Inner *vs.* Outer-sphere Ru-catalyzed Formic Acid Dehydrogenation: A Computational Study.

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Supporting Information

1. Variable Temperature (VT) NMR experimental procedure

Complex [Ru(κ^4-NP_3)(H)Cl] (**4**, 20 mg, 2.53 x 10^{-2} mmol) was dissolved in CD_2Cl_2 (0.6 mL) under nitrogen at 233 K (acetone-liquid nitrogen bath). HCO_2NHEt_3 (4.0 μL, ca. 1 equiv.) was then syringed into the tube, which was then inserted into the NMR probehead pre-cooled at 233 K. Subsequently, the probe was warmed slowly to room temperature in steps of 20 K each, and new sets of ^{31}P $\{^1H\}$ and ^1H NMR data were collected at each step. The probe was cooled at 233 K and a second equiv. of HCO_2NHEt_3 was added, then the same heating sequence and NMR recording was applied. Finally, neat HCOOH (1.0 μL, ca. 1 equiv.) was added at 233 K, applying again the same heating sequence and NMR recording.

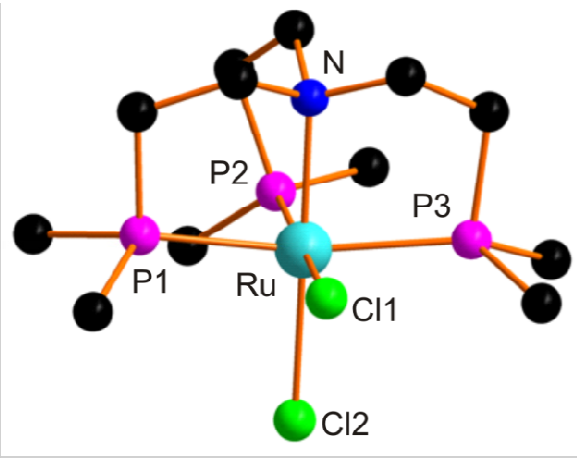
2. DFT Calculations and Optimized Structures

The model systems reported herein were optimized at the hybrid density functional theory (DFT) level using the B3LYP functional. All the DFT calculations were carried out using the Gaussian 09 package.[1] The nature of stationary point (minima or transition state) was confirmed for all of the fully optimized structures through vibrational frequencies calculations. The pseudo-potential Stuttgart-Dresden[2] was used for the Ru center while the 6-31G basis set with the important addition

of the polarization functions (d, p) for all atoms including hydrogens. All the structures were optimized in solution using the Conductor-Like Polarizable Continuum Model (CPCM)[3] as implemented in the Gaussian 09 package,[1] and in particular in dichloromethane solution for **1** and in acetone for **2.PF$_6$**.

The coordinates of all the optimized structures and the associated thermal parameters are reported below the drawing of the corresponding molecule (blue, green, dark blue, black, violet, red and grey colors stand for Ru, Cl, N, C, P, O and Hs, respectively).

Compound **1m**



Cartesian coordinates

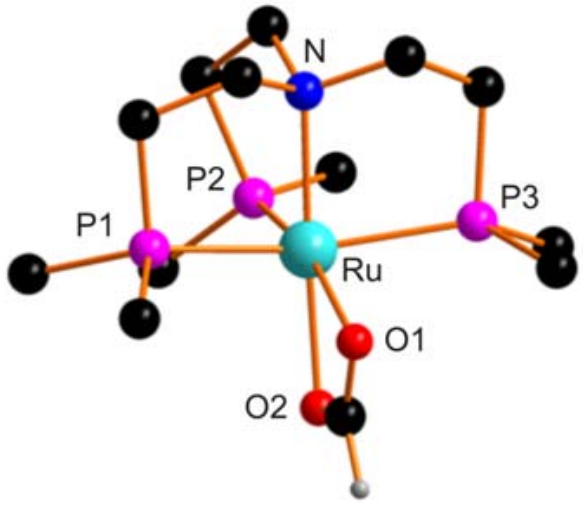
Ru -6.759428 -0.128236 -0.247452
P -6.841497 2.140239 -0.089077
N -4.553856 0.134606 -0.139343
C -5.169810 2.520536 0.638918
C -4.139357 1.593605 -0.019252
P -6.412228 -0.256799 -2.595336
P -6.569606 -0.394121 2.130950
C -4.012905 -0.657668 1.025353
C -4.710221 -0.360632 2.353199
C -3.911354 -0.433035 -1.385267
C -4.570438 0.034995 -2.687070
H -2.933219 -0.470692 1.108450
H -4.162093 -1.707566 0.773062
H -4.423861 0.618519 2.749209

H -4.397046 -1.102596 3.095637
H -4.401239 1.101884 -2.868303
H -4.120716 -0.501887 -3.529799
H -2.842368 -0.177928 -1.380767
H -3.998976 -1.518001 -1.309867
H -3.182439 1.638187 0.514351
H -3.949264 1.958904 -1.029741
H -5.209289 2.382515 1.721342
H -4.880340 3.562485 0.460088
Cl -6.410903 -2.711540 -0.283222
C -8.099663 3.004884 0.951813
H -7.782888 4.031573 1.161295
H -9.035235 3.031877 0.385822
H -8.287115 2.482188 1.887132
C -6.872952 3.300400 -1.536596
H -7.792491 3.162463 -2.110174
H -6.837335 4.331687 -1.170629
H -6.014789 3.139633 -2.192412
C -7.107180 0.847092 -3.912114
H -6.736243 0.532045 -4.892593
H -8.197916 0.761179 -3.905335
H -6.840606 1.890855 -3.756103
C -6.652184 -1.876204 -3.456042
H -7.720331 -2.112094 -3.478775
H -6.277442 -1.807197 -4.482290
H -6.140090 -2.671582 -2.916464
C -7.125315 0.759768 3.475742
H -6.748085 0.400904 4.438867
H -6.761831 1.777275 3.321373
H -8.218301 0.778022 3.516578
C -7.122292 -1.981475 2.898631
H -6.732352 -2.824750 2.330046
H -6.787864 -2.032123 3.939624
H -8.215543 -2.019767 2.870588
Cl -9.253404 -0.391227 -0.354547

Energy and thermal parameters

HF=-2569.7422592
Zero-point vibrational energy 1088822.3 (Joules/Mol)
Zero-point correction= 0.414710 (Hartree/Particle)
Thermal correction to Energy= 0.441789
Thermal correction to Enthalpy= 0.442733
Thermal correction to Gibbs Free Energy= 0.361262
Sum of electronic and zero-point Energies= -2569.327549
Sum of electronic and thermal Energies= -2569.300470
Sum of electronic and thermal Enthalpies= -2569.299526
Sum of electronic and thermal Free Energies= -2569.380997

Compound η^2-**3m**$^+$



Cartesian coordinates

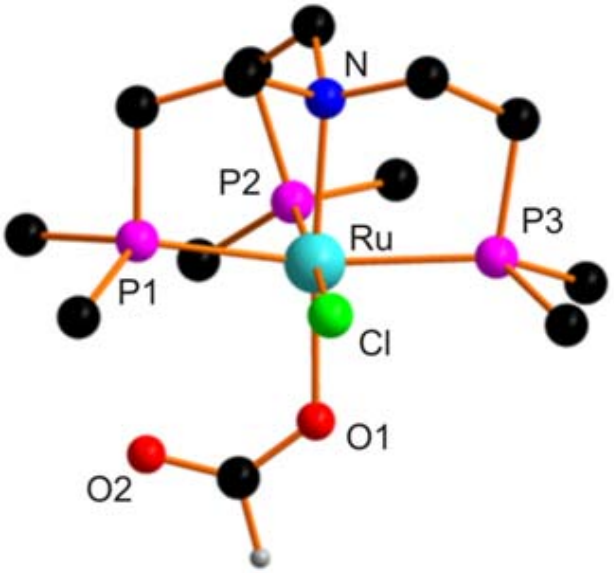
Ru -6.716770 -0.110370 -0.237197
P -6.795914 2.156003 -0.092148
N -4.509839 0.198472 -0.133072
C -5.142295 2.583439 0.636003
C -4.093140 1.660118 0.007212
P -6.336329 -0.287051 -2.574637
P -6.494624 -0.439432 2.132462
C -3.966120 -0.604015 1.022255
C -4.648646 -0.291141 2.351030
C -3.850772 -0.346344 -1.380683
C -4.524366 0.118680 -2.672879
H -2.883159 -0.436257 1.093924
H -4.120147 -1.656952 0.772806
H -4.403325 0.714157 2.704720
H -4.293596 -0.989954 3.115640
H -4.412920 1.197099 -2.824233
H -4.049689 -0.372987 -3.528897
H -2.788884 -0.067199 -1.372211
H -3.900942 -1.435893 -1.316443
H -3.153217 1.697402 0.569057
H -3.871242 2.027871 -0.995357
H -5.198864 2.466517 1.720579
H -4.870891 3.626512 0.439957
C -8.074114 2.965612 0.960445
H -7.834326 4.024170 1.100962
H -9.039022 2.887817 0.450505
H -8.160756 2.481563 1.932094
C -6.887476 3.252858 -1.578412
H -7.824330 3.075674 -2.112648
H -6.855391 4.299978 -1.261574

H -6.051357 3.071205 -2.257152
C -7.113612 0.642706 -3.968430
H -6.654185 0.343917 -4.915866
H -8.180577 0.403988 -4.002329
H -7.002525 1.719609 -3.843870
C -6.419368 -2.009072 -3.239879
H -7.461864 -2.334938 -3.284564
H -5.992315 -2.039152 -4.247135
H -5.878967 -2.695867 -2.586378
C -7.168502 0.555993 3.538512
H -6.815456 0.138983 4.486913
H -6.846056 1.597555 3.477389
H -8.261543 0.522611 3.524361
C -6.859854 -2.150832 2.723451
H -6.377068 -2.881815 2.072900
H -6.505305 -2.272637 3.751484
H -7.938615 -2.328441 2.695965
O -7.246505 -2.355838 -0.312206
C -8.465302 -2.016553 -0.345370
H -9.253478 -2.782015 -0.392130
O -8.792041 -0.788351 -0.324426

Energy and thermal parameters

HF=-1838.3076225
Zero-point vibrational energy 1147331.1 (Joules/Mol)
Zero-point correction= 0.436995 (Hartree/Particle)
Thermal correction to Energy= 0.463647
Thermal correction to Enthalpy= 0.464592
Thermal correction to Gibbs Free Energy= 0.384593
Sum of electronic and zero-point Energies= -1837.870627
Sum of electronic and thermal Energies= -1837.843975
Sum of electronic and thermal Enthalpies= -1837.843031
Sum of electronic and thermal Free Energies= -1837.923030

Compound η^1-**3m$_N$**



Cartesian coordinates

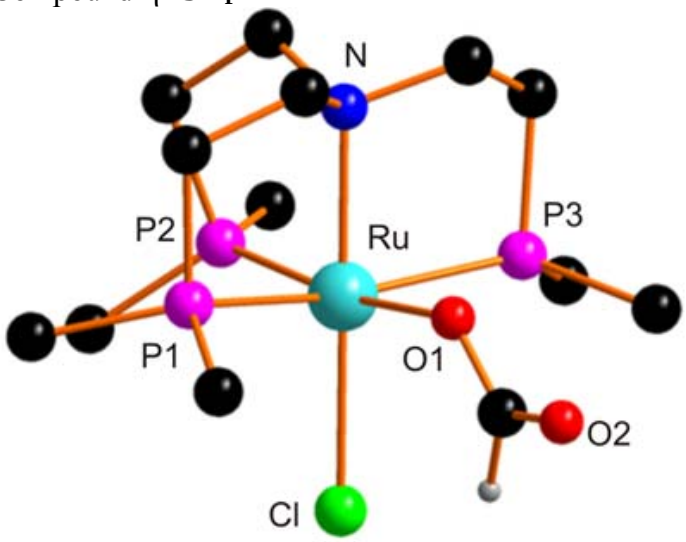
Ru -6.754715 -0.154282 -0.233417
P -6.850538 2.112617 -0.067157
N -4.546316 0.130056 -0.140586
C -5.176777 2.507085 0.649432
C -4.141766 1.590762 -0.017196
P -6.413775 -0.277454 -2.588978
P -6.551992 -0.398884 2.146098
C -3.995720 -0.660564 1.019173
C -4.684283 -0.357802 2.349123
C -3.906713 -0.428426 -1.390440
C -4.577330 0.039029 -2.686802
H -2.914472 -0.475415 1.091788
H -4.148282 -1.710955 0.769609
H -4.392378 0.623121 2.737179
H -4.362004 -1.094799 3.092874
H -4.423038 1.109412 -2.860676
H -4.124746 -0.485919 -3.535540
H -2.839174 -0.166379 -1.392782
H -3.985176 -1.514634 -1.318532
H -3.182759 1.641278 0.512519
H -3.958688 1.961756 -1.027011
H -5.206713 2.367795 1.731548
H -4.900401 3.552230 0.468587
Cl -6.426106 -2.737139 -0.266795
O -8.863687 -0.452913 -0.463748
C -9.753315 -0.450187 0.459918
H -10.774148 -0.649628 0.069582
O -9.608831 -0.257622 1.681274
C -8.118340 2.945623 0.989058
H -7.766984 3.929631 1.316252

H -9.018673 3.080312 0.381574
H -8.382521 2.332819 1.847833
C -6.898129 3.286255 -1.504601
H -7.817439 3.145479 -2.078226
H -6.872991 4.314231 -1.127814
H -6.039770 3.141295 -2.164176
C -7.124976 0.819672 -3.903606
H -6.732698 0.529769 -4.883734
H -8.212761 0.700352 -3.912452
H -6.893920 1.869285 -3.729782
C -6.629593 -1.898984 -3.453381
H -7.693857 -2.152231 -3.477260
H -6.255729 -1.823735 -4.479596
H -6.105673 -2.687513 -2.914639
C -7.073208 0.766256 3.492047
H -6.649681 0.426861 4.443112
H -6.732887 1.787346 3.309830
H -8.162983 0.757362 3.557949
C -7.048925 -1.987389 2.948187
H -6.662649 -2.830459 2.376314
H -6.669273 -2.018339 3.974661
H -8.140298 -2.033935 2.959308

Energy and thermal parameters

HF=-2298.6929311
Zero-point vibrational energy 1146098.2 (Joules/Mol)
Zero-point correction= 0.436526 (Hartree/Particle)
Thermal correction to Energy= 0.465607
Thermal correction to Enthalpy= 0.466551
Thermal correction to Gibbs Free Energy= 0.380572
Sum of electronic and zero-point Energies= -2298.256405
Sum of electronic and thermal Energies= -2298.227324
Sum of electronic and thermal Enthalpies= -2298.226380
Sum of electronic and thermal Free Energies= -2298.312360

