

Supporting Information

Factors Controlling Reactivity in the Hydrogen Atom Transfer and Radical Addition Steps of A Radical Relay Cascade

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General Computation Procedure **S3**

**Cartesian Coordinates of the Computed Structures and the
Corresponding Energies (in hartree)** **S3**

General Computation Procedure

All calculations were performed using Gaussian 09.¹ Conformational search was performed using Spartan 16 software package. The structure of each species was submitted for geometry optimization at uM062X(D3)/6-31G(d) level followed by frequency calculation at the same theoretical level. Each optimized structure was then used for single point energy calculation at uM062X(D3)/6-311++G(2d,p) level. All reported Gibbs free energies are for 298K.

Cartesian Coordinates of the Computed Structures and the Corresponding Energies (in hartree)

10a

Geometry optimization + frequency calculation: $E[\text{uM062X(D3)/6-31G(d)}] = -460.633819530$

Zero-point correction= 0.172113

Thermal correction to Energy= 0.181223

Thermal correction to Enthalpy= 0.182168

Thermal correction to Gibbs Free Energy= 0.135967

Single point energy calculation: $E[\text{uM062X(D3)/6-311++G(2d,p)}] = -460.787586766$

H 0.017341 0.442833 -1.030067

C 0.651163 -1.265776 0.169017

H 0.169553 -1.909438 0.911915

C 2.688843 0.190654 -0.287094

H 3.649358 0.524811 0.151603

O 2.066771 1.366847 -0.631659

H 0.887740 -1.886319 -0.703655

H 2.949837 -0.406122 -1.178339

C 1.922337 -0.640496 0.743615

H 2.580655 -1.436299 1.109610

H 1.667824 0.003774 1.591154
C -0.374619 -0.237427 -0.251139
C -2.658003 -0.109058 -0.338941
C -2.037398 1.045155 0.467983
H -3.215720 0.244127 -1.212295
H -3.313115 -0.735228 0.275282
H -1.894572 1.936315 -0.158819
H -2.598927 1.315922 1.363187
O -1.535812 -0.879909 -0.744767
O -0.787697 0.513977 0.858899

10b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -499.926793807

Zero-point correction = 0.201832

Thermal correction to Energy = 0.212008

Thermal correction to Enthalpy = 0.212952

Thermal correction to Gibbs Free Energy = 0.164717

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -500.091105414

C 0.249979 1.704747 -0.060554
H -0.294950 2.358079 0.628639
H 0.386178 2.253752 -0.999247
C 1.606197 1.330969 0.545169
H 2.179070 2.257100 0.661707
C 2.181392 -1.155205 0.060903
H 3.059725 -1.759793 -0.241253
O 1.148813 -1.752301 -0.619674
H 1.443274 0.937884 1.555689
H 2.067167 -1.322880 1.144698

C 2.456417 0.322847 -0.247169
H -0.279133 -0.065488 -1.210021
H 2.350070 0.478326 -1.328513
H 3.510650 0.506317 -0.007476
C -0.629070 0.509074 -0.337314
C -1.788512 -1.161967 0.555135
C -2.767527 -0.217821 -0.186504
H -1.506912 -2.018307 -0.070794
H -2.161736 -1.518198 1.516692
H -3.190031 -0.694818 -1.078396
H -3.583781 0.133436 0.450317
O -0.659191 -0.341470 0.785652
O -1.968728 0.901114 -0.540984

10c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1106.57286285

Zero-point correction = 0.165562

Thermal correction to Energy = 0.175437

Thermal correction to Enthalpy = 0.176381

Thermal correction to Gibbs Free Energy = 0.128217

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1106.73741647

H 0.558297 -0.445800 -1.178939
C 0.878137 -0.867590 0.927529
H 0.305521 -0.770921 1.856717
C 3.059093 -0.210179 -0.207778
H 4.055174 0.234469 -0.017757
O 2.554629 0.551587 -1.236752
H 1.054247 -1.941855 0.776792

H 3.243629 -1.249742 -0.528927
C 2.219202 -0.144757 1.067899
H 2.783350 -0.597640 1.891265
H 2.052833 0.908752 1.315554
C 0.015575 -0.363040 -0.232569
C -2.721567 -0.033909 -0.220363
C -2.089749 1.061210 0.623462
H -2.983313 0.346164 -1.210105
H -3.615486 -0.444623 0.257370
H -2.665782 1.989347 0.575519
H -2.004625 0.749199 1.668132
S -1.511507 -1.389857 -0.367975
S -0.450056 1.399828 -0.085818

10d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1145.86315009

Zero-point correction = 0.194528

Thermal correction to Energy = 0.205718

Thermal correction to Enthalpy = 0.206662

Thermal correction to Gibbs Free Energy = 0.154674

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1146.03960685

C 0.609560 0.106332 1.206956
H -0.080633 -0.180633 2.008280
H 1.015483 1.091499 1.467676
C 1.751739 -0.920641 1.133542
H 1.959706 -1.270371 2.150680
C 2.963818 0.098842 -0.894357
H 3.977661 0.253099 -1.313346

O 2.380450 1.339706 -1.014282
H 1.417184 -1.807728 0.579543
H 2.475759 -0.634330 -1.560599
C 3.068603 -0.408680 0.541774
H 0.383248 0.648961 -0.896920
H 3.461847 0.411938 1.153754
H 3.806096 -1.219629 0.572620
C -0.221840 0.266485 -0.072130
C -2.707667 -0.843634 -0.541968
C -2.843077 0.249376 0.505083
H -3.028953 -0.480465 -1.520438
H -3.289983 -1.730258 -0.275848
H -3.814472 0.747503 0.445015
H -2.710752 -0.154369 1.512752
S -0.954438 -1.344595 -0.603445
S -1.566976 1.489511 0.135801

11a+12a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1585.72951394

Zero-point correction = 0.393558

Thermal correction to Energy = 0.420145

Thermal correction to Enthalpy = 0.421089

Thermal correction to Gibbs Free Energy = 0.331719

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1586.17745707

C 2.876957 -3.416680 -0.765493
H 3.432255 -3.793373 -1.623000
H 2.243585 -4.197814 -0.341742
H 3.564458 -3.033448 -0.005281

O 2.068940 -2.350547 -1.273768
C 1.174187 -1.853822 -0.415737
O 0.990953 -2.297796 0.697797
C 0.464174 -0.654188 -0.944106
C 0.912283 0.014878 -2.008411
H 1.779334 -0.329375 -2.560924
H 0.407126 0.914462 -2.346283
C -0.730873 -0.208160 -0.155088
H -0.746773 0.875342 -0.005254
H -0.784602 -0.731569 0.802699
S -2.223576 -0.637707 -1.078377
C -3.530975 -0.220958 0.059849
C -3.952882 -1.180100 0.975932
C -4.082888 1.055443 0.019369
C -4.951864 -0.842168 1.883607
H -3.512297 -2.172259 0.955460
C -5.082038 1.380382 0.932246
H -3.741773 1.762907 -0.729909
C -5.510858 0.434773 1.861941
H -5.299062 -1.576602 2.603028
H -5.530626 2.368350 0.913971
H -6.291500 0.692588 2.570897
O -2.315697 0.271651 -2.220665
O -2.231303 -2.085911 -1.267829
C 2.416455 0.963167 1.217071
H 1.512342 0.360485 1.363805
H 2.610091 1.485712 2.168540
C 3.593880 0.057367 0.860067
H 3.393855 -0.449579 -0.092323

H 4.500946 0.654059 0.716676
C 3.840354 -0.983921 1.936132
H 2.927174 -1.576532 2.089422
H 4.089062 -0.484799 2.885331
C 2.136544 1.967596 0.148539
C 1.117517 3.977478 -0.170311
C 2.508764 3.940630 -0.803914
H 0.327928 4.275230 -0.862972
H 1.090037 4.617505 0.718391
H 2.455820 3.689356 -1.870349
H 3.092005 4.850364 -0.661411
O 4.913999 -1.806941 1.503963
H 5.070132 -2.476727 2.183355
O 0.916207 2.621947 0.223030
O 3.131310 2.883687 -0.088559

11a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -460.647981394

Zero-point correction = 0.173563

Thermal correction to Energy = 0.182733

Thermal correction to Enthalpy = 0.183677

Thermal correction to Gibbs Free Energy = 0.137890

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -460.808485329

H 1.083110 1.173400 -0.862379
C 0.667357 -1.303159 0.134689
H 0.257654 -2.043931 0.839663
C 2.667355 0.226182 -0.290927
H 3.636424 0.526111 0.118799

O 1.970867 1.424833 -0.554886
H 0.881620 -1.833651 -0.800039
H 2.864904 -0.333182 -1.220943
C 1.948913 -0.685218 0.702607
H 2.626473 -1.494862 0.997196
H 1.712169 -0.107845 1.603056
C -0.397448 -0.289479 -0.152962
C -2.647710 -0.115201 -0.397667
C -2.100281 0.963395 0.538434
H -3.240146 0.280774 -1.224527
H -3.227500 -0.871745 0.142059
H -1.930293 1.908823 0.009248
H -2.706081 1.136682 1.427776
O -1.462728 -0.719618 -0.912506
O -0.856570 0.404823 0.938023

11b+12b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1625.02245037

Zero-point correction = 0.422675

Thermal correction to Energy = 0.450392

Thermal correction to Enthalpy = 0.451336

Thermal correction to Gibbs Free Energy = 0.359827

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1625.48271050

C -3.118877 -3.211498 0.404114
H -3.835120 -3.484024 1.178865
H -2.459251 -4.051047 0.177406
H -3.642934 -2.899680 -0.503014
O -2.359203 -2.129625 0.954756

C -1.286017 -1.770650 0.237419
O -1.019625 -2.243289 -0.844354
C -0.466998 -0.708657 0.894138
C -0.819938 -0.147055 2.052138
H -1.717799 -0.459403 2.574031
H -0.204625 0.625980 2.501710
C 0.785592 -0.327493 0.160795
H 0.934962 0.755494 0.115837
H 0.796488 -0.758228 -0.843211
S 2.203889 -1.015190 1.045053
C 3.564093 -0.664274 -0.052378
C 3.857175 -1.571391 -1.066616
C 4.285095 0.513102 0.117507
C 4.899631 -1.280510 -1.940908
H 3.284140 -2.490140 -1.147987
C 5.326823 0.791018 -0.762767
H 4.037013 1.178931 0.938036
C 5.628813 -0.101961 -1.789121
H 5.147568 -1.975889 -2.736146
H 5.906707 1.700631 -0.644406
H 6.442771 0.118847 -2.472653
O 2.392233 -0.224280 2.261910
O 2.035564 -2.464119 1.112481
C -1.987532 1.546405 -1.029397
H -1.330219 0.710416 -1.300376
H -2.215152 2.082316 -1.965246
C -3.273544 1.016454 -0.396465
H -3.034595 0.601584 0.590626
H -3.964575 1.850989 -0.226670

C -3.934215 -0.062436 -1.248700
H -3.215513 -0.865892 -1.457386
H -4.241838 0.340768 -2.221040
C -1.237740 2.445636 -0.102203
C 0.186060 4.220746 -0.141367
C -0.953555 4.434679 0.854476
H 1.179120 4.357265 0.290762
H 0.078269 4.855635 -1.027680
H -0.652433 4.158511 1.872454
H -1.374065 5.440347 0.847440
O 0.018634 2.856646 -0.519865
O -1.936099 3.527054 0.377392
C -5.143275 -0.663813 -0.557894
H -4.848578 -1.018012 0.443329
H -5.920364 0.103857 -0.422978
O -5.615714 -1.733235 -1.359223
H -6.408066 -2.099229 -0.943950

