Supporting Information for

QM/MM Calculated Reactivity Networks Reveal How Cytochrome P450cam and Its T252A Mutant Select Their Oxidation Pathways

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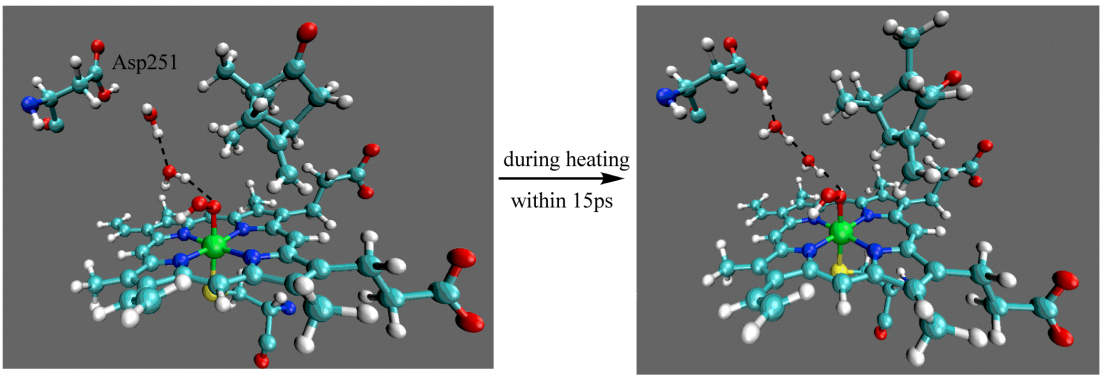

Figure S1. Fast active structure change during the MD simulation for Cpd 0 of T252A. Left: the initial structure; Right: the equilibrated one.

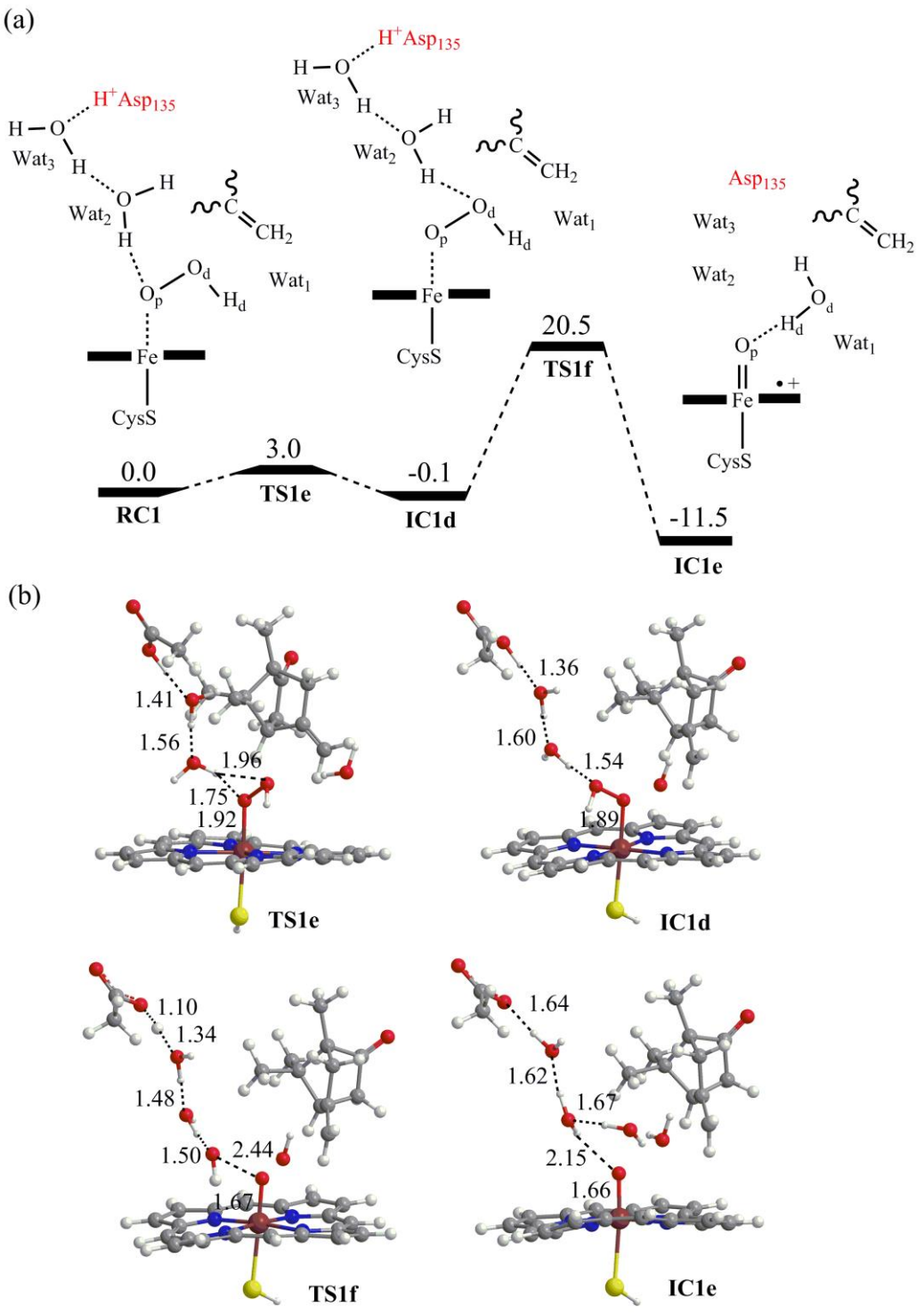

Figure S2. (a) QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the Cpd I formation from Cpd 0 in T252A. (b) Geometrical parameters (in Å) of optimized structures of the species at QM/MM (UB3LYP/B1) calculations.

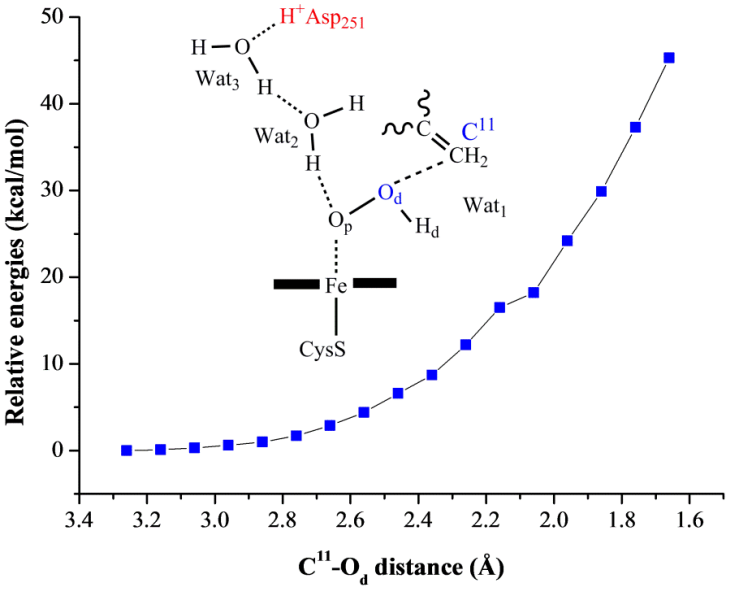

Figure S3. QM/MM(UB3LYP/B1) scanned energy profile (in kcal mol^{-1}) for the concerted nucleophilic attack mechanism of Cpd 0/**S1** in T252A.

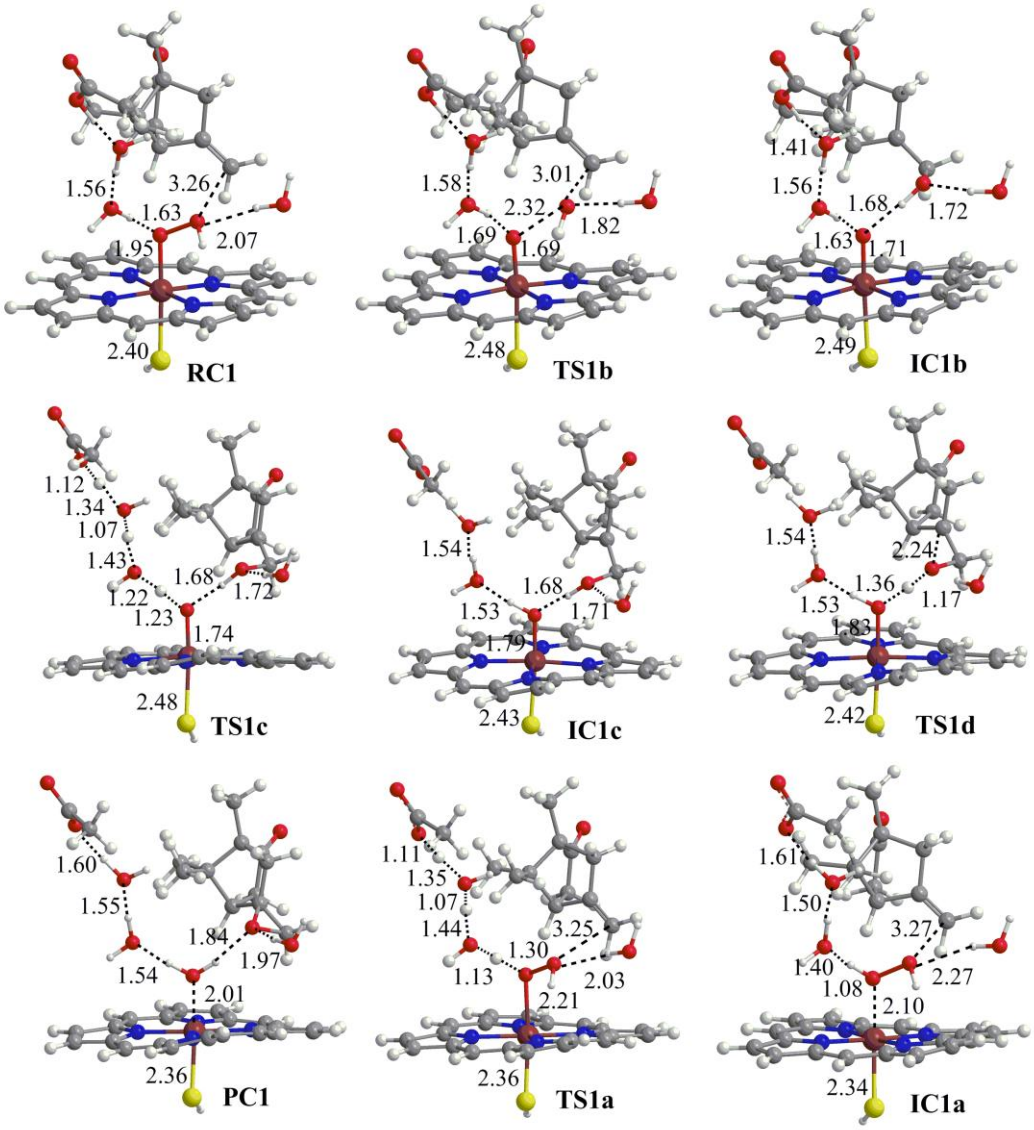

Figure S4. Geometrical parameters (in Å) of optimized structures of the key species at QM/MM(UB3LYP/B1) for the epoxidation of **S1** by the Cpd 0 in T252A.

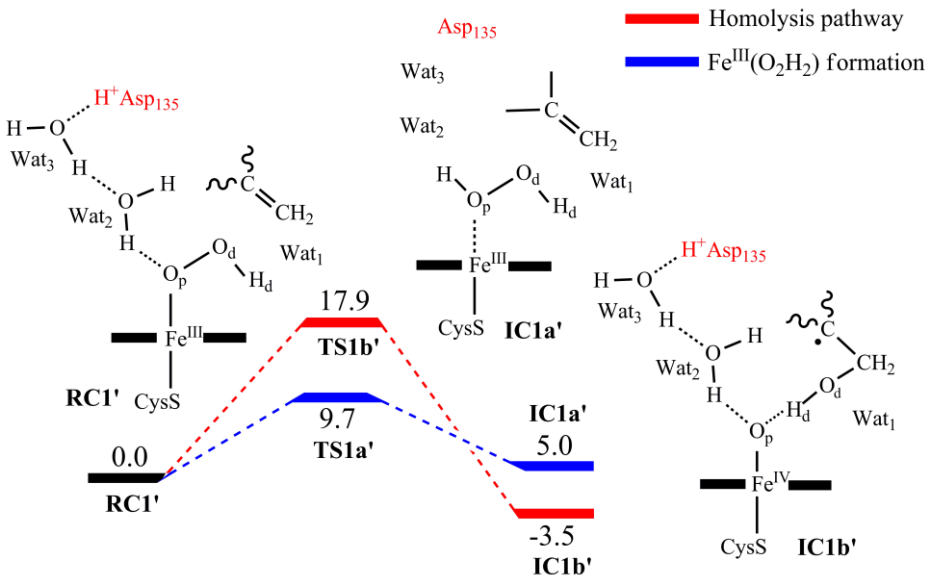

Figure S5. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the competing reactions of Cpd 0 in the presence of **S1** in the second snapshot. Key intermediates along the reaction energy profile are schematically drawn. The blue energy profile generates $Fe^{III}(O_2H_2)$, while the red energy profile corresponds to the homolytic mechanism.

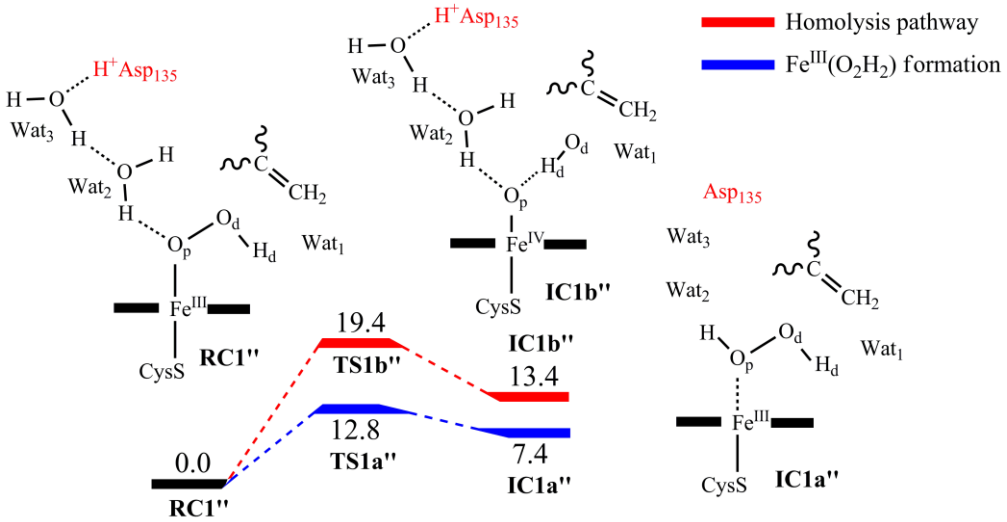

Figure S6. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the competing reactions of Cpd 0 in the presence of **S1** in the third snapshot. Key intermediates along the reaction energy profile are schematically drawn. The blue energy profile generates $Fe^{III}(O_2H_2)$, while the red energy profile corresponds to the homolytic mechanism.

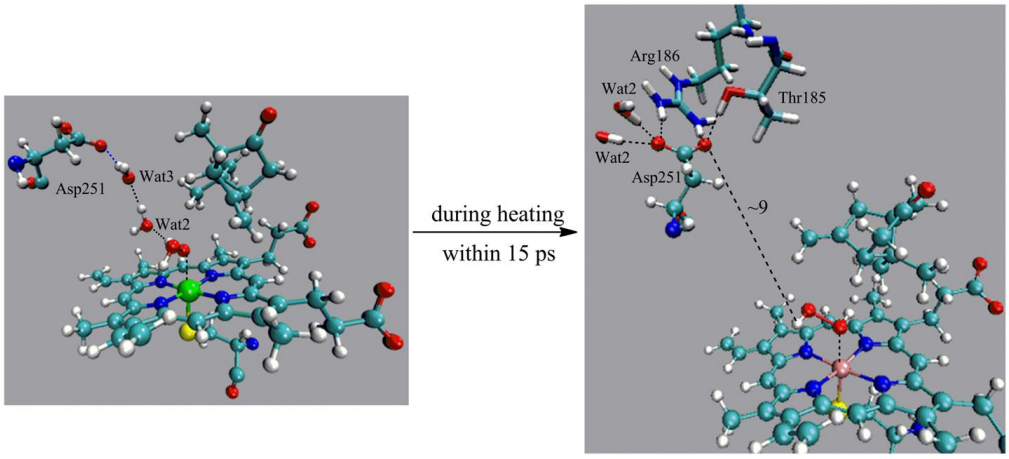

Figure S7. Fast active-site structural change during the MD simulation for $Fe^{III}(O_2H_2)$ in T252A. Left: the initial structure. Right: the equilibrated final structure (the distance is given in Å). In the equilibrated structure, the carboxyl group of Asp251 are strongly H-bonded to Arg186, Thr185 and the nearby water molecules, and the water chain between Op of H_2O_2 and the carboxyl group of Asp251 is completely broken. Using much smoother heating (by increasing the heating time from 15 ps to 150 ps) leads to the same equilibrated structure as the right one.

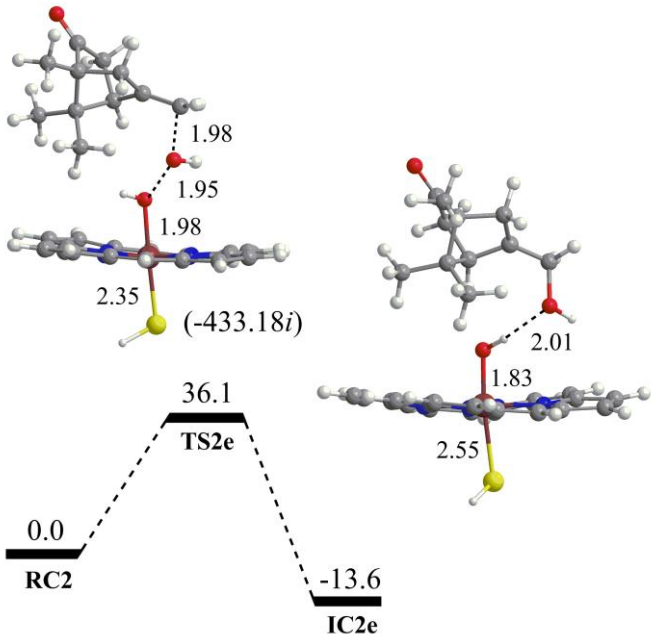

Figure S8. QM/MM(UB3LYP/B2) relative energies (kcal/mol) and geometrical parameters (in Å) of optimized structures of the species at QM/MM (UB3LYP/B1) for the epoxidation of **S1** in T252A via the nucleophilic attack mechanism. The imaginary

frequencies in cm^{-1} are shown underneath the transition state structure.