Compound η^1-**3m$_P$**



Cartesian coordinates

Ru -6.826429 -0.018692 -0.238481
P -6.806293 2.254618 -0.086352
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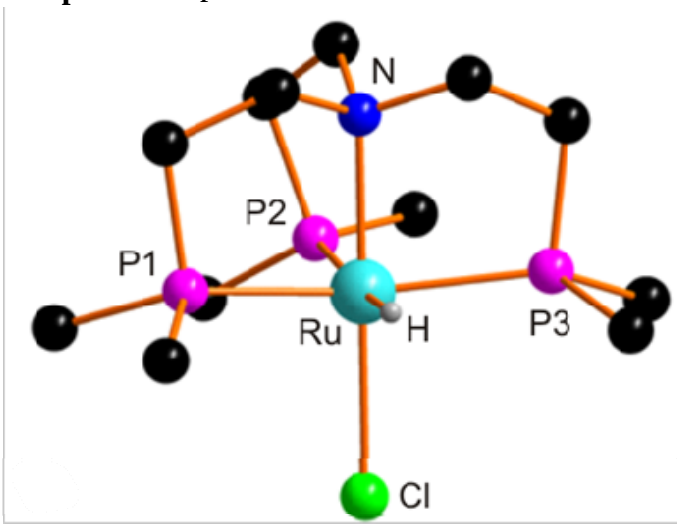
C -5.116119 2.550977 0.637551
C -4.127501 1.573277 -0.012290
P -6.486804 -0.195012 -2.570781
P -6.641345 -0.334274 2.128453
C -4.116606 -0.689627 1.023716
C -4.785459 -0.341379 2.353436
C -4.003656 -0.461325 -1.384313
C -4.641860 0.045500 -2.681998
H -3.026175 -0.577529 1.098682
H -4.339906 -1.727459 0.772699
H -4.466101 0.636854 2.725095
H -4.489959 -1.077340 3.109059
H -4.432410 1.106252 -2.854590
H -4.217123 -0.502712 -3.530386
H -2.922144 -0.267537 -1.382348
H -4.150134 -1.540604 -1.310251
H -3.173184 1.570809 0.528062
H -3.912957 1.928473 -1.021494
H -5.172186 2.413655 1.720124
H -4.771249 3.576669 0.462305
C -7.994928 3.188940 0.975176
H -7.637368 4.208789 1.149353
H -8.952879 3.234430 0.449064
H -8.158111 2.691663 1.929831
C -6.800012 3.396434 -1.548405
H -7.744287 3.308660 -2.092044
H -6.684985 4.430307 -1.206968
H -5.977661 3.164599 -2.229032

C -7.187018 0.848111 -3.927918
H -6.782226 0.529914 -4.893949
H -8.273687 0.721389 -3.941866
H -6.964958 1.904452 -3.781293
C -6.726816 -1.870286 -3.317601
H -7.782796 -2.149561 -3.261444
H -6.414492 -1.857304 -4.366459
H -6.144487 -2.613892 -2.772561
C -7.210101 0.755669 3.514939
H -6.875590 0.342121 4.471826
H -6.811471 1.767753 3.417692
H -8.302802 0.806922 3.518591
C -7.172828 -1.979050 2.780126
H -6.682690 -2.775712 2.220198
H -6.919397 -2.063361 3.841372
H -8.255045 -2.083564 2.659801
Cl -9.331175 -0.197171 -0.343738
O -6.485200 -2.211216 -0.243091
C -7.370244 -3.129223 -0.392407
H -8.403648 -2.775661 -0.561806
O -7.140592 -4.354870 -0.358985

Energy and thermal parameters

HF=-2298.6964268
Zero-point vibrational energy 1147073.9 (Joules/Mol)
Zero-point correction= 0.436897 (Hartree/Particle)
Thermal correction to Energy= 0.466001
Thermal correction to Enthalpy= 0.466945
Thermal correction to Gibbs Free Energy= 0.381011
Sum of electronic and zero-point Energies= -2298.259529
Sum of electronic and thermal Energies= -2298.230426
Sum of electronic and thermal Enthalpies= -2298.229482
Sum of electronic and thermal Free Energies= -2298.315415

Compound 4m$_P$



Cartesian coordinates

Ru -6.784499 -0.025839 -0.235530
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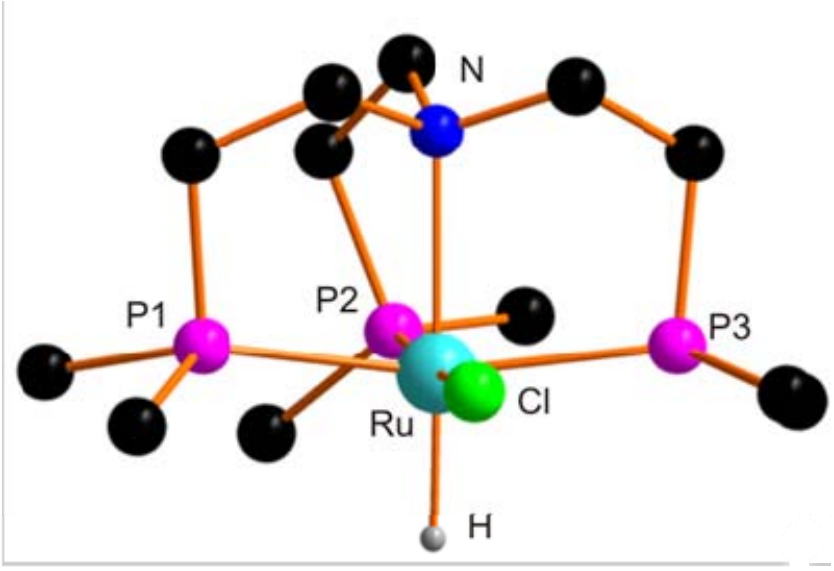
N -4.576139 0.197919 -0.132121
C -5.093502 2.636484 0.567811
C -4.123265 1.649867 -0.089888
P -6.440710 -0.317094 -2.516011
P -6.624136 -0.464172 2.055794
C -4.042834 -0.551906 1.066048
C -4.791655 -0.271459 2.367070
C -3.933043 -0.441455 -1.344657
C -4.598301 -0.061591 -2.668878
H -2.971997 -0.329561 1.177159
H -4.138212 -1.613549 0.830588
H -4.601839 0.742047 2.732358
H -4.438192 -0.960589 3.142755
H -4.417282 0.986745 -2.928897
H -4.166980 -0.666300 -3.475197
H -2.863922 -0.184741 -1.357409
H -4.011673 -1.521147 -1.206373
H -3.141096 1.689947 0.398685
H -3.969452 1.965734 -1.123510
H -5.119061 2.519253 1.654485
H -4.745731 3.657147 0.364928
C -7.881437 3.344344 1.068518
H -7.515651 4.373055 1.157821
H -8.900757 3.367302 0.670128
H -7.917696 2.887918 2.058698
C -6.867806 3.508579 -1.540839
H -7.835575 3.422429 -2.044161
H -6.728109 4.546024 -1.217423
H -6.083045 3.261513 -2.260373
C -7.123755 0.684511 -3.920841

H -6.674285 0.383762 -4.873547
H -8.204997 0.524485 -3.976681
H -6.943740 1.748584 -3.758845
C -6.694706 -2.017816 -3.205127
H -7.756855 -2.273863 -3.144052
H -6.370755 -2.076467 -4.249847
H -6.136852 -2.739698 -2.604170
C -7.366564 0.466586 3.482200
H -7.068671 0.020485 4.437118
H -7.044505 1.510460 3.470028
H -8.457769 0.440196 3.405144
C -6.987688 -2.196255 2.599358
H -6.406682 -2.895269 1.993665
H -6.757314 -2.343066 3.660029
H -8.049171 -2.402508 2.431184
Cl -9.323606 -0.350518 -0.338538
H -6.555322 -1.654276 -0.275890

Energy and thermal parameters

HF=-2110.0816462
Zero-point vibrational energy 1100050.4 (Joules/Mol)
Zero-point correction= 0.418987 (Hartree/Particle)
Thermal correction to Energy= 0.445004
Thermal correction to Enthalpy= 0.445948
Thermal correction to Gibbs Free Energy= 0.366186
Sum of electronic and zero-point Energies= -2109.662659
Sum of electronic and thermal Energies= -2109.636642
Sum of electronic and thermal Enthalpies= -2109.635698
Sum of electronic and thermal Free Energies= -2109.715460

Compound $4m_N$



Cartesian coordinates

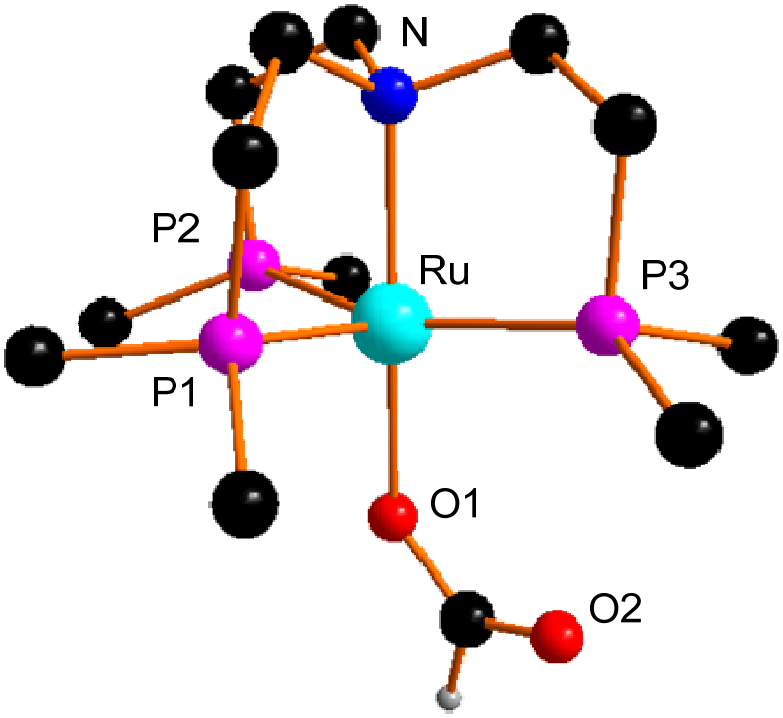
Ru -6.836953 -0.126418 -0.244657
P -6.846807 2.126691 -0.091889
N -4.503737 0.136920 -0.138103
C -5.166764 2.506790 0.638808
C -4.109052 1.587193 0.005083
P -6.458630 -0.261257 -2.571172
P -6.604491 -0.398281 2.108831
C -4.009756 -0.675394 1.016395
C -4.735426 -0.381316 2.333459
C -3.911057 -0.413361 -1.401046
C -4.617217 0.077656 -2.673384
H -2.926940 -0.516938 1.143709
H -4.170186 -1.721356 0.749672
H -4.447694 0.595536 2.735132
H -4.435661 -1.124956 3.080484
H -4.477215 1.154686 -2.818618
H -4.172032 -0.415877 -3.545464
H -2.838072 -0.169392 -1.446446
H -4.000401 -1.500447 -1.342155
H -3.169514 1.645431 0.571732
H -3.887421 1.966147 -0.994607
H -5.218865 2.371356 1.721657
H -4.883059 3.551763 0.464534
C -8.066087 3.048310 0.957774
H -7.715869 4.064476 1.167930
H -9.004650 3.110402 0.397988
H -8.266694 2.531920 1.894774
C -6.857750 3.299367 -1.536010
H -7.797784 3.210866 -2.086572
H -6.761603 4.326612 -1.168926
H -6.027485 3.099381 -2.216780
C -7.160333 0.805564 -3.918982

H -6.675896 0.574080 -4.873438
H -8.230143 0.592616 -4.009197
H -7.038430 1.866693 -3.710384
C -6.610838 -1.889424 -3.443896
H -7.660630 -2.196249 -3.460044
H -6.248572 -1.790405 -4.472456
H -6.043902 -2.655645 -2.916290
C -7.125090 0.756148 3.471957
H -6.730967 0.395200 4.427764
H -6.759885 1.772204 3.311687
H -8.217192 0.782032 3.533827
C -7.137743 -1.979954 2.911685
H -6.778851 -2.829624 2.332197
H -6.758059 -2.028451 3.937422
H -8.231459 -2.012879 2.933404
H -8.449463 -0.256619 -0.296117
Cl -6.543374 -2.725395 -0.279171

Energy and thermal parameters

HF=-2110.0833137
Zero-point vibrational energy 1103095.5 (Joules/Mol)
Zero-point correction= 0.420147 (Hartree/Particle)
Thermal correction to Energy= 0.445631
Thermal correction to Enthalpy= 0.446576
Thermal correction to Gibbs Free Energy= 0.368988
Sum of electronic and zero-point Energies= -2109.663167
Sum of electronic and thermal Energies= -2109.637682
Sum of electronic and thermal Enthalpies= -2109.636738
Sum of electronic and thermal Free Energies= -2109.714325

Compound [Ru(κ^4-NP_3)(η^1-HCO_2)]



Cartesian coordinates

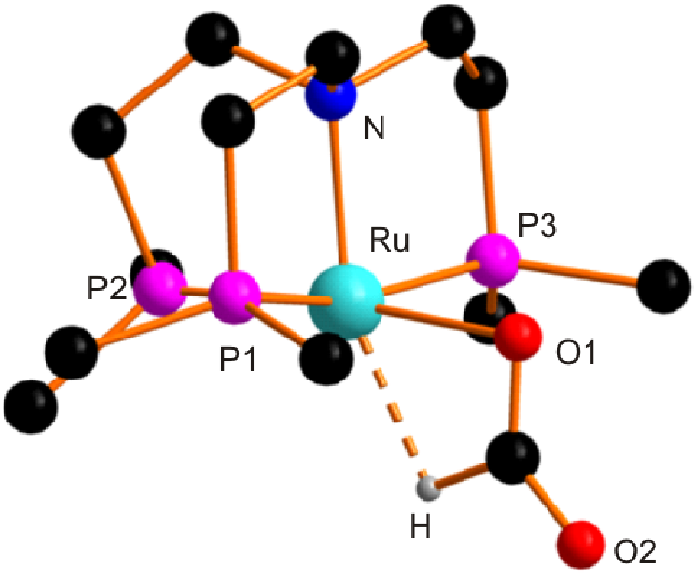
Ru -6.784377 0.084901 -0.216358
P -6.744985 2.305517 -0.051948
N -4.551552 0.225540 -0.121662
C -5.028428 2.664975 0.556323
C -4.058461 1.664285 -0.080755
P -6.416982 -0.180476 -2.534458
P -6.605286 -0.355486 2.121106
C -4.045949 -0.541832 1.076877
C -4.763630 -0.205124 2.381697
C -3.943129 -0.438927 -1.338937
C -4.572039 -0.006341 -2.667235
H -2.964346 -0.378418 1.173025
H -4.193791 -1.601497 0.852552
H -4.532829 0.808741 2.720877
H -4.418307 -0.886550 3.167245
H -4.330004 1.031405 -2.916997
H -4.167535 -0.626719 -3.474561
H -2.861236 -0.250795 -1.345466
H -4.082976 -1.514976 -1.211118
H -3.088939 1.686458 0.429961
H -3.877734 1.971380 -1.111573
H -5.030719 2.599614 1.646462
H -4.722582 3.684327 0.296243
O -8.840856 -0.279540 -0.520643
C -9.766036 -0.440591 0.365299
H -10.747701 -0.681087 -0.089734

O -9.671314 -0.360677 1.597844
C -7.896622 3.153211 1.105441
H -7.648891 4.217684 1.164069
H -8.917279 3.044913 0.728327
H -7.847234 2.714525 2.101517
C -6.931551 3.361032 -1.554529
H -7.899642 3.165519 -2.022973
H -6.882304 4.416101 -1.267583
H -6.139635 3.161344 -2.279284
C -7.114854 0.681676 -4.006262
H -6.711238 0.248073 -4.926448
H -8.201909 0.561566 -4.002064
H -6.883285 1.747669 -3.981568
C -6.731585 -1.955402 -2.947314
H -7.809746 -2.137199 -2.928562
H -6.339635 -2.202254 -3.939225
H -6.262276 -2.607050 -2.205084
C -7.306789 0.433500 3.633993
H -6.974230 -0.115908 4.520631
H -6.974388 1.470176 3.726472
H -8.395247 0.404924 3.568088
C -6.937091 -2.147939 2.426659
H -6.442522 -2.762145 1.669087
H -6.575406 -2.441603 3.417327
H -8.014818 -2.313321 2.365117

Energy and thermal parameters

HF=-1838.3016511
Zero-point vibrational energy 1145293.6 (Joules/Mol)
Zero-point correction= 0.436219 (Hartree/Particle)
Thermal correction to Energy= 0.463331
Thermal correction to Enthalpy= 0.464275
Thermal correction to Gibbs Free Energy= 0.382753
Sum of electronic and zero-point Energies= -1837.865432
Sum of electronic and thermal Energies= -1837.838320
Sum of electronic and thermal Enthalpies= -1837.837376
Sum of electronic and thermal Free Energies= -1837.918898

