.602065 |
| H | -4.130391 | -0.086353 | 2.795217 |
| H | -6.022143 | -0.946608 | 1.441414 |
| H | -1.871970 | 0.554029 | -0.198664 |
| C | -0.639387 | -0.117894 | -2.604141 |
| H | -1.518124 | -0.744182 | -2.425730 |
| H | -0.571811 | 0.052883 | -3.680559 |
| H | 0.259731 | -0.662469 | -2.303559 |
| C | 0.409760 | 2.131920 | -2.286527 |
| H | 0.445759 | 3.042769 | -1.683204 |
| H | 1.361128 | 1.606995 | -2.202672 |
| H | 0.300415 | 2.429015 | -3.331583 |
| C | -2.073415 | 1.892658 | -2.382085 |
| H | -2.952190 | 1.342516 | -2.032664 |
| H | -2.158235 | 2.930920 | -2.062305 |
| H | -2.086861 | 1.885478 | -3.473679 |
| C | 1.274610 | -1.887866 | 0.950207 |
| H | 1.724162 | -1.355104 | 1.785558 |
| H | 0.925374 | -2.857956 | 1.297087 |
| H | 2.057172 | -2.040278 | 0.200693 |

**17J-*E***

Imaginary frequency: None

Electronic energies: -1077.867796

Free energies: -1077.458784

Corrected Free energies: -1077.454206

| | | | |
|---|---|---|---|
| C | 3.094925 | 0.389618 | -1.052498 |
| C | 1.640877 | 0.662717 | -0.712270 |
| C | 2.565727 | -0.994561 | 0.791783 |
| H | 1.055126 | 0.499045 | -1.620799 |
| N | 1.350093 | -0.306845 | 0.324875 |
| C | 0.043547 | -0.812652 | 0.540535 |
| C | -0.719053 | -1.268904 | -0.473992 |
| N | 3.533276 | -0.594991 | -0.242813 |
| O | 3.740122 | 0.973856 | -1.907390 |
| C | 4.906400 | -1.055464 | -0.253662 |
| H | 5.421318 | -0.787768 | 0.671793 |
| H | 4.950770 | -2.137229 | -0.389293 |

| | | | |
|---|---|---|---|
| H | 5.405045 | -0.568146 | -1.089463 |
| C | 1.454494 | 2.131866 | -0.294727 |
| H | 2.026525 | 2.321106 | 0.617453 |
| H | 1.880326 | 2.748720 | -1.092424 |
| C | 0.005979 | 2.498153 | -0.087000 |
| C | -0.503913 | 2.739956 | 1.187950 |
| C | -0.856285 | 2.609454 | -1.182702 |
| C | -1.839638 | 3.096282 | 1.367966 |
| H | 0.155234 | 2.662867 | 2.046888 |
| C | -2.188023 | 2.966884 | -1.008864 |
| H | -0.473103 | 2.428428 | -2.182772 |
| C | -2.683813 | 3.216872 | 0.269652 |
| H | -2.216670 | 3.285423 | 2.366489 |
| H | -2.840025 | 3.054710 | -1.870213 |
| H | -3.720911 | 3.499522 | 0.406674 |
| C | 2.399631 | -2.511536 | 0.806074 |
| H | 1.620645 | -2.802679 | 1.512143 |
| H | 2.126575 | -2.871832 | -0.187193 |
| H | 3.328900 | -2.990885 | 1.119697 |
| C | 3.040903 | -0.478027 | 2.156476 |
| H | 2.301874 | -0.699547 | 2.926178 |
| H | 3.981490 | -0.950382 | 2.448969 |
| H | 3.184789 | 0.603147 | 2.110855 |
| C | -0.190230 | -1.538327 | -1.859249 |
| H | -0.606251 | -2.475400 | -2.236354 |
| H | -0.490690 | -0.755340 | -2.565759 |
| H | 0.896873 | -1.623220 | -1.870578 |
| C | -2.183520 | -1.472378 | -0.303178 |
| C | -2.807965 | -2.677060 | -0.641591 |
| C | -2.976072 | -0.419187 | 0.166354 |
| C | -4.183154 | -2.829181 | -0.495588 |
| H | -2.213300 | -3.508939 | -1.003712 |
| C | -4.351239 | -0.566858 | 0.306157 |
| H | -2.496365 | 0.522003 | 0.415181 |
| C | -4.960121 | -1.774887 | -0.023427 |
| H | -4.649382 | -3.773907 | -0.750180 |
| H | -4.947430 | 0.263740 | 0.667280 |
| H | -6.031853 | -1.894139 | 0.083893 |
| C | -0.412477 | -0.780484 | 1.977466 |
| H | 0.292861 | -1.334947 | 2.602192 |
| H | -0.435600 | 0.247055 | 2.350002 |
| H | -1.393220 | -1.233176 | 2.107745 |

**17J-*E*** radical cation

Imaginary frequency: None

Electronic energies: -1077.674236

Free energies: -1077.262008

Corrected Free energies: -1077.258140

| | | | |
|---|---|---|---|
| C | 3.087911 | 1.126605 | -0.669423 |
| C | 1.600443 | 0.864610 | -0.571350 |
| C | 2.891940 | -0.974087 | 0.433450 |
| H | 1.160146 | 0.950242 | -1.561578 |
| N | 1.531428 | -0.514248 | -0.045681 |
| C | 0.404357 | -1.217266 | 0.034554 |
| C | -0.672918 | -0.969938 | -0.887597 |
| N | 3.732397 | 0.132531 | -0.031868 |
| O | 3.577755 | 2.107834 | -1.187832 |
| C | 5.184192 | 0.085054 | 0.027374 |
| H | 5.520877 | -0.183829 | 1.027844 |
| H | 5.585577 | -0.625132 | -0.697698 |
| H | 5.544926 | 1.082496 | -0.213691 |
| C | 0.999201 | 1.923053 | 0.375291 |
| H | 1.421411 | 1.785713 | 1.373639 |
| H | 1.374560 | 2.877421 | -0.006588 |
| C | -0.504561 | 1.963756 | 0.441311 |
| C | -1.164661 | 1.783519 | 1.655710 |
| C | -1.257115 | 2.243117 | -0.703326 |
| C | -2.552436 | 1.871907 | 1.726129 |
| H | -0.588824 | 1.577183 | 2.552204 |
| C | -2.643082 | 2.304990 | -0.639963 |
| H | -0.754012 | 2.424349 | -1.648721 |
| C | -3.295210 | 2.119815 | 0.577453 |
| H | -3.052964 | 1.727387 | 2.676595 |
| H | -3.214977 | 2.510046 | -1.537339 |
| H | -4.376536 | 2.166720 | 0.627656 |
| C | 3.323540 | -2.244397 | -0.301268 |
| H | 2.700260 | -3.104711 | -0.075423 |
| H | 3.313207 | -2.067803 | -1.377753 |
| H | 4.340595 | -2.494016 | 0.005358 |
| C | 2.976072 | -1.088614 | 1.954821 |
| H | 2.496747 | -1.990075 | 2.327169 |
| H | 4.026311 | -1.142035 | 2.242446 |
| H | 2.530964 | -0.213894 | 2.430185 |
| C | -0.326748 | -0.733201 | -2.331679 |
| H | -0.791359 | -1.524659 | -2.924487 |
| H | -0.716568 | 0.218806 | -2.703381 |
| H | 0.742902 | -0.793318 | -2.515238 |

| | | | |
|---|---|---|---|
| C | -2.064332 | -1.116054 | -0.517186 |
| C | -3.065115 | -1.151214 | -1.514968 |
| C | -2.485365 | -1.153363 | 0.829347 |
| C | -4.402848 | -1.254918 | -1.179812 |
| H | -2.798264 | -1.100629 | -2.561624 |
| C | -3.824995 | -1.270737 | 1.158593 |
| H | -1.766470 | -1.046025 | 1.628878 |
| C | -4.789813 | -1.325890 | 0.158034 |
| H | -5.149156 | -1.285139 | -1.963878 |
| H | -4.118188 | -1.293411 | 2.201052 |
| H | -5.838286 | -1.411686 | 0.416435 |
| C | 0.279569 | -2.344623 | 1.025093 |
| H | 1.134207 | -3.012818 | 0.979088 |
| H | 0.228271 | -1.947171 | 2.042002 |
| H | -0.612325 | -2.927408 | 0.818814 |