11b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -499.941001497

Zero-point correction = 0.202511

Thermal correction to Energy = 0.212960

Thermal correction to Enthalpy = 0.213904

Thermal correction to Gibbs Free Energy = 0.164624

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -500.112778239

C 0.346313 1.311347 -0.633924
H -0.199257 2.268021 -0.654649
H 0.686144 1.114274 -1.656694

C 1.537421 1.417843 0.327319
 H 1.989210 2.405926 0.187637
 C 2.220104 -1.090985 0.394405
 H 3.115784 -1.695179 0.569135
 O 1.573365 -1.679338 -0.715567
 H 1.159169 1.393891 1.356725
 H 1.597515 -1.157386 1.301384
 C 2.635755 0.362508 0.158825
 H 0.664840 -1.329733 -0.730974
 H 3.063387 0.422831 -0.849957
 H 3.442539 0.608472 0.861018
 C -0.631214 0.241600 -0.256882
 C -2.272335 -0.514527 1.041425
 C -2.850830 -0.231479 -0.345202
 H -2.009671 -1.572676 1.159836
 H -2.904094 -0.189609 1.867953
 H -3.378330 -1.080891 -0.782669
 H -3.502857 0.648630 -0.346233
 O -1.090007 0.275280 1.036210
 O -1.687815 0.052257 -1.120431

11c+12c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2231.67331876

Zero-point correction = 0.386431

Thermal correction to Energy = 0.414277

Thermal correction to Enthalpy = 0.415221

Thermal correction to Gibbs Free Energy = 0.321221

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2232.13463868

C 1.926372 -3.829930 -1.126928
H 2.447142 -4.180013 -2.016663
H 1.111308 -4.506727 -0.864745
H 2.623020 -3.735304 -0.288644
O 1.401168 -2.544587 -1.475155
C 0.588403 -1.997484 -0.569542
O 0.263741 -2.542085 0.463735
C 0.152738 -0.618005 -0.935686
C 0.767613 0.090785 -1.883662
H 1.598162 -0.323588 -2.444664
H 0.440535 1.101252 -2.111370
C -1.010398 -0.088705 -0.153976
H -0.940040 0.986800 0.029197
H -1.139825 -0.638402 0.781631
S -2.506363 -0.352905 -1.138750
C -3.816320 0.057370 -0.002658
C -4.310697 -0.937312 0.836274
C -4.296301 1.362561 0.034135
C -5.311073 -0.606512 1.744854
H -3.923527 -1.948616 0.756445
C -5.297718 1.679694 0.947383
H -3.898866 2.099478 -0.656719
C -5.799170 0.698285 1.800342
H -5.714700 -1.367552 2.404685
H -5.690933 2.690235 0.988992
H -6.581119 0.950428 2.509875
O -2.508458 0.641312 -2.210883
O -2.590881 -1.780530 -1.435987
C 2.404905 0.230735 1.499070

H 1.364093 -0.123864 1.569365
H 2.692742 0.524135 2.522926
C 3.291938 -0.926930 1.037957
H 3.017658 -1.230341 0.020269
H 4.342913 -0.615389 1.000705
C 3.176593 -2.117711 1.972987
H 2.134550 -2.463833 2.004242
H 3.471106 -1.816422 2.990162
C 2.441617 1.416475 0.587544
C 2.196107 3.968595 -0.113070
C 3.048181 3.242410 -1.146525
H 1.477235 4.641216 -0.586547
H 2.826297 4.537715 0.574472
H 2.427613 2.839152 -1.951249
H 3.810089 3.900230 -1.570812
O 4.037359 -3.134411 1.481725
H 3.942442 -3.908987 2.052396
S 1.271266 2.712380 0.835454
S 3.886468 1.873330 -0.288731

11c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1106.59193026

Zero-point correction = 0.166878

Thermal correction to Energy = 0.177078

Thermal correction to Enthalpy = 0.178022

Thermal correction to Gibbs Free Energy = 0.129013

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1106.76484416

H 1.287402 -0.336610 1.452009

C 1.081501 0.906108 -1.020016
H 0.801148 0.960923 -2.084087
C 2.941098 0.091552 0.539284
H 3.946215 -0.340290 0.534941
O 2.185426 -0.703080 1.426847
H 1.262671 1.938158 -0.690865
H 3.031704 1.126928 0.907818
C 2.384485 0.107765 -0.882912
H 3.129661 0.550278 -1.554772
H 2.230136 -0.927788 -1.211409
C -0.071049 0.351006 -0.228766
C -2.504690 0.119201 0.740219
C -2.340456 -1.024963 -0.250447
H -2.248719 -0.200269 1.753710
H -3.521263 0.519373 0.731295
H -2.808829 -1.942070 0.114227
H -2.766716 -0.759902 -1.221350
S -1.371559 1.443161 0.214426
S -0.551700 -1.334917 -0.435080

11d+12d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2270.97061289

Zero-point correction = 0.416119

Thermal correction to Energy = 0.444718

Thermal correction to Enthalpy = 0.445663

Thermal correction to Gibbs Free Energy = 0.354180

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2271.44295923

C -3.646756 -3.121608 0.530631

H -4.400944 -3.201135 1.313131
H -3.127957 -4.072812 0.398006
H -4.111535 -2.821515 -0.411407
O -2.726998 -2.125008 0.992683
C -1.597150 -2.021593 0.280510
O -1.398834 -2.635194 -0.744408
C -0.599747 -1.079015 0.875687
C -0.876749 -0.377052 1.975657
H -1.833481 -0.492672 2.472294
H -0.160072 0.314678 2.405813
C 0.687185 -1.015115 0.094167
H 0.673613 -0.222953 -0.663215
H 0.875302 -1.971329 -0.400411
S 2.125216 -0.672975 1.122393
C 3.468795 -0.879708 -0.028931
C 4.191510 -2.067923 -0.008915
C 3.753083 0.147178 -0.924667
C 5.230673 -2.230063 -0.920879
H 3.943156 -2.833232 0.719553
C 4.790374 -0.031023 -1.834119
H 3.167167 1.061714 -0.901064
C 5.524955 -1.216102 -1.830290
H 5.812093 -3.146200 -0.919372
H 5.028435 0.755629 -2.542548
H 6.335230 -1.348768 -2.540409
O 2.082665 0.741339 1.512618
O 2.236033 -1.711165 2.143072
C -1.867154 1.261451 -1.307778
H -1.375621 0.315633 -1.591991

H -2.100914 1.767508 -2.258657
C -3.174663 0.937887 -0.582552
H -2.948092 0.542186 0.414134
H -3.748335 1.862308 -0.431144
C -4.011739 -0.078912 -1.351444
H -3.430869 -0.998308 -1.503674
H -4.265464 0.298162 -2.349524
C -0.908984 2.075170 -0.493739
C 1.196941 3.569299 0.185730
C 0.307673 3.327217 1.402902
H 2.233143 3.320039 0.427226
H 1.132564 4.605160 -0.154202
H 0.635737 2.428714 1.925632
H 0.331559 4.184031 2.080056
S 0.651458 2.490570 -1.191568
S -1.408616 3.098434 0.831316
C -5.291032 -0.428184 -0.615004
H -5.942130 0.456745 -0.553552
H -5.045655 -0.731514 0.415811
O -5.925262 -1.480993 -1.320836
H -6.769980 -1.671774 -0.891565

11d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1145.88010053

Zero-point correction = 0.194938

Thermal correction to Energy = 0.207073

Thermal correction to Enthalpy = 0.208017

Thermal correction to Gibbs Free Energy = 0.153646

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1146.06710205

C -0.418041 -0.752897 -0.403028
H -0.550682 -1.798226 -0.096212
H -0.511197 -0.735462 -1.502200
C -1.544396 0.092508 0.201348
H -1.451908 0.080257 1.294476
C -4.045641 0.435387 0.361678
H -3.980573 0.430403 1.461116
H -1.422620 1.138531 -0.112827
H -3.932297 1.479482 0.029917
C -2.924097 -0.406768 -0.218183
H -3.067374 -1.444699 0.105996
H -3.015070 -0.399831 -1.311119
C 0.944785 -0.301400 0.019549
C 3.497569 -0.182581 0.532529
C 3.187805 1.093481 -0.239869
H 3.404399 -0.020241 1.609248
H 4.498291 -0.556875 0.304551
H 3.711686 1.954883 0.180936
H 3.460541 0.981648 -1.292214
S 1.392987 1.399372 -0.114664
S 2.284153 -1.429815 0.000962
O -5.271665 -0.113555 -0.081988
H -5.992033 0.419271 0.279329

12

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1125.06797263

Zero-point correction = 0.218938

Thermal correction to Energy = 0.234403

Thermal correction to Enthalpy= 0.235347

Thermal correction to Gibbs Free Energy= 0.173177

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)]= -1125.35684707

C 4.728801 -1.401865 0.325712

H 5.699054 -1.034546 0.655414

H 4.834981 -2.038957 -0.554958

H 4.239492 -1.969737 1.119455

O 3.962435 -0.240316 0.008787

C 2.715923 -0.491419 -0.408009

O 2.264898 -1.605048 -0.538044

C 1.942181 0.750224 -0.714855

C 2.488603 1.965147 -0.664841

H 3.533606 2.096801 -0.408961

H 1.894311 2.851146 -0.866383

C 0.490412 0.515518 -1.002611

H 0.318863 -0.508368 -1.341445

H 0.069413 1.236510 -1.706298

S -0.420828 0.730087 0.551007

C -2.018503 0.032986 0.185364

C -3.052969 0.874915 -0.208245

C -2.182160 -1.346109 0.288214

C -4.289498 0.312909 -0.514519

H -2.884995 1.946428 -0.250642

C -3.421743 -1.894178 -0.024048

H -1.352959 -1.963463 0.621527

C -4.469497 -1.065852 -0.425414

H -5.113116 0.951401 -0.816983

H -3.573261 -2.965884 0.052575

H -5.435724 -1.498899 -0.664809

O 0.223863 -0.109021 1.556648

O -0.586911 2.167198 0.763225

13a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1585.77164439

Zero-point correction = 0.395595

Thermal correction to Energy = 0.421074

Thermal correction to Enthalpy = 0.422018

Thermal correction to Gibbs Free Energy = 0.335496

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1586.21655887

C -1.363035 4.437131 -1.075915

H -2.203032 4.678123 -1.725327

H -0.435774 4.858634 -1.469952

H -1.530822 4.826945 -0.069167

O -1.289890 3.015117 -1.049112

C -0.292835 2.520884 -0.298168

O 0.502927 3.219930 0.301393

C -0.282777 1.058021 -0.255451

C -1.466977 0.246319 -0.648425

H -2.027431 0.745841 -1.443279

H -1.144927 -0.738698 -1.001970

C 0.927157 0.416284 0.307569

H 0.686071 -0.474429 0.895533

H 1.530188 1.131427 0.873347

S 1.970518 -0.158276 -1.073853

C 3.428941 -0.765611 -0.251232

C 4.465720 0.123183 0.018266

C 3.483927 -2.104748 0.122616
C 5.588720 -0.348327 0.690899
H 4.389587 1.154297 -0.313465
C 4.613690 -2.562839 0.794143
H 2.662116 -2.767213 -0.131004
C 5.658864 -1.685695 1.078656
H 6.411760 0.325210 0.906303
H 4.681433 -3.604936 1.089022
H 6.538385 -2.048578 1.601358
O 1.289666 -1.296278 -1.691351
O 2.341290 1.013242 -1.861976
C -3.728597 -0.606971 0.190989
H -4.290318 0.088229 -0.444143
H -4.296531 -0.714940 1.124542
C -3.565418 -1.963220 -0.488430
H -3.133461 -1.852473 -1.489264
H -2.881754 -2.591436 0.093384
C -4.894647 -2.683509 -0.627705
H -5.598012 -2.054559 -1.196449
H -5.332045 -2.846063 0.370217
C -2.407047 0.057158 0.559490
C -2.030845 1.379278 2.410003
C -1.921567 -0.089332 2.795072
H -1.039584 1.840145 2.296755
H -2.634277 1.977520 3.095725
H -1.073947 -0.323408 3.442217
H -2.848884 -0.452144 3.257839
O -4.652157 -3.909308 -1.287902
H -5.494168 -4.371211 -1.393157