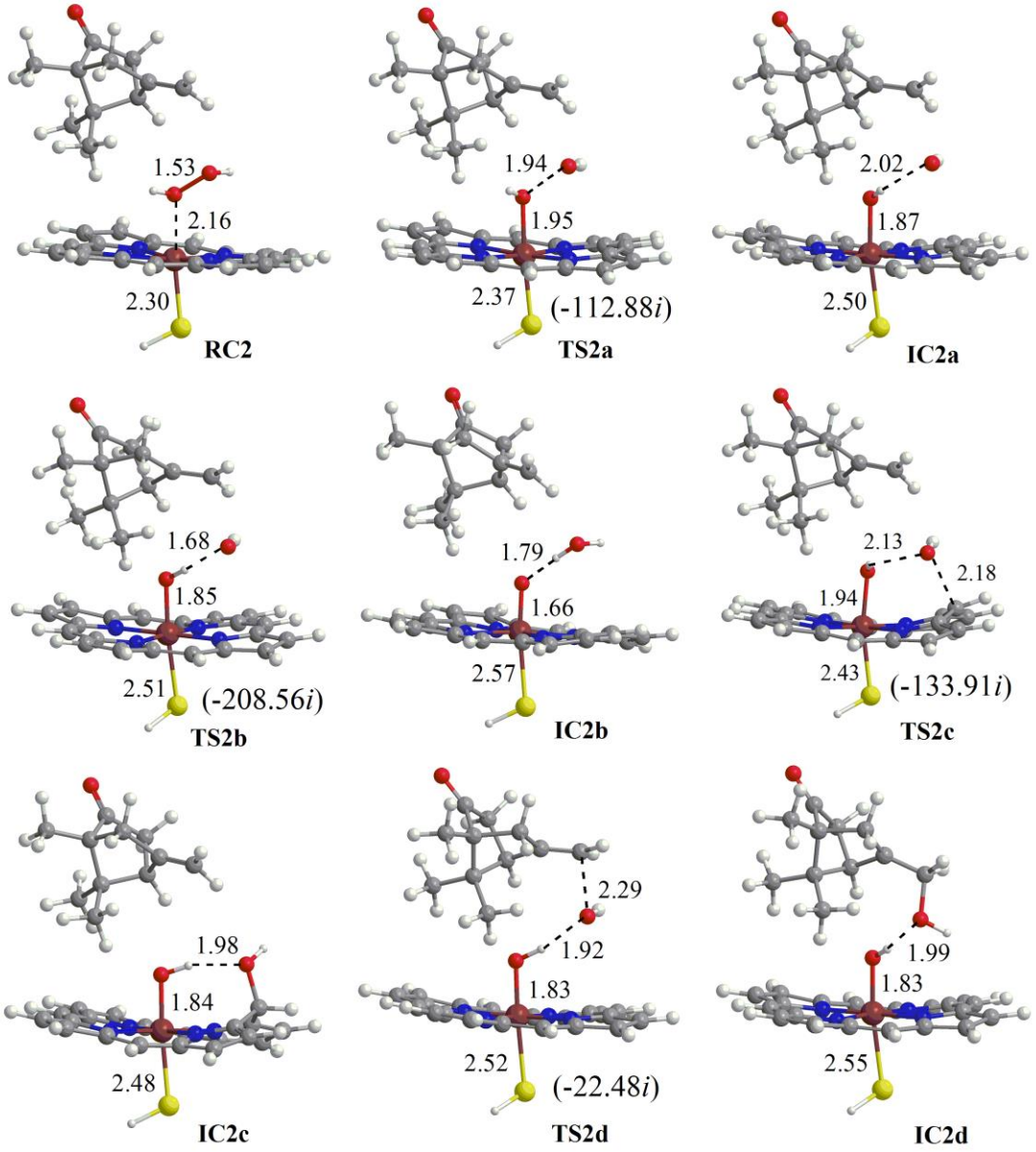

Figure S9. Geometrical parameters (in Å) of optimized structures of the species using QM/MM (UB3LYP/B1) calculations for the reactivity of $Fe^{III}(O_2H_2)$ complex in the presence of **S1** in T252A. The imaginary frequencies in cm^{-1} are shown underneath the transition state structures.

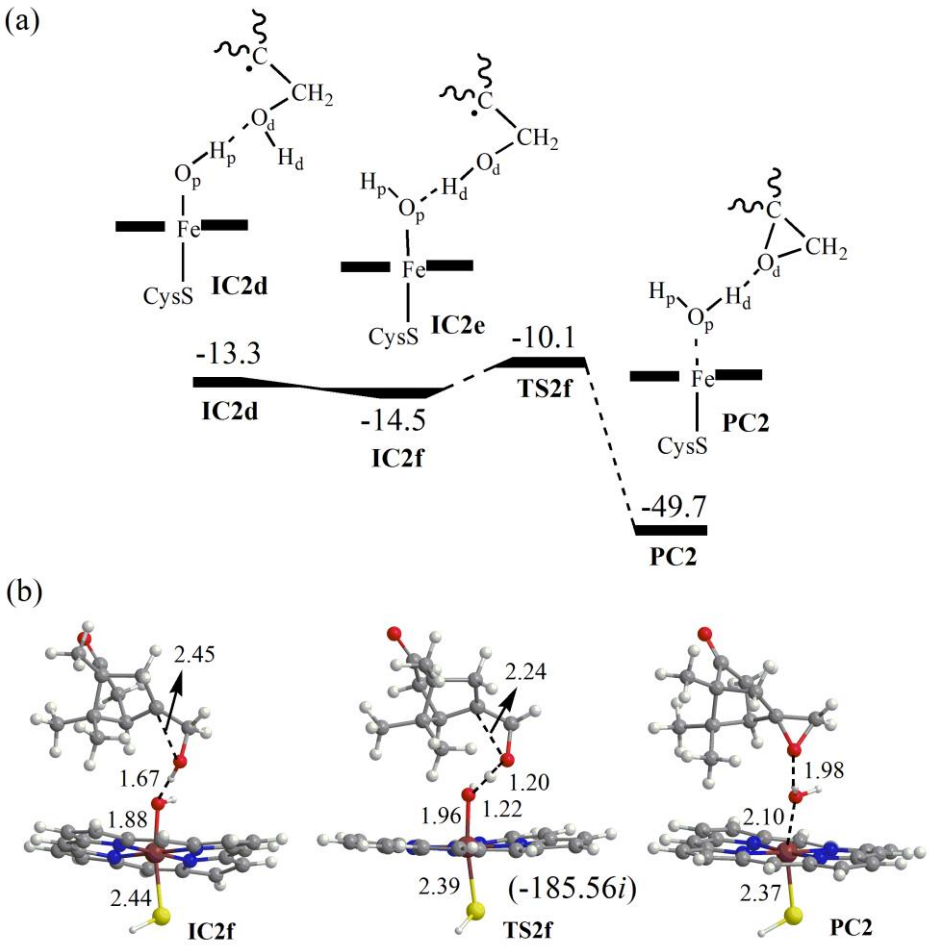

Figure S10. (a) QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the epoxide formation from **IC2d** intermediate in T252A. (b) Geometrical parameters (in Å) of optimized structures of the species at QM/MM (UB3LYP/B1) calculations. The imaginary frequencies in cm^{-1} are shown underneath the transition state structure.

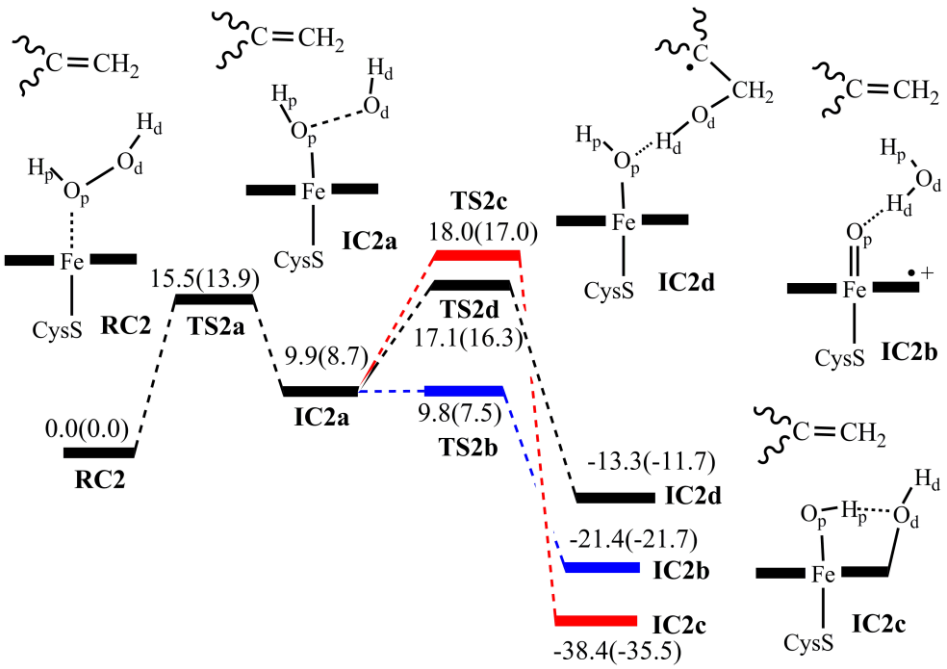

Figure S11. Calculated relative QM/MM energies (kcal/mol) for the reactions of the $Fe^{III}(O_2H_2)$ species in T252A. The relative energies are given as B3LYP/B2//B1(B3LYP/B2//B1+ZPE) in kcal/mol.

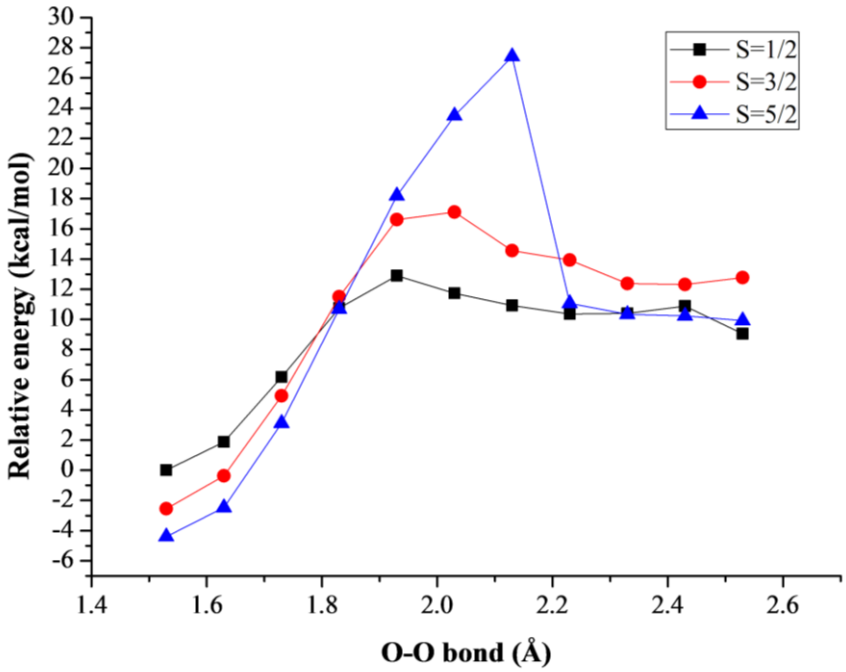

Figure S12. Scanned QM/MM(B3LYP/B1) energy profile (in kcal mol^{-1}) for the O-O homolysis of $Fe^{III}(O_2H_2)$ in its various spin states in T252A.

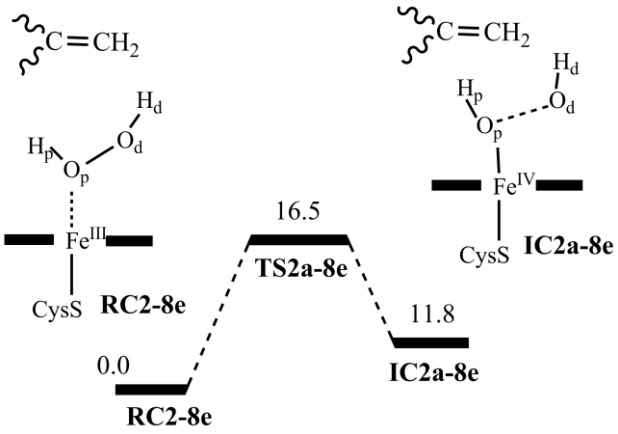

Figure S13. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the O-O homolysis of $Fe^{III}(O_2H_2)$ in T252A without protonation of the surface titratable residues (with a net charge of 8^-).

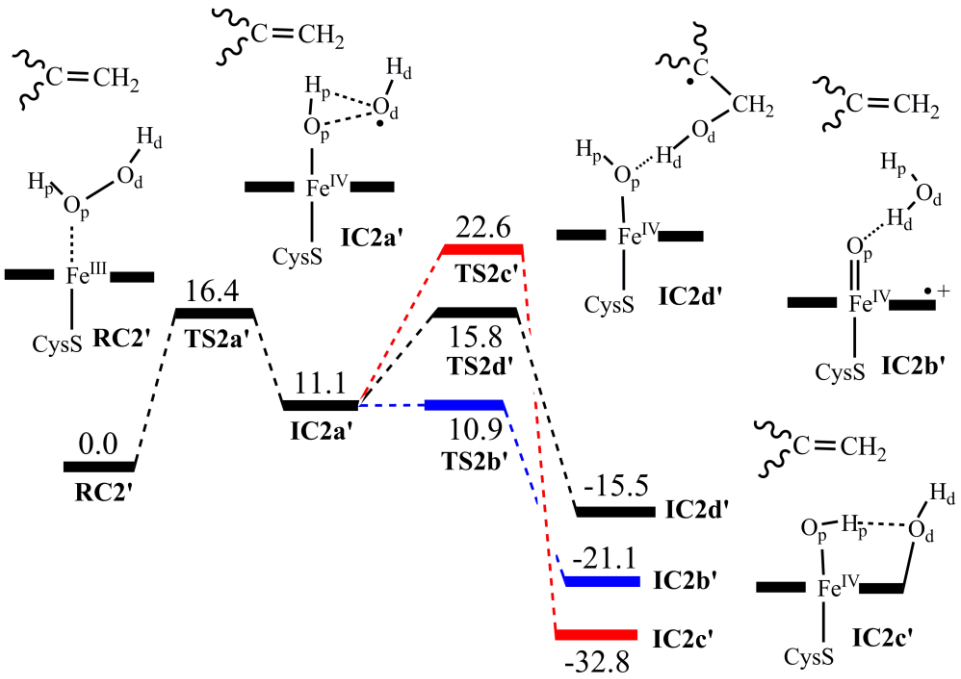

Figure S14. UB3LYP/B2 relative QM/MM energies (kcal/mol) for the reactions of the $Fe^{III}(O_2H_2)$/**S1** in the second snapshot, with schematic drawings of key intermediates along the reaction pathways.

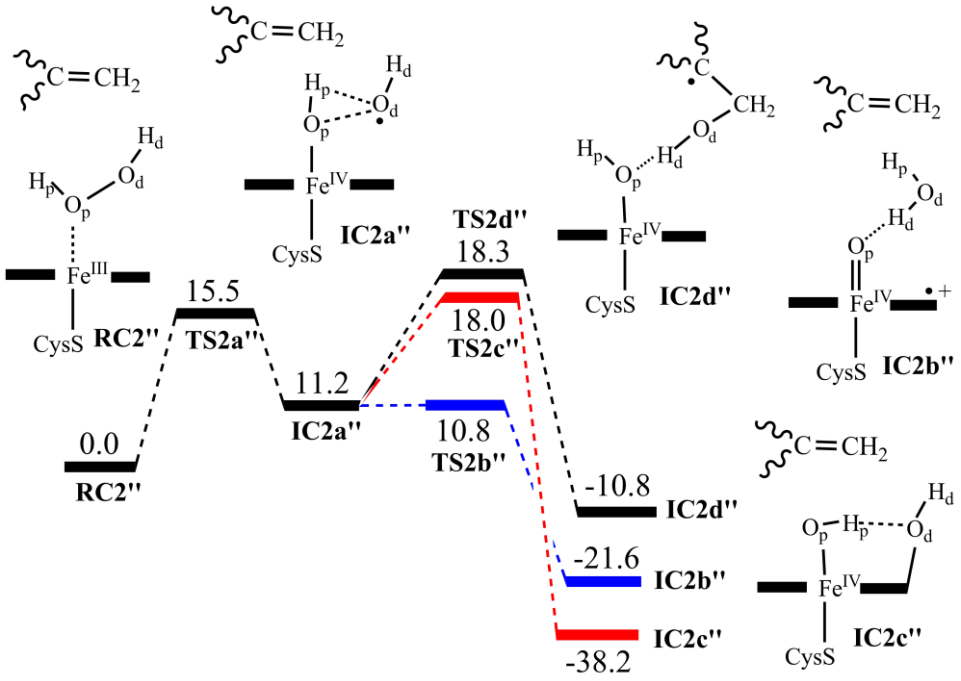

Figure S15. UB3LYP/B2 relative QM/MM energies (kcal/mol) for the reactions of the $Fe^{III}(O_2H_2)$/**S1** in the third snapshot, with schematic drawings of key intermediates along the reaction pathways.

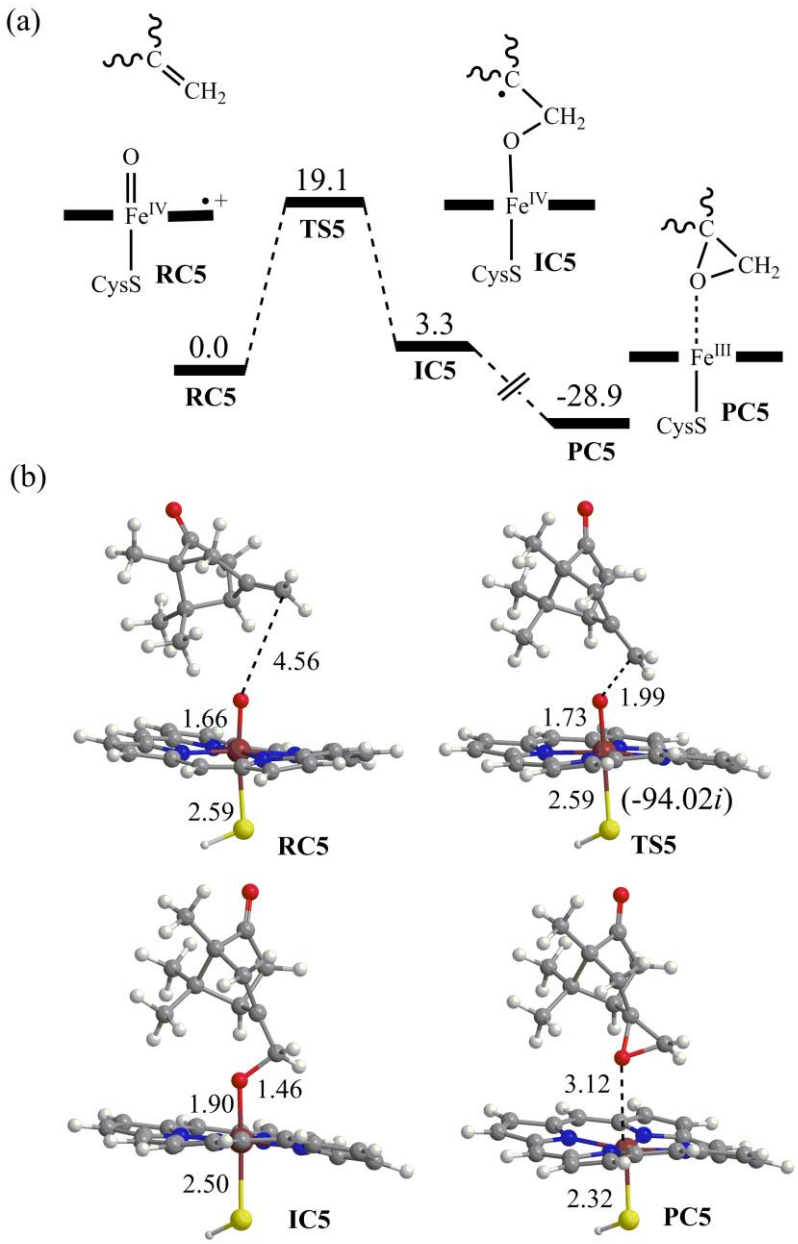

Figure S16. (a) QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the epoxidation of **S1** by Cpd I in T252A. (b) Geometrical parameters (in Å) of optimized structures of the species at QM/MM (UB3LYP/B1) calculations. The imaginary frequencies in cm^{-1} are shown underneath the transition state structure.