**17J-*Z***

Imaginary frequency: None

Electronic energies: -1077.865720

Free energies: -1077.454189

Corrected Free energies: -1077.450510

| | | | |
|---|---|---|---|
| C | -1.938163 | 0.214759 | -1.722030 |
| C | -0.716019 | -0.167546 | -0.907156 |
| C | -2.742506 | -0.459487 | 0.390803 |
| H | -0.044637 | 0.699124 | -0.933147 |
| N | -1.274658 | -0.389540 | 0.412494 |
| C | -0.483605 | -0.716344 | 1.536509 |
| C | 0.586313 | 0.026954 | 1.885063 |
| C | 1.583988 | -0.438594 | 2.927892 |
| H | 1.109548 | -0.600092 | 3.898583 |
| H | 2.071994 | -1.373710 | 2.634725 |
| H | 2.362770 | 0.311258 | 3.066020 |
| N | -3.017979 | 0.143857 | -0.920967 |
| O | -1.925568 | 0.538834 | -2.898394 |
| C | -4.357669 | 0.406463 | -1.403856 |
| H | -4.922605 | 0.970830 | -0.661279 |
| H | -4.268261 | 0.998037 | -2.313062 |
| H | -4.892905 | -0.517410 | -1.637784 |
| C | 0.023768 | -1.366421 | -1.548716 |
| H | -0.450941 | -2.293114 | -1.215159 |
| H | -0.116620 | -1.285414 | -2.630482 |
| C | 1.504242 | -1.388834 | -1.255329 |
| C | 2.374608 | -0.622243 | -2.033585 |

| | | | |
|---|---|---|---|
| C | 2.037299 | -2.144602 | -0.210301 |
| C | 3.741676 | -0.606391 | -1.775664 |
| H | 1.972845 | -0.031269 | -2.851323 |
| C | 3.403679 | -2.129827 | 0.055217 |
| H | 1.376042 | -2.749679 | 0.403245 |
| C | 4.261325 | -1.360406 | -0.727485 |
| H | 4.399870 | -0.006247 | -2.393541 |
| H | 3.799765 | -2.724938 | 0.870334 |
| H | 5.325651 | -1.352959 | -0.524156 |
| C | -3.345872 | 0.381414 | 1.512924 |
| H | -3.106343 | 1.434126 | 1.358240 |
| H | -4.430367 | 0.262211 | 1.553416 |
| H | -2.936923 | 0.062798 | 2.473865 |
| C | -3.332949 | -1.880565 | 0.397872 |
| H | -3.263406 | -2.342963 | 1.380642 |
| H | -4.392026 | -1.838050 | 0.133497 |
| H | -2.815013 | -2.506549 | -0.331808 |
| C | 0.906760 | 1.307824 | 1.205003 |
| C | 2.160885 | 1.486446 | 0.613768 |
| C | -0.021790 | 2.351220 | 1.133797 |
| C | 2.469973 | 2.665283 | -0.058142 |
| H | 2.887074 | 0.680435 | 0.658869 |
| C | 0.287272 | 3.532143 | 0.468920 |
| H | -0.989930 | 2.224737 | 1.604178 |
| C | 1.532943 | 3.690666 | -0.136627 |
| H | 3.441822 | 2.778873 | -0.525601 |
| H | -0.443029 | 4.331918 | 0.422851 |
| H | 1.771146 | 4.609088 | -0.660002 |
| C | -0.815377 | -2.001483 | 2.257787 |
| H | -0.970327 | -2.808497 | 1.537505 |
| H | -0.017308 | -2.295259 | 2.936082 |
| H | -1.729595 | -1.910748 | 2.851756 |

**17J-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -1077.675059

Free energies: -1077.263279

Corrected Free energies: -1077.259566

| | | | |
|---|---|---|---|
| C | 1.872832 | -1.731580 | 0.587453 |
| C | 0.816044 | -0.798642 | 0.043232 |
| C | 3.063966 | 0.213435 | -0.087905 |
| H | 0.131460 | -0.590145 | 0.864810 |
| N | 1.580597 | 0.416836 | -0.310325 |

| | | | |
|---|---|---|---|
| C | 1.017768 | 1.484274 | -0.850240 |
| C | -0.407957 | 1.694439 | -0.797494 |
| C | -1.074949 | 2.274894 | -2.007861 |
| H | -1.461433 | 3.276106 | -1.792873 |
| H | -0.411644 | 2.322903 | -2.868105 |
| H | -1.929109 | 1.652945 | -2.286032 |
| N | 3.071265 | -1.130687 | 0.493023 |
| O | 1.631074 | -2.838817 | 1.022861 |
| C | 4.283244 | -1.748257 | 1.005361 |
| H | 4.701592 | -1.160995 | 1.823700 |
| H | 4.001512 | -2.730795 | 1.377411 |
| H | 5.028172 | -1.866304 | 0.218594 |
| C | 0.060179 | -1.434631 | -1.150038 |
| H | 0.312958 | -0.898346 | -2.066935 |
| H | 0.437126 | -2.454603 | -1.265006 |
| C | -1.438631 | -1.492303 | -0.970047 |
| C | -1.987260 | -1.965492 | 0.223781 |
| C | -2.294548 | -1.101256 | -1.998172 |
| C | -3.364961 | -2.014614 | 0.396837 |
| H | -1.329934 | -2.302597 | 1.020459 |
| C | -3.676355 | -1.157298 | -1.829880 |
| H | -1.879090 | -0.751087 | -2.937985 |
| C | -4.214401 | -1.605139 | -0.628230 |
| H | -3.776322 | -2.374895 | 1.332567 |
| H | -4.329286 | -0.845258 | -2.636582 |
| H | -5.288532 | -1.640735 | -0.491553 |
| C | 3.595635 | 1.210406 | 0.941565 |
| H | 3.102124 | 1.051760 | 1.901560 |
| H | 4.667852 | 1.052705 | 1.066700 |
| H | 3.450937 | 2.243520 | 0.635369 |
| C | 3.853669 | 0.201614 | -1.396612 |
| H | 4.021439 | 1.198203 | -1.795000 |
| H | 4.834038 | -0.232972 | -1.199757 |
| H | 3.344385 | -0.413004 | -2.140449 |
| C | -1.176988 | 1.521262 | 0.419946 |
| C | -2.581594 | 1.425257 | 0.370803 |
| C | -0.554823 | 1.529832 | 1.686482 |
| C | -3.322432 | 1.295823 | 1.534037 |
| H | -3.096120 | 1.410058 | -0.580678 |
| C | -1.301220 | 1.405850 | 2.844760 |
| H | 0.519045 | 1.658854 | 1.760171 |
| C | -2.688412 | 1.279389 | 2.773278 |
| H | -4.399018 | 1.194706 | 1.471866 |
| H | -0.803989 | 1.418618 | 3.806526 |

| | | | |
|---|---|---|---|
| H | -3.270071 | 1.176919 | 3.681215 |
| C | 1.816784 | 2.512704 | -1.601902 |
| H | 2.022663 | 2.140164 | -2.610186 |
| H | 1.249001 | 3.436022 | -1.680400 |
| H | 2.765065 | 2.735946 | -1.126098 |

## Calculated Cartesian coordinates for other pyrrolidine derived enamines

**9K**

Imaginary frequency: None

Electronic energies: -327.958771

Free energies: -327.824989

Corrected Free energies: -327.824006

| | | | |
|---|---|---|---|
| C | -2.200728 | 0.666795 | 0.252762 |
| C | -2.130650 | -0.778033 | -0.257770 |
| C | -0.711484 | -1.203542 | 0.119940 |
| C | -0.818376 | 1.226347 | -0.093740 |
| H | -3.007741 | 1.242935 | -0.198723 |
| H | -2.339487 | 0.668948 | 1.336762 |
| H | -2.243152 | -0.794850 | -1.344829 |
| H | -2.889877 | -1.425357 | 0.179943 |
| H | -0.672419 | -1.557354 | 1.156929 |
| H | -0.308532 | -1.982298 | -0.529171 |
| H | -0.474198 | 1.984527 | 0.614517 |
| H | -0.800191 | 1.661834 | -1.099367 |
| N | 0.040878 | 0.042484 | -0.037260 |
| C | 1.372967 | 0.124211 | -0.014494 |
| C | 2.602782 | -0.714870 | 0.051268 |
| C | 2.492546 | 0.792937 | -0.044268 |
| H | 2.892570 | -1.302658 | -0.823242 |
| H | 2.873019 | -1.188919 | 0.997825 |
| H | 3.041520 | 1.712737 | -0.112010 |

**9K** radical cation

Imaginary frequency: None

Electronic energies: -327.767978

Free energies: -327.633474

Corrected Free energies: -327.633051

| | | | |
|---|---|---|---|
| C | -2.188357 | 0.681084 | 0.260127 |

| | | | |
|---|---|---|---|
| C | -2.141654 | -0.757506 | -0.266628 |
| C | -0.735357 | -1.217872 | 0.108085 |
| C | -0.809927 | 1.228039 | -0.100713 |
| H | -2.982634 | 1.273517 | -0.189359 |
| H | -2.318889 | 0.683998 | 1.343860 |
| H | -2.259905 | -0.768093 | -1.351837 |
| H | -2.902231 | -1.398479 | 0.174351 |
| H | -0.680680 | -1.558580 | 1.144999 |
| H | -0.304610 | -1.973651 | -0.546283 |
| H | -0.432021 | 2.004316 | 0.562065 |
| H | -0.766591 | 1.576128 | -1.135204 |
| N | 0.056747 | 0.029313 | 0.003944 |
| C | 1.342888 | 0.067056 | -0.000157 |
| C | 2.609050 | -0.689442 | 0.051888 |
| C | 2.492107 | 0.788910 | -0.063298 |
| H | 2.914062 | -1.263015 | -0.824403 |
| H | 2.925915 | -1.117951 | 1.003686 |
| H | 2.997854 | 1.734999 | -0.145302 |