O -2.701439 1.310560 1.162247

O -1.708209 -0.706001 1.536491

13b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1625.06523287

Zero-point correction = 0.424375

Thermal correction to Energy = 0.451264

Thermal correction to Enthalpy = 0.452208

Thermal correction to Gibbs Free Energy = 0.361847

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1625.52186335

C -0.288196 4.675525 -1.353975

H -1.110008 5.025332 -1.976554

H 0.672650 4.873487 -1.833932

H -0.306767 5.169006 -0.379458

O -0.487414 3.273555 -1.201577

C 0.445473 2.653484 -0.461767

O 1.400186 3.227116 0.029288

C 0.177792 1.225558 -0.287360

C -1.154801 0.626987 -0.572022

H -1.652349 1.166730 -1.382254

H -1.037526 -0.423234 -0.859097

C 1.271060 0.409063 0.288290

H 0.897541 -0.350571 0.981797

H 2.039094 1.039688 0.743726

S 2.086731 -0.505227 -1.062971

C 3.479725 -1.263628 -0.252310

C 4.671002 -0.549276 -0.160896

C 3.334906 -2.536561 0.290259

C 5.746740 -1.130930 0.502599
H 4.745759 0.432144 -0.619398
C 4.419512 -3.106501 0.950589
H 2.394582 -3.066251 0.173191
C 5.618261 -2.403382 1.057611
H 6.686865 -0.594797 0.580991
H 4.331626 -4.101113 1.375460
H 6.461525 -2.853213 1.572383
O 1.173904 -1.567521 -1.487203
O 2.590041 0.477028 -2.018542
C -3.491498 0.269353 0.407002
H -3.951650 1.015482 -0.251396
H -4.024267 0.319088 1.365296
C -3.616603 -1.131085 -0.187873
H -3.197001 -1.145594 -1.202169
H -3.016608 -1.826746 0.412890
C -5.067457 -1.603691 -0.237750
H -5.678521 -0.899039 -0.814953
H -5.491084 -1.636147 0.773279
C -2.054827 0.698641 0.678714
C -1.345453 2.046367 2.407925
C -1.492768 0.613397 2.899854
H -0.292434 2.300245 2.220640
H -1.788430 2.794152 3.068776
H -0.672317 0.267242 3.531712
H -2.447250 0.465709 3.421994
O -2.082389 2.021785 1.196959
O -1.461522 -0.116391 1.684663
C -5.205081 -2.980852 -0.860287

H -4.810375 -2.962259 -1.888172
H -4.602596 -3.705150 -0.289769
O -6.576558 -3.327738 -0.843327
H -6.674851 -4.198052 -1.251139

13c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2231.70066036

Zero-point correction = 0.388851

Thermal correction to Energy = 0.415455

Thermal correction to Enthalpy = 0.416399

Thermal correction to Gibbs Free Energy = 0.327126

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2232.15902599

C -1.104772 4.099485 -1.821428
H -1.831769 4.211742 -2.623996
H -0.137256 4.512035 -2.114210
H -1.450753 4.603132 -0.915298
O -0.996962 2.698035 -1.589480
C -0.120913 2.356170 -0.634388
O 0.586534 3.156375 -0.052277
C -0.115488 0.916424 -0.346042
C -1.273428 0.038481 -0.682521
H -1.750256 0.406827 -1.597961
H -0.908881 -0.977041 -0.876614
C 1.122605 0.381447 0.266269
H 0.937236 -0.460662 0.938544
H 1.697360 1.173067 0.754837
S 2.177763 -0.265960 -1.076252
C 3.674963 -0.727462 -0.229890

C 4.672405 0.228928 -0.062579
C 3.797709 -2.022270 0.264632
C 5.825889 -0.126856 0.629392
H 4.543029 1.220382 -0.485934
C 4.957249 -2.364210 0.954303
H 3.004238 -2.742054 0.089011
C 5.964179 -1.417950 1.137085
H 6.619382 0.600431 0.766617
H 5.077808 -3.370173 1.342807
H 6.867159 -1.690590 1.674441
O 1.542047 -1.484434 -1.577662
O 2.478246 0.847382 -1.972195
C -3.621542 -0.733519 -0.122111
H -4.062462 -0.090596 -0.897549
H -4.348002 -0.795625 0.695701
C -3.368202 -2.124101 -0.701528
H -2.763259 -2.070992 -1.612913
H -2.821671 -2.746580 0.017657
C -4.672592 -2.823213 -1.043965
H -5.250400 -2.203187 -1.747866
H -5.278416 -2.939163 -0.131805
C -2.367385 -0.028500 0.420536
C -1.772277 1.728742 2.411162
C -1.877038 0.393710 3.131956
H -0.748169 1.938293 2.086838
H -2.113842 2.551706 3.045257
H -1.076226 0.269407 3.866400
H -2.842040 0.305752 3.635491
O -4.348777 -4.076787 -1.609659

H -5.170772 -4.531998 -1.834461

S -2.891961 1.644651 0.984949

S -1.698859 -0.938099 1.898171

13d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2270.99432550

Zero-point correction = 0.417712

Thermal correction to Energy = 0.445701

Thermal correction to Enthalpy = 0.446645

Thermal correction to Gibbs Free Energy = 0.353619

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2271.46440628

C -0.275512 4.134505 -2.259504

H -1.033512 4.274904 -3.028221

H 0.722435 4.324501 -2.659601

H -0.456696 4.802470 -1.413750

O -0.393046 2.777136 -1.843006

C 0.483047 2.404347 -0.899602

O 1.362222 3.129223 -0.473545

C 0.262145 1.035616 -0.416844

C -1.045174 0.338089 -0.586824

H -1.511730 0.672104 -1.520492

H -0.866379 -0.740695 -0.664168

C 1.427423 0.374123 0.214905

H 1.146012 -0.307330 1.022451

H 2.168720 1.108348 0.541918

S 2.246924 -0.658456 -1.048690

C 3.714235 -1.228678 -0.216607

C 4.867197 -0.451819 -0.284695

C 3.662904 -2.419148 0.501972
C 6.001238 -0.883122 0.396370
H 4.867746 0.458642 -0.876276
C 4.804767 -2.838266 1.178331
H 2.748980 -3.004984 0.507050
C 5.966780 -2.070222 1.126573
H 6.913182 -0.296800 0.352389
H 4.789800 -3.766589 1.739955
H 6.854980 -2.402478 1.654895
O 1.382637 -1.813798 -1.293724
O 2.649114 0.221965 -2.142155
C -3.450284 0.054393 0.161299
H -3.829110 0.671516 -0.666037
H -4.125927 0.205246 1.009915
C -3.473378 -1.414847 -0.260047
H -2.894708 -1.554061 -1.181714
H -2.989849 -2.025746 0.514948
C -4.900737 -1.910157 -0.482358
H -5.405112 -1.292818 -1.235766
H -5.481663 -1.820926 0.443173
C -2.064795 0.589643 0.560169
C -1.060256 2.433794 2.289434
C -1.342158 1.230276 3.175485
H -0.037809 2.421892 1.898969
H -1.217495 3.371547 2.829723
H -0.529582 1.054488 3.886104
H -2.275474 1.370112 3.724846
S -2.265720 2.381686 0.933664
S -1.466772 -0.245983 2.110553

C -4.944143 -3.356524 -0.940421
H -4.384501 -3.462254 -1.882921
H -4.451141 -3.995640 -0.191129
O -6.302366 -3.714629 -1.106906
H -6.340348 -4.632579 -1.405821

14a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -805.754731778

Zero-point correction = 0.292499

Thermal correction to Energy = 0.309546

Thermal correction to Enthalpy = 0.310490

Thermal correction to Gibbs Free Energy = 0.246674

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -806.026476245

C 3.199367 -2.204541 -1.085470
H 2.822241 -3.171727 -1.414248
H 4.189275 -2.307486 -0.636151
H 3.259982 -1.509241 -1.926137
O 2.261373 -1.725670 -0.126776
C 2.562856 -0.529343 0.401777
O 3.593587 0.057731 0.165347
C 1.485989 -0.029812 1.312921
C 0.074256 -0.457090 1.029724
H 0.031776 -1.523284 0.789574
H -0.565695 -0.267251 1.895963
C 1.826629 0.853689 2.249592
H 1.083804 1.275832 2.919255
H 2.858839 1.171809 2.357488
C -1.749735 -0.238061 -0.752814

H -1.491935 -1.194062 -1.224210
H -2.070707 0.437973 -1.556187
C -2.869140 -0.415381 0.268540
H -2.609316 -1.186965 1.002496
H -3.021074 0.519895 0.818769
C -4.176727 -0.816463 -0.389495
H -4.031004 -1.742745 -0.967883
H -4.488692 -0.032484 -1.097351
C -0.475453 0.350608 -0.156709
C 0.954646 1.775990 -1.286563
C -0.214815 2.556266 -0.701332
H 1.868723 1.908755 -0.695482
H 1.156995 2.003224 -2.335667
H 0.069541 3.496096 -0.224581
H -0.987997 2.747885 -1.458149
O -5.136431 -0.996442 0.633349
H -5.974362 -1.248581 0.223824
O -0.691334 1.675059 0.298848
O 0.496852 0.432719 -1.197309

14b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -845.047751402

Zero-point correction = 0.321303

Thermal correction to Energy = 0.339740

Thermal correction to Enthalpy = 0.340684

Thermal correction to Gibbs Free Energy = 0.273238

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -845.331167189

C 3.424401 -2.394870 -1.081231

H 2.970581 -3.330009 -1.405652
H 4.405844 -2.574246 -0.637350
H 3.533868 -1.707812 -1.923694
O 2.532365 -1.842215 -0.118195
C 2.929005 -0.671896 0.405216
O 4.002377 -0.168808 0.165227
C 1.896583 -0.085510 1.316299
C 0.455335 -0.400058 1.034024
H 0.328400 -1.461036 0.800286
H -0.167219 -0.154235 1.898955
C 2.307536 0.770567 2.250164
H 1.601643 1.252872 2.919220
H 3.361930 1.005734 2.356158
C -1.341846 -0.047820 -0.756650
H -1.162355 -1.025798 -1.219023
H -1.607440 0.643573 -1.566485
C -2.482727 -0.128088 0.254578
H -2.260140 -0.896583 1.007101
H -2.548949 0.828747 0.788445
C -3.819208 -0.447880 -0.410301
H -3.754811 -1.395258 -0.959304
H -4.072283 0.326708 -1.144135
C -0.028115 0.442044 -0.157991
C 1.511444 1.748886 -1.287580
C 0.403266 2.619036 -0.710044
H 2.430918 1.813698 -0.693417
H 1.734210 1.955414 -2.336802
H 0.757325 3.536755 -0.236835
H -0.350852 2.865118 -1.470178

O -0.141995 1.781574 0.293003
O 0.951977 0.445110 -1.194513
C -4.954939 -0.548866 0.591150
H -4.730358 -1.338389 1.325757
H -5.043586 0.399478 1.144281
O -6.139961 -0.837887 -0.125326
H -6.869248 -0.900199 0.505281

14c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1451.68481063

Zero-point correction = 0.286015

Thermal correction to Energy = 0.304044

Thermal correction to Enthalpy = 0.304988

Thermal correction to Gibbs Free Energy = 0.239352

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1451.96968793

C 3.296571 -2.463325 -0.996945
H 2.940967 -3.404610 -1.413075
H 4.236712 -2.607168 -0.460697
H 3.445151 -1.723699 -1.787820
O 2.275925 -2.020187 -0.106881
C 2.541465 -0.860467 0.514600
O 3.602579 -0.286839 0.425055
C 1.390042 -0.391245 1.348418
C -0.010110 -0.715102 0.905477
H -0.041351 -1.730242 0.493877
H -0.681096 -0.685634 1.770423
C 1.678624 0.338678 2.426142
H 0.895363 0.717336 3.075067