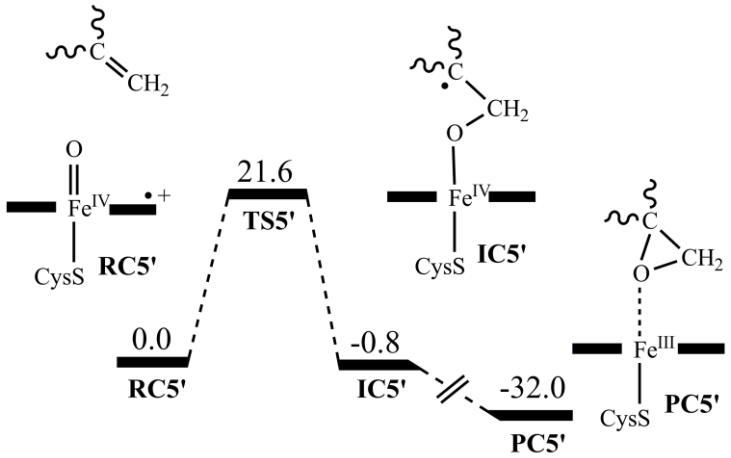

Figure S17. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the epoxidation of **S1** by Cpd I in T252A in the second snapshot.

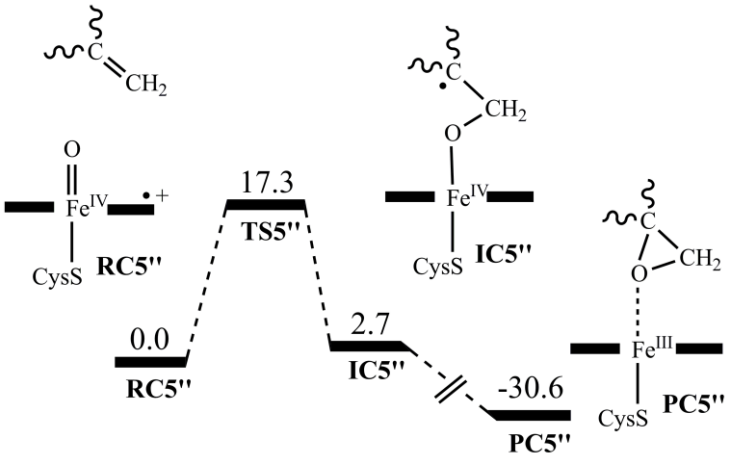

Figure S18. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the epoxidation of **S1** by Cpd I in T252A in the third snapshot.

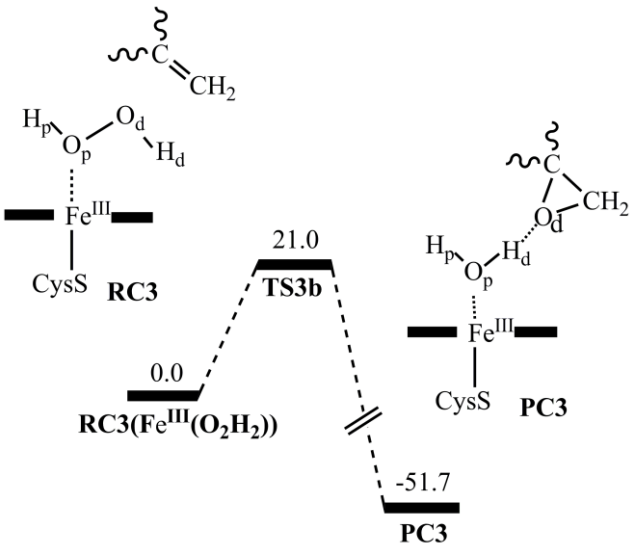

Figure S19. QM/MM(UB3LYP/B2) relative energies (kcal/mol) for the concerted epoxidation of **S1** by the constrained-$Fe^{III}(O_2H_2)$ complex in T252A.

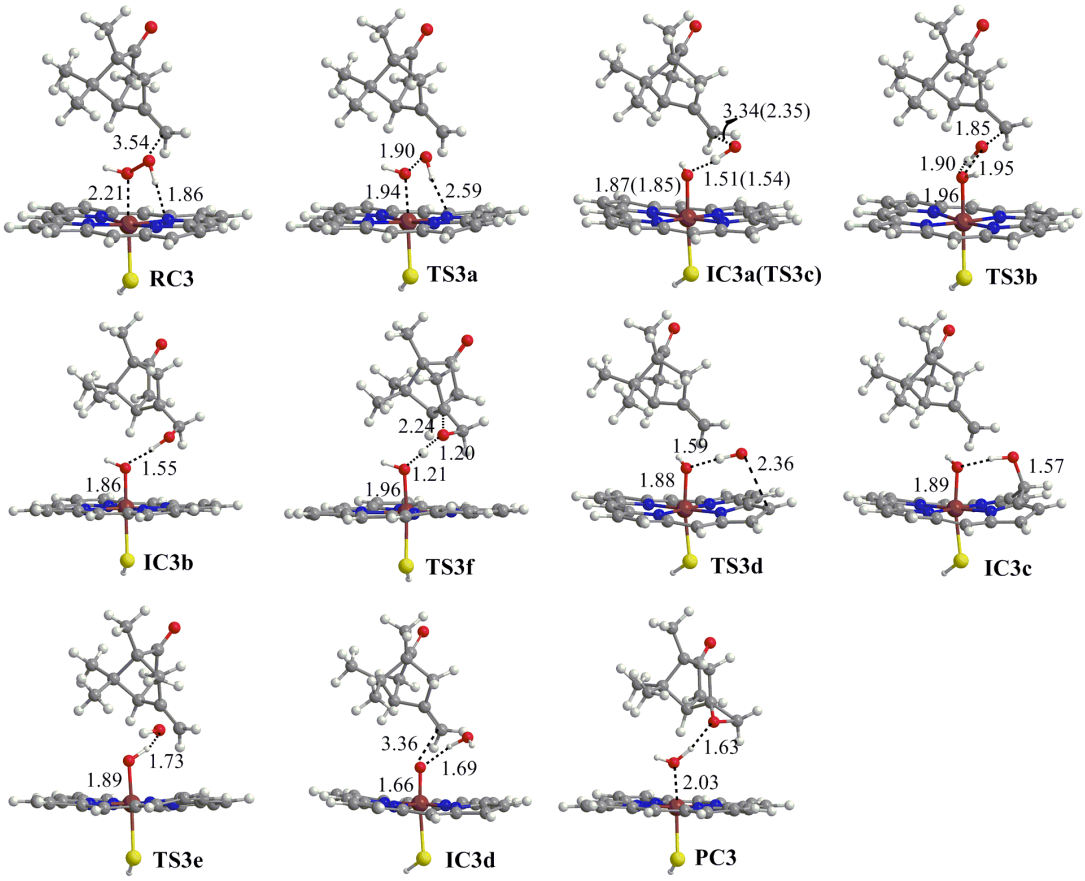

Figure S20. Geometrical parameters (in Å) of optimized structures of the key species using QM/MM (UB3LYP/B1) calculations for the reactions of the constrained-$Fe^{III}(O_2H_2)$ complex in the presence of **S1** in T252A**.**

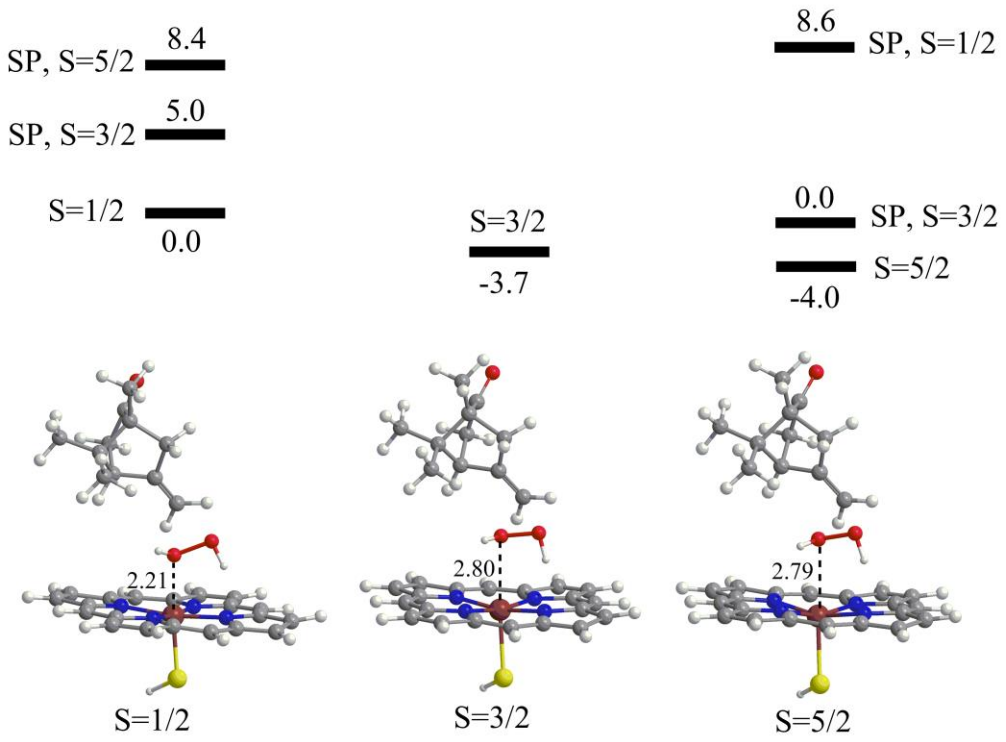

Figure S21. The relative QM/MM(UB3LYP/B2) energies (in kcal/mol) of the various spin states for $Fe^{III}(O_2H_2)$ in the T252A mutant in the presence of **S1**. SP is the single-point energy based on the optimized structure of the lowest energy species.

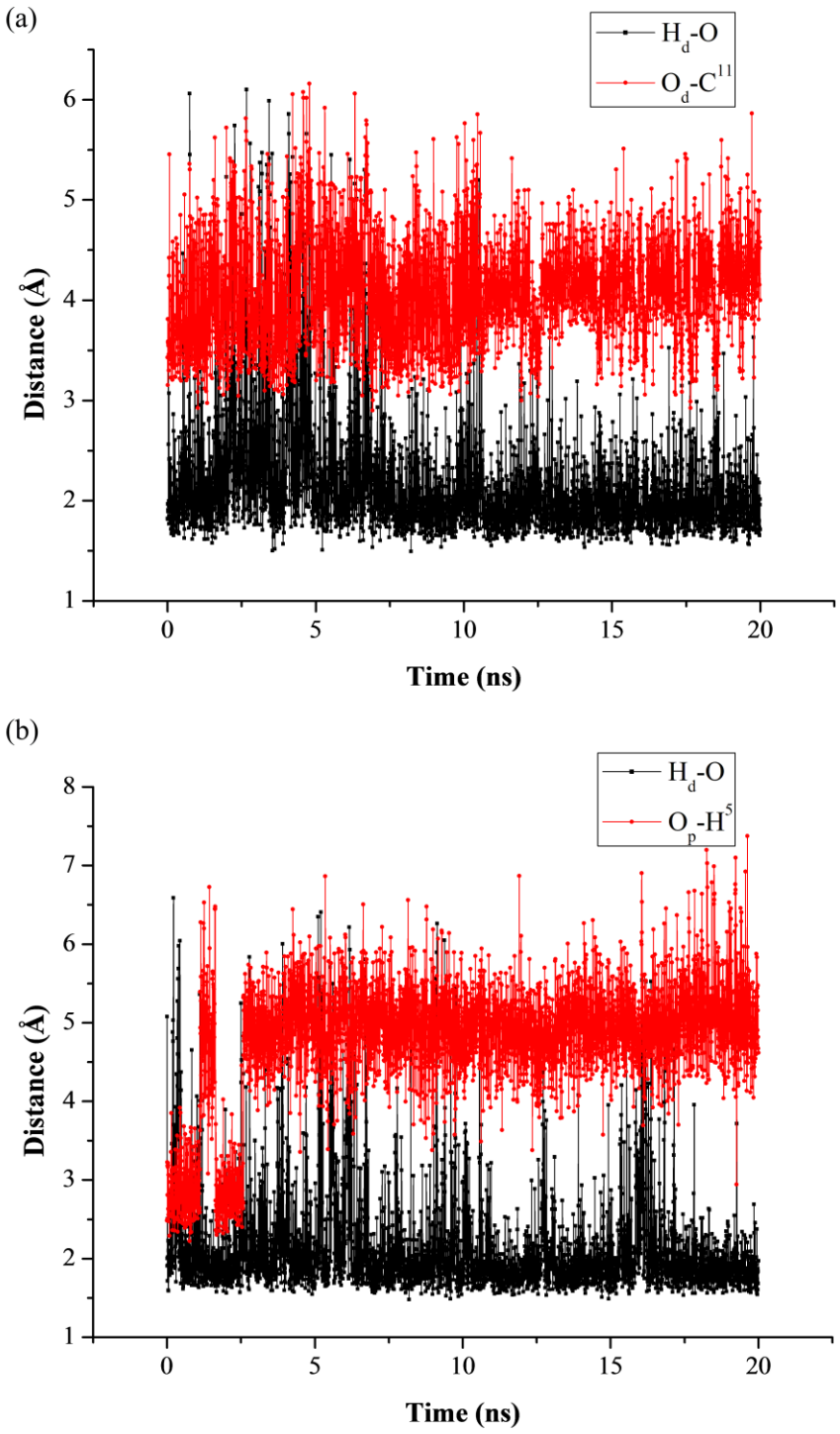

Figure S22. The mobility of substrates and the fluctuation of the H-bond between H_d and the carbonyl oxygen of Gly248 in the P450cam T252A binding pocket: (a) for **S1**, the bulkier **S1** maintains a stable conformation relative to H_2O_2 moiety. (b) for **S2**, the substrate **S2** overturns completely after a short period of MD simulations.

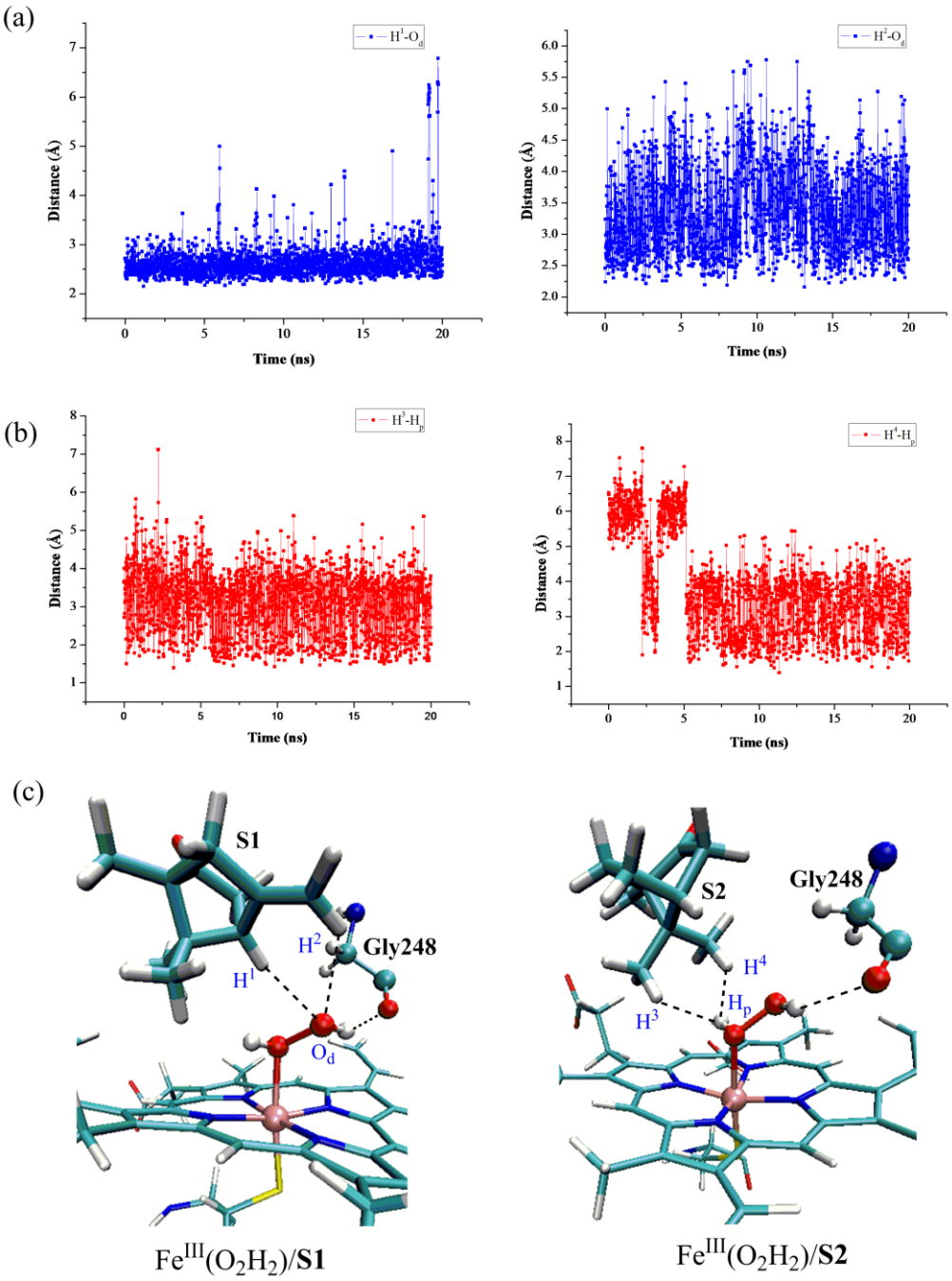

Figure S23. The mobility of substrates and the fluctuation of the key distances in the P450cam T252A binding pocket: (a) for **S1**. (b) for **S2**. (c) the atom labels for substrates.