Transition State $3m_{TS}^{+}$



Imaginary frequency at -89.9 cm^{-1}

Cartesian coordinates

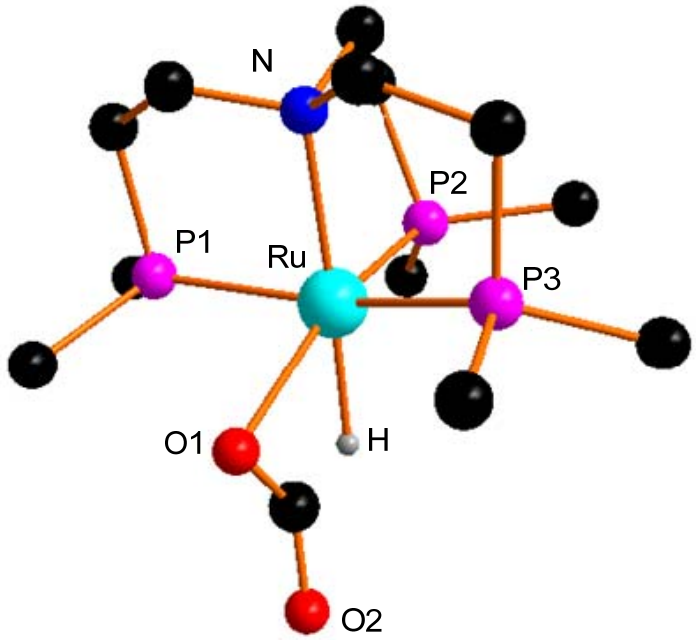
Ru -6.836932 0.044498 -0.263030
P -6.756159 2.333441 -0.109166
N -4.667549 0.148625 -0.154876
C -5.079690 2.568161 0.653755
C -4.121124 1.567473 0.001254
P -6.497009 -0.137876 -2.613419
P -6.671553 -0.274881 2.134145
C -4.202708 -0.721233 0.992587
C -4.821428 -0.343745 2.334427
C -4.049712 -0.449879 -1.404791
C -4.655323 0.083323 -2.702502
H -3.107537 -0.675462 1.039307
H -4.483986 -1.745091 0.735890
H -4.452734 0.619385 2.697520
H -4.542796 -1.091676 3.083755
H -4.425463 1.141430 -2.860514
H -4.229966 -0.463672 -3.550505
H -2.967766 -0.271442 -1.373766
H -4.206176 -1.529078 -1.345682
H -3.177569 1.508849 0.554192
H -3.877451 1.925700 -0.999555
H -5.162622 2.413022 1.731768
H -4.697182 3.583121 0.501562
C -7.967194 3.252742 0.932477
H -7.621140 4.276039 1.108004
H -8.918600 3.290632 0.393330
H -8.135698 2.757526 1.887316
C -6.706767 3.459995 -1.574470
H -7.651747 3.398109 -2.120153

H -6.563125 4.490624 -1.235030
H -5.889259 3.202226 -2.251016
C -7.190216 0.903818 -3.968130
H -6.792308 0.568995 -4.931109
H -8.278497 0.794696 -3.977612
H -6.947093 1.956806 -3.830418
C -6.758909 -1.827063 -3.311382
H -7.829146 -2.047048 -3.354120
H -6.345210 -1.873266 -4.323176
H -6.282036 -2.577551 -2.679098
C -7.219489 0.824549 3.514544
H -6.896931 0.397672 4.469291
H -6.795701 1.826584 3.422915
H -8.310438 0.900220 3.514835
C -7.246151 -1.916424 2.749477
H -6.856752 -2.710808 2.111156
H -6.908160 -2.064140 3.779329
H -8.338824 -1.956130 2.723406
O -7.146440 -2.142443 -0.304784
C -8.413303 -2.013950 -0.381471
H -8.764987 -0.906419 -0.406084
O -9.304944 -2.856782 -0.435180

Energy and thermal parameters

HF=-1838.2783774
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 1142721.9 (Joules/Mol)
Zero-point correction= 0.435240 (Hartree/Particle)
Thermal correction to Energy= 0.461386
Thermal correction to Enthalpy= 0.462330
Thermal correction to Gibbs Free Energy= 0.383443
Sum of electronic and zero-point Energies= -1837.843138
Sum of electronic and thermal Energies= -1837.816992
Sum of electronic and thermal Enthalpies= -1837.816048
Sum of electronic and thermal Free Energies= -1837.894934

Compound [Ru(κ^4-NP_3)(H)(CO_2)]$^+$



Cartesian coordinates

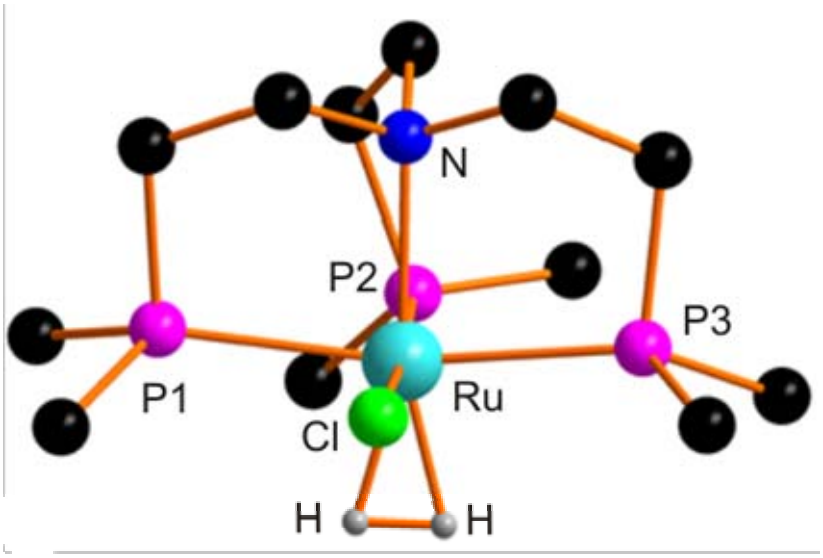
Ru -6.834076 0.010059 -0.251858
P -6.761218 2.278060 -0.097830
N -4.597606 0.171606 -0.148020
C -5.082061 2.587487 0.626423
C -4.095360 1.604345 -0.012601
P -6.452868 -0.194246 -2.593494
P -6.628805 -0.348333 2.117417
C -4.111888 -0.665048 1.009452
C -4.779095 -0.316379 2.336513
C -3.978572 -0.421037 -1.394343
C -4.617962 0.081302 -2.688942
H -3.021386 -0.563700 1.086554
H -4.329066 -1.705533 0.755508
H -4.475526 0.670215 2.696793
H -4.470892 -1.039390 3.098876
H -4.425770 1.145856 -2.855027
H -4.183441 -0.454500 -3.539693
H -2.900610 -0.213500 -1.387119
H -4.101312 -1.504340 -1.324709
H -3.149780 1.586911 0.540626
H -3.862996 1.958201 -1.017718
H -5.143857 2.464915 1.710274
H -4.743489 3.612299 0.438922
C -7.977140 3.167886 0.960545
H -7.675560 4.212775 1.082396
H -8.951418 3.136559 0.464119
H -8.075966 2.704034 1.940628
C -6.792294 3.369078 -1.588475

H -7.743401 3.250084 -2.113598
H -6.690075 4.412970 -1.275964
H -5.975776 3.132081 -2.273538
C -7.165816 0.775603 -3.990678
H -6.733253 0.434821 -4.936453
H -8.247491 0.616605 -4.017685
H -6.973572 1.842124 -3.876087
C -6.656520 -1.919041 -3.220827
H -7.718676 -2.171091 -3.271880
H -6.219622 -2.000289 -4.220645
H -6.172601 -2.627880 -2.546521
C -7.247186 0.674366 3.525919
H -6.931968 0.222968 4.471776
H -6.852599 1.691633 3.480262
H -8.339624 0.715467 3.501484
C -7.114956 -2.041844 2.664923
H -6.690722 -2.791114 1.994582
H -6.765008 -2.214819 3.686988
H -8.203703 -2.138188 2.638783
O -7.646715 -2.122106 -0.341610
C -8.695091 -1.431289 -0.401017
H -8.570547 -0.181255 -0.286754
O -9.886165 -1.671388 -0.528678

Energy and thermal parameters

HF=-1838.2827082
Zero-point vibrational energy 1140101.5 (Joules/Mol)
Zero-point correction= 0.434242 (Hartree/Particle)
Thermal correction to Energy= 0.461220
Thermal correction to Enthalpy= 0.462164
Thermal correction to Gibbs Free Energy= 0.380401
Sum of electronic and zero-point Energies= -1837.848467
Sum of electronic and thermal Energies= -1837.821489
Sum of electronic and thermal Enthalpies= -1837.820544
Sum of electronic and thermal Free Energies= -1837.902308

Compound $6m_N^+$



Cartesian coordinates

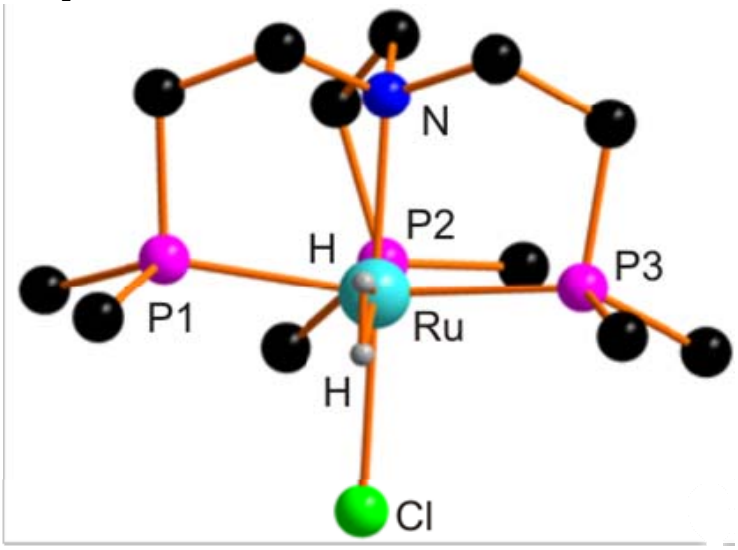
Ru -6.782153 -0.130089 -0.236206
P -6.839590 2.167587 -0.079593
N -4.562935 0.125128 -0.138237
C -5.169382 2.508813 0.660392
C -4.141598 1.582237 -0.001365
P -6.413883 -0.263285 -2.602885
P -6.552982 -0.401802 2.157555
C -4.022211 -0.686640 1.014516
C -4.696145 -0.379594 2.349963
C -3.925511 -0.432014 -1.392538
C -4.583544 0.061472 -2.682873
H -2.939746 -0.518600 1.084150
H -4.190634 -1.733087 0.758721
H -4.396415 0.596453 2.742411
H -4.384623 -1.124084 3.089793
H -4.425330 1.132973 -2.841179
H -4.133165 -0.453264 -3.538281
H -2.856617 -0.182453 -1.384832
H -4.015778 -1.517991 -1.332339
H -3.190082 1.615430 0.540704
H -3.939602 1.955916 -1.005878
H -5.217596 2.360576 1.740718
H -4.870433 3.550051 0.496356
C -8.105313 3.022378 0.953626
H -7.793908 4.050581 1.161654
H -9.038562 3.047327 0.382872
H -8.292877 2.502954 1.890861
C -6.853986 3.310794 -1.533726
H -7.781780 3.191236 -2.097538
H -6.793712 4.341695 -1.170746
H -6.004353 3.131058 -2.195155
C -7.162656 0.824782 -3.892575

H -6.768686 0.545599 -4.874425
H -8.246525 0.677562 -3.893530
H -6.953983 1.877906 -3.717799
C -6.619982 -1.896227 -3.435252
H -7.675632 -2.180674 -3.423875
H -6.279735 -1.810927 -4.471797
H -6.052965 -2.666475 -2.914675
C -7.114435 0.771160 3.473280
H -6.732269 0.426361 4.439007
H -6.755045 1.787177 3.305025
H -8.207076 0.782255 3.515902
C -7.118739 -1.984792 2.912374
H -6.713395 -2.832032 2.361541
H -6.801459 -2.022141 3.958752
H -8.210719 -2.028564 2.866131
H -8.400866 -0.302732 -0.734377
Cl -6.543079 -2.661442 -0.273982
H -8.431310 -0.327950 0.136955

Energy and thermal parameters

HF=-2110.5461101
Zero-point vibrational energy 1133216.4 (Joules/Mol)
Zero-point correction= 0.431619 (Hartree/Particle)
Thermal correction to Energy= 0.457350
Thermal correction to Enthalpy= 0.458294
Thermal correction to Gibbs Free Energy= 0.380189
Sum of electronic and zero-point Energies= -2110.114491
Sum of electronic and thermal Energies= -2110.088760
Sum of electronic and thermal Enthalpies= -2110.087816
Sum of electronic and thermal Free Energies= -2110.165921

Compound $6m_P^+$



Cartesian coordinates

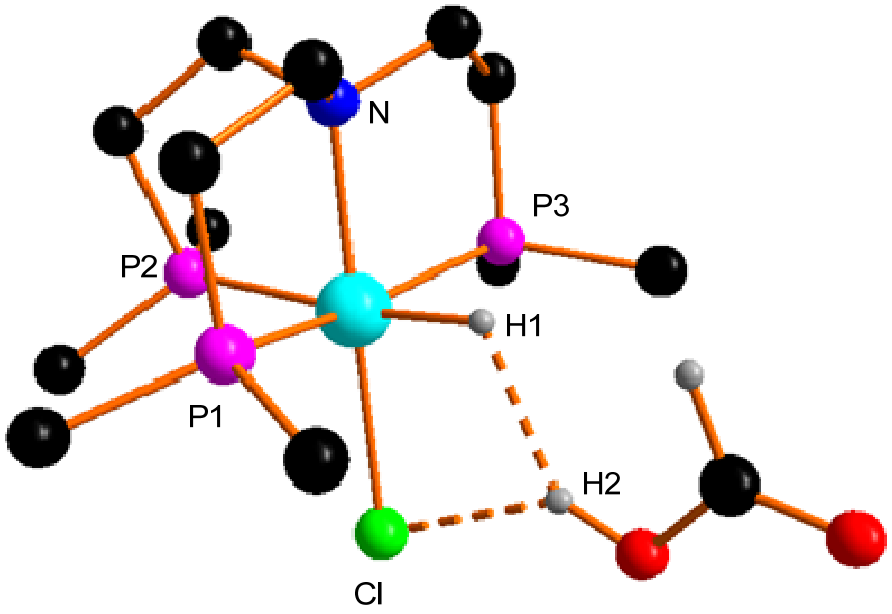
Ru -6.760504 -0.041936 -0.235965
P -6.781637 2.277899 -0.085710
N -4.545300 0.186072 -0.132840
C -5.101402 2.598466 0.627807
C -4.100002 1.641455 -0.026832
P -6.408840 -0.225994 -2.570913
P -6.575115 -0.377137 2.126100
C -4.016247 -0.601062 1.044549
C -4.725235 -0.292989 2.364026
C -3.905622 -0.394131 -1.378511
C -4.572503 0.060860 -2.680927
H -2.938178 -0.417308 1.137963
H -4.145454 -1.657881 0.799135
H -4.463032 0.700676 2.737602
H -4.397898 -1.009842 3.124437
H -4.398653 1.123983 -2.875691
H -4.132095 -0.487636 -3.520632
H -2.838919 -0.135169 -1.381989
H -3.973864 -1.480997 -1.294518
H -3.140708 1.666872 0.501688
H -3.906270 1.991497 -1.041351
H -5.152310 2.467375 1.710938
H -4.780068 3.630127 0.446584
C -8.008858 3.129678 0.984379
H -7.742113 4.184866 1.094798
H -8.988035 3.053558 0.504560
H -8.074306 2.665378 1.966839
C -6.834535 3.368915 -1.574121
H -7.778989 3.225336 -2.104708
H -6.762584 4.414418 -1.258987
H -6.007386 3.155076 -2.254267
C -7.148518 0.756566 -3.944095