**9L**

Imaginary frequency: None

Electronic energies: -367.297532

Free energies: -367.134252

Corrected Free energies: -367.133493

| | | | |
|---|---|---|---|
| C | 2.534951 | 0.702531 | -0.289560 |
| C | 2.528465 | -0.755934 | 0.184944 |
| C | 1.096917 | -1.192765 | -0.116836 |
| C | 1.146450 | 1.220989 | 0.113178 |
| H | 3.342208 | 1.291742 | 0.144591 |
| H | 2.638883 | 0.731559 | -1.376921 |
| H | 2.706177 | -0.803396 | 1.262301 |
| H | 3.271780 | -1.373254 | -0.318877 |
| H | 0.989485 | -1.460542 | -1.177528 |
| H | 0.767013 | -2.040031 | 0.487744 |
| H | 0.725760 | 1.905895 | -0.632407 |
| H | 1.166486 | 1.745304 | 1.074870 |
| N | 0.334630 | 0.009048 | 0.214512 |
| C | -1.013803 | 0.075987 | 0.075645 |
| C | -2.022675 | -1.044675 | -0.020280 |
| C | -1.934600 | 1.062857 | 0.017667 |
| C | -3.097245 | 0.090802 | -0.083464 |
| H | -2.085235 | -1.688687 | 0.859999 |
| H | -1.950866 | -1.664106 | -0.917468 |

| | | | |
|---|---|---|---|
| H | -3.795436 | 0.080482 | 0.758380 |
| H | -3.670570 | 0.110247 | -1.014367 |
| H | -1.878855 | 2.142703 | 0.060329 |

**9L** radical cation

Imaginary frequency: None

Electronic energies: -367.116200

Free energies: -366.952141

Corrected Free energies: -366.951735

| | | | |
|---|---|---|---|
| C | -2.544061 | 0.696634 | 0.273188 |
| C | -2.516945 | -0.734641 | -0.272690 |
| C | -1.111374 | -1.213181 | 0.084114 |
| C | -1.158559 | 1.230115 | -0.084400 |
| H | -3.332572 | 1.305715 | -0.164003 |
| H | -2.669715 | 0.686160 | 1.357530 |
| H | -2.642969 | -0.729201 | -1.357059 |
| H | -3.280996 | -1.373919 | 0.164759 |
| H | -1.053882 | -1.579371 | 1.112959 |
| H | -0.697945 | -1.963513 | -0.588883 |
| H | -0.776484 | 1.993507 | 0.592023 |
| H | -1.116119 | 1.599712 | -1.112062 |
| N | -0.308097 | 0.023371 | -0.001645 |
| C | 0.992804 | 0.039639 | -0.003333 |
| C | 2.030142 | -1.052690 | 0.069958 |
| C | 1.948590 | 1.071776 | -0.072194 |
| C | 3.087288 | 0.097425 | -0.003852 |
| H | 2.022870 | -1.732534 | -0.781928 |
| H | 2.017051 | -1.618878 | 1.001114 |
| H | 3.722533 | 0.085580 | -0.891737 |
| H | 3.716807 | 0.204409 | 0.881840 |
| H | 1.880802 | 2.148274 | -0.147777 |

**9M**

Imaginary frequency: None

Electronic energies: -406.637266

Free energies: -406.444367

Corrected Free energies: -406.443688

| | | | |
|---|---|---|---|
| C | -2.874761 | 0.709880 | 0.300794 |
| C | -2.866128 | -0.734406 | -0.212760 |
| C | -1.443930 | -1.186763 | 0.106349 |
| C | -1.466194 | 1.225588 | -0.031189 |
| H | -3.658678 | 1.320220 | -0.146735 |

| | | | |
|---|---|---|---|
| H | -3.021871 | 0.710435 | 1.383436 |
| H | -3.019479 | -0.752709 | -1.294692 |
| H | -3.623275 | -1.361367 | 0.257782 |
| H | -1.359270 | -1.480048 | 1.163387 |
| H | -1.114959 | -2.025739 | -0.509655 |
| H | -1.061506 | 1.854582 | 0.771590 |
| H | -1.444944 | 1.816436 | -0.954110 |
| N | -0.667103 | 0.014007 | -0.190114 |
| C | 0.696633 | 0.071594 | -0.090430 |
| C | 1.479157 | 1.169300 | -0.049830 |
| C | 1.526217 | -1.195711 | -0.122088 |
| C | 2.943619 | 0.797759 | -0.084853 |
| C | 2.923424 | -0.699059 | 0.288676 |
| H | 1.518151 | -1.611199 | -1.136980 |
| H | 1.142334 | -1.969904 | 0.546515 |
| H | 3.371025 | 0.946057 | -1.085598 |
| H | 3.557939 | 1.381182 | 0.606545 |
| H | 3.728469 | -1.268446 | -0.177631 |
| H | 3.027427 | -0.796136 | 1.372117 |
| H | 1.120144 | 2.189501 | -0.093187 |

**9M** radical cation

Imaginary frequency: None

Electronic energies: -406.460742

Free energies: -406.266751

Corrected Free energies: -406.266461

| | | | |
|---|---|---|---|
| C | -2.867560 | 0.688319 | 0.338829 |
| C | -2.852702 | -0.705471 | -0.294970 |
| C | -1.444928 | -1.206769 | 0.014153 |
| C | -1.483890 | 1.236969 | 0.000144 |
| H | -3.657639 | 1.327788 | -0.049302 |
| H | -2.981225 | 0.610215 | 1.422023 |
| H | -2.990906 | -0.632153 | -1.375625 |
| H | -3.613148 | -1.369769 | 0.110308 |
| H | -1.376693 | -1.637283 | 1.017850 |
| H | -1.049092 | -1.920927 | -0.707378 |
| H | -1.097361 | 1.951359 | 0.725757 |
| H | -1.454357 | 1.680755 | -0.998485 |
| N | -0.633994 | 0.026959 | -0.009862 |
| C | 0.675592 | 0.033314 | -0.040494 |
| C | 1.484382 | 1.182664 | -0.105542 |
| C | 1.524916 | -1.209591 | -0.046854 |
| C | 2.918261 | 0.795923 | -0.159081 |

| | | | |
|---|---|---|---|
| C | 2.927250 | -0.676302 | 0.299552 |
| H | 1.493327 | -1.641679 | -1.053489 |
| H | 1.157958 | -1.964062 | 0.649977 |
| H | 3.267508 | 0.896032 | -1.196573 |
| H | 3.548635 | 1.451623 | 0.444356 |
| H | 3.717658 | -1.256133 | -0.171916 |
| H | 3.071705 | -0.715594 | 1.379964 |
| H | 1.113664 | 2.196779 | -0.162852 |

**9N**

Imaginary frequency: None

Electronic energies: -485.244339

Free energies: -484.994452

Corrected Free energies: -484.993691

| | | | |
|---|---|---|---|
| C | 3.131247 | -0.834468 | -0.309713 |
| C | 1.801747 | -1.581752 | -0.171378 |
| C | 0.872142 | -1.000000 | 0.905752 |
| C | 3.032480 | 0.632145 | -0.735450 |
| C | 2.245471 | 1.521349 | 0.243391 |
| C | 0.745154 | 1.369996 | 0.159968 |
| H | 3.651341 | -0.881445 | 0.655507 |
| H | 1.277855 | -1.596575 | -1.133605 |
| H | 1.477221 | -0.722305 | 1.776854 |
| H | 2.567587 | 0.700547 | -1.724979 |
| H | 2.496051 | 2.565566 | 0.042084 |
| H | 3.761977 | -1.370200 | -1.025986 |
| H | 2.022785 | -2.622602 | 0.083289 |
| H | 0.177449 | -1.765868 | 1.250865 |
| H | 4.050253 | 1.024199 | -0.833210 |
| H | 2.607978 | 1.315711 | 1.260825 |
| C | 0.100500 | 0.221765 | 0.449698 |
| H | 0.181093 | 2.235091 | -0.168333 |
| C | -1.926944 | -1.196135 | 0.074261 |
| C | -2.097818 | 1.206717 | -0.044427 |
| C | -3.221770 | -0.791916 | -0.641254 |
| H | -2.145317 | -1.761277 | 0.986489 |
| H | -1.292804 | -1.818095 | -0.563538 |
| C | -3.500714 | 0.612518 | -0.101195 |
| H | -1.784021 | 1.557485 | -1.041111 |
| H | -2.006441 | 2.047953 | 0.648005 |
| H | -3.047295 | -0.737432 | -1.718810 |
| H | -4.031542 | -1.498963 | -0.461711 |
| H | -4.176902 | 1.191229 | -0.730259 |