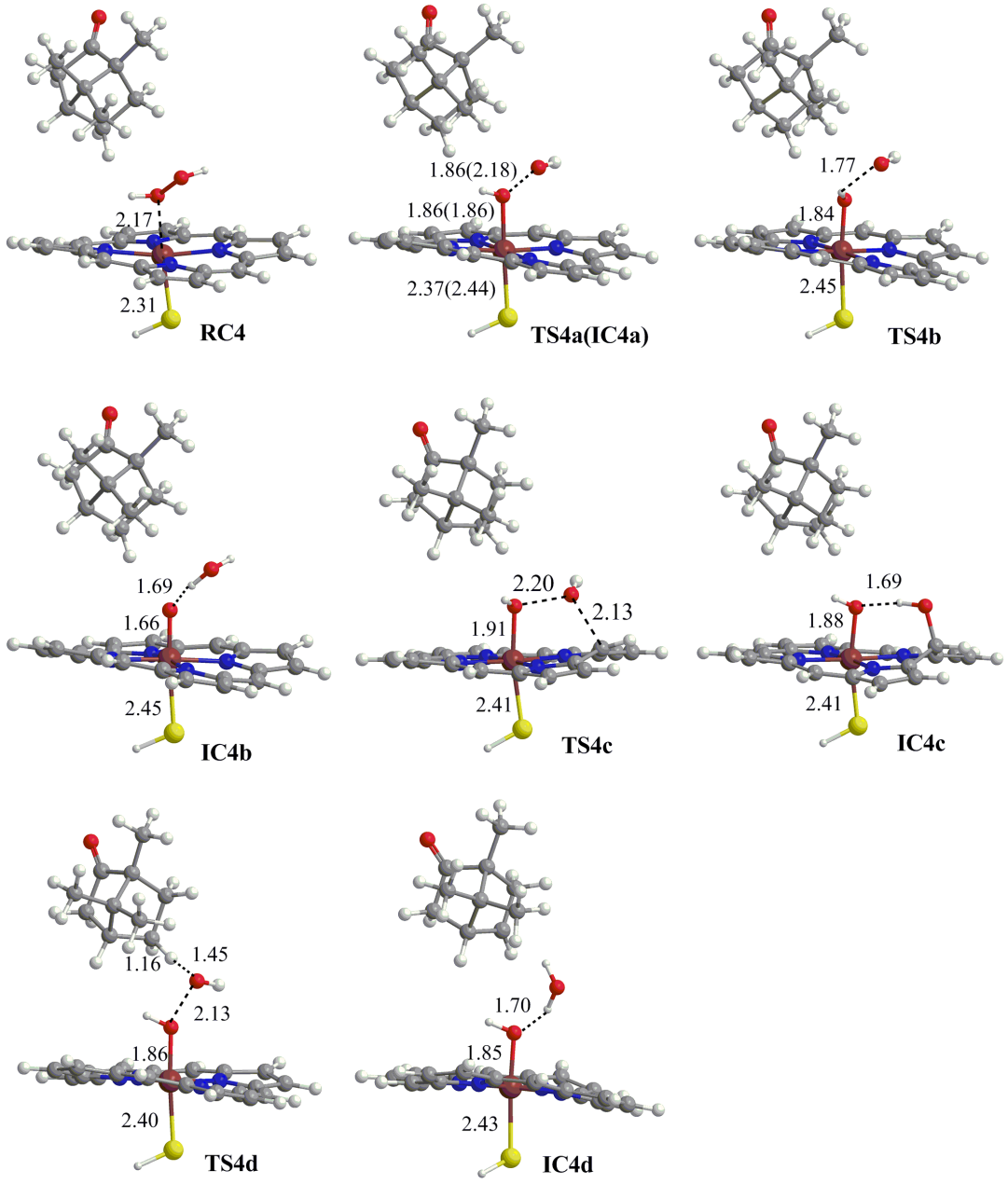

Figure S24. QM/MM(UB3LYP/B1) geometrical parameters (in Å) of optimized structures of the key species for the reactivity of $Fe^{III}(O_2H_2)$ in the presence of **S2** in the WT P450cam.

Total QM/MM energies, as well as Cartesian coordinates of all computed species

RC1

Total QM energy at B2: -3764.202492 (a.u.)

Total QM/MM energy at B2: -3875.029076 (a.u.)

C	2.453420 -6.612238 -1.627079	C	3.718741 -3.577753 5.691743
H	3.049416 -5.781040 -1.249056	C	3.624337 -2.707407 6.940878
H	2.999798 -7.539698 -1.431294	O	3.550778 -3.121534 8.115676
C	1.106329 -6.697243 -0.923138	C	3.726196 -1.252892 6.502636
O	0.342090 -7.683258 -1.073757	H	4.537490 -0.738984 7.030366
O	0.782279 -5.682759 -0.128283	H	2.796144 -0.721725 6.740748
H	1.498047 -4.887063 -0.010705	C	3.043826 -2.633450 4.619618
S	5.094476 4.154667 0.239905	C	3.961772 -1.401632 4.969892
O	4.404064 0.098618 1.628521	H	3.795805 -0.500679 4.379183
O	5.563834 -0.847005 1.304018	C	5.359270 -1.998588 4.831615
H	5.851410 -0.468616 0.437143	C	6.453275 -1.375377 4.390475
Fe	4.741484 1.946676 1.116531	H	6.415296 -0.353872 4.031830
N	3.654476 2.497250 2.738798	H	7.417901 -1.872212 4.334731
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N	5.833330 1.351579 -0.508310	H	5.464257 -4.162042 4.500699
N	6.433514 2.029485 2.217972	H	5.904838 -3.698385 6.145319
C	4.134685 2.780652 4.011307	C	1.544938 -2.409440 4.889144
C	3.028807 3.134380 4.903471	H	1.313561 -2.087397 5.909900
C	1.881734 3.072026 4.144158	H	0.986518 -3.334765 4.702635
C	2.283305 2.677153 2.797015	H	1.159789 -1.648726 4.201014
C	1.745861 2.239290 0.404087	C	3.202837 -3.114963 3.171261
C	0.817047 2.241684 -0.728268	H	2.768994 -4.114180 3.037603
C	1.553556 1.938267 -1.860508	H	4.244179 -3.131954 2.839117
C	2.946200 1.754678 -1.393501	H	2.666911 -2.435474 2.504302
C	5.358785 1.218264 -1.803010	C	3.200529 -4.995632 5.843135
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C	8.662539 1.865833 2.891104	H	3.379898 -4.335112 0.432691
C	7.949994 2.316566 3.982287	H	2.526440 -2.915210 0.214943
C	6.551106 2.402491 3.552424	O	2.583877 -1.367412 0.380378
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H	5.711567 3.020239 5.394118	H	3.276111 -0.828120 0.896035
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H	0.366358 2.731356 1.939623	H	8.431733 -2.675018 2.134219
C	4.041466 1.437552 -2.195966	H	7.478270 -1.420615 1.841272
H	3.855923 1.322252 -3.259313	h	4.731118 5.100796 1.176472
C	8.048113 1.245361 0.520815	h	3.107041 3.366500 5.965575
H	9.102453 1.060435 0.361982	h	0.849971 3.276826 4.429794
		h	-0.234450 2.510454 -0.627351
		h	1.267865 1.835643 -2.907368
		h	6.262113 0.557429 -3.746106

h 8.462888 0.056076 -2.232677
h 9.707682 1.564805 2.819521
h 8.314530 2.530098 4.987068
h 2.436679 -6.533176 -2.714064

TS1a

Total QM energy at B2: -3764.191436 (a.u.)

Total QM/MM energy at B2: -3875.017220 (a.u.)

C 2.448563 -6.600360 -1.622785
H 3.053967 -5.771371 -1.253713
H 2.986502 -7.531073 -1.418854
C 1.103381 -6.659585 -0.908816
O 0.331646 -7.645953 -1.048564
O 0.800396 -5.634043 -0.129832
H 1.546857 -4.818022 -0.009911
S 5.088742 4.163867 0.228201
O 4.354272 -0.124623 1.601289
O 5.603480 -0.932358 1.283478
H 5.893703 -0.489156 0.449429
Fe 4.724844 1.998134 1.099688
N 3.640483 2.513266 2.731283
N 3.012986 1.951032 -0.020793
N 5.811390 1.373432 -0.507540
N 6.407547 2.032185 2.216239
C 4.118682 2.795165 4.007006
C 3.013124 3.141902 4.899746
C 1.865507 3.077148 4.141394
C 2.266323 2.688636 2.793462
C 1.730304 2.257326 0.402028
C 0.802560 2.257496 -0.729689
C 1.539963 1.957940 -1.861949
C 2.931931 1.779788 -1.396154
C 5.340236 1.237599 -1.804410
C 6.402942 0.758114 -2.682854
C 7.525690 0.553003 -1.895357
C 7.169193 1.028664 -0.553613
C 7.686681 1.703786 1.793915
C 8.638604 1.866623 2.889002
C 7.927147 2.320869 3.979691
C 6.530298 2.409819 3.551043
C 5.461218 2.767617 4.366544
H 5.693929 3.031398 5.392519
C 1.394543 2.558999 1.718028
H 0.348353 2.738737 1.938838
C 4.025309 1.462879 -2.199155
H 3.839527 1.344272 -3.261839
C 8.025455 1.248647 0.521968
H 9.078538 1.057338 0.364636
C 3.718681 -3.579362 5.701208
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H 3.793646 -0.511603 4.369736
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H 6.409994 -0.361800 4.021381
H 7.416922 -1.875272 4.332160
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H 5.469442 -4.167504 4.518640
H 5.904078 -3.691448 6.161309
C 1.545286 -2.413578 4.886805
H 1.312294 -2.082398 5.904398
H 0.984794 -3.338486 4.705637
H 1.164392 -1.657638 4.190940
C 3.202332 -3.139974 3.177872
H 2.750990 -4.132632 3.046746
H 4.245359 -3.179905 2.853051
H 2.688400 -2.455419 2.499043
C 3.202930 -4.997598 5.854936
H 3.275909 -5.541566 4.908474
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H 3.775888 -5.547075 6.611540
O 2.535998 -3.919372 0.144116
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H 2.567747 -2.856433 0.233883
O 2.684386 -1.432643 0.413388
H 2.066271 -0.845341 -0.053823
H 3.457061 -0.825927 0.972202
O 8.376842 -1.838948 1.682108
H 8.482481 -2.710709 2.115005
H 7.469785 -1.495199 1.850837
h 4.726733 5.104516 1.170791
h 3.093214 3.371993 5.962154
h 0.833580 3.276248 4.430446
h -0.251069 2.517534 -0.628139

h 1.253933 1.851327 -2.908317
h 6.240290 0.560783 -3.742415
h 8.436936 0.054659 -2.226038
h 9.682507 1.561108 2.818335
h 8.293662 2.531954 4.984269
h 2.431350 -6.529105 -2.710302

IC1a

Total QM energy at B2: -3764.211235 (a.u.)

Total QM/MM energy at B2: -3875.029333 (a.u.)

C 2.389498 -6.678972 -1.680658
H 3.001271 -5.870441 -1.276933
H 2.913319 -7.623856 -1.502358
C 1.026511 -6.730978 -0.972582
O 0.277237 -7.754158 -1.172161
O 0.731443 -5.730473 -0.211638
H 1.784728 -4.537273 0.004008
S 5.080020 4.149513 0.227542
O 4.332692 -0.004908 1.583171
O 5.511099 -0.906613 1.282066
H 5.880509 -0.434060 0.492734
Fe 4.694647 2.008455 1.094282
N 3.612940 2.526597 2.723821
N 2.985494 1.956499 -0.022726
N 5.783908 1.362974 -0.508922
N 6.378689 2.022215 2.211628
C 4.092682 2.803733 4.000625
C 2.988423 3.149329 4.893805
C 1.839745 3.086755 4.136735
C 2.238081 2.702186 2.787932
C 1.701492 2.264122 0.398775
C 0.774554 2.254105 -0.731961
C 1.511889 1.947739 -1.863275
C 2.904444 1.778035 -1.398481
C 5.313207 1.235985 -1.807611
C 6.373058 0.754256 -2.686254
C 7.493519 0.535607 -1.898488
C 7.141463 1.008112 -0.554861
C 7.657758 1.680952 1.793384
C 8.608119 1.843857 2.888746
C 7.897986 2.309603 3.975729
C 6.503011 2.407252 3.545161
C 5.435199 2.771792 4.359407
H 5.668926 3.035766 5.384911
C 1.365952 2.571842 1.713267
H 0.320238 2.752975 1.933248
C 3.998509 1.463448 -2.201457
H 3.812760 1.345906 -3.263810
C 7.996637 1.216559 0.524410
H 9.047450 1.010708 0.371897
C 3.727768 -3.603339 5.713399
C 3.621422 -2.722283 6.953896
O 3.546009 -3.121648 8.133234
C 3.709305 -1.270663 6.501241
H 4.519319 -0.746015 7.020378
H 2.776574 -0.744377 6.739054
C 3.036423 -2.679691 4.633866
C 3.940172 -1.432557 4.968781
H 3.757915 -0.536462 4.375477
C 5.345528 -2.011279 4.830691
C 6.433116 -1.378378 4.385088
H 6.385404 -0.358249 4.023087
H 7.404291 -1.864139 4.336418
C 5.249061 -3.458915 5.323155
H 5.482718 -4.177071 4.528910
H 5.915682 -3.682589 6.166023
C 1.535730 -2.467662 4.907575
H 1.305933 -2.129823 5.923570
H 0.986397 -3.401160 4.738436
H 1.138684 -1.723756 4.207700
C 3.191646 -3.181140 3.192630
H 2.733796 -4.169548 3.066129
H 4.232237 -3.232330 2.861983
H 2.674192 -2.500921 2.513550
C 3.231566 -5.027550 5.874380
H 3.320578 -5.579663 4.934393
H 2.177011 -5.045126 6.174839
H 3.804964 -5.561391 6.641603
O 2.557296 -3.875274 0.132908
H 3.371044 -4.369107 0.379694
H 2.572719 -2.384874 0.301550
O 2.587545 -1.350972 0.434590
H 1.954635 -0.877433 -0.127488
H 3.538692 -0.566098 1.107303
O 8.461137 -1.916282 1.678375
H 8.650991 -2.791664 2.082086
H 7.559978 -1.626812 1.931497
h 4.720522 5.096950 1.164277
h 3.069994 3.376435 5.956742

h 0.807856 3.282075 4.428490
h -0.280724 2.507962 -0.631902
h 1.224460 1.831192 -2.908200
h 6.210715 0.564296 -3.747210
h 8.398793 0.028195 -2.231772
h 9.652002 1.537811 2.820103
h 8.265074 2.522576 4.979699
h 2.390175 -6.575446 -2.765715

TS1b

Total QM energy at B2: -3764.177141 (a.u.)

Total QM/MM energy at B2: -3875.000421 (a.u.)

C 2.457820 -6.625535 -1.636119
H 3.061945 -5.799781 -1.259408
H 3.000498 -7.556807 -1.448312
C 1.117624 -6.706526 -0.919649
O 0.342354 -7.683278 -1.069960
O 0.812963 -5.698053 -0.107486
H 1.538086 -4.917445 0.008832
S 5.059483 4.218591 0.229005
O 4.304945 0.359554 1.592867
O 5.954461 -1.275337 1.462573
H 5.820045 -0.611561 0.743576
Fe 4.663096 1.952730 1.158658
N 3.611687 2.635269 2.753168
N 2.966396 2.025676 -0.010937
N 5.751924 1.392713 -0.475723
N 6.359727 2.075768 2.254776
C 4.088150 2.897326 4.030478
C 2.979277 3.230839 4.921255
C 1.834174 3.172042 4.158484
C 2.238306 2.797828 2.806949
C 1.689909 2.332353 0.421097
C 0.752454 2.303821 -0.704976
C 1.482018 1.986060 -1.836986
C 2.878521 1.824400 -1.377736
C 5.279950 1.262250 -1.770950
C 6.338805 0.762379 -2.642971
C 7.451051 0.531720 -1.849225
C 7.093158 1.009793 -0.505133
C 7.623780 1.698941 1.835616
C 8.581073 1.851012 2.929825
C 7.884285 2.341015 4.013224
C 6.489850 2.463689 3.584213
C 5.428943 2.851801 4.394696
H 5.663564 3.114629 5.420288
C 1.364586 2.656481 1.734111
H 0.319870 2.839141 1.957962
C 3.971332 1.497376 -2.176575
H 3.788199 1.374624 -3.239145
C 7.950971 1.213352 0.572351
H 8.996739 0.983208 0.425145
C 3.721864 -3.543833 5.715209
C 3.610624 -2.697641 6.979730
O 3.537540 -3.133612 8.146899
C 3.693310 -1.233565 6.570969
H 4.496393 -0.719882 7.111136
H 2.755422 -0.719534 6.816701
C 3.039780 -2.588590 4.656999
C 3.940276 -1.351634 5.038332
H 3.763112 -0.440262 4.466246
C 5.345553 -1.929515 4.889526
C 6.426926 -1.291864 4.439734
H 6.374590 -0.267659 4.092770
H 7.390453 -1.783592 4.334831
C 5.245280 -3.392185 5.335603
H 5.480130 -4.085022 4.518743
H 5.906528 -3.646575 6.174220
C 1.536407 -2.390429 4.922560
H 1.294786 -2.090293 5.947616
H 0.991251 -3.319208 4.714306
H 1.145535 -1.621809 4.246438
C 3.213783 -3.041769 3.200747
H 2.804692 -4.049223 3.050240
H 4.254065 -3.021280 2.865921
H 2.659399 -2.367166 2.542913
C 3.220471 -4.970773 5.841413
H 3.307609 -5.500082 4.887728
H 2.166344 -4.993679 6.143982
H 3.794295 -5.524266 6.594429
O 2.592664 -3.979939 0.161546
H 3.447917 -4.384930 0.430619
H 2.613485 -2.960704 0.216538
O 2.714035 -1.392250 0.335724
H 2.128522 -0.772675 -0.132951
H 3.380310 -0.852587 0.864331
O 8.657324 -1.875692 1.671409
H 8.753686 -2.766163 2.070515
H 7.725879 -1.555433 1.780434