H -6.753534 0.408954 -4.903593
H -8.232923 0.615596 -3.932759
H -6.935264 1.819636 -3.836010
C -6.633240 -1.942755 -3.219234
H -7.692229 -2.211399 -3.165349
H -6.300320 -2.003640 -4.259657
H -6.065266 -2.658048 -2.619338
C -7.240497 0.625199 3.527116
H -6.941676 0.172173 4.477475
H -6.860282 1.648365 3.497056
H -8.332441 0.649426 3.474708
C -7.043450 -2.080931 2.663307
H -6.529153 -2.828709 2.055138
H -6.789895 -2.237590 3.715902
H -8.121351 -2.210539 2.530282
H -7.181312 -1.768151 -0.313668
H -6.364433 -1.791557 -0.257045
Cl -9.248153 -0.110321 -0.344374

Energy and thermal parameters

HF=-2110.5381377
Zero-point vibrational energy 1131379.3 (Joules/Mol)
Zero-point correction= 0.430920 (Hartree/Particle)
Thermal correction to Energy= 0.457037
Thermal correction to Enthalpy= 0.457981
Thermal correction to Gibbs Free Energy= 0.378402
Sum of electronic and zero-point Energies= -2110.107218
Sum of electronic and thermal Energies= -2110.081101
Sum of electronic and thermal Enthalpies= -2110.080157
Sum of electronic and thermal Free Energies= -2110.159736

Transition State 4m$_{TS}$



Imaginary frequency at -93.1 cm^{-1}

Cartesian coordinates

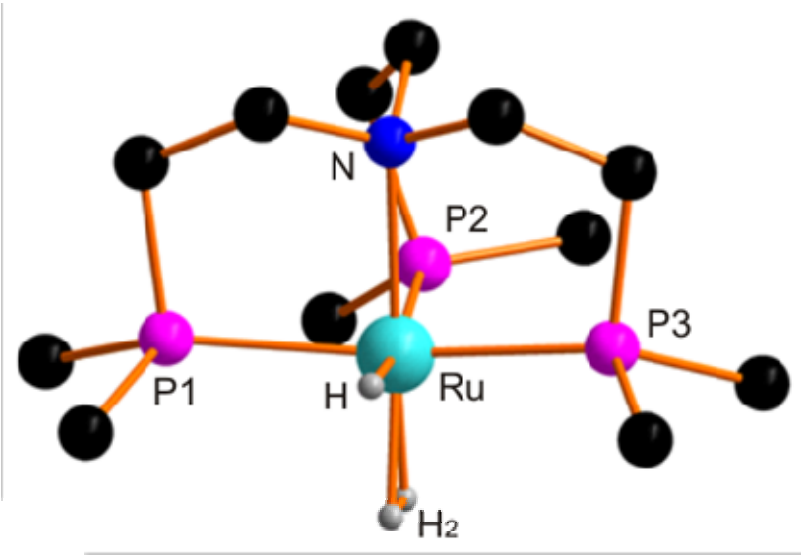
Ru -7.109170 0.343887 -0.093746
P -6.459897 2.630041 -0.191187
N -4.915224 -0.050960 -0.024561
C -4.732225 2.475549 0.497574
C -4.071970 1.214690 -0.067661
P -6.914682 -0.212234 -2.353623
P -6.975424 0.136104 2.238624
C -4.594450 -0.844489 1.218556
C -5.161055 -0.237675 2.499617
C -4.502805 -0.911787 -1.197444
C -5.071550 -0.434644 -2.535221
H -3.504305 -0.964777 1.293516
H -5.031101 -1.834118 1.072386
H -4.641500 0.685419 2.772283
H -5.015832 -0.939304 3.328698
H -4.636989 0.522809 -2.841533
H -4.821394 -1.161759 -3.316317
H -3.405217 -0.960212 -1.235241
H -4.869317 -1.919446 -0.992715
H -3.122175 1.012290 0.443557
H -3.827188 1.400908 -1.114991
H -4.811566 2.438509 1.587012
H -4.109179 3.343128 0.248102
C -7.215679 3.993822 0.813201
H -6.582373 4.887375 0.811888
H -8.185818 4.249598 0.375697
H -7.384997 3.674254 1.842249
C -6.151235 3.590211 -1.755063
H -7.099987 3.772670 -2.268522

H -5.682522 4.554267 -1.529771
H -5.495561 3.034151 -2.430131
C -7.380667 0.822384 -3.819472
H -7.051924 0.352227 -4.752409
H -8.469776 0.927243 -3.842688
H -6.942817 1.818930 -3.746455
C -7.583196 -1.846738 -2.910453
H -8.673608 -1.842977 -2.823100
H -7.309308 -2.049433 -3.951239
H -7.189779 -2.641288 -2.272076
C -7.307389 1.412744 3.545726
H -7.095818 1.009872 4.541819
H -6.687245 2.298606 3.389644
H -8.358830 1.712609 3.502908
C -7.824966 -1.316302 3.010283
H -7.502843 -2.232839 2.510990
H -7.598513 -1.385763 4.079302
H -8.906242 -1.214276 2.879465
Cl -9.620702 0.721868 -0.153256
H -7.363720 -1.282981 0.040505
H -9.262848 -1.693288 -0.018518
O -9.844275 -2.494124 -0.003520
C -9.137225 -3.615809 0.113831
H -8.049202 -3.460086 0.173035
O -9.659019 -4.713754 0.151146

Energy and thermal parameters

HF=-2299.8687361
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 1192657.1 (Joules/Mol)
Zero-point correction= 0.454259 (Hartree/Particle)
Thermal correction to Energy= 0.484120
Thermal correction to Enthalpy= 0.485064
Thermal correction to Gibbs Free Energy= 0.395206
Sum of electronic and zero-point Energies= -2299.414477
Sum of electronic and thermal Energies= -2299.384616
Sum of electronic and thermal Enthalpies= -2299.383672
Sum of electronic and thermal Free Energies= -2299.473530

Compound $5m_P^+$



Cartesian coordinates

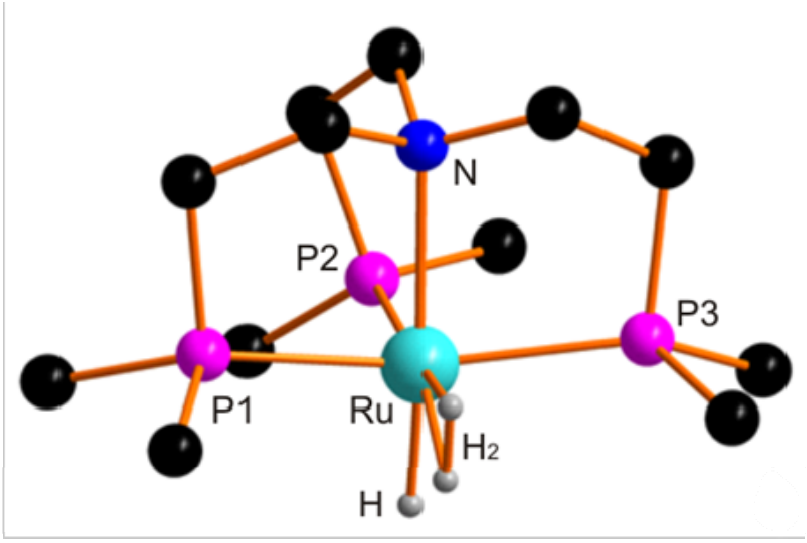
Ru -6.792646 -0.003264 -0.231667
P -6.797453 2.390386 -0.081019
N -4.560757 0.224489 -0.130085
C -5.077222 2.659612 0.577376
C -4.107964 1.675573 -0.085044
P -6.439480 -0.291146 -2.529620
P -6.619480 -0.436906 2.079958
C -4.035987 -0.530050 1.069620
C -4.786086 -0.244436 2.368481
C -3.926973 -0.416757 -1.347397
C -4.598949 -0.034339 -2.667214
H -2.966088 -0.311385 1.186039
H -4.132656 -1.591351 0.833207
H -4.594159 0.768340 2.733404
H -4.435193 -0.932046 3.146020
H -4.417216 1.013183 -2.928224
H -4.171989 -0.637604 -3.476285
H -2.859337 -0.159394 -1.368827
H -4.002249 -1.496399 -1.208060
H -3.128388 1.714228 0.406564
H -3.950857 1.994357 -1.116888
H -5.107007 2.537819 1.662997
H -4.730376 3.681118 0.381546
C -7.891326 3.342582 1.064268
H -7.527583 4.367719 1.187391
H -8.897925 3.375271 0.636258
H -7.952821 2.861094 2.040250
C -6.855342 3.524686 -1.547581
H -7.812975 3.411679 -2.063289
H -6.748510 4.564614 -1.222221
H -6.051500 3.299965 -2.252129
C -7.136135 0.715555 -3.915075

H -6.687809 0.419799 -4.869227
H -8.216386 0.549718 -3.966811
H -6.959057 1.779079 -3.749966
C -6.703542 -1.996267 -3.190393
H -7.768108 -2.242839 -3.136788
H -6.370463 -2.068061 -4.230719
H -6.155333 -2.715291 -2.577545
C -7.361196 0.496771 3.496317
H -7.046948 0.055975 4.447897
H -7.049270 1.543126 3.478862
H -8.452345 0.456112 3.431555
C -6.986449 -2.172244 2.596380
H -6.423226 -2.866684 1.969249
H -6.731530 -2.333955 3.648584
H -8.052864 -2.370396 2.452612
H -8.290742 -0.727762 -0.314933
H -8.460583 0.176671 -0.295738
H -6.488520 -1.604643 -0.265390

Energy and thermal parameters

HF=-1650.8989196
Zero-point vibrational energy 1144796.7 (Joules/Mol)
Zero-point correction= 0.436030 (Hartree/Particle)
Thermal correction to Energy= 0.460515
Thermal correction to Enthalpy= 0.461459
Thermal correction to Gibbs Free Energy= 0.386086
Sum of electronic and zero-point Energies= -1650.462890
Sum of electronic and thermal Energies= -1650.438405
Sum of electronic and thermal Enthalpies= -1650.437461
Sum of electronic and thermal Free Energies= -1650.512834

Compound $5m_N^+$



Cartesian coordinates

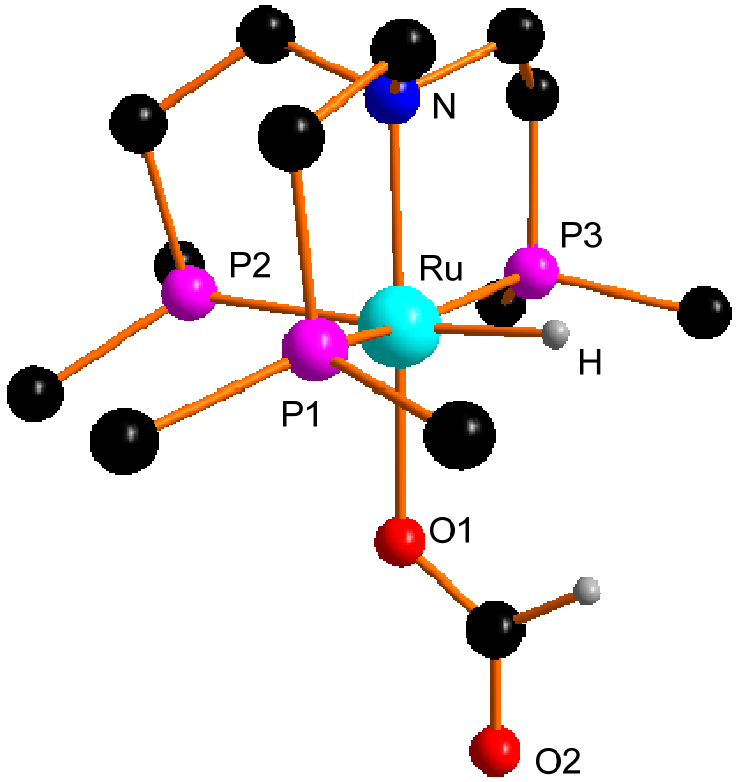
Ru -6.820613 -0.042675 -0.231574
P -6.780520 2.285979 -0.087814
N -4.496310 0.203007 -0.126575
C -5.085323 2.614852 0.601562
C -4.070884 1.654754 -0.036341
P -6.430559 -0.250878 -2.542798
P -6.593841 -0.409596 2.095808
C -3.993549 -0.569083 1.059302
C -4.745494 -0.266018 2.357566
C -3.890375 -0.390434 -1.370732
C -4.591137 0.050785 -2.661922
H -2.919455 -0.375121 1.194527
H -4.105046 -1.628809 0.817868
H -4.522646 0.740971 2.721370
H -4.412759 -0.959715 3.137706
H -4.433694 1.116268 -2.860602
H -4.157952 -0.491156 -3.510379
H -2.821269 -0.137484 -1.416687
H -3.962448 -1.476324 -1.274679
H -3.114650 1.706530 0.499435
H -3.873891 1.998629 -1.053016
H -5.131107 2.500773 1.687345
H -4.771801 3.646758 0.405371
C -7.956838 3.191552 1.004403
H -7.644997 4.233464 1.125700
H -8.945459 3.169606 0.536837
H -8.032683 2.719168 1.983163
C -6.837964 3.379023 -1.578875
H -7.791001 3.247097 -2.097609
H -6.742304 4.426038 -1.274603
H -6.025390 3.143570 -2.269843
C -7.137181 0.705741 -3.956928
H -6.664308 0.398262 -4.895133
H -8.210278 0.502613 -4.017790

H -6.996204 1.778249 -3.822364
C -6.617811 -1.975203 -3.189728
H -7.675059 -2.255207 -3.174607
H -6.243941 -2.044287 -4.215923
H -6.067222 -2.677453 -2.558752
C -7.283108 0.538609 3.526961
H -6.940410 0.098023 4.468564
H -6.964115 1.582602 3.497691
H -8.375757 0.503341 3.496504
C -6.976927 -2.139973 2.626191
H -6.442703 -2.853320 1.993823
H -6.690455 -2.300283 3.670122
H -8.050363 -2.320364 2.518319
H -7.493677 -1.587881 -0.318536
H -6.613894 -1.756316 -0.270667
H -8.425325 0.066520 -0.277463

Energy and thermal parameters

HF=-1650.8944813
Zero-point vibrational energy 1146436.9 (Joules/Mol)
Zero-point correction= 0.436655 (Hartree/Particle)
Thermal correction to Energy= 0.460846
Thermal correction to Enthalpy= 0.461790
Thermal correction to Gibbs Free Energy= 0.387437
Sum of electronic and zero-point Energies= -1650.457827
Sum of electronic and thermal Energies= -1650.433635
Sum of electronic and thermal Enthalpies= -1650.432691
Sum of electronic and thermal Free Energies= -1650.507045