| | | | |
|---|---|---|---|
| H | -3.921997 | 0.556646 | 0.905986 |
| N | -1.279177 | 0.088431 | 0.401960 |

**9N** radical cation

Imaginary frequency: None

Electronic energies: -485.068945

Free energies: -484.818542

Corrected Free energies: -484.817768

| | | | |
|---|---|---|---|
| C | 3.140412 | -0.820757 | -0.332546 |
| C | 1.810705 | -1.575365 | -0.282616 |
| C | 0.855346 | -1.077154 | 0.822895 |
| C | 3.043649 | 0.670562 | -0.653128 |
| C | 2.248056 | 1.496112 | 0.389746 |
| C | 0.776995 | 1.366333 | 0.217975 |
| H | 3.646232 | -0.942623 | 0.632071 |
| H | 1.307251 | -1.524240 | -1.253683 |
| H | 1.436612 | -0.818265 | 1.713033 |
| H | 2.599047 | 0.817273 | -1.642311 |
| H | 2.515094 | 2.547935 | 0.299479 |
| H | 3.779055 | -1.294303 | -1.082725 |
| H | 2.016189 | -2.629855 | -0.089382 |
| H | 0.169884 | -1.867218 | 1.118410 |
| H | 4.052700 | 1.085974 | -0.694557 |
| H | 2.541629 | 1.169183 | 1.394458 |
| C | 0.092754 | 0.146971 | 0.402375 |
| H | 0.224041 | 2.230585 | -0.125741 |
| C | -1.996724 | -1.177830 | 0.191341 |
| C | -2.059087 | 1.228394 | -0.203603 |
| C | -3.309452 | -0.787850 | -0.480397 |
| H | -2.147900 | -1.465067 | 1.235617 |
| H | -1.457823 | -1.969625 | -0.325989 |
| C | -3.476146 | 0.678382 | -0.081373 |
| H | -1.825153 | 1.518509 | -1.231577 |
| H | -1.856067 | 2.062556 | 0.465537 |
| H | -3.212758 | -0.877922 | -1.564412 |
| H | -4.130259 | -1.421117 | -0.149745 |
| H | -4.171291 | 1.222744 | -0.717411 |
| H | -3.816203 | 0.753586 | 0.953396 |
| N | -1.204189 | 0.073586 | 0.160217 |

**9O**

Imaginary frequency: None

Electronic energies: -524.533795

Free energies: -524.257305

Corrected Free energies: -524.256175

| | | | |
|---|---|---|---|
| C | 3.666399 | 0.626224 | -0.763778 |
| C | 3.838506 | -0.536825 | 0.216536 |
| C | 2.428942 | -1.137834 | 0.319399 |
| C | 2.297743 | 1.163740 | -0.366530 |
| H | 4.453654 | 1.375860 | -0.683503 |
| H | 3.635833 | 0.259226 | -1.792885 |
| H | 4.146582 | -0.146644 | 1.189660 |
| H | 4.577981 | -1.270679 | -0.103847 |
| H | 2.321361 | -2.003656 | -0.341402 |
| H | 2.211732 | -1.464909 | 1.340787 |
| H | 1.815659 | 1.757722 | -1.147381 |
| H | 2.378589 | 1.794292 | 0.534231 |
| N | 1.530209 | -0.046375 | -0.106372 |
| C | 0.225975 | 0.054704 | 0.373798 |
| C | -0.378655 | 1.239282 | 0.592524 |
| C | -0.514746 | -1.258934 | 0.530587 |
| C | -1.851266 | 1.390648 | 0.874474 |
| H | 0.172134 | 2.158220 | 0.427427 |
| H | -0.969977 | -1.302223 | 1.524429 |
| H | 0.206046 | -2.074495 | 0.495048 |
| C | -1.610141 | -1.539630 | -0.535157 |
| C | -2.708421 | 1.330464 | -0.418814 |
| H | -2.193741 | 0.621489 | 1.574704 |
| H | -2.016314 | 2.346186 | 1.377018 |
| C | -3.053276 | -1.232736 | -0.088485 |
| H | -1.369153 | -1.003582 | -1.458625 |
| H | -1.556718 | -2.603055 | -0.780311 |
| C | -3.646209 | 0.119660 | -0.515495 |
| H | -3.311255 | 2.237870 | -0.517302 |
| H | -2.029548 | 1.323608 | -1.275529 |
| H | -3.103437 | -1.328067 | 1.000779 |
| H | -3.715615 | -2.011659 | -0.476726 |
| H | -4.537978 | 0.301053 | 0.094076 |
| H | -3.996404 | 0.045494 | -1.550396 |

9O radical cation

Imaginary frequency: None

Electronic energies: -524.359702

Free energies: -524.082093

Corrected Free energies: -524.081075

| | | | |
|---|---|---|---|
| C | 3.520679 | -0.638096 | 0.837677 |
| C | 3.735074 | 0.665597 | 0.071120 |
| C | 2.316214 | 1.186201 | -0.136303 |
| C | 2.292475 | -1.234118 | 0.158689 |
| H | 4.372396 | -1.313622 | 0.787745 |
| H | 3.298950 | -0.431402 | 1.886729 |
| H | 4.200076 | 0.464102 | -0.895942 |
| H | 4.348244 | 1.386175 | 0.608611 |
| H | 1.966099 | 1.773170 | 0.717177 |
| H | 2.205486 | 1.772745 | -1.046199 |
| H | 1.706425 | -1.876867 | 0.812177 |
| H | 2.556801 | -1.780389 | -0.750884 |
| N | 1.494173 | -0.044994 | -0.224484 |
| C | 0.215006 | -0.080414 | -0.563553 |
| C | -0.434156 | -1.327337 | -0.694198 |
| C | -0.536412 | 1.202095 | -0.794025 |
| C | -1.907070 | -1.462162 | -0.796174 |
| H | 0.153140 | -2.232674 | -0.612605 |
| H | -1.103815 | 1.102512 | -1.721853 |
| H | 0.173227 | 2.007890 | -0.957399 |
| C | -1.499194 | 1.609983 | 0.360146 |
| C | -2.523404 | -1.266574 | 0.628603 |
| H | -2.324841 | -0.725121 | -1.485779 |
| H | -2.154004 | -2.448810 | -1.183076 |
| C | -2.978564 | 1.247540 | 0.134200 |
| H | -1.136924 | 1.213128 | 1.313633 |
| H | -1.426054 | 2.695227 | 0.441508 |
| C | -3.473965 | -0.072924 | 0.743354 |
| H | -3.052915 | -2.177962 | 0.910049 |
| H | -1.717526 | -1.153743 | 1.359271 |
| H | -3.178182 | 1.260991 | -0.941639 |
| H | -3.595829 | 2.046401 | 0.551603 |
| H | -4.429701 | -0.324113 | 0.274171 |
| H | -3.680352 | 0.078576 | 1.806876 |

**9P**

Imaginary frequency: None

Electronic energies: -329.231745

Free energies: -329.073897

Corrected Free energies: -329.073180

| | | | |
|---|---|---|---|
| C | -2.172164 | 0.669647 | 0.239637 |
| C | -2.101116 | -0.770333 | -0.277892 |
| C | -0.690062 | -1.196620 | 0.121554 |

| | | | |
|---|---|---|---|
| C | -0.767707 | 1.218269 | -0.036377 |
| H | -2.952550 | 1.261504 | -0.237853 |
| H | -2.359982 | 0.662930 | 1.316189 |
| H | -2.191169 | -0.783861 | -1.367194 |
| H | -2.869309 | -1.418716 | 0.143030 |
| H | -0.668366 | -1.527794 | 1.169608 |
| H | -0.307885 | -2.007843 | -0.499741 |
| H | -0.433629 | 1.907909 | 0.747519 |
| H | -0.712402 | 1.755708 | -0.991644 |
| N | 0.077254 | 0.031145 | -0.073968 |
| C | 1.443998 | 0.124535 | -0.018773 |
| C | 2.183903 | -1.186235 | 0.055828 |
| C | 2.110488 | 1.299116 | -0.054204 |
| H | 1.987801 | -1.793695 | -0.831514 |
| H | 1.869529 | -1.767562 | 0.926565 |
| H | 1.606489 | 2.252973 | -0.128857 |
| H | 3.255551 | -1.008728 | 0.123838 |
| H | 3.191103 | 1.298888 | -0.030805 |