h	4.724687 5.182973 1.157565	C	6.480839 2.370947 3.577917
h	3.057192 3.441954 5.987757	C	5.423096 2.773182 4.387412
h	0.800145 3.355073 4.450632	H	5.664359 3.070926 5.402173
h	-0.303393 2.554343 -0.602544	C	1.344453 2.519336 1.751412
h	1.191236 1.857640 -2.879589	H	0.300254 2.703724 1.976866
h	6.180694 0.581915 -3.706221	C	3.959644 1.460280 -2.183293
h	8.355356 0.025208 -2.186486	H	3.780857 1.366378 -3.249581
h	9.616915 1.518723 2.861409	C	7.902807 1.020090 0.588787
h	8.255668 2.555217 5.015351	H	8.938885 0.747533 0.450771
h	2.435119 -6.542186 -2.722675	C	3.712752 -3.532779 5.640951
IC1b		C	3.659795 -2.676391 6.903462
Total QM energy at B2: -3764.214610 (a.u.)		O	3.637495 -3.105241 8.074339
Total QM/MM energy at B2: -3875.040422 (a.u.)		C	3.710667 -1.213140 6.484148
C	2.445450 -6.617411 -1.639866	H	4.529586 -0.688304 6.988124
H	3.044508 -5.793696 -1.251537	H	2.779024 -0.705984 6.766073
H	2.988912 -7.549093 -1.456811	C	2.969768 -2.588391 4.614056
C	1.099835 -6.707394 -0.935663	C	3.892598 -1.342657 4.938613
O	0.337964 -7.695156 -1.084952	H	3.678978 -0.434861 4.372049
O	0.773858 -5.695201 -0.137308	C	5.277787 -1.927859 4.738343
H	1.489528 -4.902078 -0.020368	C	6.379018 -1.325122 3.948331
S	5.078945 4.105381 0.272944	H	6.458389 -0.248345 4.127257
O	4.384803 0.177350 1.548067	H	7.343373 -1.787103 4.183736
O	6.204737 -1.554058 2.491850	C	5.213984 -3.376723 5.176647
H	5.558244 -0.875648 2.114140	H	5.414714 -4.070024 4.346921
Fe	4.640208 1.819426 1.158790	H	5.921546 -3.639362 5.978897
N	3.594468 2.493354 2.763698	C	1.482326 -2.388865 4.953680
N	2.948499 1.919116 -0.003571	H	1.291731 -2.058437 5.979832
N	5.726856 1.295254 -0.479246	H	0.931166 -3.324926 4.801706
N	6.338567 1.942675 2.262591	H	1.054852 -1.642767 4.274997
C	4.079516 2.797298 4.031367	C	3.068692 -3.054062 3.155261
C	2.975545 3.157788 4.917704	H	2.608327 -4.041916 3.026446
C	1.825747 3.076571 4.163329	H	4.098394 -3.091425 2.788749
C	2.221585 2.663821 2.821229	H	2.524804 -2.357727 2.510629
C	1.671118 2.218448 0.433038	C	3.220215 -4.958940 5.806337
C	0.739365 2.233700 -0.696805	H	3.252639 -5.495900 4.853534
C	1.473199 1.954136 -1.837107	H	2.185045 -4.978147 6.168642
C	2.866084 1.769579 -1.379589	H	3.835015 -5.506848 6.530562
C	5.261078 1.191752 -1.773351	O	2.529569 -3.960758 0.135612
C	6.312076 0.670803 -2.646567	H	3.388106 -4.364285 0.397735
C	7.404710 0.385965 -1.845949	H	2.551926 -2.937615 0.182085
C	7.045107 0.852522 -0.493593	O	2.656654 -1.383834 0.302554
C	7.595091 1.545478 1.842243	H	2.095732 -0.780091 -0.214243
C	8.563458 1.730409 2.920719	H	3.348761 -0.826926 0.798441
C	7.879428 2.259429 3.996582	O	8.716958 -2.062764 1.614985

H 8.943728 -2.920371 2.038716
H 7.773346 -1.827211 1.834048
h 4.726339 5.069726 1.194928
h 3.057396 3.394089 5.978613
h 0.795019 3.284370 4.450534
h -0.315219 2.487680 -0.589973
h 1.186814 1.865766 -2.885077
h 6.157266 0.515318 -3.714240
h 8.298247 -0.133741 -2.191730
h 9.602166 1.408848 2.844886
h 8.254780 2.491993 4.993121
h 2.432812 -6.521750 -2.725571

TS1c

Total QM energy at B2: -3764.202459 (a.u.)

Total QM/MM energy at B2: -3875.028357 (a.u.)

C 2.452337 -6.574254 -1.625469
H 3.062427 -5.748750 -1.257753
H 2.986587 -7.508001 -1.424751
C 1.108401 -6.626368 -0.908328
O 0.336345 -7.614597 -1.035770
O 0.808136 -5.590928 -0.140071
H 1.562512 -4.777268 -0.021665
S 5.079082 4.063921 0.288761
O 4.337331 0.111366 1.495887
O 6.197349 -1.565802 2.481399
H 5.532565 -0.910401 2.098392
Fe 4.613931 1.789882 1.149167
N 3.576268 2.462717 2.758346
N 2.932760 1.907792 -0.009071
N 5.706823 1.284247 -0.487720
N 6.311597 1.897867 2.261000
C 4.062769 2.769664 4.026832
C 2.961597 3.139318 4.910235
C 1.810761 3.059450 4.156621
C 2.203046 2.640551 2.817029
C 1.655772 2.209119 0.428658
C 0.727238 2.235898 -0.701674
C 1.460667 1.960387 -1.842769
C 2.851307 1.766909 -1.386756
C 5.242393 1.186538 -1.782806
C 6.292560 0.666510 -2.655320
C 7.383122 0.374026 -1.853966
C 7.023827 0.833891 -0.500737
C 7.571730 1.510026 1.837258
C 8.541477 1.705192 2.910723
C 7.858328 2.236566 3.986771
C 6.458958 2.337601 3.573479
C 5.404848 2.745014 4.383469
H 5.647693 3.047969 5.396004
C 1.326503 2.503248 1.747030
H 0.282940 2.688952 1.972317
C 3.942732 1.460526 -2.192493
H 3.763514 1.370348 -3.258512
C 7.880900 0.991413 0.582629
H 8.916361 0.717901 0.444227
C 3.718086 -3.527704 5.647539
C 3.661643 -2.668864 6.906965
O 3.633115 -3.092782 8.079832
C 3.714097 -1.206684 6.483302
H 4.533714 -0.681861 6.986491
H 2.782684 -0.698487 6.763861
C 2.974975 -2.587589 4.616049
C 3.895823 -1.340154 4.938081
H 3.679595 -0.434335 4.369542
C 5.281763 -1.923643 4.738944
C 6.376446 -1.328270 3.934050
H 6.459617 -0.251041 4.108106
H 7.341807 -1.790607 4.163824
C 5.219476 -3.370681 5.183500
H 5.421313 -4.066229 4.356151
H 5.927156 -3.628591 5.987093
C 1.487157 -2.386549 4.953241
H 1.294076 -2.054853 5.978794
H 0.936446 -3.322698 4.800794
H 1.061485 -1.642251 4.271492
C 3.077147 -3.058357 3.160470
H 2.603719 -4.039648 3.033707
H 4.108154 -3.115021 2.800993
H 2.557682 -2.357184 2.500558
C 3.228557 -4.954463 5.813776
H 3.264871 -5.491132 4.861178
H 2.192177 -4.975218 6.172467
H 3.842425 -5.500414 6.540367
O 2.560623 -3.892560 0.138414
H 3.400783 -4.334346 0.397205
H 2.634010 -2.824497 0.221256
O 2.784839 -1.408629 0.372538
H 2.140745 -0.864654 -0.115647

H	3.566233 -0.654385 0.923852	C	7.007447 0.847778 -0.513410
O	8.711850 -2.057394 1.617870	C	7.560808 1.519919 1.820302
H	8.943687 -2.916666 2.035722	C	8.527874 1.692271 2.896439
H	7.762233 -1.836147 1.827551	C	7.851124 2.233373 3.972427
h	4.723131 5.030863 1.206731	C	6.457089 2.362462 3.559574
h	3.045547 3.381360 5.969685	C	5.409860 2.778072 4.372996
h	0.781460 3.273372 4.444447	H	5.655964 3.070715 5.387393
h	-0.326864 2.491565 -0.594109	C	1.320910 2.511804 1.752235
h	1.172870 1.874678 -2.890573	H	0.276812 2.681773 1.984190
h	6.139286 0.514439 -3.723706	C	3.924240 1.477944 -2.199487
h	8.275564 -0.146742 -2.200975	H	3.740083 1.382947 -3.263455
h	9.581689 1.388784 2.833837	C	7.866011 0.993807 0.569026
h	8.235921 2.473008 4.981550	H	8.894550 0.694521 0.437185
h	2.435083 -6.500019 -2.712786	C	3.714497 -3.550790 5.655936
IC1c		C	3.651662 -2.687511 6.912830
Total QM energy at B2: -3764.228359 (a.u.)		O	3.623684 -3.105290 8.087481
Total QM/MM energy at B2: -3875.046745 (a.u.)		C	3.699404 -1.225574 6.484989
C	2.374927 -6.673129 -1.690715	H	4.516640 -0.697686 6.989081
H	2.971965 -5.861823 -1.272300	H	2.765838 -0.719523 6.762164
H	2.908247 -7.614029 -1.519429	C	2.969618 -2.616753 4.620703
C	1.007141 -6.751724 -0.996528	C	3.885520 -1.364926 4.940767
O	0.275621 -7.785490 -1.211379	H	3.667572 -0.462176 4.367844
O	0.685906 -5.763485 -0.231281	C	5.274431 -1.943771 4.749247
H	1.748500 -4.560279 0.001856	C	6.377562 -1.337880 3.965063
S	5.036744 4.068461 0.253972	H	6.462621 -0.263432 4.159249
O	4.345302 0.119147 1.539709	H	7.339503 -1.806193 4.196382
O	6.215373 -1.549363 2.506739	C	5.216057 -3.390064 5.194981
H	5.532249 -0.910992 2.131688	H	5.421497 -4.086670 4.369525
Fe	4.613411 1.845892 1.139684	H	5.923148 -3.644231 6.000280
N	3.580973 2.510308 2.745568	C	1.480652 -2.421141 4.957381
N	2.923213 1.913720 -0.007332	H	1.285694 -2.090582 5.982962
N	5.695427 1.318145 -0.499615	H	0.934198 -3.359227 4.803999
N	6.304229 1.931407 2.242759	H	1.051517 -1.679043 4.275294
C	4.068715 2.808580 4.017415	C	3.071250 -3.089356 3.164691
C	2.967180 3.156915 4.905641	H	2.599353 -4.070310 3.033722
C	1.813854 3.069614 4.155824	H	4.100617 -3.144836 2.800595
C	2.203436 2.667065 2.812796	H	2.540005 -2.390405 2.513565
C	1.645068 2.210266 0.435108	C	3.230091 -4.978863 5.824306
C	0.712449 2.224811 -0.689092	H	3.271846 -5.518195 4.873722
C	1.443025 1.953497 -1.834544	H	2.192435 -5.002743 6.178603
C	2.835922 1.773430 -1.387098	H	3.843040 -5.520386 6.554891
C	5.225356 1.210940 -1.793897	O	2.516393 -3.897834 0.123366
C	6.265776 0.672085 -2.663346	H	3.339434 -4.387068 0.350324
C	7.354952 0.371317 -1.861636	H	2.555389 -2.364295 0.258571

O 2.587942 -1.340083 0.367042
H 1.947304 -0.887175 -0.204732
H 3.620832 -0.438368 1.044235
O 8.727834 -2.015048 1.638571
H 8.969772 -2.884561 2.028932
H 7.774772 -1.814147 1.852453
h 4.694163 5.036033 1.176354
h 3.050481 3.390292 5.967085
h 0.782848 3.265668 4.450194
h -0.344019 2.469058 -0.578249
h 1.149951 1.863162 -2.880496
h 6.106393 0.506787 -3.728869
h 8.236260 -0.167627 -2.209344
h 9.561810 1.354964 2.823864
h 8.230633 2.460571 4.968630
h 2.384895 -6.555936 -2.774335

TS1d

Total QM energy at B2: -3764.219483 (a.u.)

Total QM/MM energy at B2: -3875.039825 (a.u.)

C 2.359201 -6.701677 -1.716348
H 2.962960 -5.898184 -1.292649
H 2.884330 -7.647935 -1.550175
C 0.991182 -6.771421 -1.022226
O 0.252766 -7.800497 -1.237467
O 0.675975 -5.781515 -0.257113
H 1.743113 -4.573100 -0.023665
S 5.034411 4.040425 0.255400
O 4.396646 0.069854 1.578202
O 6.051908 -1.540782 2.611235
H 5.316976 -0.765426 2.139237
Fe 4.628997 1.833528 1.159286
N 3.597042 2.494867 2.760352
N 2.932792 1.875680 0.018492
N 5.702810 1.297930 -0.477920
N 6.317930 1.926402 2.256148
C 4.087931 2.811046 4.027891
C 2.987417 3.160503 4.916487
C 1.831606 3.059909 4.171594
C 2.217411 2.645239 2.832372
C 1.653442 2.170461 0.461222
C 0.719884 2.184840 -0.661517
C 1.450549 1.920484 -1.808891
C 2.844229 1.744456 -1.363941
C 5.233851 1.191535 -1.773288
C 6.271970 0.644913 -2.639456
C 7.353775 0.330099 -1.832647
C 7.009837 0.813811 -0.488116
C 7.572328 1.503115 1.837175
C 8.542442 1.688280 2.907537
C 7.870706 2.246771 3.978068
C 6.476527 2.375558 3.566644
C 5.430527 2.797376 4.378440
H 5.679381 3.104744 5.387652
C 1.331263 2.478056 1.777069
H 0.287589 2.647506 2.011272
C 3.932797 1.459101 -2.179105
H 3.749169 1.369153 -3.243657
C 7.870778 0.959852 0.592263
H 8.896549 0.652016 0.460653
C 3.735532 -3.566538 5.610242
C 3.679584 -2.683642 6.855062
O 3.684836 -3.084360 8.035901
C 3.670950 -1.227096 6.404724
H 4.485910 -0.667044 6.876518
H 2.730491 -0.743736 6.700446
C 2.937004 -2.669290 4.582886
C 3.825743 -1.390989 4.858014
H 3.575324 -0.503952 4.273494
C 5.229485 -1.930530 4.660336
C 6.328871 -1.240798 4.005077
H 6.347158 -0.162099 4.189959
H 7.316229 -1.652823 4.242604
C 5.217267 -3.376578 5.101617
H 5.408166 -4.072190 4.270465
H 5.953924 -3.616384 5.884560
C 1.452504 -2.509743 4.960046
H 1.277676 -2.168084 5.985576
H 0.928553 -3.465029 4.837170
H 0.983858 -1.790834 4.279112
C 3.010062 -3.162280 3.132620
H 2.569498 -4.161318 3.029791
H 4.029849 -3.181092 2.740508
H 2.435138 -2.491652 2.488915
C 3.287734 -5.001302 5.817367
H 3.311447 -5.555741 4.875063
H 2.261720 -5.039088 6.202602
H 3.932537 -5.517857 6.538586
O 2.518047 -3.920419 0.094326

H 3.331202 -4.423000 0.328460
H 2.590834 -2.386473 0.255528
O 2.644124 -1.364141 0.373333
H 2.028754 -0.893504 -0.211749
H 3.673609 -0.483319 1.075373
O 8.545688 -2.048924 1.697367
H 8.821449 -2.900752 2.102970
H 7.588665 -1.859447 1.928280
h 4.687583 5.013803 1.170054
h 3.071026 3.394215 5.977833
h 0.801017 3.256127 4.467315
h -0.338091 2.421726 -0.549097
h 1.156378 1.832827 -2.854761
h 6.115730 0.478302 -3.705240
h 8.227895 -0.226033 -2.171315
h 9.573143 1.340746 2.837229
h 8.250969 2.476807 4.973332
h 2.373067 -6.577466 -2.799143

PC1

Total QM energy at B2: -3764.297611 (a.u.)

Total QM/MM energy at B2: -3875.116575 (a.u.)

C 2.348642 -6.730345 -1.733379
H 2.948907 -5.927004 -1.304432
H 2.878261 -7.675852 -1.577438
C 0.982879 -6.816392 -1.037118
O 0.244124 -7.839770 -1.269857
O 0.669159 -5.845571 -0.246249
H 1.713366 -4.646181 -0.035813
S 4.994036 4.115959 0.253002
O 4.243971 0.044557 1.621889
O 5.917944 -1.703291 3.044699
H 4.948513 -0.479649 2.064513
Fe 4.588205 1.960148 1.127256
N 3.553128 2.545725 2.771224
N 2.895438 1.933362 -0.007188
N 5.638590 1.293865 -0.475145
N 6.267370 1.954378 2.284238
C 4.031484 2.844562 4.044381
C 2.924769 3.191165 4.930941
C 1.777061 3.108499 4.172578
C 2.179711 2.709701 2.827468
C 1.622225 2.243150 0.436361
C 0.677786 2.236841 -0.684839
C 1.398730 1.936522 -1.827242
C 2.795579 1.759716 -1.380004
C 5.182370 1.161894 -1.772002
C 6.226927 0.598726 -2.624480
C 7.306462 0.311841 -1.806675
C 6.950035 0.827196 -0.470945
C 7.521569 1.546764 1.860023
C 8.500465 1.734395 2.928580
C 7.827939 2.279897 4.005942
C 6.428955 2.401449 3.594531
C 5.374923 2.816427 4.404752
H 5.618735 3.120964 5.417358
C 1.304410 2.560047 1.754151
H 0.260746 2.743554 1.981870
C 3.882321 1.432364 -2.186701
H 3.697071 1.314066 -3.249265
C 7.811991 1.000882 0.609005
H 8.847198 0.724291 0.464213
C 3.808883 -3.502581 5.512585
C 3.806260 -2.579644 6.728683
O 3.799935 -2.938416 7.920166
C 3.855004 -1.144657 6.215805
H 4.715328 -0.605023 6.629156
H 2.958539 -0.598567 6.528166
C 2.990831 -2.624216 4.482115
C 3.906398 -1.357105 4.676697
H 3.657728 -0.483466 4.074147
C 5.302224 -1.925589 4.412730
C 6.514234 -1.093943 4.293633
H 6.445855 -0.013240 4.332475
H 7.485142 -1.514692 4.533661
C 5.277130 -3.359464 4.953629
H 5.434804 -4.077233 4.144779
H 6.035712 -3.546316 5.722212
C 1.526931 -2.404889 4.907644
H 1.401799 -2.012347 5.921987
H 0.973188 -3.348632 4.846226
H 1.053377 -1.703016 4.212959
C 2.986143 -3.184504 3.053808
H 2.438805 -4.132672 3.009273
H 3.984027 -3.353897 2.642094
H 2.477918 -2.487565 2.383494
C 3.349049 -4.922199 5.780682
H 3.330176 -5.507006 4.856777

H 2.337546 -4.926204 6.202786
H 4.009531 -5.426458 6.496145
O 2.484376 -3.982809 0.077625
H 3.302340 -4.472716 0.319941
H 2.540220 -2.440766 0.168424
O 2.607158 -1.424694 0.299158
H 2.019693 -0.925813 -0.291552
H 3.612822 -0.533411 1.057888
O 8.516699 -2.184686 1.785524
H 8.846122 -3.040014 2.148525
H 7.575300 -2.073315 2.036698
h 4.678805 5.080096 1.188638
h 3.007274 3.418963 5.993658
h 0.744366 3.302030 4.462668
h -0.378533 2.481295 -0.573044
h 1.102316 1.826134 -2.870324
h 6.077816 0.407932 -3.687226
h 8.184840 -0.250054 -2.124153
h 9.537332 1.407884 2.848806
h 8.212148 2.514029 4.998732
h 2.361216 -6.596857 -2.815085

TS1e

Total QM energy at B2: -3764.198606 (a.u.)