Compound 9m$_P$



Cartesian coordinates

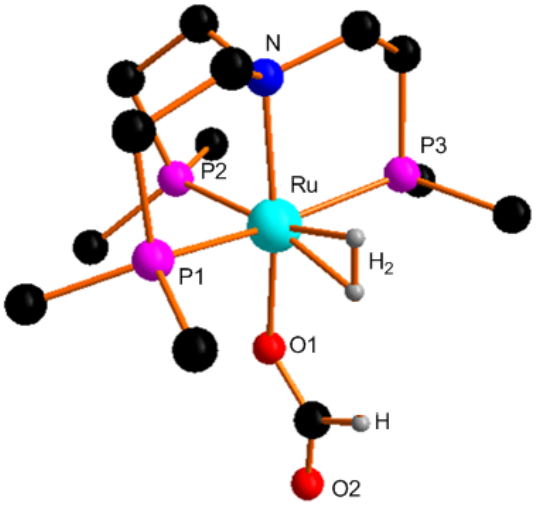
Ru -6.739401 -0.063804 -0.245127
P -6.833114 2.312723 -0.094249
N -4.528057 0.226688 -0.132998
C -5.117031 2.650386 0.560273
C -4.118522 1.690535 -0.095709
P -6.369844 -0.345972 -2.526367
P -6.564191 -0.497736 2.051046
C -3.976862 -0.500086 1.069435
C -4.740990 -0.237210 2.364996
C -3.864478 -0.398720 -1.340423
C -4.534904 -0.041302 -2.668535
H -2.913905 -0.244486 1.185918
H -4.037542 -1.565584 0.839310
H -4.587404 0.784003 2.725579
H -4.369022 -0.909520 3.146720
H -4.380650 1.010032 -2.933363
H -4.085411 -0.637858 -3.470954
H -2.802123 -0.114666 -1.352357
H -3.915500 -1.479821 -1.199238
H -3.137053 1.762909 0.390867
H -3.976527 2.008905 -1.130237
H -5.138744 2.536523 1.647305
H -4.800129 3.680239 0.353913
C -7.927354 3.278003 1.053846

H -7.592597 4.317190 1.144305
H -8.945726 3.271200 0.652210
H -7.953300 2.821067 2.044174
C -6.904927 3.470941 -1.552157
H -7.869091 3.365583 -2.058631
H -6.787822 4.510919 -1.228056
H -6.112871 3.240418 -2.269162
C -7.073385 0.636566 -3.934808
H -6.599961 0.359883 -4.883204
H -8.146692 0.433984 -4.006133
H -6.938752 1.705899 -3.763994
C -6.572312 -2.052566 -3.219124
H -7.626329 -2.341263 -3.163007
H -6.243512 -2.099044 -4.262926
H -5.995027 -2.759242 -2.618333
C -7.341416 0.401017 3.479970
H -7.011151 -0.023206 4.434264
H -7.076212 1.460553 3.459211
H -8.430493 0.316474 3.414496
C -6.849105 -2.243682 2.601177
H -6.246216 -2.918485 1.989292
H -6.596193 -2.376411 3.658583
H -7.902408 -2.500238 2.452191
H -6.492417 -1.688987 -0.290859
O -8.896772 -0.288137 -0.359376
C -9.517786 -1.406308 -0.390249
H -8.875620 -2.310848 -0.356447
O -10.757446 -1.547557 -0.453560

Energy and thermal parameters

HF=-1839.0310429
Zero-point vibrational energy 1157154.9 (Joules/Mol)
Zero-point correction= 0.440737 (Hartree/Particle)
Thermal correction to Energy= 0.468960
Thermal correction to Enthalpy= 0.469904
Thermal correction to Gibbs Free Energy= 0.384640
Sum of electronic and zero-point Energies= -1838.590306
Sum of electronic and thermal Energies= -1838.562083
Sum of electronic and thermal Enthalpies= -1838.561139
Sum of electronic and thermal Free Energies= -1838.646403

Compound 10m$_P$



Cartesian coordinates

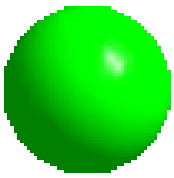
Ru -6.730935 -0.117030 -0.236378
P -6.815657 2.212559 -0.090768
N -4.518102 0.183918 -0.133925
C -5.145651 2.584358 0.618042
C -4.117238 1.652753 -0.032765
P -6.365775 -0.298251 -2.576644
P -6.524366 -0.449210 2.131874
C -3.962449 -0.579748 1.045881
C -4.679704 -0.284782 2.363514
C -3.859085 -0.378205 -1.377387
C -4.541006 0.052172 -2.680240
H -2.890460 -0.362791 1.137070
H -4.060162 -1.641822 0.807930
H -4.455809 0.722240 2.725948
H -4.323152 -0.979893 3.130965
H -4.405036 1.120687 -2.875219
H -4.081541 -0.480309 -3.519939
H -2.801791 -0.083388 -1.382667
H -3.890165 -1.466681 -1.291023
H -3.159580 1.708489 0.496277
H -3.932340 2.004876 -1.048074
H -5.190623 2.460150 1.702006
H -4.855314 3.623572 0.428686
C -8.077714 3.009921 0.979076
H -7.888869 4.085327 1.045067
H -9.058849 2.842847 0.526795
H -8.085130 2.581262 1.980041
C -6.908121 3.294299 -1.582669
H -7.848158 3.116778 -2.110862
H -6.870659 4.342774 -1.271777
H -6.075153 3.105064 -2.262936
C -7.132740 0.655019 -3.955603

H -6.703523 0.335266 -4.910133
H -8.208461 0.457917 -3.965845
H -6.977159 1.726944 -3.836818
C -6.525941 -2.023108 -3.222039
H -7.575620 -2.327955 -3.184254
H -6.176489 -2.074597 -4.257555
H -5.943024 -2.718101 -2.612813
C -7.233071 0.510986 3.540424
H -6.908010 0.068264 4.486992
H -6.903998 1.551770 3.514536
H -8.325030 0.481874 3.492248
C -6.899978 -2.179518 2.657352
H -6.342091 -2.891431 2.044282
H -6.637079 -2.328752 3.708759
H -7.968533 -2.371809 2.525151
H -6.241862 -1.818305 -0.256619
O -8.859353 -0.058865 -0.325731
C -9.657457 -1.065871 -0.426380
H -9.171785 -2.066342 -0.456933
O -10.891697 -0.993768 -0.489361
H -7.069208 -1.853255 -0.304999

Energy and thermal parameters

HF=-1839.4842974
Zero-point vibrational energy 1190174.4 (Joules/Mol)
Zero-point correction= 0.453314 (Hartree/Particle)
Thermal correction to Energy= 0.481273
Thermal correction to Enthalpy= 0.482217
Thermal correction to Gibbs Free Energy= 0.398681
Sum of electronic and zero-point Energies= -1839.030984
Sum of electronic and thermal Energies= -1839.003025
Sum of electronic and thermal Enthalpies= -1839.002081
Sum of electronic and thermal Free Energies= -1839.085616

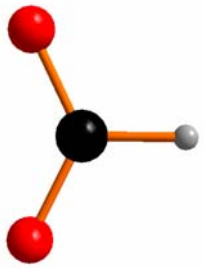
Cl^-



Cartesian coordinates
Cl 0.000000 0.000000 0.000000

Energy and thermal parameters
HF=-460.3702521
Zero-point vibrational energy 0.0 (Joules/Mol)
Zero-point correction= 0.000000 (Hartree/Particle)
Thermal correction to Energy= 0.001416
Thermal correction to Enthalpy= 0.002360
Thermal correction to Gibbs Free Energy= -0.015023
Sum of electronic and zero-point Energies= -460.370252
Sum of electronic and thermal Energies= -460.368836
Sum of electronic and thermal Enthalpies= -460.367892
Sum of electronic and thermal Free Energies= -460.385275

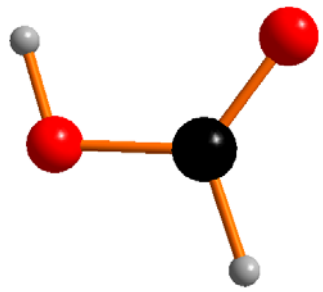
$HCOO^-$



Cartesian coordinates
C -0.905736 0.820893 0.000000
H -2.027366 0.816472 -0.000000
O -0.360046 1.958412 -0.000000
O -0.351551 -0.312877 -0.000000

Energy and thermal parameters
HF=-189.3118481
Zero-point vibrational energy 53399.7 (Joules/Mol)
Zero-point correction= 0.020339 (Hartree/Particle)
Thermal correction to Energy= 0.023321
Thermal correction to Enthalpy= 0.024266
Thermal correction to Gibbs Free Energy= -0.003489
Sum of electronic and zero-point Energies= -189.291509
Sum of electronic and thermal Energies= -189.288527
Sum of electronic and thermal Enthalpies= -189.287583
Sum of electronic and thermal Free Energies= -189.315337

HCOOH



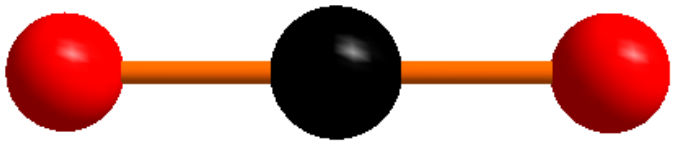
Cartesian coordinates

H -7.784398 -2.733725 -0.392363
O -8.393782 -3.486642 -0.505006
C -7.734156 -4.624697 -0.245867
H -8.400532 -5.487686 -0.366046
O -6.566632 -4.693150 0.075782

Energy and thermal parameters

HF=-189.7797631
Zero-point vibrational energy 88462.2 (Joules/Mol)
Zero-point correction= 0.033693 (Hartree/Particle)
Thermal correction to Energy= 0.036873
Thermal correction to Enthalpy= 0.037817
Thermal correction to Gibbs Free Energy= 0.009598
Sum of electronic and zero-point Energies= -189.746070
Sum of electronic and thermal Energies= -189.742890
Sum of electronic and thermal Enthalpies= -189.741946
Sum of electronic and thermal Free Energies= -189.770165

CO_2



Cartesian coordinates

C -0.539198 0.822142 0.000000
O -0.543422 1.991717 0.000000
O -0.534713 -0.347431 0.000000

Energy and thermal parameters

HF=-188.5900297
Zero-point vibrational energy 26293.7 (Joules/Mol)
Zero-point correction= 0.010015 (Hartree/Particle)
Thermal correction to Energy= 0.012990
Thermal correction to Enthalpy= 0.013935
Thermal correction to Gibbs Free Energy= -0.004963
Sum of electronic and zero-point Energies= -188.580015
Sum of electronic and thermal Energies= -188.577039
Sum of electronic and thermal Enthalpies= -188.576095

Sum of electronic and thermal Free Energies= -188.594993

H_2

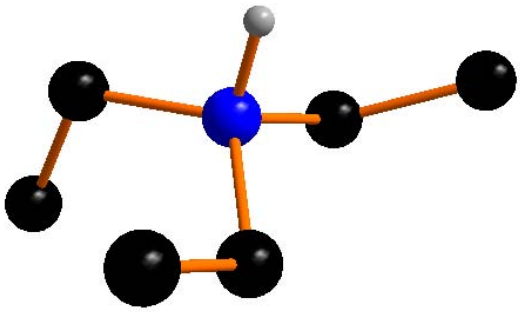
Cartesian coordinates

H 0.000000 0.000000 -0.021564
H 0.000000 0.000000 0.721564

Energy and thermal parameters

HF=-1.1786618
Zero-point vibrational energy 26671.9 (Joules/Mol)
Zero-point correction= 0.010159 (Hartree/Particle)
Thermal correction to Energy= 0.012519
Thermal correction to Enthalpy= 0.013463
Thermal correction to Gibbs Free Energy= -0.001329
Sum of electronic and zero-point Energies= -1.168503
Sum of electronic and thermal Energies= -1.166143
Sum of electronic and thermal Enthalpies= -1.165198
Sum of electronic and thermal Free Energies= -1.179991

NEt_3H^+



Cartesian coordinates

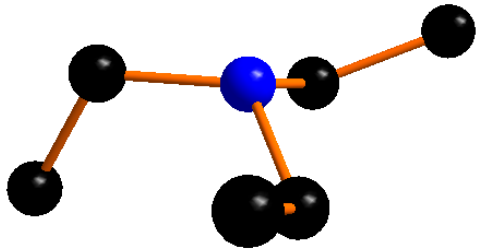
N -2.062945 -0.206565 -0.107235
H -1.700784 0.253928 0.733843
C -3.575306 -0.250064 0.078776
C -4.329245 -0.900191 -1.072579
H -3.879704 0.789844 0.213608
H -3.754283 -0.774095 1.018043
H -5.396753 -0.840025 -0.842735
H -4.168133 -0.384198 -2.022382
H -4.081345 -1.957477 -1.195252
C -1.651948 0.666655 -1.284843
C -0.237662 1.215719 -1.143697
H -2.374337 1.483825 -1.326640
H -1.764136 0.058131 -2.183259
H -0.044235 1.876782 -1.993035

H -0.126451 1.808880 -0.230061
H 0.526231 0.434491 -1.155476
C -1.407557 -1.576007 -0.160647
C -1.588574 -2.378289 1.121323
H -0.349205 -1.394769 -0.348455
H -1.822573 -2.087981 -1.029657
H -0.981426 -3.284214 1.042125
H -1.240169 -1.821578 1.997575
H -2.623059 -2.688405 1.286061

Energy and thermal parameters

HF=-292.8967836
Zero-point vibrational energy 582630.7 (Joules/Mol)
Zero-point correction= 0.221912 (Hartree/Particle)
Thermal correction to Energy= 0.231265
Thermal correction to Enthalpy= 0.232210
Thermal correction to Gibbs Free Energy= 0.188200
Sum of electronic and zero-point Energies= -292.674871
Sum of electronic and thermal Energies= -292.665518
Sum of electronic and thermal Enthalpies= -292.664574
Sum of electronic and thermal Free Energies= -292.708584

NEt_3



Cartesian coordinates

N -2.052253 -0.216099 -0.143735
C -3.512826 -0.240573 0.046602
C -4.358914 -0.894111 -1.062511
H -3.834270 0.800219 0.173643
H -3.722336 -0.740589 0.998185
H -5.421600 -0.816864 -0.805686
H -4.213803 -0.400535 -2.029583
H -4.126505 -1.957058 -1.186609
C -1.641485 0.629632 -1.275218
C -0.231886 1.209894 -1.119520
H -2.352254 1.461298 -1.339901
H -1.709008 0.086556 -2.236641
H 0.000339 1.860457 -1.970523
H -0.158313 1.803327 -0.201813
H 0.537337 0.431692 -1.083562
C -1.428428 -1.546066 -0.193016
C -1.568352 -2.346797 1.104128
H -0.362516 -1.397644 -0.390103

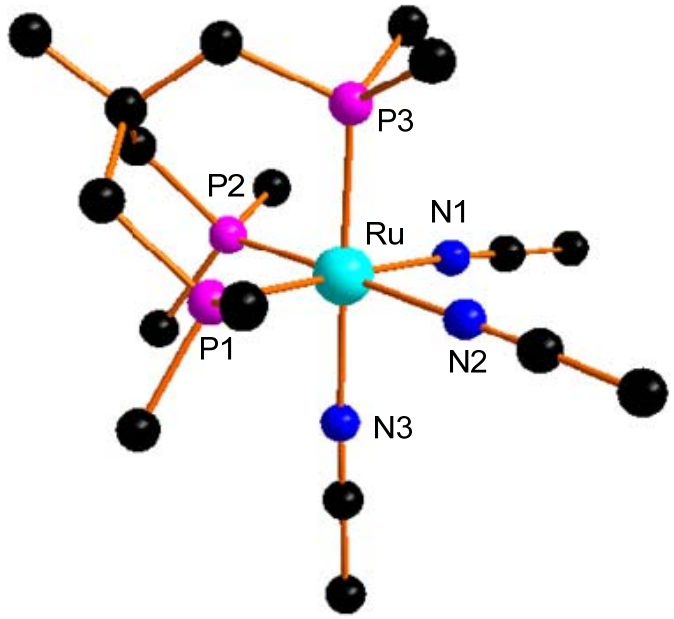
H -1.814709 -2.145317 -1.039346
H -0.980060 -3.268236 1.033646
H -1.199194 -1.769480 1.959048
H -2.604061 -2.635706 1.309313