**9P** radical cation

Imaginary frequency: None

Electronic energies: -329.045002

Free energies: -328.886549

Corrected Free energies: -328.886367

| | | | |
|---|---|---|---|
| C | -2.166459 | 0.640157 | 0.289883 |
| C | -2.091243 | -0.770444 | -0.296274 |
| C | -0.671336 | -1.207558 | 0.049665 |
| C | -0.798345 | 1.226854 | -0.043444 |
| H | -2.970111 | 1.239147 | -0.133321 |
| H | -2.296657 | 0.594352 | 1.372852 |
| H | -2.215263 | -0.739701 | -1.380491 |
| H | -2.830983 | -1.450497 | 0.120964 |
| H | -0.603668 | -1.604978 | 1.067507 |
| H | -0.242274 | -1.930666 | -0.642483 |
| H | -0.457847 | 1.978670 | 0.666002 |
| H | -0.766720 | 1.637962 | -1.055948 |
| N | 0.101237 | 0.050828 | 0.001031 |
| C | 1.420043 | 0.098602 | 0.001012 |
| C | 2.191585 | -1.182155 | 0.089644 |
| C | 2.083466 | 1.332036 | -0.098851 |
| H | 2.075968 | -1.754102 | -0.834313 |
| H | 1.828136 | -1.795792 | 0.915470 |
| H | 1.553643 | 2.267632 | -0.200230 |

| | | | |
|---|---|---|---|
| H | 3.247718 | -0.973626 | 0.238395 |
| H | 3.163132 | 1.350849 | -0.091430 |

**9Q**

Imaginary frequency: None

Electronic energies: -289.923700

Free energies: -289.792657

Corrected Free energies: -289.791962

| | | | |
|---|---|---|---|
| C | -1.657896 | 0.964744 | 0.172851 |
| C | -1.927273 | -0.447568 | -0.359248 |
| C | -0.725913 | -1.237681 | 0.163068 |
| C | -0.143895 | 1.113564 | 0.001571 |
| H | -2.214684 | 1.738800 | -0.354383 |
| H | -1.916524 | 1.016776 | 1.233695 |
| H | -1.915356 | -0.440507 | -1.452214 |
| H | -2.878726 | -0.860225 | -0.024345 |
| H | -0.914301 | -1.605279 | 1.179509 |
| H | -0.473126 | -2.092441 | -0.468266 |
| H | 0.303448 | 1.778624 | 0.747692 |
| H | 0.118595 | 1.506093 | -0.991794 |
| N | 0.347626 | -0.246151 | 0.152277 |
| C | 1.668088 | -0.552765 | 0.035895 |
| C | 2.681208 | 0.319584 | -0.122775 |
| H | 2.520771 | 1.389138 | -0.172807 |
| H | 3.694353 | -0.048499 | -0.196946 |
| H | 1.876263 | -1.618687 | 0.085752 |

**9Q** radical cation

Imaginary frequency: None

Electronic energies: -289.733168

Free energies: -289.600865

Corrected Free energies: -289.600701

| | | | |
|---|---|---|---|
| C | -1.649096 | 0.961973 | 0.208628 |
| C | -1.941341 | -0.446961 | -0.316003 |
| C | -0.723609 | -1.236604 | 0.149640 |
| C | -0.150834 | 1.128555 | -0.042296 |
| H | -2.223338 | 1.735316 | -0.296993 |
| H | -1.854779 | 1.017554 | 1.279025 |
| H | -1.990588 | -0.447352 | -1.406575 |
| H | -2.865057 | -0.866040 | 0.077567 |
| H | -0.809811 | -1.527939 | 1.200599 |
| H | -0.477807 | -2.112134 | -0.448746 |

| | | | |
|---|---|---|---|
| H | 0.354761 | 1.763838 | 0.684080 |
| H | 0.058871 | 1.493549 | -1.051231 |
| N | 0.372632 | -0.250611 | 0.052364 |
| C | 1.643980 | -0.585085 | 0.033015 |
| C | 2.678445 | 0.337733 | -0.076534 |
| H | 2.494389 | 1.399767 | -0.158996 |
| H | 3.698875 | -0.014862 | -0.086646 |
| H | 1.860789 | -1.645088 | 0.102664 |

**9R-*E***

Imaginary frequency: None

Electronic energies: -788.830526

Free energies: -788.684682

Corrected Free energies: -788.683454

| | | | |
|---|---|---|---|
| C | -2.785028 | -1.067023 | -0.235067 |
| C | -3.050714 | 0.331211 | 0.329955 |
| C | -1.802986 | 1.106672 | -0.088407 |
| C | -1.284099 | -1.262713 | 0.000239 |
| H | -3.384051 | -1.844622 | 0.237484 |
| H | -2.994141 | -1.077388 | -1.307611 |
| H | -3.106578 | 0.290573 | 1.420720 |
| H | -3.967290 | 0.782098 | -0.049390 |
| H | -1.903263 | 1.482914 | -1.115181 |
| H | -1.600485 | 1.954097 | 0.568036 |
| H | -0.815318 | -1.857158 | -0.792183 |
| H | -1.077770 | -1.761987 | 0.956304 |
| N | -0.752323 | 0.093479 | 0.010583 |
| C | 0.590973 | 0.347721 | -0.017086 |
| C | 1.484896 | -0.665057 | 0.034119 |
| H | 1.230596 | -1.708652 | 0.103080 |
| Cl | 3.225089 | -0.408653 | 0.035830 |
| C | 0.985224 | 1.796689 | -0.088868 |
| H | 0.706334 | 2.310680 | 0.834185 |
| H | 2.055818 | 1.907402 | -0.234638 |
| H | 0.466288 | 2.289806 | -0.913306 |

**9R-*Z***

Imaginary frequency: None

Electronic energies: -788.827688

Free energies: -788.680627

Corrected Free energies: -788.679994

| | | | |
|---|---|---|---|
| C | 2.131569 | -1.314561 | 0.571523 |

| | | | |
|---|---|---|---|
| C | 2.740838 | -0.361523 | -0.457391 |
| C | 1.806905 | 0.841785 | -0.374104 |
| C | 0.630853 | -1.165389 | 0.318373 |
| H | 2.468271 | -2.345308 | 0.464084 |
| H | 2.375993 | -0.972643 | 1.580708 |
| H | 2.689958 | -0.804813 | -1.455343 |
| H | 3.776155 | -0.095696 | -0.245814 |
| H | 2.101785 | 1.490505 | 0.459731 |
| H | 1.806409 | 1.437131 | -1.289113 |
| H | 0.032128 | -1.325213 | 1.217874 |
| H | 0.292057 | -1.871851 | -0.444365 |
| N | 0.492801 | 0.227070 | -0.141201 |
| C | -0.632183 | 0.982840 | 0.074366 |
| C | -1.900472 | 0.534752 | 0.146039 |
| C | -0.426893 | 2.469471 | 0.243535 |
| H | 0.030758 | 2.897693 | -0.651027 |
| H | -1.379674 | 2.968545 | 0.408764 |
| H | 0.232625 | 2.677799 | 1.088838 |
| Cl | -2.426662 | -1.103300 | -0.215021 |
| H | -2.726510 | 1.186212 | 0.375369 |

**9R-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -788.636490

Free energies: -788.488839

Corrected Free energies: -788.488234

| | | | |
|---|---|---|---|
| C | 2.110017 | -1.438763 | 0.361618 |
| C | 2.759266 | -0.287876 | -0.403932 |
| C | 1.847217 | 0.885669 | -0.075462 |
| C | 0.619639 | -1.211043 | 0.130032 |
| H | 2.417791 | -2.420977 | 0.008893 |
| H | 2.336412 | -1.362078 | 1.427003 |
| H | 2.742509 | -0.483992 | -1.477772 |
| H | 3.785000 | -0.091267 | -0.098841 |
| H | 2.092316 | 1.325876 | 0.896020 |
| H | 1.834010 | 1.670064 | -0.829997 |
| H | -0.007959 | -1.575052 | 0.939759 |
| H | 0.285948 | -1.645987 | -0.814564 |
| N | 0.503040 | 0.266716 | 0.030750 |
| C | -0.594542 | 0.995087 | 0.071462 |
| C | -1.912313 | 0.495832 | 0.081107 |
| C | -0.461829 | 2.491792 | 0.085902 |
| H | -0.115086 | 2.842159 | -0.889197 |

| | | | |
|---|---|---|---|
| H | -1.420857 | 2.957812 | 0.295718 |
| H | 0.259910 | 2.806186 | 0.840595 |
| Cl | -2.424247 | -1.098504 | -0.129316 |
| H | -2.723803 | 1.200610 | 0.181144 |

**9R-*E*** radical cation

Imaginary frequency: None

Electronic energies: -788.640788

Free energies: -788.493893

Corrected Free energies: -788.493258

| | | | |
|---|---|---|---|
| C | 2.765918 | -1.052774 | 0.268110 |
| C | 3.025214 | 0.319998 | -0.353451 |
| C | 1.780860 | 1.110135 | 0.035111 |
| C | 1.280011 | -1.279146 | 0.003213 |
| H | 3.371388 | -1.843989 | -0.168997 |
| H | 2.950396 | -1.023941 | 1.343535 |
| H | 3.089620 | 0.240928 | -1.440423 |
| H | 3.930829 | 0.795084 | 0.017807 |
| H | 1.857829 | 1.516158 | 1.048481 |
| H | 1.526093 | 1.914361 | -0.652989 |
| H | 0.793930 | -1.897741 | 0.756272 |
| H | 1.102757 | -1.700821 | -0.989772 |
| N | 0.710402 | 0.089461 | 0.032265 |
| C | -0.575634 | 0.385958 | 0.043835 |
| C | -1.499382 | -0.672944 | -0.042652 |
| H | -1.200015 | -1.705635 | -0.131746 |
| Cl | -3.166654 | -0.427315 | -0.049348 |
| C | -0.991875 | 1.820272 | 0.118946 |
| H | -0.825805 | 2.300938 | -0.848856 |
| H | -2.044355 | 1.908124 | 0.370542 |
| H | -0.403041 | 2.345663 | 0.870548 |