Total QM/MM energy at B2: -3875.024346 (a.u.)

C 2.442593 -6.642618 -1.642634
H 3.037952 -5.815976 -1.254600
H 2.988786 -7.572376 -1.458505
C 1.096397 -6.737850 -0.940544
O 0.332784 -7.722186 -1.101465
O 0.770425 -5.734421 -0.131090
H 1.488976 -4.946267 -0.006419
S 5.095391 4.170175 0.234576
O 4.387936 0.203101 1.751187
O 5.393314 -0.876087 1.232034
H 5.720966 -0.409742 0.421272
Fe 4.734417 1.985569 1.128366
N 3.649368 2.545490 2.747278
N 3.021413 1.953944 -0.011538
N 5.820806 1.352335 -0.494173
N 6.428593 2.068717 2.224391
C 4.129009 2.821116 4.021060
C 3.021306 3.162824 4.914708
C 1.874640 3.100325 4.155440
C 2.278396 2.716046 2.805322
C 1.740960 2.266078 0.412984
C 0.811261 2.261810 -0.719162
C 1.546915 1.954401 -1.850686
C 2.939315 1.772998 -1.384552
C 5.348838 1.222627 -1.791292
C 6.414317 0.751629 -2.672030
C 7.537948 0.548329 -1.885649
C 7.180540 1.018641 -0.540525
C 7.699682 1.718270 1.804749
C 8.651892 1.874685 2.902469
C 7.942178 2.334922 3.991916
C 6.546039 2.437442 3.560266
C 5.473999 2.792618 4.376090
H 5.707382 3.052606 5.403278
C 1.407901 2.579432 1.727664
H 0.361660 2.762459 1.946887
C 4.033545 1.449367 -2.186058
H 3.848121 1.332478 -3.249203
C 8.034453 1.243875 0.535748
H 9.086940 1.045053 0.382101
C 3.720187 -3.575357 5.694259
C 3.625458 -2.697866 6.938186
O 3.552355 -3.105280 8.115397
C 3.725756 -1.246098 6.490124
H 4.538998 -0.729112 7.011667
H 2.796945 -0.713163 6.728986
C 3.040136 -2.639743 4.618114
C 3.956491 -1.403649 4.957028
H 3.788634 -0.506385 4.361317
C 5.354362 -1.998493 4.815972
C 6.442422 -1.376968 4.357402
H 6.395756 -0.359314 3.988247
H 7.409165 -1.869538 4.301108
C 5.243823 -3.446418 5.306422
H 5.471151 -4.165880 4.511229
H 5.905806 -3.680135 6.150372
C 1.541862 -2.412956 4.889788
H 1.313858 -2.082621 5.908546
H 0.980794 -3.338178 4.711155
H 1.156816 -1.655631 4.197683
C 3.194830 -3.134928 3.174582
H 2.747079 -4.128876 3.047391
H 4.236232 -3.170243 2.844306

H	2.670971	-2.453668 2.500211
C	3.206454	-4.994031 5.852875
H	3.279034	-5.542294 4.908701
H	2.154937	-4.999619 6.164962
H	3.781345	-5.539639 6.610745
O	2.534929	-4.011027 0.147705
H	3.386528	-4.416426 0.428528
H	2.565654	-2.989396 0.193275
O	2.740344	-1.447336 0.351259
H	2.162186	-0.751089 -0.003742
H	3.471982	-1.006453 0.876003
O	8.312718	-1.833381 1.654156
H	8.393832	-2.686584 2.125958
H	7.406362	-1.472506 1.783932
h	4.734949	5.122963 1.165501
h	3.098895	3.386780 5.978612
h	0.841340	3.295235 4.442438
h	-0.241542	2.525651 -0.618872
h	1.260752	1.845634 -2.896797
h	6.252868	0.561517 -3.733094
h	8.450636	0.054821 -2.219591
h	9.694125	1.563418 2.832252
h	8.308142	2.543671 4.997182
h	2.428405	-6.549401 -2.728533

IC1d

Total QM energy at B2: -3764.203954 (a.u.)

Total QM/MM energy at B2: -3875.029244 (a.u.)

C	2.389121	-6.763061 -1.723741
H	2.947848	-5.947927 -1.264383
H	2.959968	-7.686493 -1.590890
C	1.033982	-6.954882 -1.061988
O	0.294273	-7.935353 -1.328372
O	0.671350	-6.050699 -0.161838
H	1.369928	-5.236586 0.024510
S	5.068036	4.234604 0.246617
O	4.350643	0.331118 1.833271
O	4.488154	-0.762287 0.759293
H	4.976222	-0.249010 0.063660
Fe	4.695573	2.061229 1.157026
N	3.649206	2.642921 2.784489
N	3.010974	2.019419 -0.003049
N	5.761891	1.364977 -0.462274
N	6.387062	2.119855 2.282900
C	4.120089	2.931253 4.057997
C	3.003936	3.254047 4.946787
C	1.860719	3.165408 4.183928
C	2.275426	2.783732 2.835398
C	1.732008	2.302316 0.440432
C	0.787680	2.276429 -0.682200
C	1.516974	1.989669 -1.822868
C	2.916874	1.839642 -1.372635
C	5.320517	1.294332 -1.780824
C	6.392636	0.818367 -2.645028
C	7.489300	0.554751 -1.835934
C	7.109391	0.987524 -0.482084
C	7.636937	1.696713 1.869469
C	8.603317	1.845146 2.960322
C	7.919443	2.365039 4.039343
C	6.526756	2.512908 3.609525
C	5.464350	2.905530 4.419231
H	5.698790	3.178997 5.442713
C	1.407413	2.616343 1.758412
H	0.359375	2.780478 1.983762
C	4.012277	1.540759 -2.184026
H	3.831325	1.448800 -3.250265
C	7.950856	1.171414 0.612693
H	8.996401	0.930357 0.474387
C	3.823038	-3.498614 5.627038
C	3.743356	-2.544492 6.815414
O	3.666162	-2.881319 8.013951
C	3.850581	-1.125009 6.272513
H	4.674894	-0.581452 6.747262
H	2.930299	-0.567703 6.485298
C	3.131033	-2.630146 4.503448
C	4.056600	-1.379893 4.747793
H	3.884306	-0.523843 4.095417
C	5.449133	-1.990725 4.623441
C	6.537147	-1.401671 4.119192
H	6.488588	-0.401997 3.700744
H	7.505621	-1.896124 4.111390
C	5.340380	-3.401905 5.211669
H	5.557109	-4.174412 4.465097
H	6.011394	-3.579344 6.061785
C	1.636884	-2.376872 4.779526
H	1.424785	-1.996267 5.784235
H	1.065912	-3.304854 4.654036
H	1.247996	-1.649874 4.057310

C	3.265025 -3.216368 3.093015	N	2.951877 2.149632 0.051262
H	2.783398 -4.200267 3.028914	N	5.707647 1.480401 -0.413727
H	4.304325 -3.308172 2.766251	N	6.352933 2.192185 2.305484
H	2.764487 -2.557663 2.379726	C	4.101413 3.089412 4.070139
C	3.306687 -4.900707 5.883733	C	2.993846 3.394153 4.972659
H	3.372832 -5.513356 4.979533	C	1.842092 3.315034 4.221056
H	2.256904 -4.880306 6.200747	C	2.240238 2.953570 2.865586
H	3.883177 -5.395144 6.674718	C	1.672782 2.426947 0.494737
O	2.323625 -4.286148 0.221935	C	0.722012 2.360312 -0.619636
H	3.208462 -4.597064 0.510201	C	1.447705 2.065035 -1.758274
H	2.223045 -3.260276 0.197769	C	2.852944 1.948616 -1.313934
O	2.195896 -1.757189 0.224840	C	5.255703 1.421587 -1.726398
H	1.450575 -1.136661 0.241363	C	6.313200 0.930641 -2.599502
H	3.083937 -1.288438 0.428898	C	7.404027 0.626639 -1.797734
O	8.692656 -2.014895 1.593993	C	7.040728 1.054685 -0.439433
H	8.843677 -2.863001 2.068993	C	7.590728 1.728672 1.904547
H	7.828572 -1.643159 1.854638	C	8.555386 1.862233 2.997042
h	4.737736 5.195880 1.179996	C	7.881457 2.413952 4.065510
h	3.076230 3.467238 6.013271	C	6.495769 2.599479 3.627269
h	0.823103 3.337538 4.469919	C	5.445059 3.034422 4.427927
h	-0.271630 2.510205 -0.576005	H	5.686297 3.308115 5.449355
h	1.224009 1.871075 -2.866024	C	1.358060 2.768901 1.805378
h	6.247627 0.668975 -3.714944	H	0.313726 2.934240 2.041005
h	8.399949 0.063592 -2.178788	C	3.947568 1.667708 -2.127422
h	9.638435 1.511541 2.887480	H	3.764861 1.575803 -3.192867
h	8.295413 2.582886 5.038971	C	7.891832 1.195223 0.651262
h	2.399546 -6.599947 -2.801401	H	8.927401 0.917214 0.513079
		C	3.866258 -3.432355 5.594545
TS1f		C	3.774796 -2.486496 6.788575
Total QM energy at B2: -3764.17546 (a.u.)		O	3.686358 -2.831353 7.983903
Total QM/MM energy at B2: -3874.996402 (a.u.)		C	3.891129 -1.063426 6.256733
C	2.388292 -6.789938 -1.747292	H	4.710177 -0.525515 6.746748
H	2.937264 -5.972867 -1.278019	H	2.969638 -0.505497 6.462884
H	2.968373 -7.708330 -1.618600	C	3.191870 -2.555662 4.465493
C	1.032890 -6.999974 -1.091720	C	4.115144 -1.308066 4.732817
O	0.287896 -7.967484 -1.392771	H	3.948043 -0.444123 4.088425
O	0.674188 -6.131922 -0.158489	C	5.505668 -1.923183 4.612295
H	1.386852 -5.327634 0.064719	C	6.592623 -1.345175 4.093760
S	5.095049 4.349330 0.238826	H	6.551519 -0.345150 3.676064
O	4.302135 0.578513 1.832326	H	7.555603 -1.848427 4.066324
O	4.490699 -1.174346 0.146379	C	5.390318 -3.334245 5.201168
H	4.827144 -0.273427 -0.076269	H	5.625009 -4.109931 4.462806
Fe	4.641670 2.090731 1.211742	H	6.045733 -3.505025 6.064641
N	3.615156 2.827038 2.796947	C	1.693601 -2.300490 4.716891

H	1.466721	-1.916713 5.717189
H	1.124109	-3.228242 4.584578
H	1.315609	-1.574060 3.987805
C	3.352697	-3.134962 3.055356
H	2.801820	-4.078030 2.956366
H	4.395578	-3.306092 2.776537
H	2.944557	-2.435827 2.322387
C	3.346971	-4.836375 5.837979
H	3.419192	-5.441776 4.929253
H	2.295704	-4.817963 6.150174
H	3.919093	-5.336229 6.628878
O	2.316570	-4.389413 0.296162
H	3.215275	-4.672595 0.563442
H	2.175963	-3.362763 0.247404
O	2.080439	-1.887707 0.170413
H	1.416014	-1.288968 0.544585
H	3.022499	-1.460222 0.146483
O	8.712138	-2.042419 1.589501
H	8.866482	-2.915920 2.016319
H	7.797827	-1.751531 1.769239
h	4.764135	5.336536 1.144512
h	3.073012	3.578042 6.044099
h	0.805661	3.462541 4.524569
h	-0.345261	2.552104 -0.509135
h	1.150061	1.910576 -2.795393
h	6.164967	0.805129 -3.672041
h	8.298387	0.115203 -2.153571
h	9.581964	1.501972 2.930594
h	8.258870	2.631009 5.064766
h	2.400200	-6.620718 -2.823995

IC1e

Total QM energy at B2: -3764.17546 (a.u.)

Total QM/MM energy at B2: -3874.996402 (a.u.)

C	2.410415	-6.696122 -1.645621
H	2.946055	-5.843747 -1.224543
H	3.011367	-7.592840 -1.454543
C	1.053566	-6.877912 -0.945708
O	0.294446	-7.849848 -1.309600
O	0.780847	-6.049391 0.003259
H	1.908808	-4.935701 0.419905
S	5.076186	4.368316 0.193508
O	4.144991	0.558459 1.679420
O	5.914287	-1.645780 1.695542
H	5.618949	-0.856263 2.187006
Fe	4.522661	2.096442 1.175130
N	3.514569	2.864034 2.752555
N	2.850761	2.229614 0.014740
N	5.593013	1.485334 -0.436497
N	6.234447	2.182718 2.263434
C	3.999152	3.126791 4.024259
C	2.903045	3.431935 4.933618
C	1.745558	3.359686 4.186426
C	2.138776	3.001560 2.832954
C	1.566401	2.488731 0.451442
C	0.620140	2.420373 -0.661694
C	1.353294	2.146694 -1.801913
C	2.752804	2.031642 -1.349795
C	5.152131	1.427832 -1.738394
C	6.181014	0.868311 -2.610050
C	7.235069	0.487718 -1.797661
C	6.879652	0.947877 -0.444080
C	7.453437	1.661832 1.888546
C	8.427300	1.801519 2.967208
C	7.780124	2.420922 4.016689
C	6.401489	2.630940 3.577314
C	5.352129	3.074631 4.370413
H	5.597675	3.358348 5.388118
C	1.257620	2.818875 1.768801
H	0.214088	2.982255 2.006413
C	3.854928	1.733901 -2.148661
H	3.680094	1.653085 -3.216137
C	7.721899	1.051319 0.655016
H	8.718655	0.649033 0.563052
C	3.661917	-3.397171 5.785165
C	3.589853	-2.727870 7.155442
O	3.590290	-3.307493 8.259664
C	3.607073	-1.218538 6.949288
H	4.415067	-0.749947 7.522279
H	2.665275	-0.775826 7.296381
C	2.899519	-2.333631 4.900505
C	3.781751	-1.126171 5.407840
H	3.543082	-0.152486 4.976112
C	5.192975	-1.629640 5.111988
C	6.240524	-0.909774 4.704823
H	6.161949	0.159785 4.543801
H	7.197435	-1.362549 4.459883
C	5.156900	-3.140772 5.351435

H	5.370339 -3.696694 4.431005	S	5.252346 4.451404 0.247773
H	5.873246 -3.480381 6.110219	O	4.516161 0.363697 1.494590
C	1.407877 -2.226871 5.254523	O	5.580466 -0.626792 1.013132
H	1.198634 -2.065040 6.316801	H	5.852083 -0.188289 0.169306
H	0.881285 -3.136875 4.943254	Fe	4.849125 2.213274 1.016064
H	0.974764 -1.392242 4.695801	N	3.730752 2.679443 2.651629
C	3.016230 -2.564952 3.390455	N	3.143944 2.222041 -0.133049
H	2.540700 -3.499511 3.074935	N	5.949719 1.666740 -0.611295
H	4.044904 -2.569996 3.028131	N	6.526583 2.276818 2.131622
H	2.505266 -1.749493 2.865483	C	4.195080 2.907180 3.940653
C	3.212740 -4.846974 5.740741	C	3.073621 3.167399 4.845042
H	3.297156 -5.247095 4.725292	C	1.931232 3.100471 4.078892
H	2.168066 -4.949514 6.058173	C	2.353898 2.804877 2.712912
H	3.823373 -5.467811 6.407560	C	1.853582 2.483015 0.295058
O	2.708703 -4.351224 0.650481	C	0.925851 2.479909 -0.838149
H	3.516340 -4.910181 0.721664	C	1.668378 2.199685 -1.971980
H	3.149734 -2.808834 0.427342	C	3.065770 2.057560 -1.507507
O	3.669210 -1.945777 0.318966	C	5.483324 1.546828 -1.911182
H	3.264818 -1.164237 0.737880	C	6.553092 1.082764 -2.790068
H	5.164449 -1.867503 1.054508	C	7.674061 0.879088 -1.999801
O	8.560854 -1.918484 1.721363	C	7.312020 1.342729 -0.653231
H	8.833520 -2.793950 2.070634	C	7.815896 2.012128 1.701668
H	7.559104 -1.861459 1.690962	C	8.759919 2.196425 2.802914
h	4.754923 5.358007 1.099955	C	8.022522 2.573202 3.906400
h	2.990527 3.604142 6.006352	C	6.623617 2.613428 3.476373
h	0.711940 3.510727 4.497692	C	5.538176 2.904146 4.300298
h	-0.455004 2.559447 -0.548605	H	5.760529 3.137627 5.336282
h	1.061642 2.005253 -2.842586	C	1.496850 2.713699 1.620975
h	6.034787 0.749862 -3.683668	H	0.440544 2.841721 1.834415
h	8.095960 -0.083140 -2.145591	C	4.167994 1.766601 -2.309941
h	9.436662 1.393685 2.913113	H	3.987327 1.658695 -3.375005
h	8.163628 2.634716 5.014328	C	8.164704 1.578000 0.422704
h	2.421344 -6.601268 -2.731415	H	9.221717 1.409633 0.262287
		C	3.904246 -3.497454 5.520704
RC1'		C	3.416341 -2.476991 6.544079
Total QM energy at B2: -3764.211791 (a.u.)		O	3.079614 -2.699364 7.723415
Total QM/MM energy at B2: -3875.055150 (a.u.)		C	3.452807 -1.110489 5.863564
C	2.487000 -6.343017 -1.691480	H	4.123536 -0.432264 6.400545
H	3.208422 -5.642046 -1.267461	H	2.454761 -0.656486 5.865434
H	2.886530 -7.347172 -1.515085	C	3.323772 -2.872038 4.186690
C	1.143583 -6.233748 -0.989530	C	3.972489 -1.461878 4.438306
O	0.283986 -7.140686 -1.071971	H	3.789754 -0.704127 3.676290
O	0.930473 -5.139244 -0.272548	C	5.439105 -1.822899 4.622602
H	1.666165 -4.368082 -0.276017	C	6.476336 -1.105185 4.184758

H 6.316067 -0.194587 3.619248
H 7.507418 -1.403621 4.339058
C 5.441004 -3.153342 5.386647
H 5.941683 -3.952847 4.826224
H 5.928140 -3.097075 6.367929
C 1.786720 -2.848756 4.148152
H 1.401251 -3.872038 4.066229
H 1.451455 -2.290109 3.266367
H 1.330291 -2.396312 5.035098
C 3.833169 -3.569829 2.917838
H 3.458395 -4.600093 2.859080
H 4.924360 -3.592455 2.857886
H 3.467043 -3.047462 2.031143
C 3.600156 -4.950505 5.826777
H 3.980799 -5.602370 5.033300
H 2.519832 -5.116745 5.917409
H 4.063294 -5.256191 6.770520
O 2.604457 -3.302124 -0.305210
H 2.491300 -2.352462 0.088105
H 3.435026 -3.388296 -0.809527
O 2.419610 -0.952144 0.636653
H 3.229763 -0.456228 1.006994
H 1.764029 -0.308155 0.319976
O 8.451375 -1.396930 1.575100
H 8.551223 -2.269174 2.012741
H 7.524786 -1.081498 1.668935
h 4.907893 5.345845 1.240583
h 3.140303 3.365037 5.914883
h 0.890092 3.226913 4.375721
h -0.126468 2.738825 -0.721299
h 1.379135 2.063077 -3.013970
h 6.395992 0.896814 -3.852522
h 8.584636 0.378453 -2.328866
h 9.821435 1.961353 2.725509
h 8.361042 2.748580 4.927533
h 2.497208 -6.229951 -2.775537

TS1a’

Total QM energy at B2: -3764.196747 (a.u.)