H 2.709907 0.573482 2.671394
 C -1.852185 -0.317694 -0.789908
 H -1.582022 -1.217231 -1.361978
 H -2.234483 0.416875 -1.507021
 C -2.939043 -0.672882 0.223208
 H -2.631647 -1.514200 0.853928
 H -3.138924 0.177977 0.886080
 C -4.236243 -1.056776 -0.466906
 H -4.051124 -1.886165 -1.168113
 H -4.606597 -0.203131 -1.055118
 C -0.566368 0.254272 -0.169028
 C 1.357170 2.047442 -0.903644
 C 0.207316 2.919437 -0.422951
 H 2.062641 1.820055 -0.100651
 H 1.896138 2.521929 -1.728514
 H 0.566889 3.745319 0.197243
 H -0.348970 3.323792 -1.271345
 O -5.159211 -1.430071 0.536756
 H -5.997302 -1.655121 0.111979
 S -0.898087 1.902915 0.612396
 S 0.623210 0.517909 -1.553389

14d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1490.97786361

Zero-point correction = 0.314767

Thermal correction to Energy = 0.334185

Thermal correction to Enthalpy = 0.335129

Thermal correction to Gibbs Free Energy = 0.265817

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1491.27447352

C 3.355979 -2.763270 -0.992160
H 2.889654 -3.659414 -1.398424
H 4.280463 -3.011339 -0.466899
H 3.577252 -2.048668 -1.789017
O 2.404331 -2.202129 -0.092193
C 2.807359 -1.075013 0.514855
O 3.926415 -0.627977 0.410985
C 1.725100 -0.467795 1.352518
C 0.293111 -0.633375 0.924262
H 0.140421 -1.644136 0.529276
H -0.361131 -0.512788 1.794200
C 2.105631 0.236471 2.418685
H 1.377389 0.710801 3.068839
H 3.159310 0.354072 2.652614
C -1.503395 -0.053288 -0.770080
H -1.343051 -0.989902 -1.323582
H -1.802827 0.704435 -1.501643
C -2.629580 -0.260290 0.242691
H -2.385996 -1.092608 0.915473
H -2.727705 0.638246 0.867546
C -3.960025 -0.547719 -0.449805
H -3.872660 -1.434674 -1.089170
H -4.235607 0.288934 -1.102445
C -0.157984 0.377785 -0.161355
C 1.952274 1.932139 -0.927272
C 0.912006 2.935379 -0.453161
H 2.632108 1.636262 -0.124460
H 2.536789 2.332282 -1.760531

H 1.366752 3.722636 0.154633
H 0.399718 3.389399 -1.304066
S -0.295267 2.063361 0.600095
S 1.045543 0.488505 -1.554251
C -5.088519 -0.778522 0.538486
H -4.836829 -1.626149 1.195583
H -5.205962 0.110363 1.178090
O -6.264821 -1.036812 -0.202959
H -6.991668 -1.177270 0.417830

15

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -779.994003750

Zero-point correction = 0.100172

Thermal correction to Energy = 0.107670

Thermal correction to Enthalpy = 0.108614

Thermal correction to Gibbs Free Energy = 0.066616

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -780.167885100

S 1.697645 -0.000002 -0.252825
C -0.091419 0.000000 -0.084690
C -0.757135 1.220481 -0.054499
C -0.757137 -1.220482 -0.054507
C -2.145910 1.210558 0.032113
H -0.193458 2.147152 -0.077806
C -2.145911 -1.210557 0.032108
H -0.193460 -2.147153 -0.077819
C -2.835705 0.000001 0.073291
H -2.688921 2.149157 0.070599
H -2.688925 -2.149154 0.070590

H -3.919073 0.000001 0.138821

O 2.182551 -1.290737 0.266127

O 2.182552 1.290739 0.266113

16

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -613.004910642

Zero-point correction = 0.196646

Thermal correction to Energy = 0.207511

Thermal correction to Enthalpy = 0.208455

Thermal correction to Gibbs Free Energy = 0.158480

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -613.196893126

H -0.115326 -2.290783 -0.868442

C 0.629253 -1.601385 -0.483750

C 2.514246 0.193191 0.459462

C 0.286969 -0.257597 -0.354969

C 1.900991 -2.053967 -0.134593

C 2.845931 -1.155550 0.343407

C 1.245862 0.654298 0.118103

H 2.149038 -3.105515 -0.240641

H 3.840397 -1.495250 0.615465

H 3.257146 0.902668 0.816554

C 0.944059 2.134229 0.259217

H 0.215749 2.296404 1.076907

H 1.850380 2.695250 0.540115

O 0.330902 2.703805 -0.826707

C -1.122116 0.203431 -0.720371

O -1.988234 -0.888523 -0.922265

C -2.576678 -1.199527 0.334680

C -2.167875 -0.022202 1.244595
O -1.698825 0.951624 0.327894
H -3.658236 -1.269547 0.193321
H -2.199358 -2.156231 0.712931
H -1.370085 -0.316017 1.939174
H -2.998190 0.409819 1.804871
H -1.126105 0.824421 -1.616306

17

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -613.031275719

Zero-point correction = 0.197385

Thermal correction to Energy = 0.208614

Thermal correction to Enthalpy = 0.209558

Thermal correction to Gibbs Free Energy = 0.159384

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -613.231507320

H -0.426555 -2.596091 0.203103
C -1.061353 -1.722937 0.101793
C -2.660459 0.529855 -0.154265
C -0.447065 -0.445952 -0.057117
C -2.434590 -1.850163 0.128415
C -3.253688 -0.724553 0.002867
C -1.285997 0.708817 -0.195256
H -2.875587 -2.834979 0.250809
H -4.333785 -0.820433 0.027096
H -3.292483 1.409214 -0.252642
C -0.731810 2.104407 -0.385400
H -0.037566 2.122253 -1.237461
H -1.562197 2.774128 -0.625762

O -0.118222 2.644092 0.770184
C 0.949361 -0.402351 -0.076655
O 1.725960 -1.518076 -0.022311
C 3.058824 -1.096375 0.250745
C 3.067248 0.313350 -0.328960
O 1.718869 0.726542 -0.099604
H 3.229771 -1.091861 1.333124
H 3.747774 -1.785481 -0.237185
H 3.266954 0.312323 -1.405713
H 3.733259 1.009310 0.180161
H 0.734728 2.196560 0.861307

18a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1738.15025105

Zero-point correction = 0.421155

Thermal correction to Energy = 0.447869

Thermal correction to Enthalpy = 0.448813

Thermal correction to Gibbs Free Energy = 0.361098

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1738.63063357

H 1.263098 0.638792 2.498576
C 2.197421 0.291806 2.071866
C 4.576629 -0.581158 0.969346
C 2.518909 0.654350 0.760609
C 3.055664 -0.501462 2.825877
C 4.254895 -0.940663 2.272488
C 3.725421 0.212612 0.195438
H 2.786647 -0.772910 3.841893
H 4.933931 -1.558935 2.851817

H 5.503024 -0.929673 0.518954
C 4.152125 0.453454 -1.243791
H 3.523785 1.198795 -1.736086
H 5.176735 0.837620 -1.250853
C 1.484662 1.419108 -0.057384
O 0.506214 1.962723 0.807300
C 0.143949 3.235513 0.283819
C 1.475498 3.715741 -0.270304
O 2.046362 2.513103 -0.765700
H -0.618077 3.126617 -0.496173
H -0.242967 3.838664 1.106751
H 2.108213 4.140512 0.518401
H 1.386637 4.422364 -1.097300
O 4.195216 -0.759272 -1.980465
H 3.304531 -1.141177 -1.940673
C 0.792721 0.490137 -1.093862
H 0.079747 1.112140 -1.645680
H 1.544312 0.129242 -1.799003
C 0.095219 -0.647989 -0.427822
C -1.229515 -0.461839 0.219786
H -1.582615 -1.403745 0.645656
H -1.204090 0.328277 0.978947
S -2.466948 0.087192 -0.990534
C -4.003507 -0.136637 -0.118785
C -6.351028 -0.507962 1.273158
C -4.508890 0.914613 0.639637
C -4.648085 -1.367437 -0.203800
C -5.833193 -1.547854 0.502236
C -5.695179 0.719907 1.340834

H -3.986248 1.865732 0.656181
H -4.229899 -2.152584 -0.826335
H -6.355616 -2.497144 0.446255
H -6.110809 1.527629 1.934320
H -7.276723 -0.654092 1.820900
O -2.279795 1.526584 -1.201075
O -2.431967 -0.838940 -2.118649
C 0.712304 -1.959730 -0.237876
O 0.212318 -2.864541 0.400135
O 1.927623 -2.064445 -0.817984
C 2.666338 -3.239226 -0.469054
H 2.186522 -4.125337 -0.889122
H 2.719057 -3.331574 0.617481
H 3.660065 -3.087680 -0.889354

18b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -958.131808548

Zero-point correction = 0.318026

Thermal correction to Energy = 0.336378

Thermal correction to Enthalpy = 0.337322

Thermal correction to Gibbs Free Energy = 0.271848

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -958.439642989

H 0.770730 0.431114 2.245745
C 0.256036 -0.402407 1.778750
C -1.080213 -2.483312 0.545705
C 0.477940 -0.648210 0.420872
C -0.619666 -1.192195 2.518383
C -1.285328 -2.246406 1.900664

C -0.208476 -1.698201 -0.213120
H -0.778367 -0.982335 3.571498
H -1.966999 -2.873724 2.467086
H -1.617927 -3.285545 0.045575
C -0.180411 -1.965869 -1.708869
H 0.673565 -1.484194 -2.189846
H -0.093130 -3.042978 -1.880877
C 1.412362 0.298199 -0.342769
O 2.228930 1.027269 0.551291
C 3.352567 0.208908 0.845612
C 3.332787 -0.869024 -0.263013
O 2.329705 -0.407650 -1.151161
H 4.243348 0.840390 0.816410
H 3.256394 -0.236602 1.842279
H 3.065179 -1.852129 0.142567
H 4.267629 -0.946050 -0.820093
O -1.404746 -1.581050 -2.317998
H -1.546173 -0.647378 -2.095624
C 0.663956 1.304126 -1.222243
H 1.431026 1.890488 -1.734830
H 0.094340 0.757037 -1.978519
C -0.221451 2.212972 -0.407169
C 0.190982 3.395522 0.049165
H -0.462626 4.003620 0.665773
H 1.186397 3.765428 -0.174441
C -1.599462 1.783901 -0.008635
O -2.272307 2.318037 0.837480
O -2.031735 0.714455 -0.709329
C -3.266361 0.149544 -0.253492