Energy and thermal parameters

HF=-292.4409113
Zero-point vibrational energy 539020.1 (Joules/Mol)
Zero-point correction= 0.205302 (Hartree/Particle)
Thermal correction to Energy= 0.214710
Thermal correction to Enthalpy= 0.215655
Thermal correction to Gibbs Free Energy= 0.171341
Sum of electronic and zero-point Energies= -292.235609
Sum of electronic and thermal Energies= -292.226201
Sum of electronic and thermal Enthalpies= -292.225257
Sum of electronic and thermal Free Energies= -292.269570

Reactivity of [Ru(κ^3-triphos)$(MeCN)_3]^{2+}$ in acetone solution

Compound $2m^{2+}$



Cartesian coordinates

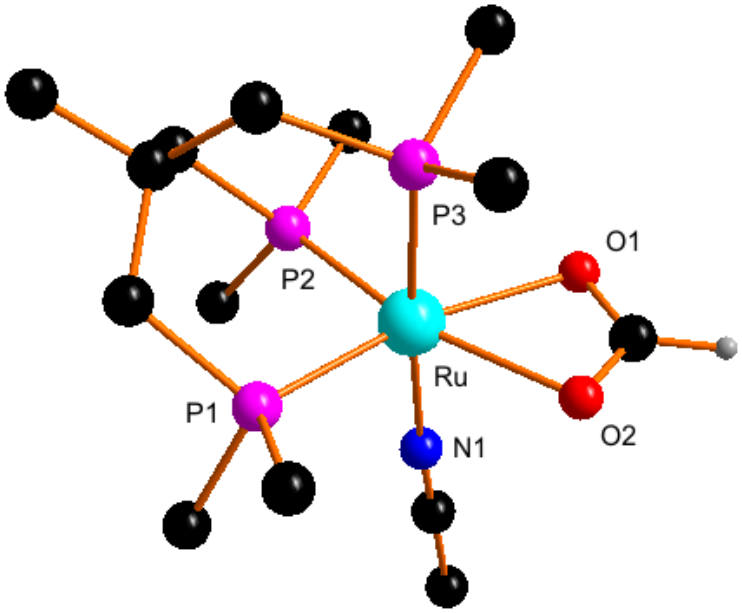
Ru 0.554110 -0.163102 -0.086627
P 0.659589 -0.282390 2.246059
P 0.612288 -2.498037 -0.158064
P 2.887875 -0.150732 -0.137957
C 1.794042 -3.257688 1.070331
C 3.667790 -1.490980 0.904406
C 1.998940 -1.423823 2.873618
C 2.754888 -2.318767 1.852385
H 2.731107 -0.801974 3.401281
H 1.539725 -2.068089 3.631923
H 4.454137 -1.014954 1.500692
H 4.174432 -2.179965 0.219424
H 2.390521 -3.997950 0.525464
H 1.190459 -3.818115 1.793276
N 0.412285 -0.015779 -2.193375
N -1.565197 -0.136086 -0.071507
N 0.452339 1.952410 -0.056460
C 0.264616 0.126061 -3.332225
C -2.720086 -0.071517 -0.101527
C 0.332267 3.103009 -0.080596
C 0.184648 4.551295 -0.100022
H -0.648499 4.845939 0.543803
H 1.102428 5.021780 0.262958
H -0.013324 4.889960 -1.120425
C -4.173841 0.000586 -0.129347
H -4.538029 0.472351 0.787324
H -4.499473 0.590227 -0.990375
H -4.592070 -1.006829 -0.204816
C 0.081559 0.301096 -4.765854

H -0.908260 0.721652 -4.962692
H 0.844096 0.980461 -5.156105
H 0.168143 -0.664670 -5.271138
C 3.669320 -0.362832 -1.795661
H 3.397717 0.487143 -2.426930
H 4.757675 -0.394913 -1.689795
H 3.331191 -1.277605 -2.283821
C 3.740554 1.391932 0.412336
H 4.818987 1.280508 0.264428
H 3.384411 2.234980 -0.184418
H 3.554602 1.605645 1.465739
C 0.976090 1.295848 3.146988
H 0.139518 1.978448 2.978184
H 1.061757 1.096085 4.219275
H 1.891885 1.776674 2.801262
C -0.859144 -0.850189 3.128381
H -0.680199 -0.829736 4.207543
H -1.687111 -0.177853 2.891156
H -1.139289 -1.864372 2.839996
C 1.081486 -3.274853 -1.765626
H 1.025232 -4.363616 -1.673095
H 0.385476 -2.946706 -2.541246
H 2.094372 -3.001820 -2.065765
C -0.977620 -3.376101 0.165290
H -1.701609 -3.104067 -0.606908
H -0.813819 -4.457547 0.136253
H -1.389778 -3.106811 1.138365
C 3.693851 -3.234756 2.676309
H 4.372808 -2.639835 3.296460
H 3.117843 -3.891099 3.337326
H 4.300789 -3.864631 2.017143

Energy and thermal parameters

HF=-1952.6670911
Zero-point vibrational energy 1333138.3 (Joules/Mol)
Zero-point correction= 0.507766 (Hartree/Particle)
Thermal correction to Energy= 0.543741
Thermal correction to Enthalpy= 0.544685
Thermal correction to Gibbs Free Energy= 0.440596
Sum of electronic and zero-point Energies= -1952.159326
Sum of electronic and thermal Energies= -1952.123350
Sum of electronic and thermal Enthalpies= -1952.122406
Sum of electronic and thermal Free Energies= -1952.226495

Compound 7m^{+}



Cartesian coordinates

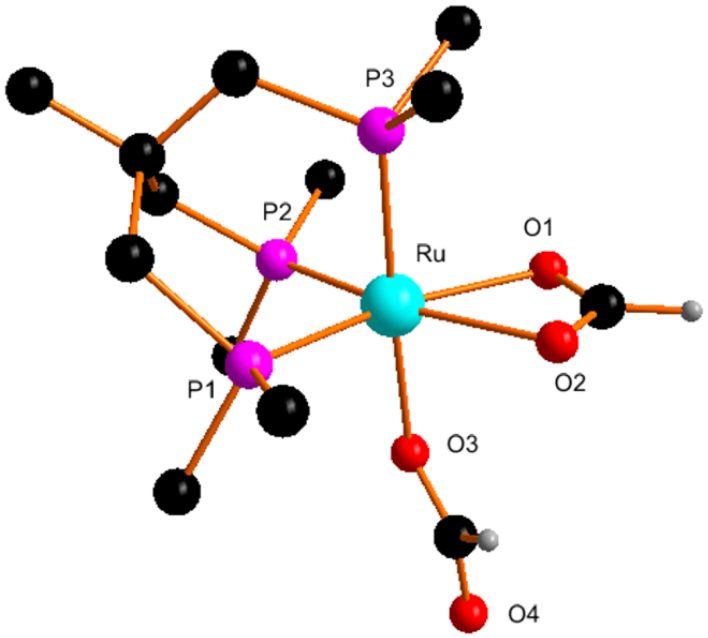
Ru 0.700900 -0.078068 0.099071
P 0.820786 -0.388974 2.362434
P 0.643884 -2.382206 -0.181712
P 2.983879 -0.157324 0.025072
C 1.791041 -3.316001 0.960849
C 3.737186 -1.619147 0.917425
C 2.094195 -1.649470 2.905170
C 2.802436 -2.490379 1.805289
H 2.858044 -1.110225 3.477324
H 1.601367 -2.328831 3.610308
H 4.550935 -1.230185 1.539927
H 4.205464 -2.262350 0.163605
H 2.344430 -4.035240 0.346121
H 1.166655 -3.906061 1.641418
O -1.500691 0.087503 -0.437529
O 0.010678 0.248041 -2.041500
C -1.196817 0.281733 -1.653661
H -1.994693 0.480142 -2.385588
N 0.637113 2.016902 0.252613
C 0.537307 3.170436 0.273759
C 0.417442 4.621158 0.307314
H 0.353646 5.011262 -0.712025
H -0.483928 4.905990 0.856764
H 1.290891 5.053939 0.802671
C 1.058365 -3.027197 -1.863398
H 0.858197 -4.102189 -1.903493
H 0.437796 -2.514442 -2.602142
H 2.107595 -2.858882 -2.111684
C -0.994480 -3.197072 0.070041

H -1.692667 -2.832282 -0.687183
H -0.888895 -4.281740 -0.029366
H -1.405280 -2.965155 1.053184
C -0.745332 -0.945534 3.171876
H -1.022299 -1.953972 2.861154
H -0.620795 -0.937512 4.259147
H -1.552266 -0.260234 2.898130
C 1.202906 1.087277 3.404304
H 0.399855 1.820380 3.291314
H 1.271542 0.792130 4.455699
H 2.141762 1.553631 3.102123
C 3.678229 -0.248497 -1.683478
H 4.768947 -0.329286 -1.643697
H 3.274874 -1.101775 -2.229851
H 3.406120 0.664701 -2.220210
C 3.937290 1.285758 0.673741
H 5.003776 1.139750 0.476725
H 3.602239 2.195624 0.169640
H 3.794129 1.408063 1.748211
C 3.708754 -3.510885 2.537393
H 3.111847 -4.191884 3.153895
H 4.276948 -4.113169 1.819897
H 4.423191 -2.999453 3.191607

Energy and thermal parameters

HF=-1876.4462627
Zero-point vibrational energy 1145740.9 (Joules/Mol)
Zero-point correction= 0.436390 (Hartree/Particle)
Thermal correction to Energy= 0.466324
Thermal correction to Enthalpy= 0.467269
Thermal correction to Gibbs Free Energy= 0.379009
Sum of electronic and zero-point Energies= -1876.009873
Sum of electronic and thermal Energies= -1875.979938
Sum of electronic and thermal Enthalpies= -1875.978994
Sum of electronic and thermal Free Energies= -1876.067254

Compound 8m



Cartesian coordinates

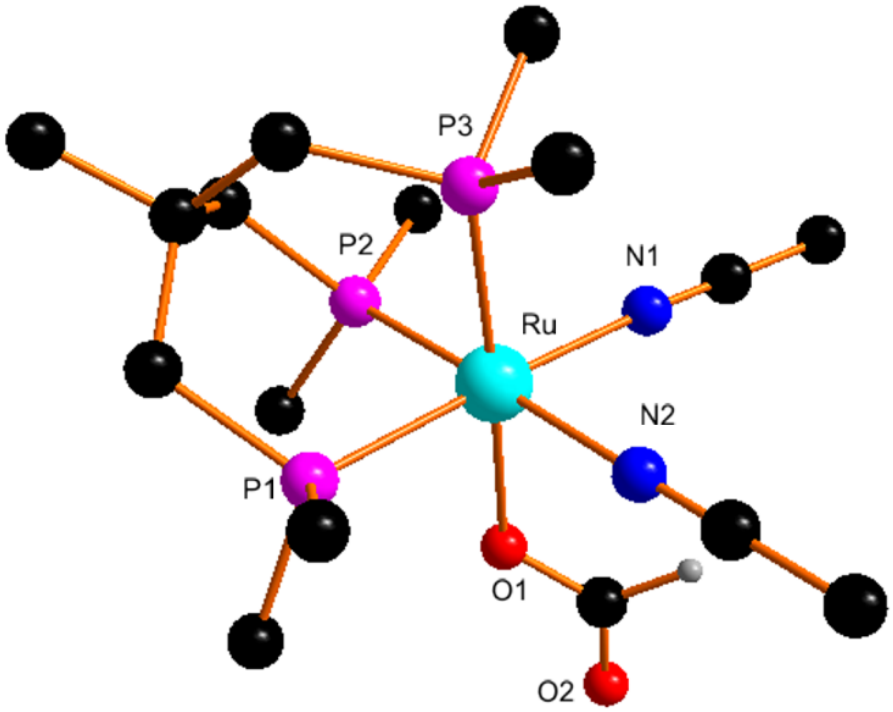
Ru 0.598583 -0.237530 -0.224732
P 0.716249 -0.170955 2.045843
P 0.601262 -2.534707 -0.139348
P 2.873352 -0.247914 -0.286254
C 1.942215 -3.253645 0.948878
C 3.684246 -1.349330 0.989700
C 1.846632 -1.455788 2.800493
C 2.758508 -2.270776 1.836873
H 2.480480 -0.943973 3.533955
H 1.223006 -2.156680 3.367758
H 4.248574 -0.701368 1.670550
H 4.423167 -1.971810 0.471826
H 2.638389 -3.797429 0.299602
H 1.474080 -4.005279 1.595243
O -1.602232 -0.188332 -0.789325
O -0.084787 -0.226413 -2.397338
C -1.292709 -0.160619 -2.019729
H -2.091984 -0.079856 -2.773576
O 0.603003 1.933317 -0.440732
C -0.397456 2.707264 -0.229935
H -1.316195 2.223802 0.158039
O -0.408778 3.939580 -0.425239
C 3.685426 -3.135824 2.725066
H 3.099639 -3.783472 3.386624
H 4.330763 -3.773511 2.110962
H 4.327723 -2.505290 3.349604
C 0.819001 -3.437562 -1.740171
H 0.880921 -4.515759 -1.561956
H -0.039906 -3.230041 -2.383569
H 1.721006 -3.106823 -2.257067

C -0.934878 -3.371694 0.469484
H -1.788663 -3.031460 -0.122035
H -0.833275 -4.456658 0.365616
H -1.125703 -3.139874 1.518775
C -0.895330 -0.416817 2.918826
H -0.748510 -0.416536 4.003569
H -1.566728 0.403510 2.649782
H -1.363810 -1.355481 2.620464
C 1.263557 1.402327 2.851729
H 0.622428 2.221975 2.519435
H 1.189064 1.306242 3.939539
H 2.295070 1.644169 2.590461
C 3.740506 1.370152 -0.089057
H 4.823763 1.223323 -0.139902
H 3.423714 2.036885 -0.894312
H 3.484022 1.839118 0.861525
C 3.609078 -0.802413 -1.891337
H 3.171352 -0.214782 -2.703227
H 4.693002 -0.649502 -1.881408
H 3.407762 -1.858361 -2.079069

Energy and thermal parameters

HF=-1933.000544
Zero-point vibrational energy 1078574.6 (Joules/Mol)
Zero-point correction= 0.410807 (Hartree/Particle)
Thermal correction to Energy= 0.440396
Thermal correction to Enthalpy= 0.441340
Thermal correction to Gibbs Free Energy= 0.354038
Sum of electronic and zero-point Energies= -1932.589737
Sum of electronic and thermal Energies= -1932.560148
Sum of electronic and thermal Enthalpies= -1932.559204
Sum of electronic and thermal Free Energies= -1932.646507