Total QM/MM energy at B2: -3875.039733 (a.u.)

C 2.461979 -6.310249 -1.709396
H 3.190460 -5.614665 -1.288155
H 2.848577 -7.318206 -1.525976
C 1.116185 -6.176635 -1.008800
O 0.255136 -7.089757 -1.088783
O 0.912808 -5.073197 -0.318457
H 1.687835 -4.269407 -0.301525
S 5.236279 4.472712 0.224411
O 4.463139 0.113705 1.501920
O 5.577958 -0.750611 0.938417
H 5.830286 -0.209733 0.151524
Fe 4.813579 2.291775 0.998692
N 3.702249 2.711029 2.640062
N 3.115160 2.258438 -0.133011
N 5.908499 1.693205 -0.607543
N 6.484535 2.296926 2.125148
C 4.165184 2.935703 3.932693
C 3.044542 3.180306 4.838601
C 1.900984 3.107123 4.074436
C 2.321463 2.822885 2.707887
C 1.820740 2.507442 0.293771
C 0.895236 2.505793 -0.838564
C 1.638666 2.235357 -1.973120
C 3.035642 2.099469 -1.509780
C 5.446732 1.579144 -1.911350
C 6.511181 1.100561 -2.785960
C 7.627089 0.880797 -1.992380
C 7.268895 1.349465 -0.648766
C 7.776005 2.019609 1.699450
C 8.719195 2.197167 2.799459
C 7.984388 2.582047 3.902179
C 6.588042 2.634933 3.471475
C 5.506209 2.932529 4.295021
H 5.728590 3.161339 5.331637
C 1.462300 2.728696 1.619372
H 0.405539 2.845737 1.834884
C 4.135914 1.811710 -2.313183
H 3.956455 1.707106 -3.378291
C 8.123956 1.578201 0.424604
H 9.178275 1.393963 0.266711
C 3.912827 -3.521236 5.544970
C 3.415535 -2.496961 6.559757
O 3.084843 -2.709846 7.742850
C 3.434052 -1.136153 5.865619
H 4.098518 -0.444732 6.394405
H 2.430664 -0.693936 5.865898
C 3.322082 -2.916513 4.206701
C 3.953924 -1.496730 4.442303

H 3.760534 -0.754549 3.669080
C 5.424957 -1.837766 4.626437
C 6.452962 -1.115580 4.174079
H 6.279755 -0.214795 3.596660
H 7.488246 -1.400418 4.326829
C 5.444649 -3.160040 5.403483
H 5.951649 -3.958769 4.847867
H 5.934429 -3.088951 6.382514
C 1.785284 -2.906446 4.169922
H 1.407520 -3.931870 4.078901
H 1.449540 -2.343512 3.291222
H 1.324971 -2.464971 5.060836
C 3.834484 -3.620939 2.942417
H 3.488661 -4.662061 2.907735
H 4.925367 -3.615456 2.869617
H 3.442077 -3.120834 2.054421
C 3.627237 -4.975404 5.860606
H 4.037201 -5.629352 5.083801
H 2.547973 -5.158476 5.926673
H 4.072779 -5.262946 6.817966
O 2.569627 -3.280720 -0.285284
H 2.502295 -2.283719 0.183313
H 3.392883 -3.385575 -0.796792
O 2.506172 -1.065188 0.745561
H 3.462074 -0.487332 1.112424
H 1.777857 -0.462394 0.522561
O 8.426484 -1.405527 1.580168
H 8.549233 -2.283910 2.000339
H 7.480835 -1.140670 1.641539
h 4.895343 5.358274 1.226353
h 3.112578 3.373189 5.909224
h 0.859886 3.224242 4.375207
h -0.160191 2.750832 -0.719830
h 1.349876 2.097703 -3.015097
h 6.353892 0.912397 -3.847996
h 8.530813 0.366861 -2.319823
h 9.778700 1.952751 2.723451
h 8.324940 2.752765 4.923427
h 2.475477 -6.202383 -2.793946

IC1a'

Total QM energy at B2: -3764.209028 (a.u.)

Total QM/MM energy at B2: -3875.047173 (a.u.)

C 2.382710 -6.309849 -1.770173
H 3.118657 -5.625150 -1.340341
H 2.749267 -7.325947 -1.585395
C 1.026627 -6.136700 -1.071937
O 0.152371 -7.053987 -1.213393
O 0.866847 -5.059534 -0.377421
H 1.841736 -3.961956 -0.273429
S 5.245781 4.439375 0.244465
O 4.451273 0.287670 1.459067
O 5.506956 -0.679830 0.960049
H 5.835704 -0.174664 0.172515
Fe 4.803901 2.259394 1.004021
N 3.688399 2.699674 2.641958
N 3.103307 2.248173 -0.132901
N 5.902318 1.674998 -0.607750
N 6.474756 2.265565 2.130509
C 4.152771 2.923714 3.933747
C 3.032892 3.178637 4.838123
C 1.889333 3.113708 4.073433
C 2.308830 2.825086 2.707192
C 1.809676 2.509620 0.292041
C 0.886120 2.506258 -0.841712
C 1.630429 2.227975 -1.974886
C 3.026427 2.088481 -1.510176
C 5.440082 1.568891 -1.912485
C 6.505960 1.098470 -2.789359
C 7.622707 0.876168 -1.997117
C 7.264520 1.335831 -0.650627
C 7.767069 1.995394 1.703350
C 8.709586 2.181123 2.802914
C 7.973637 2.568667 3.904141
C 6.576571 2.614145 3.473936
C 5.494138 2.915568 4.295933
H 5.716834 3.149211 5.331318
C 1.450823 2.737193 1.617053
H 0.395047 2.865351 1.830284
C 4.128197 1.800392 -2.312674
H 3.948671 1.697652 -3.377753
C 8.116932 1.557047 0.427466
H 9.171644 1.374594 0.270589
C 3.906670 -3.539128 5.548472
C 3.411160 -2.524245 6.574250
O 3.091846 -2.743933 7.758481
C 3.414652 -1.158450 5.889271
H 4.076502 -0.465858 6.419595

H	2.407436	-0.725326	5.898559
C	3.300239	-2.929424	4.218766
C	3.927131	-1.506778	4.459929
H	3.719065	-0.754653	3.699837
C	5.402142	-1.838967	4.632794
C	6.427145	-1.103455	4.193998
H	6.254079	-0.190201	3.636104
H	7.463237	-1.385116	4.349219
C	5.434436	-3.168331	5.396493
H	5.940912	-3.958427	4.828563
H	5.933116	-3.102672	6.371215
C	1.762872	-2.932206	4.202562
H	1.393833	-3.959238	4.101096
H	1.402496	-2.361484	3.338938
H	1.311033	-2.508261	5.106112
C	3.806034	-3.629365	2.948904
H	3.477253	-4.675781	2.923142
H	4.896141	-3.608687	2.864058
H	3.396586	-3.151009	2.055364
C	3.632450	-4.997468	5.855603
H	4.042462	-5.643543	5.072534
H	2.555129	-5.188669	5.926104
H	4.085228	-5.288468	6.808354
O	2.544680	-3.177314	-0.237748
H	2.468506	-1.875234	0.321442
H	3.345342	-3.388177	-0.752420
O	2.450647	-0.887869	0.712538
H	3.505371	-0.244772	1.129004
H	1.740588	-0.331828	0.355043
O	8.436202	-1.430295	1.586504
H	8.594877	-2.310283	1.995017
H	7.504553	-1.162591	1.733288
h	4.899160	5.336253	1.234319
h	3.102147	3.370966	5.908767
h	0.848844	3.235770	4.374345
h	-0.168482	2.756701	-0.727000
h	1.341130	2.086346	-3.016190
h	6.348790	0.915779	-3.852368
h	8.527470	0.365941	-2.327479
h	9.770909	1.944796	2.726689
h	8.313880	2.744294	4.924659
h	2.414876	-6.198999	-2.854029

TS1b’

Total QM energy at B2: -3764.189475 (a.u.)

Total QM/MM energy at B2: -3875.026606 (a.u.)

C	2.495982	-6.319403	-1.720735
H	3.230923	-5.627154	-1.305476
H	2.879999	-7.328717	-1.540310
C	1.157989	-6.184281	-1.013765
O	0.289774	-7.084682	-1.069401
O	0.956228	-5.069572	-0.320507
H	1.696961	-4.315988	-0.325964
S	5.221869	4.582510	0.223851
O	4.381655	0.700540	1.470582
O	5.961998	-1.015836	0.782890
H	5.357060	-0.259953	1.150909
Fe	4.752933	2.287521	1.048877
N	3.668780	2.909508	2.661735
N	3.067780	2.387137	-0.129055
N	5.847309	1.758006	-0.572032
N	6.429806	2.372119	2.175290
C	4.126997	3.100206	3.957529
C	3.000504	3.318108	4.861041
C	1.860720	3.250616	4.090392
C	2.288162	2.999102	2.718511
C	1.780308	2.637245	0.307761
C	0.844212	2.581822	-0.817388
C	1.581246	2.278744	-1.949285
C	2.981607	2.176422	-1.494059
C	5.386083	1.634404	-1.870314
C	6.451527	1.141951	-2.738140
C	7.557441	0.908199	-1.938782
C	7.187808	1.368918	-0.591534
C	7.706610	2.043261	1.752489
C	8.654295	2.202534	2.853793
C	7.932893	2.629391	3.948251
C	6.539031	2.724678	3.516376
C	5.465469	3.066381	4.330822
H	5.687497	3.293577	5.367774
C	1.429758	2.888822	1.630896
H	0.372996	3.001851	1.847978
C	4.082438	1.870606	-2.288271
H	3.906543	1.747205	-3.351992
C	8.043687	1.579538	0.484791
H	9.091707	1.361774	0.338981
C	3.946020	-3.447543	5.481981
C	3.465483	-2.423695	6.505238

O 3.140914 -2.642962 7.688009
C 3.479915 -1.060661 5.814989
H 4.154063 -0.370629 6.333389
H 2.478237 -0.614903 5.833700
C 3.327787 -2.841664 4.155964
C 3.970429 -1.420255 4.381153
H 3.753371 -0.667258 3.622074
C 5.444389 -1.773576 4.520295
C 6.472577 -1.087694 4.012786
H 6.311281 -0.177752 3.446103
H 7.504504 -1.408260 4.108425
C 5.473738 -3.088864 5.308482
H 5.974587 -3.892878 4.755206
H 5.977087 -3.006355 6.280014
C 1.790335 -2.834360 4.155547
H 1.413338 -3.860939 4.074826
H 1.423720 -2.272884 3.288131
H 1.351760 -2.394410 5.057680
C 3.816785 -3.551551 2.884511
H 3.494142 -4.600601 2.875081
H 4.904374 -3.523992 2.778250
H 3.387088 -3.080019 1.997229
C 3.669377 -4.900784 5.813460
H 4.084066 -5.562148 5.045075
H 2.591927 -5.091484 5.886105
H 4.119768 -5.169842 6.774391
O 2.662145 -3.232253 -0.329488
H 2.526143 -2.280696 0.026701
H 3.535065 -3.335355 -0.753191
O 2.378601 -0.826077 0.552277
H 3.132166 -0.274442 0.931885
H 1.709610 -0.225746 0.179981
O 8.694971 -1.373451 1.551923
H 8.765207 -2.284254 1.910181
H 7.754060 -1.183057 1.308708
h 4.901420 5.494025 1.209143
h 3.064926 3.479718 5.937052
h 0.817531 3.332142 4.395640
h -0.212774 2.821967 -0.702595
h 1.288704 2.099824 -2.983921
h 6.301865 0.971389 -3.804243
h 8.466982 0.414973 -2.281609
h 9.703935 1.918394 2.779055
h 8.277225 2.800879 4.968101
h 2.502392 -6.210562 -2.805253

IC1b'

Total QM energy at B2: -3764.221108 (a.u.)

Total QM/MM energy at B2: -3875.060790 (a.u.)

C 2.480144 -6.330396 -1.745039
H 3.215418 -5.652360 -1.307405
H 2.855137 -7.346124 -1.582674
C 1.137635 -6.199618 -1.044017
O 0.274361 -7.105016 -1.101696
O 0.932291 -5.084402 -0.355974
H 1.688532 -4.332848 -0.372698
S 5.186488 4.497124 0.259278
O 4.441294 0.538927 1.415818
O 6.266265 -1.178113 2.318711
H 5.599218 -0.516811 1.953225
Fe 4.700346 2.180922 1.057193
N 3.616175 2.777232 2.672142
N 3.022251 2.289510 -0.117699
N 5.807081 1.699723 -0.578052
N 6.382527 2.292635 2.181522
C 4.078998 3.009724 3.961848
C 2.955288 3.259761 4.860252
C 1.813597 3.175424 4.094175
C 2.236415 2.881566 2.729686
C 1.732866 2.537269 0.316575
C 0.804572 2.524138 -0.815480
C 1.546644 2.251234 -1.951743
C 2.944444 2.125623 -1.491895
C 5.349238 1.589767 -1.874480
C 6.411470 1.087481 -2.744622
C 7.508687 0.828980 -1.941564
C 7.136514 1.288813 -0.590154
C 7.657740 1.967218 1.754808
C 8.611136 2.151906 2.847018
C 7.893061 2.590502 3.941110
C 6.495162 2.665724 3.514730
C 5.418513 3.001535 4.330606
H 5.642280 3.255234 5.361302
C 1.377849 2.771226 1.641736
H 0.321435 2.890505 1.856764
C 4.047156 1.841433 -2.290947
H 3.873391 1.744936 -3.357752
C 7.989148 1.482526 0.491663

H 9.033730 1.246239 0.352308
C 3.899697 -3.413856 5.482529
C 3.475645 -2.423843 6.565424
O 3.206284 -2.684269 7.753604
C 3.436932 -1.035873 5.928354
H 4.130411 -0.358711 6.437959
H 2.431494 -0.605440 6.015521
C 3.197028 -2.760634 4.220795
C 3.861900 -1.344246 4.459288
H 3.603250 -0.570362 3.734607
C 5.330068 -1.707266 4.530766
C 6.410652 -1.016488 3.784431
H 6.429332 0.056632 4.008554
H 7.396699 -1.430460 4.014074
C 5.414278 -3.057139 5.215503
H 5.865492 -3.830732 4.573953
H 5.992163 -3.055345 6.152510
C 1.663272 -2.765351 4.328962
H 1.289615 -3.791877 4.232815
H 1.230098 -2.175154 3.513157
H 1.282239 -2.368229 5.275984
C 3.600335 -3.406240 2.887527
H 3.343460 -4.473259 2.869873
H 4.666612 -3.293852 2.676311
H 3.059190 -2.931947 2.065210
C 3.635088 -4.875398 5.788109
H 3.990061 -5.515152 4.973251
H 2.563467 -5.061818 5.928500
H 4.147619 -5.178211 6.707495
O 2.670259 -3.304790 -0.416957
H 2.564734 -2.337587 -0.080248
H 3.507772 -3.426666 -0.905956
O 2.492374 -0.900348 0.396977
H 3.262772 -0.373337 0.797109
H 1.818899 -0.280585 0.069954
O 8.839262 -1.425922 1.579667
H 9.023650 -2.342217 1.886743
H 7.870390 -1.243432 1.721363
h 4.865199 5.404556 1.248059
h 3.022948 3.451398 5.931123
h 0.771913 3.285725 4.395495
h -0.250103 2.772816 -0.697638
h 1.258130 2.108553 -2.993121
h 6.265584 0.932534 -3.813629
h 8.412212 0.325061 -2.284749
h 9.665514 1.887400 2.767086
h 8.240405 2.772011 4.958201
h 2.499856 -6.199164 -2.826915

RC1”

Total QM energy at B2: -3764.176124 (a.u.)

Total QM/MM energy at B2: -3874.852423 (a.u.)

C 2.463142 -6.377803 -1.688962
H 3.071200 -5.531308 -1.369737
H 3.050532 -7.277664 -1.479206
C 1.170015 -6.478787 -0.893122
O 0.406725 -7.461473 -1.019282
O 0.900889 -5.498007 -0.035505
H 1.514152 -4.633677 -0.020953
S 5.172796 4.306767 0.138157
O 4.430165 0.260870 1.425447
O 5.323412 -0.756458 0.704865
H 5.456159 -0.291408 -0.157107
Fe 4.772499 2.104365 0.929427
N 3.721434 2.569898 2.616413
N 3.033768 2.111044 -0.161312
N 5.815976 1.562555 -0.743336
N 6.489769 2.163382 1.990747
C 4.226409 2.789216 3.892530
C 3.142458 3.117134 4.825346
C 1.981192 3.095938 4.085274
C 2.354203 2.747995 2.712502
C 1.755216 2.337859 0.322503
C 0.781783 2.275190 -0.772372
C 1.491933 2.055660 -1.941312
C 2.907728 1.943915 -1.531604
C 5.307418 1.435765 -2.028144
C 6.351894 0.977804 -2.940853
C 7.504054 0.804986 -2.189447
C 7.181488 1.275822 -0.834295
C 7.768197 1.964419 1.497650
C 8.749269 2.135768 2.569570
C 8.039611 2.423114 3.719958
C 6.629184 2.449061 3.343141
C 5.576156 2.729498 4.212731
H 5.840676 2.930084 5.245426
C 1.458460 2.624148 1.653803
H 0.420402 2.798335 1.907572

C 3.978887 1.654778 -2.377519
H 3.759910 1.550023 -3.435489
C 8.072773 1.558042 0.197182
H 9.128225 1.441052 -0.018709
C 3.581195 -3.842343 5.468021
C 3.787338 -3.085184 6.773402
O 3.876606 -3.589768 7.908765
C 3.923063 -1.601091 6.441055
H 4.870092 -1.196308 6.814460
H 3.112542 -1.033395 6.914948
C 2.769651 -2.766612 4.640298
C 3.826982 -1.623716 4.889166
H 3.607950 -0.661260 4.424752
C 5.118640 -2.277515 4.409226
C 6.127185 -1.677418 3.776916
H 6.064580 -0.629365 3.503772
H 7.016159 -2.212408 3.454642
C 5.006461 -3.755943 4.793920
H 5.026233 -4.412672 3.915345
H 5.802470 -4.095903 5.469678
C 1.379022 -2.480338 5.236783
H 0.695824 -3.312693 5.029011
H 0.962174 -1.584504 4.766769
H 1.379227 -2.316757 6.319763
C 2.607897 -3.109291 3.155902
H 3.562032 -3.130295 2.629657
H 1.999571 -2.346859 2.660353
H 2.115737 -4.079318 3.015779
C 3.023986 -5.249557 5.598289
H 2.023148 -5.244360 6.046634
H 3.669656 -5.866789 6.235280
H 2.956619 -5.728326 4.615039
O 2.309542 -3.431204 -0.039982
H 2.143894 -2.473938 0.276284
H 3.207918 -3.477054 -0.438515
O 2.165459 -0.956855 0.677265
H 1.599169 -0.273293 0.279104
H 3.009562 -0.522169 1.027814
O 8.078887 -1.284700 1.321991
H 8.330324 -0.600326 1.971449
H 7.111735 -1.143819 1.151972
h 4.830524 5.220711 1.113812
h 3.249549 3.348702 5.885051
h 0.958484 3.304161 4.399562
h -0.293056 2.387945 -0.630690
h 1.175765 1.972204 -2.981091
h 6.161622 0.778373 -3.995410
h 8.418896 0.329242 -2.542714
h 9.822436 1.983607 2.454567
h 8.403509 2.532764 4.741536
h 2.368917 -6.349146 -2.774488

TS1a”

Total QM energy at B2: -3764.156709 (a.u.)