H -4.087574 0.845690 -0.434413

H -3.196299 -0.066219 0.814368

H -3.389867 -0.770381 -0.823980

19

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1738.15924845

Zero-point correction = 0.421177

Thermal correction to Energy = 0.447554

Thermal correction to Enthalpy = 0.448498

Thermal correction to Gibbs Free Energy = 0.362512

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1738.63974012

H -1.283283 0.207991 2.404713

C -0.981372 1.073179 1.827439

C -0.150373 3.225032 0.298450

C -1.627894 1.313596 0.618132

C 0.076175 1.863614 2.269180

C 0.506817 2.932058 1.472433

C -1.258995 2.456318 -0.168346

H 0.570592 1.638194 3.207927

H 1.351688 3.540028 1.781184

H 0.168224 4.074792 -0.299412

C -1.850800 2.920953 -1.364080

H -1.371150 3.730319 -1.904116

C -2.556103 0.241451 0.089773

O -2.783757 -0.731069 1.079397

C -4.022918 -1.355128 0.783753

C -4.804227 -0.279587 -0.006285

O -3.862206 0.779261 -0.159647

H -3.857935 -2.267268 0.200777
H -4.494461 -1.613370 1.733420
H -5.660274 0.118878 0.540809
H -5.137511 -0.646682 -0.982333
O -2.977713 2.517336 -1.961442
H -3.502447 1.934043 -1.369901
C -2.042304 -0.416860 -1.210072
H -2.788958 -1.153416 -1.529043
H -1.981630 0.340097 -1.996630
C -0.690263 -1.152984 -1.105627
C 0.504885 -0.211433 -0.965535
H 0.433809 0.636445 -1.652453
H 0.620789 0.161642 0.052691
S 2.035348 -1.072177 -1.397138
C 3.239038 -0.247533 -0.371314
C 5.062441 1.054004 1.231751
C 3.170341 -0.424920 1.008960
C 4.197445 0.561877 -0.966639
C 5.119528 1.213935 -0.150185
C 4.090300 0.238119 1.812285
H 2.404459 -1.070515 1.431715
H 4.210923 0.664755 -2.046973
H 5.880822 1.847078 -0.594192
H 4.055084 0.115992 2.890125
H 5.780961 1.566954 1.863548
O 1.906764 -2.456882 -0.941713
O 2.358111 -0.786783 -2.794802
C -0.799591 -2.202536 -0.009427
O -1.503907 -3.177073 -0.107256

O -0.105937 -1.891219 1.092858
C -0.289238 -2.794940 2.179305
H 0.025421 -3.799726 1.891892
H -1.342421 -2.811108 2.470900
H 0.328947 -2.413936 2.991672
H -0.585419 -1.724207 -2.034976

1

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -232.873493859

Zero-point correction = 0.124818

Thermal correction to Energy = 0.131211

Thermal correction to Enthalpy = 0.132156

Thermal correction to Gibbs Free Energy = 0.094479

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -232.951710816

C -2.334742 -0.119843 -0.131687
H -2.399461 -0.132790 -1.224695
H -2.705422 0.852103 0.211191
H -3.008200 -0.890702 0.253133
C -0.898752 -0.351875 0.329338
H -0.545633 -1.331802 -0.010470
H -0.859285 -0.368842 1.426748
C 0.062322 0.714230 -0.189783
H 0.001849 0.766455 -1.284289
H -0.222649 1.703765 0.190883
C 1.508001 0.425774 0.203947
H 1.602679 0.364649 1.306947
H 2.196883 1.234474 -0.094508
O 1.989783 -0.775878 -0.255728

20a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2863.27477061

Zero-point correction = 0.644619

Thermal correction to Energy = 0.687116

Thermal correction to Enthalpy = 0.688060

Thermal correction to Gibbs Free Energy = 0.563884

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2864.03812021

H	4.674657	0.151645	0.620590
C	3.925343	-0.163701	1.337314
C	2.003005	-0.981959	3.149481
C	2.951172	-1.081497	0.931764
C	3.932114	0.352494	2.628015
C	2.965933	-0.059687	3.540197
C	1.972036	-1.496883	1.850013
H	4.694138	1.068947	2.919041
H	2.964222	0.329739	4.553600
H	1.260988	-1.337288	3.857440
C	0.828537	-2.444572	1.524660
H	1.040026	-2.987714	0.597628
C	2.961855	-1.564927	-0.516501
O	4.168646	-1.139628	-1.127656
C	4.617042	-2.199932	-1.957224
C	4.192720	-3.412412	-1.141586
O	2.955809	-2.987575	-0.590171
H	4.122918	-2.156590	-2.935840
H	5.696294	-2.097877	-2.083115
H	4.914479	-3.626576	-0.344060

H 4.016440 -4.312391 -1.733619
O 0.716838 -3.346004 2.600359
H -0.010910 -3.946820 2.361077
C 1.774517 -1.072665 -1.359148
H 1.831356 -1.590410 -2.321549
H 0.832526 -1.370321 -0.888083
C 1.748629 0.437978 -1.644273
C 1.557408 1.314209 -0.396856
H 1.187345 0.748556 0.461183
H 2.466104 1.839088 -0.099131
S 0.299129 2.545108 -0.738158
C 0.114809 3.404898 0.804628
C -0.102082 4.698980 3.221992
C 0.865454 4.557652 1.017261
C -0.747617 2.883640 1.765766
C -0.849287 3.546572 2.985881
C 0.750291 5.206784 2.242198
H 1.507155 4.935934 0.227546
H -1.341450 1.995852 1.559107
H -1.519708 3.161794 3.747182
H 1.320332 6.110721 2.430345
H -0.188612 5.210295 4.175780
O 0.802405 3.471948 -1.749483
O -0.944610 1.797523 -0.991159
C 2.959745 0.791179 -2.498494
O 3.173695 0.265584 -3.564058
O 3.751949 1.719519 -1.955568
C 4.933825 1.999390 -2.703142
H 4.675887 2.340890 -3.707005

H 5.545529 1.096713 -2.775206
H 5.457342 2.778157 -2.151310
H 0.891492 0.583504 -2.314574
C -1.464886 -2.133793 0.346903
C -2.220632 -1.180022 -0.502000
H -1.624017 -0.320417 -0.828994
H -2.719218 -1.665124 -1.342689
S -3.549244 -0.469512 0.535950
C -4.541251 0.461144 -0.608289
C -6.063626 1.871889 -2.414443
C -5.727046 -0.102462 -1.070526
C -4.096210 1.713444 -1.023719
C -4.871697 2.417090 -1.940267
C -6.493257 0.618570 -1.980989
H -6.035970 -1.076331 -0.704628
H -3.160795 2.116263 -0.647507
H -4.543108 3.392776 -2.282547
H -7.425917 0.204093 -2.349577
H -6.663785 2.428787 -3.127387
O -4.347532 -1.584417 1.042472
O -2.910467 0.458277 1.472952
C -1.858601 -3.540250 0.373079
O -1.415000 -4.367199 1.155040
O -2.760508 -3.856082 -0.567381
C -3.218372 -5.206611 -0.532122
H -3.692894 -5.416024 0.428547
H -2.383188 -5.895018 -0.677225
H -3.937856 -5.294244 -1.344216
C -0.489782 -1.618535 1.354213

H -0.277966 -0.574803 1.100621

H -0.962318 -1.586934 2.348383

20b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2083.25551536

Zero-point correction = 0.541638

Thermal correction to Energy = 0.575558

Thermal correction to Enthalpy = 0.576502

Thermal correction to Gibbs Free Energy = 0.474793

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2083.83139361

H 1.628694 -1.838912 2.255767

C 0.734300 -1.227584 2.261761

C -1.547688 0.336272 2.247236

C -0.239340 -1.449754 1.281521

C 0.576264 -0.229370 3.215255

C -0.571034 0.559299 3.207972

C -1.398116 -0.659119 1.274943

H 1.347752 -0.070405 3.962421

H -0.707082 1.340644 3.949145

H -2.459481 0.928280 2.241129

C -2.543872 -0.797571 0.288481

H -2.427804 -1.702260 -0.315803

C 0.026705 -2.510864 0.218866

O 1.153310 -3.272049 0.610835

C 0.918197 -4.606687 0.195908

C -0.581270 -4.732878 0.433577

O -1.058717 -3.432918 0.117784

H 1.192504 -4.737565 -0.858240

H 1.526947 -5.265977 0.816693
H -0.798247 -4.971405 1.481440
H -1.075465 -5.455724 -0.219024
O -3.731401 -0.903271 1.065902
H -4.434191 -1.213343 0.475485
C 0.255135 -1.943416 -1.191485
H 0.372023 -2.800280 -1.863043
H -0.639945 -1.404622 -1.513739
C 1.488916 -1.041269 -1.374282
C 1.404964 0.305436 -0.651322
H 0.388721 0.710256 -0.639015
H 1.781247 0.255596 0.370816
S 2.407609 1.502375 -1.549370
C 2.609373 2.825068 -0.374338
C 2.885067 4.824890 1.499679
C 3.631126 2.729619 0.566426
C 1.726627 3.898998 -0.403233
C 1.871910 4.906501 0.546817
C 3.764329 3.742366 1.510199
H 4.307490 1.880293 0.538741
H 0.957163 3.940358 -1.167742
H 1.196907 5.756057 0.540462
H 4.556641 3.691791 2.249966
H 2.994067 5.613432 2.237791
O 3.716404 0.893011 -1.784696
O 1.610499 1.999968 -2.670982
C 2.730313 -1.856341 -1.035433
O 3.070434 -2.819431 -1.677323
O 3.357835 -1.434793 0.067967

C 4.454980 -2.250565 0.468318
H 5.201349 -2.298069 -0.326531
H 4.100448 -3.259610 0.693941
H 4.868027 -1.778819 1.358832
H 1.557541 -0.857886 -2.453608
C -3.989076 0.523877 -1.273038
C -4.339256 -0.064164 -2.417905
H -3.609095 -0.614644 -3.005574
H -5.350699 -0.000089 -2.803531
C -4.980266 1.317031 -0.477137
O -4.676254 2.133820 0.358417
O -6.254119 1.028747 -0.793942
C -7.229082 1.792352 -0.084628
H -7.101531 2.857347 -0.290172
H -7.131049 1.625383 0.990038
H -8.196350 1.444110 -0.443202
C -2.622539 0.431749 -0.652968
H -1.857491 0.357048 -1.433402
H -2.434751 1.343098 -0.078949

2

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -232.873451422

Zero-point correction = 0.125502

Thermal correction to Energy = 0.131640

Thermal correction to Enthalpy = 0.132584

Thermal correction to Gibbs Free Energy = 0.095601

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -232.951554790

C 1.502532 -0.881331 -0.032353

H 0.785977 -1.520920 0.494936
H 2.504339 -1.138140 0.324009
H 1.441778 -1.134014 -1.095687
C 1.204103 0.599216 0.195125
H 1.247741 0.822645 1.269241
C -1.313049 0.260192 0.290764
H -1.283904 0.326082 1.392233
O -1.412959 -1.040990 -0.139933
H 1.983153 1.208189 -0.277786
H -2.275357 0.710711 -0.022215
C -0.158492 1.034390 -0.348227
H -0.204359 0.873238 -1.431779
H -0.306263 2.105319 -0.165348

3

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -232.870445939

Zero-point correction = 0.124825

Thermal correction to Energy = 0.131299

Thermal correction to Enthalpy = 0.132243

Thermal correction to Gibbs Free Energy = 0.094818

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -232.957116658

C 1.543442 0.912530 -0.064333
H -0.635468 1.460906 0.225015
H 2.212024 1.479142 0.573890
H 1.378295 1.293101 -1.067537
C 1.263678 -0.525674 0.223981
H 1.272948 -0.697997 1.308551
C -1.287856 -0.363031 0.257206

H -1.259134 -0.485179 1.352623
O -1.422955 0.996638 -0.100486
H 2.082156 -1.145558 -0.180123
H -2.197188 -0.855095 -0.100160
C -0.061977 -1.032012 -0.360501
H -0.081390 -0.858337 -1.443491
H -0.132316 -2.114970 -0.203000

4

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -232.865987581

Zero-point correction = 0.123827

Thermal correction to Energy = 0.131107

Thermal correction to Enthalpy = 0.132051

Thermal correction to Gibbs Free Energy = 0.092494

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -232.954382256

C -2.555283 -0.277612 0.000248
H -2.943398 -0.686043 0.925786
H -2.943658 -0.685864 -0.925259
C -1.296861 0.521739 0.000154
H -1.268274 1.176953 0.880807
H -1.268458 1.177034 -0.880445
C -0.033591 -0.358523 -0.000014
H -0.030603 -1.010915 0.880427
H -0.030795 -1.010863 -0.880493
C 1.240397 0.467268 -0.000125
H 1.256708 1.119882 0.887412
H 1.256562 1.119868 -0.887672
O 2.336509 -0.426216 -0.000204