**9S-*E***

Imaginary frequency: None

Electronic energies: -537.228653

Free energies: -537.022364

Corrected Free energies: -537.020397

| | | | |
|---|---|---|---|
| C | 3.343635 | -1.156339 | 0.291664 |
| C | 3.733977 | 0.308738 | 0.075543 |
| C | 2.426010 | 1.047271 | 0.349901 |
| C | 1.929356 | -1.237643 | -0.292270 |
| H | 4.029294 | -1.860192 | -0.178863 |

| | | | |
|---|---|---|---|
| H | 3.312536 | -1.373971 | 1.362168 |
| H | 4.032961 | 0.469501 | -0.963413 |
| H | 4.543291 | 0.639698 | 0.725745 |
| H | 2.289441 | 1.210494 | 1.427559 |
| H | 2.381526 | 2.015492 | -0.150154 |
| H | 1.293289 | -1.933159 | 0.266619 |
| H | 1.932786 | -1.560858 | -1.340825 |
| N | 1.422012 | 0.125388 | -0.182342 |
| C | 0.098701 | 0.419700 | -0.346023 |
| C | -0.803218 | -0.518939 | -0.729862 |
| C | -0.295093 | 1.847104 | -0.083157 |
| H | 0.242272 | 2.518878 | -0.756432 |
| H | -1.362195 | 1.986186 | -0.236010 |
| H | -0.041583 | 2.134873 | 0.940610 |
| H | -0.504735 | -1.538635 | -0.939020 |
| N | -2.188395 | -0.222978 | -0.891733 |
| H | -2.563890 | -0.100759 | -1.824406 |
| C | -3.136895 | -0.235497 | 0.083410 |
| O | -4.317654 | -0.047094 | -0.173814 |
| C | -2.647386 | -0.470358 | 1.494176 |
| H | -2.072003 | -1.395159 | 1.554471 |
| H | -1.989546 | 0.342270 | 1.809231 |
| H | -3.512069 | -0.519002 | 2.151462 |

**9S-*Z***

Imaginary frequency: None

Electronic energies: -537.228317

Free energies: -537.020190

Corrected Free energies: -537.018922

| | | | |
|---|---|---|---|
| C | -2.017097 | -1.773391 | -0.704661 |
| C | -2.667619 | -1.257811 | 0.579681 |
| C | -2.301039 | 0.222347 | 0.554757 |
| C | -0.671952 | -1.044440 | -0.720167 |
| H | -1.899489 | -2.856406 | -0.728860 |
| H | -2.615771 | -1.471052 | -1.567923 |
| H | -2.213058 | -1.738332 | 1.450306 |
| H | -3.744824 | -1.416985 | 0.616086 |
| H | -3.003596 | 0.776376 | -0.080821 |
| H | -2.307736 | 0.674334 | 1.548131 |
| H | -0.310194 | -0.841678 | -1.730655 |
| H | 0.092711 | -1.634044 | -0.201513 |
| N | -0.947897 | 0.215726 | -0.014920 |
| C | -0.236027 | 1.369475 | -0.239195 |

| | | | |
|---|---|---|---|
| C | 1.047993 | 1.430339 | -0.662991 |
| C | -0.952420 | 2.661078 | 0.058160 |
| H | -1.203303 | 2.729140 | 1.119699 |
| H | -0.320051 | 3.509874 | -0.195751 |
| H | -1.884291 | 2.732301 | -0.506710 |
| H | 1.485452 | 2.401269 | -0.859442 |
| N | 1.914084 | 0.313760 | -0.816377 |
| H | 2.281056 | 0.093760 | -1.733909 |
| C | 2.362158 | -0.510757 | 0.168270 |
| O | 3.089250 | -1.462566 | -0.085753 |
| C | 1.903954 | -0.197036 | 1.572496 |
| H | 2.070737 | 0.855418 | 1.806479 |
| H | 0.831452 | -0.386303 | 1.671092 |
| H | 2.455897 | -0.832368 | 2.260800 |

**9S-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -537.045580

Free energies: -536.835375

Corrected Free energies: -536.834582

| | | | |
|---|---|---|---|
| C | -2.063155 | -1.666695 | -0.792669 |
| C | -2.671793 | -1.191503 | 0.527062 |
| C | -2.229002 | 0.265844 | 0.592974 |
| C | -0.673217 | -1.038260 | -0.761516 |
| H | -2.007269 | -2.750207 | -0.878094 |
| H | -2.632222 | -1.274585 | -1.638129 |
| H | -2.249543 | -1.752752 | 1.363530 |
| H | -3.755751 | -1.280628 | 0.559552 |
| H | -2.908944 | 0.910378 | 0.029568 |
| H | -2.119919 | 0.660296 | 1.603159 |
| H | -0.231406 | -0.862983 | -1.740827 |
| H | 0.003223 | -1.656121 | -0.166531 |
| N | -0.911416 | 0.261381 | -0.086045 |
| C | -0.192269 | 1.360471 | -0.241174 |
| C | 1.097881 | 1.357482 | -0.817781 |
| C | -0.765715 | 2.675138 | 0.189806 |
| H | -0.834367 | 2.705540 | 1.280734 |
| H | -0.120689 | 3.490026 | -0.130603 |
| H | -1.767280 | 2.820359 | -0.217759 |
| H | 1.414840 | 2.245213 | -1.351143 |
| N | 1.967544 | 0.319031 | -0.807232 |
| H | 2.663862 | 0.287531 | -1.546432 |
| C | 2.249051 | -0.592390 | 0.238848 |

| | | | |
|---|---|---|---|
| O | 2.993397 | -1.508496 | 0.003317 |
| C | 1.676684 | -0.302617 | 1.601114 |
| H | 1.605793 | 0.768096 | 1.791640 |
| H | 0.686286 | -0.744102 | 1.722103 |
| H | 2.342528 | -0.765798 | 2.325658 |

**9S-*E*** radical cation

Imaginary frequency: None

Electronic energies: -537.048677

Free energies: -536.839698

Corrected Free energies: -536.838312

| | | | |
|---|---|---|---|
| C | 3.300115 | -0.895873 | 0.733076 |
| C | 3.668041 | 0.395330 | -0.000628 |
| C | 2.333053 | 1.126073 | -0.110981 |
| C | 1.964023 | -1.276536 | 0.102600 |
| H | 4.040024 | -1.684606 | 0.612570 |
| H | 3.163311 | -0.702335 | 1.798931 |
| H | 4.048695 | 0.167136 | -0.998188 |
| H | 4.409174 | 0.992778 | 0.526410 |
| H | 2.114317 | 1.717942 | 0.782588 |
| H | 2.259485 | 1.769315 | -0.986940 |
| H | 1.314146 | -1.852159 | 0.760376 |
| H | 2.103840 | -1.819058 | -0.837262 |
| N | 1.343919 | 0.031633 | -0.196368 |
| C | 0.059758 | 0.217806 | -0.451425 |
| C | -0.770253 | -0.912558 | -0.602181 |
| C | -0.434015 | 1.615625 | -0.670592 |
| H | 0.149489 | 2.075120 | -1.470704 |
| H | -1.476337 | 1.621165 | -0.978387 |
| H | -0.314660 | 2.227105 | 0.226448 |
| H | -0.327216 | -1.866661 | -0.859008 |
| N | -2.124897 | -0.892943 | -0.586847 |
| H | -2.592637 | -1.629586 | -1.106591 |
| C | -3.034188 | -0.150908 | 0.201196 |
| O | -4.205654 | -0.239901 | -0.062513 |
| C | -2.509693 | 0.624964 | 1.377968 |
| H | -1.487739 | 0.369783 | 1.651012 |
| H | -2.579587 | 1.693999 | 1.173712 |
| H | -3.173279 | 0.404911 | 2.213429 |

**9T-*E***

Imaginary frequency: None

Electronic energies: -404.444792
Free energies: -404.283891
Corrected Free energies: -404.283014

| | | | |
|---|---|---|---|
| C | 2.478349 | -0.976915 | -0.047963 |
| C | 2.634405 | 0.558222 | -0.001292 |
| C | 1.248096 | 1.046253 | 0.406585 |
| C | 0.955212 | -1.217788 | -0.097650 |
| H | 2.983789 | -1.403670 | -0.914028 |
| H | 2.902788 | -1.442064 | 0.842232 |
| H | 2.871886 | 0.945803 | -0.993479 |
| H | 3.411549 | 0.885260 | 0.689215 |
| H | 1.112103 | 0.973172 | 1.498911 |
| H | 1.048901 | 2.073794 | 0.102187 |
| H | 0.606830 | -1.654957 | 0.852221 |
| H | 0.649456 | -1.889887 | -0.903016 |
| N | 0.372096 | 0.105172 | -0.295684 |
| C | -1.014906 | 0.245731 | -0.120185 |
| C | -1.829575 | -0.802756 | 0.064465 |
| C | -1.551369 | 1.647049 | -0.213349 |
| H | -1.103141 | 2.162418 | -1.066521 |
| H | -2.632334 | 1.626481 | -0.335156 |
| H | -1.318001 | 2.226807 | 0.684339 |
| O | -3.193226 | -0.624626 | 0.206500 |
| H | -1.477166 | -1.824762 | 0.124626 |
| H | -3.636800 | -1.416364 | -0.107409 |