Compound 11m^{+}



Cartesian coordinates

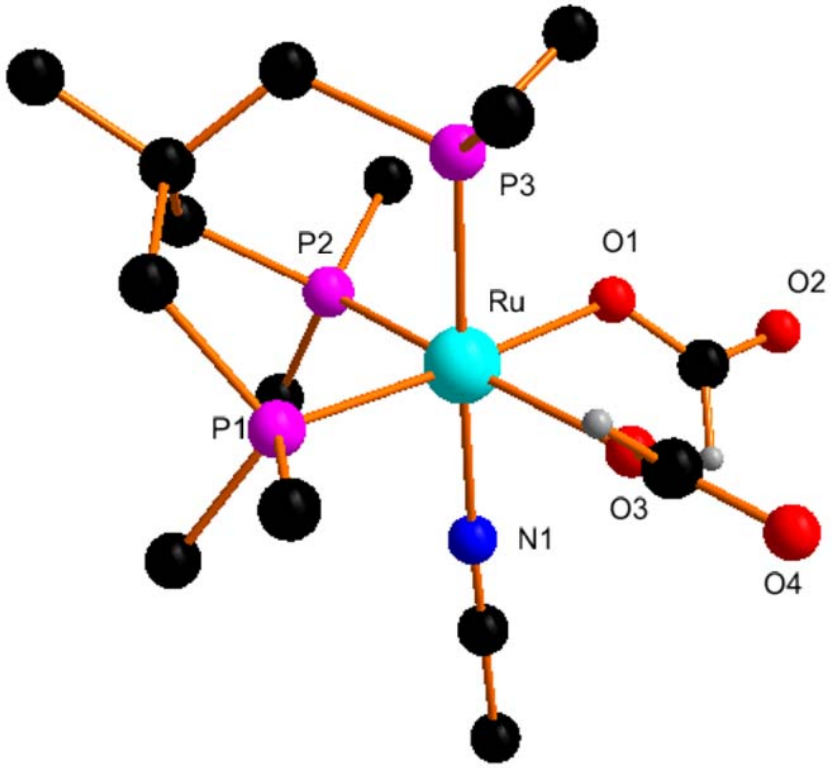
Ru 0.591168 -0.056158 -0.158037
P 0.591870 -0.340051 2.137559
P 0.676874 -2.372878 -0.394265
P 2.914532 -0.050645 -0.110514
C 1.675308 -3.209820 0.944125
C 3.634055 -1.548114 0.745360
C 2.010131 -1.395844 2.745464
C 2.704995 -2.334659 1.716157
H 2.762256 -0.723764 3.174959
H 1.629129 -1.998231 3.578376
H 4.521278 -1.209616 1.292764
H 3.998706 -2.233750 -0.028578
H 2.198192 -4.053329 0.478708
H 0.970822 -3.645660 1.661918
O 0.641797 0.090824 -2.347999
C -0.055947 0.921441 -3.032598
H -0.710895 1.602988 -2.454608
O -0.048889 1.013907 -4.275607
N 0.505923 2.047340 -0.025923
C 0.421780 3.201128 0.022807
C 0.318547 4.652099 0.089004
H 1.316606 5.097117 0.051206
H -0.270075 5.020854 -0.755394
H -0.169949 4.946693 1.021887
N -1.518595 -0.030129 -0.279771

C -2.670073 0.022879 -0.387781
C -4.118967 0.080336 -0.521895
H -4.421743 -0.379155 -1.466717
H -4.589593 -0.458232 0.305188
H -4.452391 1.121380 -0.507304
C 3.775931 -0.002556 -1.738489
H 3.582793 0.966758 -2.205250
H 4.853768 -0.127871 -1.598023
H 3.395211 -0.779270 -2.402226
C 3.740433 1.356866 0.754726
H 4.825991 1.267371 0.650480
H 3.414494 2.301135 0.312458
H 3.492011 1.364732 1.817777
C 1.421060 -3.002120 -1.960156
H 2.485396 -2.765919 -2.006397
H 1.299421 -4.087751 -2.019816
H 0.923019 -2.522994 -2.805424
C -0.919920 -3.295943 -0.381076
H -1.500197 -3.012559 -1.263295
H -0.728666 -4.372731 -0.411302
H -1.505713 -3.059432 0.508900
C -0.891883 -1.151147 2.882382
H -0.782105 -1.204441 3.969866
H -1.783181 -0.567182 2.639970
H -1.022961 -2.162653 2.494029
C 0.701537 1.169817 3.193430
H -0.202670 1.767860 3.049997
H 0.779918 0.888926 4.248180
H 1.563907 1.779661 2.918317
C 3.607210 -3.300143 2.521211
H 4.301849 -2.743491 3.159875
H 3.005150 -3.953117 3.162558
H 4.196839 -3.933560 1.849407

Energy and thermal parameters

HF=-2009.2279182
Zero-point vibrational energy 1266786.6 (Joules/Mol)
Zero-point correction= 0.482494 (Hartree/Particle)
Thermal correction to Energy= 0.517762
Thermal correction to Enthalpy= 0.518706
Thermal correction to Gibbs Free Energy= 0.417356
Sum of electronic and zero-point Energies= -2008.745425
Sum of electronic and thermal Energies= -2008.710156
Sum of electronic and thermal Enthalpies= -2008.709212
Sum of electronic and thermal Free Energies= -2008.810562

Compound 12m



Cartesian coordinates

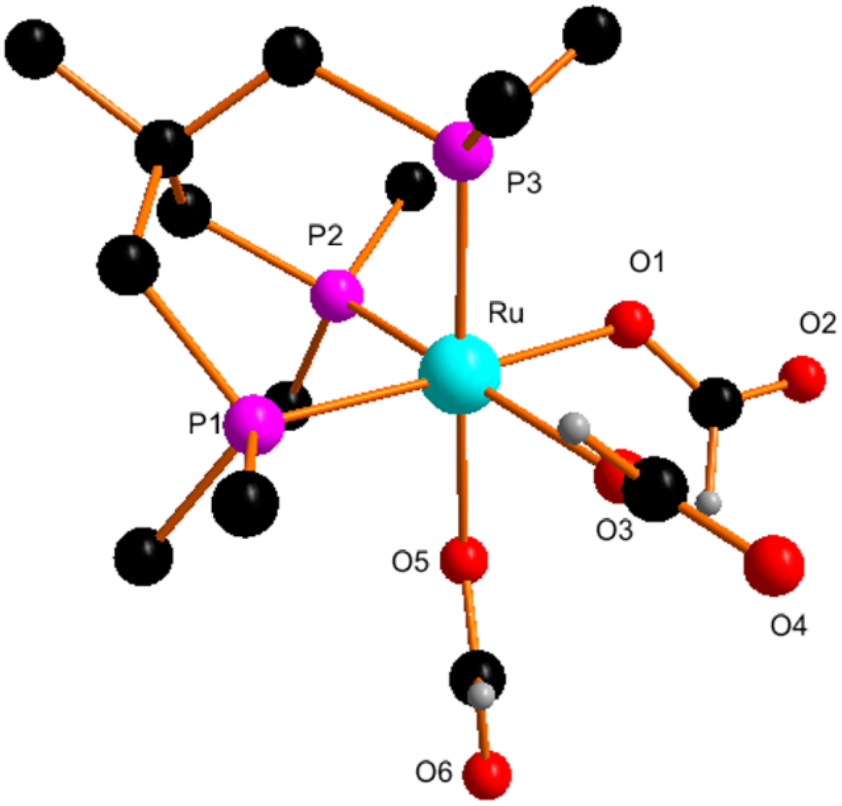
Ru 0.614692 -0.141582 -0.130318
P 0.626889 -0.453303 2.157541
P 0.772084 -2.445480 -0.400191
P 2.914483 -0.063084 -0.080665
C 2.214910 -3.189175 0.534932
C 3.687395 -1.180011 1.198335
C 1.715861 -1.878933 2.697660
C 2.815543 -2.362446 1.709898
H 2.187301 -1.586778 3.643441
H 1.058886 -2.724563 2.934434
H 3.981979 -0.560443 2.053618
H 4.617245 -1.574482 0.771870
H 3.008816 -3.399228 -0.191516
H 1.887426 -4.162926 0.916834
O -1.554999 0.016448 -0.473390
O 0.719754 0.071937 -2.314238
C -2.607786 -0.551924 -0.026360
C 0.008419 0.898957 -2.986553
H -2.459245 -1.348444 0.728070
H -0.698097 1.518313 -2.405137
O 0.057142 1.044040 -4.227194
O -3.778385 -0.284729 -0.369185
N 0.453661 1.950222 0.038752
C 0.321185 3.099308 0.092972
C 0.159641 4.545223 0.161937
H 1.139661 5.025921 0.227751

H -0.354889 4.904158 -0.733624
H -0.429641 4.812348 1.043399
C 3.703218 1.574332 0.254865
H 4.787377 1.458132 0.349374
H 3.489609 2.246464 -0.580864
H 3.308394 2.025739 1.166740
C 3.795973 -0.527343 -1.636195
H 3.391222 0.059953 -2.462698
H 4.867134 -0.331363 -1.527256
H 3.655451 -1.585313 -1.863203
C 1.005475 -3.062862 -2.122869
H 1.824288 -2.537773 -2.615336
H 1.202991 -4.139235 -2.115700
H 0.091268 -2.866722 -2.688937
C -0.643574 -3.512678 0.128419
H -1.529620 -3.262112 -0.459369
H -0.393811 -4.564971 -0.039806
H -0.874224 -3.371903 1.186354
C -0.945818 -0.814340 3.060525
H -0.740481 -0.931786 4.129127
H -1.644139 0.015059 2.920286
H -1.412403 -1.728551 2.690186
C 1.245567 0.952861 3.190492
H 0.630397 1.837050 3.005572
H 1.187070 0.691173 4.251422
H 2.281830 1.194587 2.947683
C 3.749935 -3.310548 2.498692
H 4.274826 -2.768475 3.293233
H 3.180124 -4.123997 2.961649
H 4.501693 -3.756123 1.837741

Energy and thermal parameters

HF=-2065.7770755
Zero-point vibrational energy 1202276.5 (Joules/Mol)
Zero-point correction= 0.457923 (Hartree/Particle)
Thermal correction to Energy= 0.492503
Thermal correction to Enthalpy= 0.493447
Thermal correction to Gibbs Free Energy= 0.393267
Sum of electronic and zero-point Energies= -2065.319153
Sum of electronic and thermal Energies= -2065.284573
Sum of electronic and thermal Enthalpies= -2065.283629
Sum of electronic and thermal Free Energies= -2065.383808

Compound 13m$^-$



Cartesian coordinates

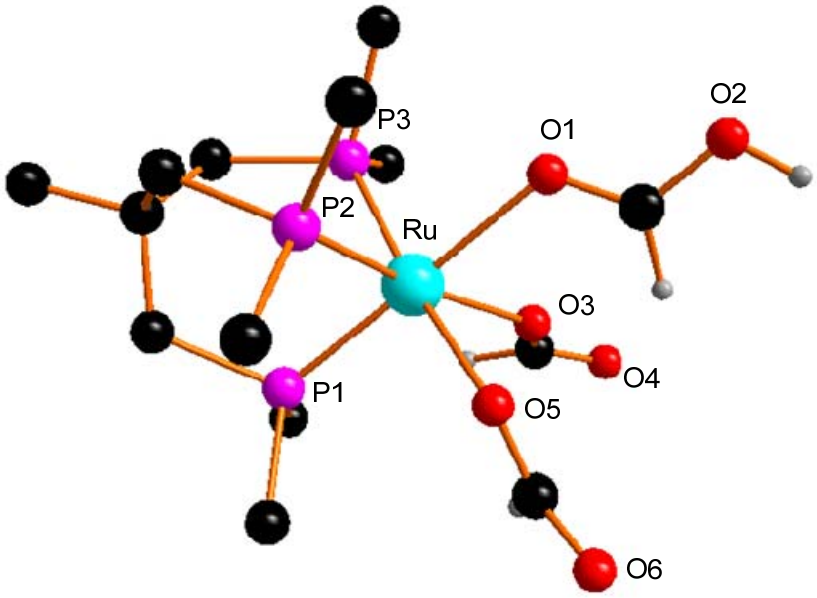
Ru 0.561459 -0.200993 -0.026354
P 0.568580 -0.621787 2.232603
P 0.836030 -2.445228 -0.417206
P 2.844302 -0.001018 0.055940
C 2.298964 -3.181421 0.501370
C 3.672457 -1.143687 1.279122
C 1.727316 -2.010550 2.723564
C 2.853939 -2.389835 1.721611
H 2.179209 -1.737014 3.684525
H 1.114708 -2.899633 2.915797
H 3.936389 -0.558099 2.167835
H 4.620322 -1.472884 0.836808
H 3.109440 -3.324022 -0.223332
H 2.006682 -4.184536 0.833498
O -1.606354 -0.087843 -0.369369
O 0.672856 0.193041 -2.191795
O 0.406116 1.979635 0.198741
C -0.574341 2.600758 0.734282
H -1.367821 1.968063 1.177864
O -0.701611 3.843814 0.791648
C -2.617483 -0.762877 0.017780
C -0.028553 1.087836 -2.778611
H -2.411239 -1.615945 0.693119

H -0.701591 1.678387 -2.133232
O -0.000332 1.332521 -4.007247
O -3.806794 -0.542548 -0.297598
C 3.532684 1.657600 0.489192
H 4.618337 1.596699 0.615082
H 3.300915 2.354791 -0.319749
H 3.076103 2.039071 1.403206
C 3.778026 -0.336834 -1.505574
H 3.347838 0.259975 -2.312395
H 4.833153 -0.078287 -1.371672
H 3.709517 -1.391064 -1.780674
C 1.136048 -2.965107 -2.166204
H 1.942802 -2.382357 -2.611981
H 1.380260 -4.031250 -2.211707
H 0.226980 -2.778418 -2.743973
C -0.518867 -3.636910 0.012534
H -1.416404 -3.398141 -0.563096
H -0.204429 -4.656685 -0.232469
H -0.764056 -3.594185 1.076190
C -0.988636 -1.111910 3.108369
H -0.785523 -1.267462 4.172681
H -1.733267 -0.318289 3.000949
H -1.400144 -2.032596 2.690059
C 1.109859 0.757399 3.348113
H 0.467391 1.627886 3.196910
H 1.043844 0.440383 4.393674
H 2.139950 1.049419 3.136320
C 3.827116 -3.332957 2.468986
H 4.321495 -2.808349 3.294512
H 3.293801 -4.194929 2.885740
H 4.603354 -3.709028 1.792915

Energy and thermal parameters

HF=-2122.3260329
Zero-point vibrational energy 1136466.5 (Joules/Mol)
Zero-point correction= 0.432857 (Hartree/Particle)
Thermal correction to Energy= 0.466836
Thermal correction to Enthalpy= 0.467780
Thermal correction to Gibbs Free Energy= 0.369941
Sum of electronic and zero-point Energies= -2121.893176
Sum of electronic and thermal Energies= -2121.859197
Sum of electronic and thermal Enthalpies= -2121.858253
Sum of electronic and thermal Free Energies= -2121.956092

Compound 14m



Cartesian coordinates

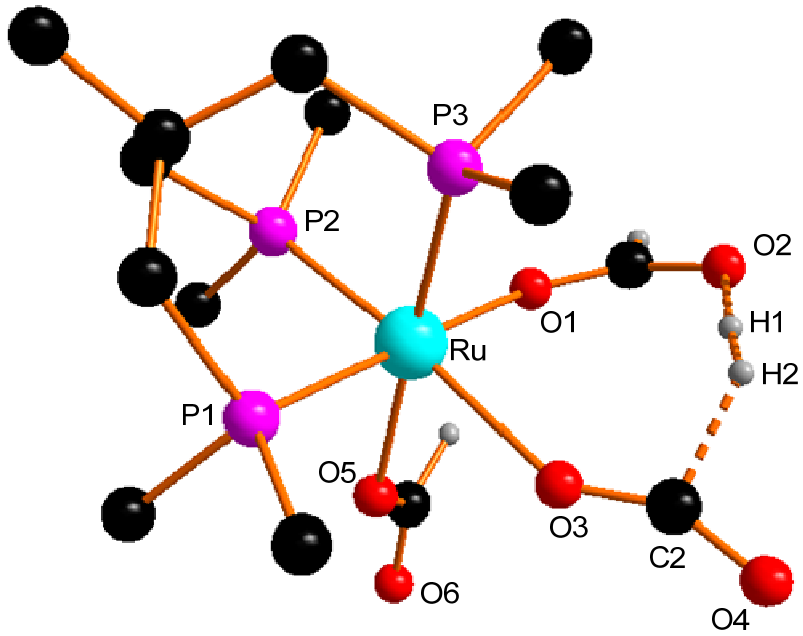
Ru 0.871248 -0.084201 -0.013521
P 0.760499 -0.552855 2.232923
P 0.960216 -2.326962 -0.440425
P 3.167029 -0.102305 0.127516
C 2.311113 -3.208696 0.517122
C 3.840734 -1.322544 1.370006
C 1.780105 -2.034971 2.744448
C 2.899470 -2.496202 1.768154
H 2.223806 -1.809189 3.721404
H 1.089836 -2.871342 2.907283
H 4.119136 -0.767144 2.273217
H 4.772860 -1.729718 0.960888
H 3.126863 -3.423665 -0.183202
H 1.906276 -4.181486 0.818987
O -1.248258 0.372660 -0.268013
O 1.034782 0.582229 -2.090327
C -2.366080 -0.227948 -0.100114
C 0.190875 0.338113 -3.025402
H -2.311456 -1.279385 0.241465
H -0.641632 -0.341943 -2.760792
O 0.240582 0.803451 -4.180956
O -3.491405 0.272308 -0.290836
C 3.961746 1.493935 0.610576
H 5.034898 1.347066 0.767271
H 3.813293 2.219640 -0.193600
H 3.511247 1.895480 1.519509
C 4.116585 -0.489669 -1.410881
H 3.746442 0.138783 -2.224286
H 5.181952 -0.297235 -1.250713
H 3.992479 -1.536607 -1.693425
C 1.291040 -2.840683 -2.185767