H 3.151864 0.092435 -0.000508

5

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -272.166387636

Zero-point correction = 0.153392

Thermal correction to Energy = 0.161164

Thermal correction to Enthalpy = 0.162108

Thermal correction to Gibbs Free Energy = 0.120744

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -272.256302026

C -1.722146 0.441188 -0.255976

H -1.897624 1.430323 0.186725

H -1.684882 0.592619 -1.342332

C -0.373871 -0.094233 0.220425

H -0.409858 -0.254912 1.307800

C 2.136055 0.231171 0.285196

H 2.975265 0.929404 0.124413

O 2.420622 -0.969812 -0.317976

H -0.183115 -1.075267 -0.232155

H 2.152649 0.012261 1.371946

C 0.791573 0.831731 -0.115108

H 0.668155 1.800134 0.386911

H 0.806972 1.033377 -1.193627

C -2.877535 -0.492846 0.094344

H -2.731760 -1.478687 -0.359351

H -3.835010 -0.098609 -0.257700

H -2.950217 -0.634215 1.177897

6

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -272.163712087

Zero-point correction = 0.154533

Thermal correction to Energy = 0.161905

Thermal correction to Enthalpy = 0.162850

Thermal correction to Gibbs Free Energy = 0.122751

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -272.253120804

C -1.405675 0.284677 -0.494396

H -2.347834 0.793867 -0.726591

H -0.979837 -0.033093 -1.453754

C -0.454321 1.288505 0.179866

H -0.690628 2.301663 -0.164641

C 1.548316 -0.315902 0.361265

H 2.653685 -0.338831 0.287788

O 1.159971 -1.359190 -0.447003

H -0.635702 1.286900 1.264023

H 1.312699 -0.520329 1.419818

C 1.036081 1.052160 -0.084136

C -1.725560 -0.943950 0.359807

H -0.835636 -1.538638 0.585849

H -2.430536 -1.602896 -0.155613

H -2.181424 -0.642948 1.309491

H 1.243625 1.149735 -1.156574

H 1.618777 1.825152 0.431791

7

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -272.162095960

Zero-point correction = 0.153769

Thermal correction to Energy = 0.161446

Thermal correction to Enthalpy= 0.162391

Thermal correction to Gibbs Free Energy= 0.121865

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)]= -272.260248219

C -1.534001 0.135829 -0.424494

H -2.566341 0.515145 -0.510896

H -1.215288 -0.084086 -1.451893

C -0.655424 1.250024 0.166917

H -1.009202 2.213298 -0.217217

C 1.551337 -0.110177 0.376098

H 2.633099 0.052626 0.346337

O 1.315499 -1.252855 -0.422621

H -0.809108 1.281023 1.254964

H 1.280208 -0.295510 1.428049

C 0.843774 1.145320 -0.132752

C -1.561854 -1.119321 0.383281

H 0.435372 -1.591515 -0.192604

H -1.948300 -2.037002 -0.047950

H -1.535384 -1.060341 1.467151

H 1.009105 1.198456 -1.216191

H 1.338856 2.020702 0.306916

8

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)]= -272.159144749

Zero-point correction= 0.152742

Thermal correction to Energy= 0.161314

Thermal correction to Enthalpy= 0.162258

Thermal correction to Gibbs Free Energy= 0.119122

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)]= -272.259289478

C 1.923884 0.540332 0.000143
H 1.864655 1.193460 -0.880004
H 1.864512 1.193478 0.880267
C 0.691486 -0.385179 0.000053
H 0.737899 -1.041254 -0.879132
C -1.837207 -0.514689 -0.000139
H -1.810689 -1.166623 -0.887628
H 0.737756 -1.041233 0.879261
H -1.810799 -1.166620 0.887355
C -0.621385 0.393677 -0.000063
H -0.675849 1.045623 -0.880449
H -0.675986 1.045651 0.880294
C 3.212961 -0.207577 0.000256
H 3.623989 -0.593460 0.925739
H 3.624145 -0.593471 -0.925154
O -2.991032 0.304093 -0.000210
H -3.769811 -0.267682 -0.000359

9a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -460.633969543

Zero-point correction = 0.171523

Thermal correction to Energy = 0.180839

Thermal correction to Enthalpy = 0.181783

Thermal correction to Gibbs Free Energy = 0.134546

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -460.787762718

C 0.666530 -0.630015 0.006579
H 0.872668 -1.703820 -0.085030

H 0.709908 -0.368703 1.068410
 C 1.694999 0.184939 -0.770134
 H 1.678509 -0.084254 -1.834329
 H 1.438521 1.247442 -0.702232
 C 3.106326 -0.025792 -0.228723
 H 3.865053 0.515860 -0.818410
 H 3.393395 -1.094168 -0.304591
 O 3.253163 0.275646 1.102910
 C -0.742010 -0.375073 -0.479181
 H -0.851562 -0.633676 -1.548146
 C -2.864244 -0.382899 0.219825
 C -2.364976 1.060239 0.298231
 H -3.381822 -0.572984 -0.731570
 H -3.502526 -0.684880 1.051232
 H -3.000034 1.768137 -0.241511
 H -2.255621 1.390223 1.337745
 O -1.089786 0.993934 -0.322392
 O -1.656658 -1.115527 0.285588

9b

Geometry optimization + frequency calculation: $E[\text{uM062X(D3)}/6\text{-31G(d)}] = -499.927469570$

Zero-point correction= 0.199527

Thermal correction to Energy= 0.210623

Thermal correction to Enthalpy= 0.211568

Thermal correction to Gibbs Free Energy= 0.159294

Single point energy calculation: $E[\text{uM062X(D3)}/6\text{-311++G(2d,p)}] = -500.092776833$

C 0.107976 1.303466 -0.155991
 H -0.086119 1.815700 -1.105643

H -0.061032 2.030861 0.647019
C -0.823999 0.105574 -0.000870
H -0.603190 -0.614023 -0.799727
C -3.218544 -0.704056 0.091813
H -3.007186 -1.471647 -0.674990
O -4.559342 -0.413118 0.086276
H -0.603236 -0.395671 0.949455
H -3.034550 -1.220309 1.055310
C -2.296923 0.502037 -0.051601
H -2.521462 1.002957 -1.001350
H -2.531143 1.216128 0.747020
C 1.570063 0.905512 -0.132391
H 2.225780 1.780099 -0.276041
C 2.931956 -0.618832 0.791363
C 2.519840 -1.144567 -0.581863
H 3.891460 -0.084488 0.740253
H 2.975677 -1.379328 1.572290
H 3.365029 -1.435916 -1.210853
H 1.824441 -1.988667 -0.491182
O 1.859903 -0.031181 -1.162809
O 1.877353 0.275487 1.087243

9c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1106.57043343

Zero-point correction = 0.165498

Thermal correction to Energy = 0.175619

Thermal correction to Enthalpy = 0.176563

Thermal correction to Gibbs Free Energy = 0.127250

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1106.73197501

C -1.021000 0.375932 0.098904
H -1.345350 1.417608 -0.004172
H -0.832133 0.208814 1.166752
C -2.124412 -0.555949 -0.394262
H -2.353132 -0.355024 -1.446933
H -1.806863 -1.601572 -0.313990
C -3.428071 -0.411728 0.426234
H -3.195698 -0.633529 1.479809
H -4.166678 -1.132398 0.045611
O -3.846936 0.885812 0.269203
C 0.286117 0.188928 -0.671809
H 0.099808 0.261206 -1.747314
C 2.812593 0.419114 0.417016
C 2.165382 -0.861925 0.917739
H 3.530627 0.201551 -0.376421
H 3.318731 0.952729 1.226219
H 2.905888 -1.645256 1.099488
H 1.601206 -0.683564 1.837280
S 1.063211 -1.445954 -0.404839
S 1.491503 1.508248 -0.212842

9d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1145.86409914

Zero-point correction = 0.193382

Thermal correction to Energy = 0.205000

Thermal correction to Enthalpy = 0.205944

Thermal correction to Gibbs Free Energy = 0.153477

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1146.03653995

C 0.316081 -0.440915 -1.313304
H 0.571523 0.154044 -2.199650
H 0.524609 -1.488886 -1.568822
C 1.203219 -0.015133 -0.148307
H 1.012540 1.042657 0.079093
C 3.573746 0.227321 0.703302
H 3.397753 1.288573 0.963850
O 4.921287 0.077254 0.492357
H 0.931557 -0.593286 0.744600
H 3.322710 -0.323401 1.629998
C 2.686321 -0.210644 -0.455982
H 2.969666 0.361513 -1.347763
H 2.893835 -1.264953 -0.675262
C -1.193521 -0.306480 -1.081639
H -1.716949 -0.547114 -2.009853
C -2.605703 -0.271157 1.291307
C -1.884901 1.059479 1.140992
H -3.656333 -0.172145 1.010122
H -2.540930 -0.646289 2.316581
H -2.461946 1.878872 1.578117
H -0.897969 1.026094 1.610620
S -1.737628 1.386602 -0.641223
S -1.780610 -1.485886 0.210678

TS1

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -232.849214110

Zero-point correction = 0.120943

Thermal correction to Energy = 0.126185

Thermal correction to Enthalpy= 0.127129

Thermal correction to Gibbs Free Energy= 0.092237

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -232.931250477

C -1.315582 -0.881615 -0.064701

H -0.092746 -1.280396 0.008022

H -1.576687 -1.118407 -1.097788

H -1.883826 -1.471934 0.654502

C -1.175470 0.594831 0.231338

H -2.012935 1.158280 -0.201324

C 1.287085 0.256085 0.241141

H 2.246756 0.574385 -0.190568

O 1.126828 -1.090149 -0.097370

H -1.198469 0.765154 1.313884

H 1.342856 0.399724 1.333123

C 0.153112 1.114701 -0.331039

H 0.307270 2.168803 -0.078000

H 0.158291 1.021573 -1.423331

TS2

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -272.143373098

Zero-point correction= 0.149888

Thermal correction to Energy= 0.156240

Thermal correction to Enthalpy= 0.157185

Thermal correction to Gibbs Free Energy= 0.119497

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -272.236439365

C -1.562993 0.165005 -0.311785

H -2.607534 0.419529 -0.083674

H -1.483658 0.129521 -1.405378
C -0.645702 1.268512 0.230702
H -1.035544 2.240687 -0.091173
C 1.545470 -0.088682 0.292396
H 2.618176 -0.004575 0.067757
O 1.148907 -1.275678 -0.339768
H -0.691360 1.264524 1.329320
H 1.453667 -0.164853 1.389085
C 0.817255 1.157594 -0.211657
C -1.250826 -1.198255 0.259342
H -0.040360 -1.431399 -0.035075
H -1.786780 -2.031444 -0.198649
H -1.273359 -1.247609 1.351585
H 0.876431 1.165401 -1.307316
H 1.359842 2.040590 0.147669

TS3a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -460.620248388

Zero-point correction = 0.168599

Thermal correction to Energy = 0.176853

Thermal correction to Enthalpy = 0.177798

Thermal correction to Gibbs Free Energy = 0.134364

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -460.776369695

H 0.349434 0.706222 -0.517643
C 0.806323 -1.313837 0.051065
H 0.431130 -2.102892 0.711976
C 2.489636 0.495194 -0.334186
H 3.370379 0.999909 0.091092

O 1.491712 1.460290 -0.451980
H 0.998426 -1.751096 -0.934817
H 2.782338 0.080360 -1.314281
C 2.069863 -0.652247 0.598738
H 2.882875 -1.380570 0.679108
H 1.870995 -0.246482 1.596304
C -0.270994 -0.268690 -0.113511
C -2.496306 -0.034487 -0.532169
C -2.055115 0.759913 0.705557
H -2.934861 0.595141 -1.310111
H -3.190355 -0.842734 -0.281770
H -1.831549 1.804580 0.455546
H -2.758926 0.719116 1.537123
O -1.281292 -0.611719 -1.005035
O -0.864210 0.089350 1.086328