**9T-*E*** radical cation
Imaginary frequency: None
Electronic energies: -404.281848
Free energies: -404.118693
Corrected Free energies: -404.118363

| | | | |
|---|---|---|---|
| C | 2.439608 | -0.940628 | 0.263382 |
| C | 2.605387 | 0.455211 | -0.340462 |
| C | 1.308604 | 1.153442 | 0.055136 |
| C | 0.971277 | -1.263361 | -0.003942 |
| H | 3.100329 | -1.682950 | -0.179911 |
| H | 2.621152 | -0.910198 | 1.339473 |
| H | 2.675264 | 0.392598 | -1.428416 |
| H | 3.478419 | 0.984455 | 0.036182 |
| H | 1.359335 | 1.554395 | 1.072297 |
| H | 1.006447 | 1.948167 | -0.625229 |
| H | 0.530715 | -1.917261 | 0.748424 |
| H | 0.823156 | -1.700068 | -0.995653 |

| | | | |
|---|---|---|---|
| N | 0.315680 | 0.061501 | 0.030683 |
| C | -0.993858 | 0.264255 | 0.028816 |
| C | -1.861659 | -0.831421 | -0.061658 |
| C | -1.529891 | 1.659548 | 0.100378 |
| H | -1.362850 | 2.171953 | -0.850462 |
| H | -2.597202 | 1.642806 | 0.301442 |
| H | -1.024199 | 2.221493 | 0.886252 |
| O | -3.160504 | -0.604648 | -0.061072 |
| H | -1.514165 | -1.852701 | -0.144004 |
| H | -3.658932 | -1.428288 | -0.136504 |

**9T-*Z***

Imaginary frequency: None

Electronic energies: -404.441936

Free energies: -404.280943

Corrected Free energies: -404.280033

| | | | |
|---|---|---|---|
| C | 2.157990 | -0.987690 | 0.446892 |
| C | 2.504160 | 0.254630 | -0.377955 |
| C | 1.275037 | 1.126410 | -0.155728 |
| C | 0.655821 | -1.177457 | 0.195987 |
| H | 2.739225 | -1.867658 | 0.171049 |
| H | 2.337108 | -0.779642 | 1.504946 |
| H | 2.588167 | -0.001862 | -1.437284 |
| H | 3.426439 | 0.741190 | -0.060465 |
| H | 1.343950 | 1.620574 | 0.825052 |
| H | 1.159047 | 1.898322 | -0.918646 |
| H | 0.125293 | -1.510774 | 1.093369 |
| H | 0.464138 | -1.913159 | -0.587690 |
| N | 0.181450 | 0.155338 | -0.216540 |
| C | -1.135692 | 0.540109 | 0.019546 |
| C | -2.180007 | -0.304257 | 0.023164 |
| C | -1.394442 | 2.009535 | 0.227537 |
| H | -1.105682 | 2.588424 | -0.653705 |
| H | -2.454280 | 2.183116 | 0.410287 |
| H | -0.827897 | 2.398397 | 1.076886 |
| H | -3.180472 | 0.061657 | 0.223402 |
| O | -2.072831 | -1.638902 | -0.335348 |
| H | -2.599745 | -2.162413 | 0.274694 |

**9T-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -404.280158

Free energies: -404.116337

Corrected Free energies: -404.116034

| | | | |
|---|---|---|---|
| C | 2.177451 | -1.013901 | 0.326279 |
| C | 2.486337 | 0.316111 | -0.360651 |
| C | 1.267347 | 1.162554 | -0.014077 |
| C | 0.687215 | -1.205833 | 0.059535 |
| H | 2.762511 | -1.845922 | -0.061008 |
| H | 2.354878 | -0.932662 | 1.400759 |
| H | 2.548455 | 0.180508 | -1.442448 |
| H | 3.407830 | 0.778238 | -0.011910 |
| H | 1.359979 | 1.613025 | 0.979026 |
| H | 1.050805 | 1.945075 | -0.739634 |
| H | 0.170404 | -1.771699 | 0.830708 |
| H | 0.500954 | -1.676188 | -0.908622 |
| N | 0.162367 | 0.180051 | 0.018481 |
| C | -1.111938 | 0.545663 | 0.039970 |
| C | -2.178319 | -0.361245 | -0.012033 |
| C | -1.447352 | 2.006539 | 0.098762 |
| H | -1.165878 | 2.499072 | -0.834651 |
| H | -2.515107 | 2.146012 | 0.250926 |
| H | -0.909533 | 2.490988 | 0.915225 |
| H | -3.191598 | 0.015092 | 0.042023 |
| O | -1.994529 | -1.659137 | -0.149828 |
| H | -2.838493 | -2.128129 | -0.177853 |

**9U-*E***

Imaginary frequency: None

Electronic energies: -443.733422

Free energies: -443.546847

Corrected Free energies: -443.545091

| | | | |
|---|---|---|---|
| C | 2.744046 | -1.219349 | 0.073977 |
| C | 3.107665 | 0.237567 | -0.254510 |
| C | 1.875830 | 1.005874 | 0.207527 |
| C | 1.202804 | -1.263051 | 0.010505 |
| H | 3.205370 | -1.928096 | -0.613236 |
| H | 3.078819 | -1.469875 | 1.081967 |
| H | 3.226731 | 0.368538 | -1.332227 |
| H | 4.021368 | 0.568404 | 0.239006 |
| H | 1.885948 | 1.137879 | 1.301654 |
| H | 1.785699 | 1.987821 | -0.257135 |
| H | 0.787837 | -1.642660 | 0.955941 |
| H | 0.823687 | -1.902346 | -0.792090 |
| N | 0.792276 | 0.119998 | -0.219900 |

| | | | |
|---|---|---|---|
| C | -0.535457 | 0.476286 | 0.008439 |
| C | -1.492608 | -0.433650 | 0.260785 |
| C | -0.855374 | 1.941938 | -0.093197 |
| H | -0.456940 | 2.350660 | -1.025249 |
| H | -1.932143 | 2.089851 | -0.067537 |
| H | -0.407572 | 2.502492 | 0.732020 |
| O | -2.805065 | -0.058930 | 0.463602 |
| H | -1.306271 | -1.501774 | 0.317005 |
| C | -3.708001 | -0.762850 | -0.373153 |
| H | -3.517410 | -0.538319 | -1.427685 |
| H | -3.619821 | -1.844231 | -0.218714 |
| H | -4.714138 | -0.443482 | -0.105473 |

**9U-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -443.731329

Free energies: -443.542405

Corrected Free energies: -443.541858

| | | | |
|---|---|---|---|
| C | -2.199140 | -1.127603 | -0.666855 |
| C | -2.630254 | -0.343670 | 0.574581 |
| C | -1.664218 | 0.836269 | 0.556655 |
| C | -0.670626 | -1.029177 | -0.626104 |
| H | -2.549489 | -2.159726 | -0.672221 |
| H | -2.581408 | -0.630705 | -1.562555 |
| H | -2.466601 | -0.942166 | 1.474850 |
| H | -3.673391 | -0.028711 | 0.549402 |
| H | -2.024729 | 1.606641 | -0.138864 |
| H | -1.541802 | 1.295318 | 1.540036 |
| H | -0.223214 | -0.985712 | -1.622645 |
| H | -0.232442 | -1.887367 | -0.105870 |
| N | -0.414082 | 0.223759 | 0.101807 |
| C | 0.719476 | 0.981612 | -0.152758 |
| C | 1.913954 | 0.433966 | -0.439154 |
| C | 0.586455 | 2.479579 | -0.088781 |
| H | 0.256011 | 2.802810 | 0.901536 |
| H | 1.547338 | 2.950147 | -0.293958 |
| H | -0.144551 | 2.844218 | -0.814805 |
| H | 2.772008 | 1.050191 | -0.685334 |
| O | 2.147719 | -0.930537 | -0.419992 |
| C | 2.240906 | -1.443823 | 0.902781 |
| H | 2.421842 | -2.515586 | 0.819771 |
| H | 3.068477 | -0.973744 | 1.443787 |
| H | 1.309457 | -1.270548 | 1.451961 |

**9U-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -443.569279

Free energies: -443.380576

Corrected Free energies: -443.379948

| | | | |
|---|---|---|---|
| C | 2.103760 | -1.586135 | 0.317064 |
| C | 2.850768 | -0.447918 | -0.378112 |
| C | 2.009904 | 0.771970 | -0.021350 |
| C | 0.637196 | -1.242367 | 0.072412 |
| H | 2.353942 | -2.569650 | -0.076246 |
| H | 2.313973 | -1.575635 | 1.388680 |
| H | 2.848728 | -0.596244 | -1.459979 |
| H | 3.879884 | -0.338234 | -0.041616 |
| H | 2.266135 | 1.161949 | 0.968848 |
| H | 2.073712 | 1.580975 | -0.747265 |
| H | -0.033712 | -1.588650 | 0.854723 |
| H | 0.280452 | -1.620555 | -0.888445 |
| N | 0.631377 | 0.238908 | 0.026281 |
| C | -0.434121 | 1.027254 | 0.048170 |
| C | -1.753071 | 0.552152 | 0.025559 |
| C | -0.236984 | 2.514045 | 0.080273 |
| H | 0.183187 | 2.863301 | -0.865761 |
| H | -1.186816 | 3.018927 | 0.240021 |
| H | 0.448893 | 2.793196 | 0.881451 |
| H | -2.570465 | 1.264116 | 0.075281 |
| O | -2.044656 | -0.720972 | -0.072962 |
| C | -3.444848 | -1.061214 | -0.086710 |
| H | -3.487335 | -2.141067 | -0.180344 |
| H | -3.904351 | -0.739594 | 0.847439 |
| H | -3.924242 | -0.584143 | -0.940898 |