H 2.142298 -2.297666 -2.598646
H 1.488186 -3.916280 -2.229293
H 0.412425 -2.619383 -2.796939
C -0.518238 -3.383738 -0.088532
H -1.354609 -3.066717 -0.715896
H -0.283573 -4.428200 -0.316539
H -0.816754 -3.312969 0.959512
C -0.887598 -0.912865 2.989352
H -0.768809 -1.158652 4.049302
H -1.523180 -0.028041 2.897372
H -1.381155 -1.746044 2.484842
C 1.349277 0.778607 3.374864
H 0.791954 1.697352 3.176226
H 1.193780 0.476368 4.415130
H 2.411625 0.979388 3.223826
C 3.759958 -3.537984 2.521825
H 4.273860 -3.076384 3.372357
H 3.137969 -4.355225 2.903860
H 4.519041 -3.969935 1.860097
O 0.869482 2.144629 0.382646
C 0.176169 2.890765 -0.293809
H -0.490550 2.533078 -1.081463
O 0.209689 4.202548 -0.069600
H -0.387532 4.669734 -0.677101

Energy and thermal parameters

HF=-2122.7778345
Zero-point vibrational energy 1171120.6 (Joules/Mol)
Zero-point correction= 0.446056 (Hartree/Particle)
Thermal correction to Energy= 0.480278
Thermal correction to Enthalpy= 0.481222
Thermal correction to Gibbs Free Energy= 0.382976
Sum of electronic and zero-point Energies= -2122.331778
Sum of electronic and thermal Energies= -2122.297557
Sum of electronic and thermal Enthalpies= -2122.296612
Sum of electronic and thermal Free Energies= -2122.394858

Transition State 14m$_{TS}$



Imaginary frequency: -884.7878 cm^{-1}

Cartesian coordinates

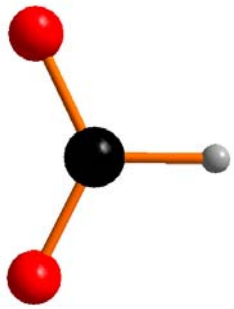
Ru 0.595134 -0.302267 0.016506
P 0.666149 -0.737109 2.243136
P 0.895646 -2.538572 -0.386710
P 2.891567 -0.036660 0.044799
C 2.393403 -3.260154 0.463576
C 3.746000 -1.206004 1.229623
C 1.840816 -2.113938 2.703830
C 2.956415 -2.467985 1.679067
H 2.303898 -1.835348 3.657502
H 1.243381 -3.010655 2.904781
H 4.027653 -0.630117 2.118985
H 4.685303 -1.519518 0.759601
H 3.186536 -3.373714 -0.284575
H 2.128081 -4.273869 0.785520
O -1.548951 -0.645021 -0.174659
O 0.339805 0.063818 -2.256955
C -2.492288 0.156097 0.164449
C 0.566566 0.772837 -3.199654
H -2.178031 1.089386 0.668330
H 1.398355 1.982794 -2.611306
O 0.496225 1.018831 -4.361841
O -3.707874 -0.045321 -0.031786
C 3.587836 1.608203 0.518130
H 4.674531 1.540972 0.629298
H 3.349051 2.334740 -0.262172
H 3.150258 1.958414 1.454683
C 3.804003 -0.335243 -1.539058
H 3.431596 0.336994 -2.315885

H 4.872433 -0.148763 -1.392390
H 3.674205 -1.365569 -1.875980
C 1.097116 -3.036714 -2.152707
H 1.885955 -2.457854 -2.636200
H 1.334421 -4.102817 -2.220156
H 0.158658 -2.843185 -2.678898
C -0.479504 -3.655231 0.131735
H -1.418357 -3.257893 -0.259275
H -0.308478 -4.664782 -0.254051
H -0.549180 -3.705319 1.220271
C -0.926335 -1.231040 3.033715
H -0.751327 -1.518038 4.075280
H -1.611131 -0.379399 3.009978
H -1.390962 -2.060468 2.498599
C 1.173950 0.652189 3.347922
H 0.548597 1.521692 3.135915
H 1.049948 0.353154 4.393222
H 2.218620 0.922395 3.183593
C 3.958622 -3.398924 2.402516
H 4.459850 -2.871920 3.221943
H 3.446848 -4.271939 2.822530
H 4.727311 -3.757533 1.709026
O 0.122760 1.812847 0.508773
C 0.318868 2.994209 0.131026
H -0.094950 3.784290 0.783134
O 0.933469 3.412607 -0.901104
H 1.229430 2.497117 -1.928237

Energy and thermal parameters

HF=-2122.7202436
****** 1 imaginary frequencies (negative Signs) ******
Zero-point vibrational energy 1149042.6 (Joules/Mol)
Zero-point correction= 0.437647 (Hartree/Particle)
Thermal correction to Energy= 0.471496
Thermal correction to Enthalpy= 0.472440
Thermal correction to Gibbs Free Energy= 0.374541
Sum of electronic and zero-point Energies= -2122.282596
Sum of electronic and thermal Energies= -2122.248748
Sum of electronic and thermal Enthalpies= -2122.247804
Sum of electronic and thermal Free Energies= -2122.345702

$HCOO^-$



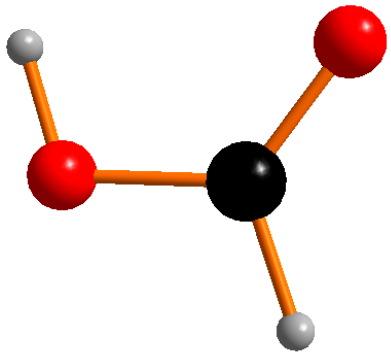
Cartesian coordinates

C -0.906953 0.820733 -0.000000
H -2.027172 0.816014 0.000000
O -0.360090 1.957934 0.000000
O -0.350486 -0.311782 0.000000

Energy and thermal parameters

HF=-189.3186702
Zero-point vibrational energy 53478.0 (Joules/Mol)
Zero-point correction= 0.020369 (Hartree/Particle)
Thermal correction to Energy= 0.023351
Thermal correction to Enthalpy= 0.024295
Thermal correction to Gibbs Free Energy= -0.003460
Sum of electronic and zero-point Energies= -189.298302
Sum of electronic and thermal Energies= -189.295319
Sum of electronic and thermal Enthalpies= -189.294375
Sum of electronic and thermal Free Energies= -189.322130

HCOOH



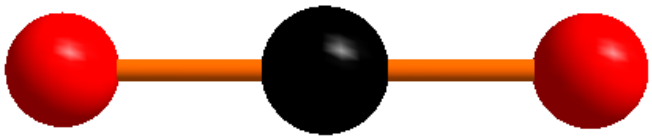
Cartesian coordinates

H -7.784878 -2.733003 -0.392548
O -8.393279 -3.486887 -0.504852
C -7.734411 -4.624652 -0.245938
H -8.400499 -5.487731 -0.366035
O -6.566432 -4.693628 0.075873

Energy and thermal parameters

HF=-189.7803264
Zero-point vibrational energy 88435.6 (Joules/Mol)
Zero-point correction= 0.033683 (Hartree/Particle)
Thermal correction to Energy= 0.036864
Thermal correction to Enthalpy= 0.037808
Thermal correction to Gibbs Free Energy= 0.009588
Sum of electronic and zero-point Energies= -189.746643
Sum of electronic and thermal Energies= -189.743463
Sum of electronic and thermal Enthalpies= -189.742518
Sum of electronic and thermal Free Energies= -189.770739

CO_2



Cartesian coordinates

C -0.539198 0.822142 0.000000
O -0.543422 1.991704 0.000000
O -0.534713 -0.347419 0.000000

Energy and thermal parameters

HF=-188.5902253
Zero-point vibrational energy 26275.0 (Joules/Mol)
Zero-point correction= 0.010008 (Hartree/Particle)
Thermal correction to Energy= 0.012984
Thermal correction to Enthalpy= 0.013928
Thermal correction to Gibbs Free Energy= -0.005624
Sum of electronic and zero-point Energies= -188.580218
Sum of electronic and thermal Energies= -188.577242
Sum of electronic and thermal Enthalpies= -188.576298
Sum of electronic and thermal Free Energies= -188.595849

H_2

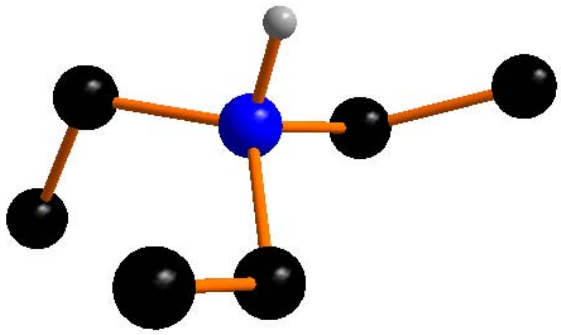
Cartesian coordinates

H 0.000000 0.000000 -0.021576
H 0.000000 0.000000 0.721576

Energy and thermal parameters

HF=-1.1786705
Zero-point vibrational energy 26669.2 (Joules/Mol)
Zero-point correction= 0.010158 (Hartree/Particle)
Thermal correction to Energy= 0.012518
Thermal correction to Enthalpy= 0.013462
Thermal correction to Gibbs Free Energy= -0.001330
Sum of electronic and zero-point Energies= -1.168513
Sum of electronic and thermal Energies= -1.166152
Sum of electronic and thermal Enthalpies= -1.165208
Sum of electronic and thermal Free Energies= -1.180001

NEt_3H^+



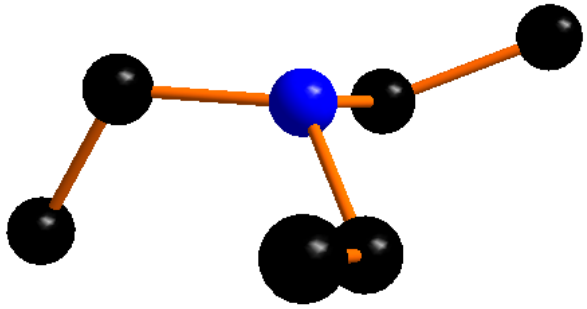
Cartesian coordinates

N -2.063015 -0.206077 -0.106599
H -1.701738 0.254748 0.734643
C -3.575202 -0.250407 0.078592
C -4.328077 -0.901335 -1.073014
H -3.880269 0.789263 0.212975
H -3.754385 -0.774214 1.017866
H -5.395663 -0.842174 -0.843217
H -4.166918 -0.385071 -2.022645
H -4.078783 -1.958301 -1.195647
C -1.652475 0.666991 -1.284212
C -0.237679 1.215097 -1.144628
H -2.374094 1.484794 -1.324836
H -1.765842 0.058830 -2.182656
H -0.045730 1.876984 -1.993686
H -0.124926 1.806798 -0.230300
H 0.525572 0.433303 -1.158487
C -1.407087 -1.574898 -0.159903
C -1.589550 -2.377798 1.121474
H -0.348537 -1.393290 -0.345771
H -1.820447 -2.086752 -1.029720
H -0.980666 -3.282637 1.043096
H -1.244104 -1.820150 1.998238
H -2.623985 -2.689307 1.283836

Energy and thermal parameters

HF=-292.9018786
Zero-point vibrational energy 582706.2 (Joules/Mol)
Zero-point correction= 0.221941 (Hartree/Particle)
Thermal correction to Energy= 0.231287
Thermal correction to Enthalpy= 0.232231
Thermal correction to Gibbs Free Energy= 0.188248
Sum of electronic and zero-point Energies= -292.679938
Sum of electronic and thermal Energies= -292.670592
Sum of electronic and thermal Enthalpies= -292.669648
Sum of electronic and thermal Free Energies= -292.713630

NEt_3



Cartesian coordinates

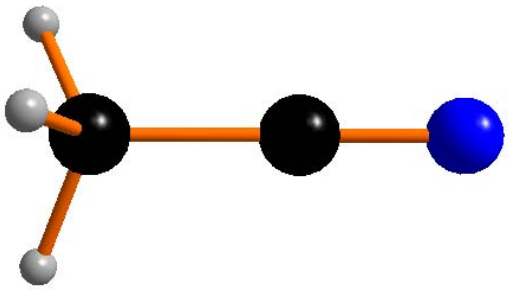
N -2.051906 -0.215134 -0.142087
C -3.512973 -0.240445 0.047201
C -4.357854 -0.894569 -1.062371
H -3.835076 0.800198 0.173695
H -3.722893 -0.740594 0.998616
H -5.420671 -0.817460 -0.806111
H -4.212248 -0.401129 -2.029422
H -4.125069 -1.957485 -1.185885
C -1.641769 0.630076 -1.274616
C -0.232129 1.210566 -1.120374
H -2.352738 1.461505 -1.339657
H -1.709732 0.085989 -2.235297
H -0.000287 1.859463 -1.972731
H -0.158061 1.806176 -0.204039
H 0.537087 0.432416 -1.083185
C -1.428136 -1.545450 -0.192337
C -1.568866 -2.347741 1.103734
H -0.362141 -1.397074 -0.388961
H -1.814415 -2.143463 -1.039377
H -0.981323 -3.269532 1.031849
H -1.199070 -1.772308 1.959715
H -2.604831 -2.636006 1.308440

Energy and thermal parameters

HF=-292.4410888

Zero-point vibrational energy 538970.8 (Joules/Mol)
Zero-point correction= 0.205283 (Hartree/Particle)
Thermal correction to Energy= 0.214690
Thermal correction to Enthalpy= 0.215634
Thermal correction to Gibbs Free Energy= 0.171327
Sum of electronic and zero-point Energies= -292.235806
Sum of electronic and thermal Energies= -292.226399
Sum of electronic and thermal Enthalpies= -292.225454
Sum of electronic and thermal Free Energies= -292.269762

CH_3CN



Cartesian coordinates

N 0.670200 1.802771 0.234430
C 0.755486 2.948207 0.411217
C 0.861571 4.387384 0.633291
H 1.098554 4.892386 -0.306767
H -0.085386 4.775183 1.017803
H 1.652676 4.594368 1.358726

Energy and thermal parameters

HF=-132.7710885
Zero-point vibrational energy 118784.0 (Joules/Mol)
Zero-point correction= 0.045242 (Hartree/Particle)
Thermal correction to Energy= 0.048839
Thermal correction to Enthalpy= 0.049784
Thermal correction to Gibbs Free Energy= 0.021230
Sum of electronic and zero-point Energies= -132.725846
Sum of electronic and thermal Energies= -132.722249
Sum of electronic and thermal Enthalpies= -132.721305
Sum of electronic and thermal Free Energies= -132.749859

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2. Dolg, M.; Stoll, H.; Preuss, H.; Pitzer, R. M. *J. Phys. Chem.* **1993**, *97*, 5852-5859.
3. (a) Barone, V.; Cossi, M. *J. Phys. Chem. A* **1998**, *102*, 1995-2001. (b) Cossi, M.; Rega, N.; Scalmani, G.; Barone, V. *J. Comput. Chem.* **2003**, *24*, 669-681.