TS3b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -499.916584465

Zero-point correction = 0.197859

Thermal correction to Energy = 0.207176

Thermal correction to Enthalpy = 0.208120

Thermal correction to Gibbs Free Energy = 0.162215

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -500.083328412

C 0.449788 1.552629 -0.275635
H -0.066518 2.426710 0.138295
H 0.677792 1.764025 -1.326089
C 1.731812 1.258962 0.512040
H 2.347407 2.164965 0.506916

C 1.910532 -1.289296 0.113211
 H 2.674152 -2.074258 -0.007830
 O 0.971250 -1.564642 -0.882061
 H 1.463538 1.067626 1.558316
 H 1.481706 -1.413874 1.121993
 C 2.572767 0.087206 -0.012471
 H 0.043336 -0.547765 -0.734000
 H 2.828266 0.242282 -1.068288
 H 3.515079 0.070445 0.548469
 C -0.511256 0.393561 -0.242145
 C -1.997507 -0.806522 0.867241
 C -2.726179 -0.111640 -0.294774
 H -1.672179 -1.816400 0.587888
 H -2.563840 -0.836186 1.798256
 H -3.176614 -0.819903 -0.994980
 H -3.487837 0.593271 0.051802
 O -0.859281 0.022451 1.051662
 O -1.692474 0.625899 -0.942795

TS3c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1106.55890164

Zero-point correction = 0.161657

Thermal correction to Energy = 0.170861

Thermal correction to Enthalpy = 0.171805

Thermal correction to Gibbs Free Energy = 0.125586

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1106.72652085

H -0.737665 -0.266843 0.878215
 C -1.143928 -0.420768 -1.212621

H -0.760949 -0.074866 -2.178455
C -2.885290 -0.191042 0.560915
H -3.778139 0.374481 0.870906
O -1.911273 0.033782 1.525180
H -1.351277 -1.495693 -1.299380
H -3.168376 -1.255727 0.494605
C -2.431392 0.304655 -0.821473
H -3.216488 0.120150 -1.561921
H -2.256258 1.386251 -0.776051
C -0.082082 -0.213130 -0.136222
C 2.462322 -0.418962 0.614859
C 2.385335 0.929525 -0.085347
H 2.274170 -0.318418 1.686795
H 3.432264 -0.899087 0.461251
H 2.959950 1.690357 0.449045
H 2.753653 0.852344 -1.111012
S 1.193348 -1.476783 -0.141485
S 0.638496 1.456479 -0.085772

TS3d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1145.85506375

Zero-point correction = 0.190697

Thermal correction to Energy = 0.201022

Thermal correction to Enthalpy = 0.201966

Thermal correction to Gibbs Free Energy = 0.153206

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1146.03440916

C -0.825764 1.403314 -0.591950
H -0.353616 1.946298 -1.418946

H -1.050042 2.138156 0.191751
C -2.134096 0.754075 -1.063643
H -2.725245 1.528698 -1.564863
C -2.351866 -1.077102 0.741509
H -3.112289 -1.596353 1.348663
O -1.355115 -0.734734 1.648465
H -1.912819 -0.002973 -1.828731
H -1.990634 -1.810491 -0.000984
C -2.991954 0.123000 0.039754
H -0.365918 -0.142359 0.864470
H -3.231484 0.873209 0.803765
H -3.940319 -0.199800 -0.406547
C 0.180832 0.413822 -0.022769
C 2.091476 -1.340143 -0.106277
C 2.845516 -0.065888 0.256600
H 1.695825 -1.830593 0.787784
H 2.726970 -2.041544 -0.652061
H 3.511337 -0.233508 1.106501
H 3.430290 0.290110 -0.594328
S 0.700462 -0.866223 -1.176156
S 1.629163 1.222007 0.717185

TS4a

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1585.72897235

Zero-point correction = 0.393632

Thermal correction to Energy = 0.419094

Thermal correction to Enthalpy = 0.420038

Thermal correction to Gibbs Free Energy = 0.335728

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1586.17466078

C 3.575805 -3.043914 -0.740287
H 4.207771 -2.598142 0.033830
H 4.174540 -3.263775 -1.623438
H 3.094503 -3.947423 -0.363777
O 2.593332 -2.098950 -1.167436
C 1.531544 -1.947466 -0.358472
O 1.349638 -2.619809 0.638074
C 0.631957 -0.857335 -0.791278
C 1.072263 0.121219 -1.611569
H 2.042787 0.037532 -2.087892
H 0.407512 0.906235 -1.951631
C -0.671039 -0.784275 -0.044351
H -0.651683 -0.021517 0.744135
H -0.922395 -1.750495 0.399652
S -2.056490 -0.318258 -1.099621
C -3.418781 -0.343045 0.051220
C -4.260307 -1.449539 0.076340
C -3.595201 0.740770 0.907369
C -5.309470 -1.469052 0.991539
H -4.093479 -2.263488 -0.622171
C -4.643465 0.706146 1.820857
H -2.925395 1.593565 0.841991
C -5.496270 -0.396595 1.861023
H -5.982435 -2.319687 1.023547
H -4.800298 1.540637 2.496578
H -6.315146 -0.417258 2.573379
O -1.868818 1.075691 -1.518761
O -2.279829 -1.363924 -2.093485

C 2.248098 1.042383 1.213669
H 1.559520 0.223422 1.457302
H 2.340894 1.659645 2.121404
C 3.607924 0.471697 0.817279
H 3.536284 -0.035639 -0.151388
H 4.344389 1.274205 0.708891
C 4.089910 -0.527938 1.853876
H 3.350829 -1.339257 1.946229
H 4.177072 -0.037297 2.835606
C 1.608359 1.854624 0.137213
C 0.065192 3.341927 -0.499430
C 1.451702 3.963459 -0.684481
H -0.347489 2.932862 -1.426149
H -0.662003 4.010845 -0.038210
H 1.632490 4.331153 -1.695946
H 1.649350 4.761872 0.038257
O 5.345312 -1.029697 1.425822
H 5.665371 -1.650184 2.094541
O 0.334778 2.278550 0.411731
O 2.337027 2.873878 -0.416434

TS4b

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1625.02192327

Zero-point correction = 0.422310

Thermal correction to Energy = 0.449118

Thermal correction to Enthalpy = 0.450062

Thermal correction to Gibbs Free Energy = 0.361971

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1625.48021654

C -3.314137 -2.976565 -0.104398
H -4.342051 -2.675424 0.097655
H -3.067411 -3.904699 0.416985
H -3.170368 -3.124408 -1.176481
O -2.481087 -1.913747 0.365338
C -1.181736 -2.025431 0.017815
O -0.763368 -2.931042 -0.670693
C -0.337010 -0.926555 0.540840
C -0.809277 -0.022380 1.417955
H -1.802006 -0.138511 1.835556
H -0.170553 0.742595 1.843434
C 1.032358 -0.874136 -0.078846
H 1.046310 -0.229239 -0.965637
H 1.364335 -1.877785 -0.357387
S 2.287802 -0.202826 1.022403
C 3.769778 -0.384849 0.047189
C 4.606312 -1.467794 0.294503
C 4.043582 0.548058 -0.949008
C 5.750063 -1.619136 -0.484783
H 4.360810 -2.161060 1.092830
C 5.186640 0.382928 -1.724015
H 3.374267 1.390004 -1.100179
C 6.035271 -0.698745 -1.491065
H 6.419401 -2.453939 -0.304607
H 5.419069 1.099507 -2.505002
H 6.927576 -0.822135 -2.096794
O 2.044899 1.236620 1.187643
O 2.408093 -1.061441 2.197039
C -2.430803 1.320030 -1.017492

H -2.053280 0.354884 -1.379391
H -2.638708 1.933185 -1.909135
C -3.702492 1.102198 -0.201114
H -3.422851 0.654649 0.758350
H -4.167949 2.068343 0.026536
C -4.686807 0.170800 -0.902095
H -4.151277 -0.714304 -1.264838
H -5.138819 0.649739 -1.778380
C -1.332604 1.935026 -0.219661
C 0.500647 3.258457 -0.427582
C -0.334183 3.644365 0.789555
H 1.545615 3.070105 -0.184821
H 0.409682 3.990642 -1.237786
H 0.063036 3.177575 1.697895
H -0.458456 4.717435 0.933515
O -0.109275 2.033764 -0.842016
O -1.606680 3.082328 0.468371
C -5.779947 -0.305367 0.037008
H -6.440459 0.531399 0.309958
H -5.316514 -0.678095 0.965097
O -6.498548 -1.337069 -0.616980
H -7.240437 -1.595964 -0.054267

TS4c

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2231.66775016

Zero-point correction = 0.387034

Thermal correction to Energy = 0.413285

Thermal correction to Enthalpy = 0.414229

Thermal correction to Gibbs Free Energy = 0.327771

Single point energy calculation: $E[\text{uM062X(D3)}/6\text{-311++G(2d,p)}] = -2232.12667949$

C -2.838441 -3.630953 0.337479
H -3.896604 -3.431258 0.509954
H -2.456768 -4.371886 1.044547
H -2.668753 -3.993840 -0.678828
O -2.181523 -2.380971 0.534088
C -0.898307 -2.320836 0.123430
O -0.338619 -3.252313 -0.416581
C -0.276165 -1.010296 0.395856
C -0.925261 -0.036693 1.098931
H -1.852711 -0.273429 1.607966
H -0.378182 0.824462 1.465338
C 1.094625 -0.842058 -0.190482
H 1.105803 -0.162107 -1.050940
H 1.496839 -1.814500 -0.486530
S 2.265498 -0.126209 0.981259
C 3.806813 -0.223918 0.089542
C 4.625521 -1.331389 0.286544
C 4.142432 0.795691 -0.796166
C 5.813719 -1.418999 -0.432873
H 4.333729 -2.092780 1.003284
C 5.332088 0.694728 -1.510937
H 3.486056 1.654162 -0.901459
C 6.161966 -0.410587 -1.329693
H 6.469762 -2.271430 -0.290123
H 5.614943 1.480408 -2.203956
H 7.089965 -0.483775 -1.888172
O 1.941042 1.298296 1.135564

O 2.361393 -0.990092 2.153718
C -2.825050 0.456936 -1.143465
H -2.168805 -0.358597 -1.479728
H -3.171491 0.978315 -2.049337
C -4.028925 -0.128204 -0.404800
H -3.719680 -0.561090 0.550139
H -4.770528 0.650950 -0.196669
C -4.678161 -1.232242 -1.220476
H -3.907083 -1.955732 -1.528807
H -5.126019 -0.813956 -2.134645
C -1.982081 1.403768 -0.326554
C -0.290539 3.355236 0.131864
C -1.628481 3.899439 0.614855
H 0.270890 2.850311 0.921420
H 0.329864 4.150605 -0.288338
H -1.529213 4.385892 1.587860
H -2.041911 4.610617 -0.104091
O -5.658795 -1.852079 -0.408022
H -6.149273 -2.483464 -0.951251
S -2.805554 2.509764 0.790977
S -0.646402 2.165297 -1.196367

TS4d

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2270.96062176

Zero-point correction = 0.416332

Thermal correction to Energy = 0.443656

Thermal correction to Enthalpy = 0.444600

Thermal correction to Gibbs Free Energy = 0.356159

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2271.43169415

C 3.052574 -3.163150 -1.122928
H 3.823422 -3.035490 -1.883090
H 2.422780 -4.023494 -1.356153
H 3.511579 -3.306329 -0.140181
O 2.279016 -1.962409 -1.158944
C 1.121722 -2.014247 -0.465615
O 0.801594 -2.982385 0.193480
C 0.293474 -0.801322 -0.613372
C 0.743834 0.324239 -1.242967
H 1.685055 0.294348 -1.780674
H 0.042729 1.095776 -1.536600
C -1.045238 -0.874889 0.060625
H -1.115877 -0.219440 0.937139
H -1.268202 -1.902936 0.356474
S -2.387256 -0.341245 -1.025150
C -3.825437 -0.608706 -0.005638
C -4.531945 -1.799462 -0.138793
C -4.191028 0.369915 0.914275
C -5.636635 -2.014600 0.680377
H -4.221187 -2.526046 -0.883108
C -5.294892 0.140760 1.729467
H -3.624111 1.294535 0.969818
C -6.012674 -1.048737 1.611949
H -6.205805 -2.933918 0.589027
H -5.599242 0.891482 2.451527
H -6.874662 -1.221892 2.248685
O -2.265868 1.107563 -1.233753
O -2.462313 -1.245097 -2.169094