**9U-*E*** radical cation

Imaginary frequency: None

Electronic energies: -443.570938

Free energies: -443.382059

Corrected Free energies: -443.381485

| | | | |
|---|---|---|---|
| C | -2.681211 | -1.248935 | -0.270610 |
| C | -3.094694 | 0.082436 | 0.359084 |
| C | -1.949019 | 1.012509 | -0.026167 |
| C | -1.177034 | -1.302965 | -0.013145 |
| H | -3.192066 | -2.106813 | 0.162091 |

| | | | |
|---|---|---|---|
| H | -2.872390 | -1.233999 | -1.345390 |
| H | -3.145431 | -0.011447 | 1.445869 |
| H | -4.051722 | 0.450963 | -0.005218 |
| H | -2.079785 | 1.420747 | -1.033079 |
| H | -1.791427 | 1.833380 | 0.671929 |
| H | -0.629228 | -1.853503 | -0.777718 |
| H | -0.947305 | -1.720738 | 0.971135 |
| N | -0.774162 | 0.119044 | -0.029234 |
| C | 0.476269 | 0.556583 | -0.040082 |
| C | 1.532886 | -0.362813 | 0.023001 |
| C | 0.745418 | 2.027298 | -0.101823 |
| H | 0.463035 | 2.499221 | 0.842444 |
| H | 1.801355 | 2.208759 | -0.279205 |
| H | 0.161149 | 2.486393 | -0.900506 |
| O | 2.762447 | 0.090204 | 0.006841 |
| H | 1.381300 | -1.434184 | 0.098350 |
| C | 3.814296 | -0.890419 | 0.074482 |
| H | 3.718879 | -1.462948 | 0.996729 |
| H | 3.758867 | -1.543297 | -0.796214 |
| H | 4.742859 | -0.329636 | 0.070257 |

**9V-*E***

Imaginary frequency: None

Electronic energies: -766.722199

Free energies: -766.541296

Corrected Free energies: -766.539267

| | | | |
|---|---|---|---|
| C | 3.160291 | -1.073217 | 0.085761 |
| C | 3.352669 | 0.297739 | -0.567135 |
| C | 2.175272 | 1.101149 | -0.017497 |
| C | 1.643037 | -1.266435 | 0.043230 |
| H | 3.694499 | -1.874350 | -0.423904 |
| H | 3.499086 | -1.039511 | 1.124316 |
| H | 3.261779 | 0.210715 | -1.653035 |
| H | 4.312959 | 0.757295 | -0.335090 |
| H | 2.418642 | 1.530445 | 0.962691 |
| H | 1.879826 | 1.913649 | -0.682213 |
| H | 1.272503 | -1.857094 | 0.886874 |
| H | 1.319709 | -1.764102 | -0.880511 |
| N | 1.117239 | 0.093560 | 0.097299 |
| C | -0.209174 | 0.359869 | 0.246653 |
| C | -1.135012 | -0.641760 | 0.295991 |
| C | -0.570668 | 1.817649 | 0.330960 |
| H | -0.395305 | 2.307209 | -0.630541 |

| | | | |
|---|---|---|---|
| H | -1.618505 | 1.936010 | 0.593672 |
| H | 0.044558 | 2.324664 | 1.077167 |
| H | -0.828370 | -1.673544 | 0.194708 |
| C | -3.436848 | -0.104866 | -1.191358 |
| H | -2.988648 | 0.805064 | -1.590050 |
| H | -3.175092 | -0.955406 | -1.819292 |
| H | -4.521332 | 0.006480 | -1.162858 |
| S | -2.867149 | -0.388951 | 0.518584 |

**9V-*Z***

Imaginary frequency: None

Electronic energies: -766.718020

Free energies: -766.533417

Corrected Free energies: -766.532797

| | | | |
|---|---|---|---|
| C | 2.251862 | -1.350812 | 0.734116 |
| C | 2.773965 | -0.720065 | -0.557209 |
| C | 2.018468 | 0.604409 | -0.595629 |
| C | 0.758562 | -1.021698 | 0.690463 |
| H | 2.436564 | -2.422676 | 0.801107 |
| H | 2.717027 | -0.864619 | 1.595795 |
| H | 2.492850 | -1.335125 | -1.416308 |
| H | 3.854335 | -0.579370 | -0.568113 |
| H | 2.532944 | 1.352238 | 0.020189 |
| H | 1.918243 | 1.004290 | -1.606555 |
| H | 0.315285 | -0.905882 | 1.681699 |
| H | 0.201038 | -1.806232 | 0.167960 |
| N | 0.706275 | 0.255773 | -0.034946 |
| C | -0.275402 | 1.194249 | 0.164760 |
| C | -1.570128 | 0.927147 | 0.471665 |
| C | 0.142812 | 2.634950 | -0.003615 |
| H | 0.486566 | 2.823787 | -1.023649 |
| H | -0.696098 | 3.297596 | 0.199808 |
| H | 0.964234 | 2.884929 | 0.672131 |
| H | -2.232165 | 1.761364 | 0.659188 |
| C | -2.105329 | -1.089102 | -1.334650 |
| H | -2.537369 | -2.077494 | -1.490934 |
| H | -2.602632 | -0.363184 | -1.976167 |
| H | -1.038930 | -1.116392 | -1.563372 |
| S | -2.357792 | -0.657382 | 0.417027 |

**9V-*Z*** radical cation

Imaginary frequency: None

Electronic energies: -766.545824
Free energies: -766.362028
Corrected Free energies: -766.361103

| | | | |
|---|---|---|---|
| C | 2.350478 | -1.638173 | 0.331418 |
| C | 3.147418 | -0.553278 | -0.392362 |
| C | 2.379710 | 0.716677 | -0.046410 |
| C | 0.901772 | -1.212684 | 0.102666 |
| H | 2.537262 | -2.639764 | -0.050804 |
| H | 2.575407 | -1.623722 | 1.399769 |
| H | 3.123651 | -0.719464 | -1.471297 |
| H | 4.185361 | -0.495234 | -0.070206 |
| H | 2.672864 | 1.110020 | 0.931928 |
| H | 2.477387 | 1.505548 | -0.790091 |
| H | 0.237434 | -1.511195 | 0.913185 |
| H | 0.514013 | -1.596170 | -0.845579 |
| N | 0.973704 | 0.259900 | 0.030283 |
| C | -0.052734 | 1.096737 | 0.061872 |
| C | -1.407389 | 0.722897 | 0.064980 |
| C | 0.252984 | 2.569231 | 0.077750 |
| H | 0.649913 | 2.880031 | -0.891914 |
| H | -0.646222 | 3.144378 | 0.281011 |
| H | 1.000235 | 2.799232 | 0.838551 |
| H | -2.118831 | 1.535898 | 0.136633 |
| C | -3.862365 | -0.385255 | -0.037762 |
| H | -4.407146 | -1.321592 | -0.134704 |
| H | -4.092532 | 0.082018 | 0.917157 |
| H | -4.102590 | 0.272663 | -0.869763 |
| S | -2.105087 | -0.821179 | -0.092423 |

**9V-*E*** radical cation
Imaginary frequency: None
Electronic energies: -766.549721
Free energies: -766.366044
Corrected Free energies: -766.365198

| | | | |
|---|---|---|---|
| C | -2.962349 | -1.341373 | -0.274658 |
| C | -3.434162 | -0.043945 | 0.383276 |
| C | -2.346271 | 0.950721 | -0.007762 |
| C | -1.453797 | -1.319671 | -0.040695 |
| H | -3.421012 | -2.232056 | 0.150256 |
| H | -3.171042 | -1.318711 | -1.346158 |
| H | -3.458808 | -0.156829 | 1.469160 |
| H | -4.415965 | 0.279457 | 0.042966 |
| H | -2.517422 | 1.364076 | -1.006530 |

| | | | |
|---|---|---|---|
| H | -2.222919 | 1.769244 | 0.699722 |
| H | -0.889361 | -1.829551 | -0.821218 |
| H | -1.185890 | -1.740280 | 0.932886 |
| N | -1.124466 | 0.120866 | -0.040932 |
| C | 0.103112 | 0.616469 | -0.052521 |
| C | 1.203686 | -0.253198 | 0.000775 |
| C | 0.268654 | 2.105676 | -0.092208 |
| H | 0.061785 | 2.527576 | 0.894811 |
| H | 1.280884 | 2.384046 | -0.376671 |
| H | -0.424618 | 2.549651 | -0.806380 |
| H | 1.059266 | -1.323333 | 0.068786 |
| C | 3.712603 | -1.264334 | 0.094561 |
| H | 3.459257 | -1.777389 | 1.019472 |
| H | 3.478849 | -1.875152 | -0.774499 |
| H | 4.768176 | -1.002786 | 0.092093 |
| S | 2.807577 | 0.302119 | -0.001048 |