C 2.250915 0.915600 1.248332
H 1.616164 0.060440 1.521017
H 2.478392 1.449723 2.182654
C 3.548249 0.401487 0.621065
H 3.370345 0.136429 -0.426603
H 4.301990 1.199525 0.628545
C 4.068621 -0.835742 1.345743
H 3.298349 -1.618027 1.329135
H 4.273035 -0.619322 2.401211
C 1.437861 1.805021 0.344089
C -0.376864 3.572846 -0.314780
C 0.944058 4.261891 -0.638151
H -0.783207 3.012911 -1.160842
H -1.125706 4.295285 0.018548
H 0.914320 4.732077 -1.623632
H 1.179374 5.017518 0.114860
S 2.286917 3.016257 -0.639898
S -0.055757 2.424494 1.055011
C 5.321058 -1.391050 0.694202
H 6.164742 -0.701225 0.847951
H 5.157042 -1.474357 -0.392303
O 5.581173 -2.658326 1.269245
H 6.401474 -3.003563 0.892432

TSS

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -612.986656724

Zero-point correction = 0.191987

Thermal correction to Energy = 0.202578

Thermal correction to Enthalpy = 0.203522

Thermal correction to Gibbs Free Energy= 0.153735

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -613.182718928

H	0.067515	-2.351809	-0.149925
C	0.846166	-1.596755	-0.089497
C	2.793970	0.384639	0.053631
C	0.480115	-0.252666	-0.013849
C	2.188559	-1.948945	-0.098398
C	3.163568	-0.952542	-0.024932
C	1.445506	0.746626	0.058764
H	2.478538	-2.992573	-0.166145
H	4.215391	-1.221541	-0.035277
H	3.556135	1.158157	0.108122
C	1.029811	2.204600	0.217241
H	1.120198	2.479810	1.281393
H	1.745627	2.825256	-0.344293
O	-0.234115	2.483708	-0.288629
C	-0.970329	0.126291	0.004886
O	-1.669253	-0.340394	-1.095902
C	-3.033821	-0.302267	-0.707004
C	-2.962318	-0.686725	0.775392
O	-1.638835	-0.312758	1.148616
H	-3.433570	0.710272	-0.842872
H	-3.589239	-1.006322	-1.326938
H	-3.077375	-1.764300	0.930978
H	-3.686207	-0.150162	1.393350
H	-0.946746	1.335233	-0.018486

TS6

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1738.10886828

Zero-point correction = 0.417157

Thermal correction to Energy = 0.444703

Thermal correction to Enthalpy = 0.445647

Thermal correction to Gibbs Free Energy = 0.356277

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1738.59371389

H	0.555119	0.300279	2.388480
C	1.533653	-0.072187	2.105657
C	4.058492	-0.969465	1.394856
C	2.229278	0.570060	1.068341
C	2.095289	-1.148001	2.780905
C	3.365422	-1.592597	2.432890
C	3.503742	0.091875	0.688574
H	1.540979	-1.632257	3.578353
H	3.816286	-2.429667	2.956671
H	5.039215	-1.325032	1.100712
C	4.252142	0.676888	-0.484945
H	3.561200	0.785617	-1.330961
H	4.615183	1.683428	-0.233579
C	1.533788	1.614714	0.341950
O	0.355781	2.069298	0.854415
C	0.085220	3.362363	0.308877
C	1.256941	3.600838	-0.657103
O	2.221736	2.629962	-0.251714
H	-0.882986	3.331256	-0.192989
H	0.070278	4.080483	1.133079
H	1.713209	4.586367	-0.561658
H	0.975511	3.424813	-1.699830

O 5.327008 -0.181953 -0.819910
H 5.807261 0.222645 -1.553661
C 0.667266 0.480072 -1.468181
H 0.030548 1.342633 -1.634613
H 1.597425 0.427270 -2.021453
C 0.141260 -0.658513 -0.938533
C -1.181128 -0.708522 -0.234008
H -1.511671 -1.744285 -0.118658
H -1.143979 -0.231599 0.753641
S -2.483400 0.171791 -1.117112
C -3.915285 -0.150522 -0.103463
C -6.096015 -0.681798 1.496685
C -4.161608 0.668221 0.994723
C -4.738989 -1.225033 -0.423131
C -5.838939 -1.487174 0.388679
C -5.262798 0.394021 1.799609
H -3.506737 1.510839 1.194458
H -4.520739 -1.824778 -1.301357
H -6.497516 -2.317014 0.153991
H -5.475029 1.022292 2.658584
H -6.955346 -0.890841 2.126196
O -2.205419 1.612310 -1.024032
O -2.696760 -0.451045 -2.419927
C 0.943398 -1.891318 -0.838442
O 0.555392 -2.929043 -0.342632
O 2.180185 -1.736024 -1.351429
C 3.056163 -2.847846 -1.191007
H 2.784324 -3.646333 -1.886773
H 3.000925 -3.226600 -0.168690

H 4.053803 -2.462670 -1.401903

TS7

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -1738.12274087

Zero-point correction = 0.415791

Thermal correction to Energy = 0.441669

Thermal correction to Enthalpy = 0.442613

Thermal correction to Gibbs Free Energy = 0.358718

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -1738.60156904

H -3.152351 -1.921519 -1.943097

C -2.735469 -2.023517 -0.945988

C -1.627030 -2.251655 1.592903

C -2.464364 -0.872178 -0.212584

C -2.456205 -3.285103 -0.418962

C -1.904075 -3.396812 0.851219

C -1.904853 -0.985323 1.078727

H -2.665400 -4.173783 -1.005962

H -1.675714 -4.374143 1.264151

H -1.187245 -2.327325 2.582101

C -1.493601 0.242968 1.822049

H -2.276095 0.991471 1.939744

C -2.737013 0.506396 -0.820053

O -3.545933 0.393227 -1.975532

C -4.901694 0.381543 -1.546281

C -4.831119 0.809714 -0.064009

O -3.507495 1.296704 0.065772

H -5.456640 1.088612 -2.167623

H -5.334363 -0.618476 -1.659673

H -4.997435 -0.042116 0.606636
H -5.515698 1.618601 0.194361
O -0.804373 0.081561 2.992228
H 0.063841 -0.309372 2.771995
C -1.483765 1.302670 -1.227944
H -1.293163 1.037836 -2.275716
H -1.773043 2.355078 -1.195047
C -0.213688 1.077928 -0.419781
C 0.592403 -0.108714 -0.891486
H -0.057109 -0.921479 -1.227255
H 1.264662 0.180190 -1.709473
S 1.662934 -0.932399 0.340097
C 3.342297 -0.651417 -0.184972
C 5.950889 -0.290575 -0.990674
C 4.072900 0.397011 0.362986
C 3.888517 -1.532304 -1.114428
C 5.204742 -1.340857 -1.522185
C 5.390598 0.570687 -0.049237
H 3.606060 1.056502 1.084674
H 3.294905 -2.361484 -1.486467
H 5.650403 -2.017173 -2.244283
H 5.980601 1.381074 0.366059
H 6.979203 -0.146652 -1.307729
O 1.505093 -0.277309 1.648047
O 1.403865 -2.365686 0.208511
C 0.621999 2.254044 -0.115071
O 1.837791 2.246575 -0.124310
O -0.102297 3.334632 0.221062
C 0.664724 4.475148 0.599491

H 1.309625 4.792214 -0.223050

H 1.285275 4.242317 1.467457

H -0.059358 5.251088 0.842267

H -0.748283 0.781361 0.895847

TS8

Geometry optimization + frequency calculation: E[uM062X(D3)/6-31G(d)] = -2863.22403452

Zero-point correction = 0.640040

Thermal correction to Energy = 0.683398

Thermal correction to Enthalpy = 0.684342

Thermal correction to Gibbs Free Energy = 0.554266

Single point energy calculation: E[uM062X(D3)/6-311++G(2d,p)] = -2863.99065891

H -2.648788 -0.605759 -2.322784

C -1.972336 0.112928 -1.874099

C -0.268523 1.951715 -0.678766

C -1.148261 -0.310496 -0.835256

C -1.970137 1.438982 -2.302572

C -1.126211 2.362218 -1.686864

C -0.251416 0.612460 -0.238871

H -2.630564 1.748960 -3.105976

H -1.126557 3.400270 -2.004116

H 0.413177 2.657050 -0.215610

C 0.756311 0.208180 0.713065

H 0.734578 -0.775613 1.167209

C -1.306169 -1.723711 -0.292136

O -2.005247 -2.504691 -1.237645

C -1.467448 -3.818400 -1.162927

C 0.007458 -3.536828 -0.898987

O -0.043261 -2.354247 -0.108002
H -1.944673 -4.379762 -0.350394
H -1.663319 -4.315279 -2.114278
H 0.555517 -3.340806 -1.827720
H 0.527915 -4.308433 -0.331468
O 1.353681 1.203869 1.421011
H 2.054078 0.807282 1.960803
C -2.010229 -1.771249 1.078901
H -1.968678 -2.812654 1.413870
H -1.429071 -1.177964 1.792629
C -3.483503 -1.325596 1.128888
C -3.691531 0.177033 0.943376
H -2.935304 0.766492 1.469729
H -3.702731 0.465622 -0.106986
S -5.286172 0.659085 1.650467
C -5.782627 2.033224 0.629100
C -6.513593 4.144788 -0.981685
C -6.262770 1.768691 -0.651471
C -5.664574 3.326003 1.123413
C -6.038525 4.389211 0.304313
C -6.626510 2.838967 -1.460442
H -6.350622 0.739774 -0.989621
H -5.297787 3.480006 2.133186
H -5.960842 5.407252 0.671881
H -7.006179 2.657217 -2.460735
H -6.802897 4.976852 -1.616096
O -6.219235 -0.442603 1.412796
O -5.061312 1.157591 3.006907
C -4.279573 -2.192540 0.163403

O -4.431036 -3.377578 0.322188
O -4.729651 -1.520436 -0.906815
C -5.365969 -2.338359 -1.885506
H -6.226509 -2.849298 -1.450050
H -4.656258 -3.078226 -2.263928
H -5.678755 -1.663288 -2.681469
H -3.845294 -1.612347 2.123030
C 3.430856 -0.732600 0.103317
C 4.469871 0.273310 0.478436
H 4.061571 1.285446 0.564078
H 5.025362 0.002208 1.378614
S 5.690005 0.365295 -0.872333
C 6.955925 1.428171 -0.204421
C 8.877042 3.073204 0.891958
C 7.983442 0.859675 0.543092
C 6.872235 2.799850 -0.422034
C 7.845506 3.624936 0.134424
C 8.949467 1.695600 1.094287
H 8.024154 -0.218512 0.665063
H 6.068983 3.197214 -1.034763
H 7.803267 4.696872 -0.029136
H 9.763095 1.272759 1.674635
H 9.634715 3.720785 1.322040
O 6.262430 -0.966190 -1.049869
O 5.051381 1.067361 -1.984585
C 3.582424 -2.139056 0.519680
O 2.843546 -3.045090 0.196025
O 4.642517 -2.320128 1.334296
C 4.887168 -3.674541 1.699457

H 5.067078 -4.278486 0.807700
H 4.031951 -4.085920 2.240571
H 5.771948 -3.656716 2.334119
C 2.361827 -0.401910 -0.683338
H 2.325505 0.573804 -1.160335
H 1.742360 -1.192927 -1.092707

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