Total QM/MM energy at B2: -3874.832102 (a.u.)

C 2.468327 -6.372840 -1.688216
H 3.107223 -5.549558 -1.371064
H 3.023784 -7.294007 -1.481160
C 1.175329 -6.427286 -0.880874
O 0.394890 -7.403891 -1.002944
O 0.941531 -5.432328 -0.042062
H 1.591462 -4.529351 -0.027786
S 5.178837 4.355925 0.112411
O 4.366039 -0.077752 1.424788
O 5.335158 -0.874407 0.565052
H 5.459822 -0.249297 -0.190238
Fe 4.755201 2.221979 0.931173
N 3.702914 2.634134 2.622599
N 3.025520 2.161400 -0.138470
N 5.794999 1.618336 -0.711326
N 6.455933 2.209276 2.010612
C 4.200960 2.857772 3.904375
C 3.113359 3.169931 4.834771
C 1.952981 3.137103 4.093457
C 2.330400 2.795197 2.723720
C 1.739870 2.365034 0.342541
C 0.770505 2.296063 -0.750846
C 1.484044 2.105260 -1.921691
C 2.899769 2.010270 -1.513190
C 5.296010 1.507581 -2.004770
C 6.337682 1.034693 -2.909131
C 7.481776 0.837180 -2.150288
C 7.160614 1.312980 -0.798666
C 7.742026 2.005280 1.526313
C 8.717044 2.179962 2.598370
C 8.004842 2.475404 3.745093
C 6.597148 2.504540 3.364726
C 5.547182 2.798635 4.230762

H	5.808670 3.003533 5.263427	h	4.837153 5.262613 1.095018
C	1.435981 2.653977 1.669008	h	3.215769 3.393273 5.896702
H	0.396487 2.821711 1.919363	h	0.926902 3.323567 4.410412
C	3.972975 1.741933 -2.360356	h	-0.307077 2.359890 -0.599821
H	3.758026 1.652562 -3.420141	h	1.166391 2.028475 -2.961531
C	8.051520 1.588739 0.232262	h	6.146495 0.829495 -3.962416
H	9.105539 1.456250 0.020381	h	8.387629 0.340606 -2.498009
C	3.603260 -3.869382 5.496644	h	9.790200 2.020682 2.493329
C	3.800355 -3.063579 6.773124	h	8.366117 2.580448 4.768085
O	3.879986 -3.522375 7.928819	h	2.374830 -6.342580 -2.773762
C	3.944525 -1.593354 6.382403		
H	4.889716 -1.177319 6.748724	**IC1a”**	
H	3.131681 -1.006440 6.828011	Total QM energy at B2: -3764.167913 (a.u.)	
C	2.800803 -2.825035 4.619946	Total QM/MM energy at B2: -3874.840595 (a.u.)	
C	3.858828 -1.676175 4.831086	C	2.436248 -6.353963 -1.724247
H	3.645890 -0.734109 4.324812	H	3.073843 -5.520048 -1.423076
C	5.151226 -2.351181 4.385980	H	2.997739 -7.270067 -1.510297
C	6.160238 -1.782218 3.726480	C	1.141421 -6.385562 -0.893878
H	6.090932 -0.750065 3.400735	O	0.365800 -7.385819 -1.046701
H	7.048400 -2.333642 3.430490	O	0.944642 -5.402154 -0.076047
C	5.036694 -3.810323 4.835045	H	1.775164 -4.140647 -0.008530
H	5.068287 -4.504359 3.986057	S	5.172007 4.319196 0.145997
H	5.825304 -4.118371 5.534508	O	4.438312 0.176966 1.388348
C	1.405536 -2.507416 5.190699	O	5.384921 -0.758980 0.661739
H	0.725837 -3.352159 5.025934	H	5.573146 -0.207519 -0.141973
H	0.989489 -1.642500 4.664437	Fe	4.773243 2.168090 0.931777
H	1.397162 -2.280480 6.262387	N	3.713083 2.594020 2.619205
C	2.647606 -3.228363 3.151488	N	3.043101 2.128567 -0.147935
H	3.608832 -3.356472 2.654908	N	5.826291 1.602550 -0.725565
H	2.122995 -2.444681 2.596639	N	6.481329 2.188008 2.003726
H	2.082690 -4.162647 3.052644	C	4.212569 2.807370 3.900630
C	3.043998 -5.271015 5.666455	C	3.126041 3.131426 4.829244
H	2.034437 -5.250824 6.094478	C	1.967456 3.118879 4.084155
H	3.677054 -5.865825 6.336872	C	2.343414 2.777385 2.713597
H	2.994265 -5.782870 4.699144	C	1.760310 2.357356 0.327987
O	2.344188 -3.427126 -0.042167	C	0.793137 2.287579 -0.767318
H	2.226659 -2.406587 0.310265	C	1.507697 2.081974 -1.935446
H	3.235253 -3.508144 -0.448916	C	2.920657 1.966758 -1.522240
O	2.291086 -1.082305 0.721002	C	5.321106 1.471651 -2.014620
H	1.674147 -0.433355 0.342297	C	6.368233 1.019107 -2.922406
H	3.302852 -0.583134 1.081811	C	7.523436 0.859220 -2.170819
O	8.057014 -1.308101 1.269335	C	7.199874 1.330465 -0.819448
H	8.226539 -0.691468 2.006183	C	7.768703 2.008366 1.515769
H	7.089571 -1.220501 1.062427	C	8.740841 2.179381 2.592649

C	8.022738	2.450644	3.742220
C	6.614879	2.468306	3.360211
C	5.559434	2.743362	4.227331
H	5.818864	2.938933	5.261865
C	1.452709	2.656059	1.652412
H	0.413494	2.846726	1.889475
C	3.993044	1.684262	-2.366535
H	3.775359	1.578430	-3.424054
C	8.084804	1.613843	0.215510
H	9.141208	1.504794	0.003522
C	3.617875	-3.861942	5.485921
C	3.827802	-3.067139	6.769368
O	3.959187	-3.540436	7.913161
C	3.914223	-1.587555	6.401617
H	4.847940	-1.142773	6.762547
H	3.085016	-1.036442	6.862760
C	2.775212	-2.825333	4.641724
C	3.809517	-1.653444	4.851850
H	3.563828	-0.708291	4.365544
C	5.115410	-2.289662	4.383920
C	6.124453	-1.679336	3.761117
H	6.053104	-0.633148	3.482834
H	7.027681	-2.204740	3.462704
C	5.031139	-3.763639	4.790065
H	5.047103	-4.430553	3.919367
H	5.843539	-4.080829	5.456736
C	1.384332	-2.554654	5.247111
H	0.709613	-3.391680	5.033351
H	0.955240	-1.659332	4.786731
H	1.386898	-2.401919	6.331920
C	2.603215	-3.205259	3.167904
H	3.546606	-3.215356	2.623381
H	1.969753	-2.468000	2.667533
H	2.128779	-4.186433	3.049432
C	3.089719	-5.275799	5.657517
H	2.082843	-5.275806	6.092395
H	3.738614	-5.856227	6.324951
H	3.043589	-5.789334	4.691189
O	2.375885	-3.285248	-0.010538
H	2.309899	-1.950435	0.448001
H	3.239709	-3.450932	-0.448965
O	2.356022	-0.922208	0.735239
H	1.709283	-0.351490	0.290276
H	3.445454	-0.321523	1.129636
O	8.186695	-1.224663	1.365114
H	8.380840	-0.566501	2.059856
H	7.218948	-1.147763	1.186545
h	4.824752	5.228637	1.124096
h	3.229372	3.355116	5.891012
h	0.942639	3.318540	4.397128
h	-0.283231	2.355019	-0.609359
h	1.192579	2.019445	-2.977011
h	6.176000	0.803285	-3.973374
h	8.439690	0.387208	-2.525432
h	9.816593	2.038435	2.487965
h	8.383224	2.555605	4.765498
h	2.336365	-6.338091	-2.809530

TS1b”

Total QM energy at B2: -3764.151508 (a.u.)

Total QM/MM energy at B2: -3874.821453 (a.u.)

C	2.464614	-6.463337	-1.721699
H	3.121424	-5.664657	-1.380945
H	2.992488	-7.403737	-1.533495
C	1.165488	-6.499329	-0.930720
O	0.374055	-7.461355	-1.031802
O	0.916082	-5.483262	-0.107111
H	1.549288	-4.638707	-0.103945
S	5.181207	4.449758	0.140776
O	4.449537	0.575663	1.447690
O	5.479637	-1.131925	0.051387
H	5.425168	-0.211296	-0.309275
Fe	4.762946	2.168661	0.993237
N	3.734138	2.775196	2.648817
N	3.042942	2.225888	-0.125833
N	5.817608	1.684834	-0.685775
N	6.485345	2.291841	2.055456
C	4.230988	2.980452	3.929202
C	3.136552	3.272862	4.857977
C	1.978812	3.236299	4.112502
C	2.361827	2.910764	2.738905
C	1.765857	2.424797	0.365160
C	0.786643	2.314477	-0.720304
C	1.494089	2.110307	-1.892061
C	2.913009	2.039174	-1.491391
C	5.313598	1.561249	-1.975592
C	6.360584	1.102129	-2.878798
C	7.507917	0.916368	-2.120641

C	7.179733 1.376719 -0.763689	O	2.304748 -0.959651 0.635084
C	7.760061 2.046413 1.572855	H	1.734928 -0.254318 0.281756
C	8.741213 2.205485 2.651292	H	3.155947 -0.547860 0.959533
C	8.033587 2.526740 3.790267	O	8.129483 -1.410395 1.051529
C	6.625012 2.587448 3.403966	H	8.156799 -0.716829 1.737229
C	5.576278 2.906328 4.262441	H	7.216571 -1.369566 0.660890
H	5.834561 3.111338 5.295576	h	4.851717 5.376543 1.108687
C	1.467831 2.743828 1.687042	h	3.232080 3.478918 5.924036
H	0.426347 2.907074 1.933209	h	0.948451 3.399308 4.428496
C	3.987309 1.769432 -2.335404	h	-0.289406 2.363527 -0.553636
H	3.773091 1.662442 -3.393784	h	1.173708 2.023371 -2.930264
C	8.066320 1.624187 0.279895	h	6.172489 0.902089 -3.933630
H	9.119772 1.478393 0.075251	h	8.422059 0.450244 -2.488254
C	3.665236 -3.824485 5.400434	h	9.811746 2.032759 2.540875
C	3.899389 -3.010069 6.666069	h	8.390863 2.627305 4.815112
O	4.039893 -3.470414 7.814300	h	2.382237 -6.402572 -2.806866
C	3.989171 -1.538798 6.268323		
H	4.939998 -1.097814 6.587613	**IC1b”**	
H	3.184227 -0.969163 6.749736	Total QM energy at B2: -3764.159552 (a.u.)	
C	2.798144 -2.804934 4.558605	Total QM/MM energy at B2: -3874.831112 (a.u.)	
C	3.834252 -1.627128 4.722418	C	2.485252 -6.432718 -1.784706
H	3.573875 -0.687586 4.232784	H	3.147120 -5.632302 -1.454348
C	5.119437 -2.270467 4.211852	H	3.016885 -7.371648 -1.600508
C	6.066216 -1.685713 3.476562	C	1.194699 -6.473319 -0.978081
H	5.950223 -0.659296 3.142396	O	0.406364 -7.439685 -1.067878
H	6.949242 -2.216917 3.131211	O	0.953010 -5.456801 -0.153049
C	5.067124 -3.729227 4.678238	H	1.596446 -4.618163 -0.163320
H	5.089825 -4.432715 3.836708	S	5.121351 4.445091 0.155068
H	5.889804 -4.005996 5.350315	O	4.450012 0.493727 1.279031
C	1.419746 -2.526672 5.187700	O	6.499909 -0.824666 0.034732
H	0.755543 -3.387907 5.046309	H	5.750020 -0.369129 0.534471
H	0.959340 -1.669083 4.686948	Fe	4.680881 2.148697 0.966824
H	1.451473 -2.306567 6.260122	N	3.671904 2.705458 2.642789
C	2.595481 -3.214788 3.096263	N	2.959912 2.225213 -0.128714
H	3.534696 -3.286212 2.547993	N	5.723879 1.717904 -0.730422
H	1.994276 -2.460136 2.580177	N	6.415342 2.264299 2.026699
H	2.077168 -4.178117 3.017188	C	4.183934 2.920355 3.921014
C	3.151333 -5.238695 5.610426	C	3.097174 3.222554 4.857865
H	2.150343 -5.238518 6.059085	C	1.933677 3.184035 4.123857
H	3.814217 -5.797324 6.282770	C	2.302471 2.849771 2.747252
H	3.098813 -5.774824 4.656466	C	1.686205 2.402880 0.374495
O	2.384138 -3.451364 -0.110947	C	0.698049 2.294746 -0.706044
H	2.248606 -2.498033 0.211717	C	1.395740 2.116892 -1.885989
H	3.273276 -3.521044 -0.527775	C	2.823432 2.059503 -1.498813

C 5.218879 1.594909 -2.000097
C 6.253401 1.113841 -2.918649
C 7.389741 0.882312 -2.169177
C 7.062876 1.319856 -0.794442
C 7.688082 2.030879 1.522767
C 8.681737 2.178106 2.589403
C 7.987953 2.490747 3.740125
C 6.573615 2.549344 3.370448
C 5.528548 2.854203 4.244282
H 5.796305 3.056528 5.275383
C 1.395450 2.693551 1.703801
H 0.356367 2.849022 1.963319
C 3.888984 1.816862 -2.355068
H 3.667757 1.727809 -3.413369
C 7.973471 1.604064 0.233748
H 9.020548 1.438066 0.025558
C 3.800022 -3.766301 5.274510
C 4.130360 -2.945016 6.514462
O 4.303727 -3.401063 7.659123
C 4.268529 -1.484987 6.090512
H 5.246990 -1.079009 6.369288
H 3.503026 -0.875157 6.586245
C 2.955938 -2.715468 4.445695
C 4.057149 -1.592071 4.551738
H 3.832171 -0.649893 4.049823
C 5.301029 -2.306450 4.029557
C 6.302424 -1.757796 3.338442
H 6.256541 -0.717213 3.033527
H 7.176575 -2.322163 3.022726
C 5.171526 -3.761222 4.492372
H 5.105026 -4.457596 3.647285
H 6.005908 -4.097215 5.120818
C 1.615472 -2.356687 5.117078
H 0.901089 -3.182140 5.004322
H 1.183227 -1.478440 4.625979
H 1.693878 -2.133147 6.186330
C 2.678318 -3.141107 3.000269
H 3.590372 -3.275661 2.419778
H 2.094482 -2.370653 2.487371
H 2.113608 -4.080343 2.962144
C 3.218373 -5.144396 5.540169
H 2.243460 -5.076756 6.038350
H 3.881566 -5.725483 6.192759
H 3.087274 -5.696384 4.602765
O 2.445410 -3.444821 -0.213704
H 2.312762 -2.479359 0.080585
H 3.325420 -3.535795 -0.644621
O 2.340527 -0.939418 0.448754
H 1.733777 -0.289678 0.053288
H 3.148490 -0.451230 0.807581
O 8.803827 -1.153041 1.338970
H 8.666412 -0.709063 2.196050
H 7.944955 -1.077670 0.825927
h 4.802957 5.357213 1.140464
h 3.204541 3.437377 5.921063
h 0.907909 3.363437 4.445853
h -0.377343 2.327829 -0.531392
h 1.066403 2.033783 -2.921700
h 6.060746 0.943885 -3.977925
h 8.299182 0.415694 -2.547664
h 9.746181 1.984821 2.456487
h 8.356410 2.592545 4.760881
h 2.386472 -6.376981 -2.868774

RC2

Total QM energy at B2: -3306.223483 (a.u.)

Total QM/MM energy at B2: -3428.680721 (a.u.)

S 2.570500 5.710531 0.081909
O 2.776923 1.559241 1.682140
H 2.091268 1.583471 2.392863
O 2.203448 0.442342 0.805055
H 2.961628 0.293117 0.171178
Fe 2.680264 3.609912 1.002191
N 1.510712 3.880550 2.668611
N 1.052757 3.093892 -0.091531
N 3.877906 3.129125 -0.558150
N 4.298902 3.860018 2.208918
C 1.901796 4.241046 3.965054
C 0.735494 4.383183 4.824239
C -0.370810 4.131347 4.036190
C 0.116279 3.846292 2.694583
C -0.266759 3.179799 0.320269
C -1.167923 2.779444 -0.763026
C -0.382342 2.460667 -1.854052
C 1.009121 2.666728 -1.411211
C 3.468177 2.708199 -1.810856
C 4.616522 2.555455 -2.694424
C 5.742158 2.931876 -1.980648

C 5.268684 3.234985 -0.619748
C 5.619560 3.673803 1.819498
C 6.509077 3.798409 2.969878
C 5.721264 4.102561 4.060426
C 4.345255 4.138929 3.578595
C 3.224495 4.368811 4.367929
H 3.396939 4.636081 5.404475
C -0.680202 3.554666 1.593732
H -1.746498 3.627694 1.754707
C 2.148592 2.486688 -2.186667
H 2.004492 2.146061 -3.206106
C 6.048106 3.431636 0.516493
H 7.115486 3.289449 0.414627
C 1.595890 -1.558083 6.029932
C 2.846977 -2.415771 5.844719
O 3.408295 -3.117239 6.705209
C 3.306830 -2.240937 4.401765
H 3.287439 -3.192767 3.861086
H 4.337240 -1.871148 4.371531
C 1.968744 -0.318278 5.113645
C 2.275998 -1.214428 3.855156
H 2.599792 -0.687030 2.958437
C 0.966455 -1.970405 3.702682
C 0.360592 -2.232417 2.542719
H 0.807278 -1.911931 1.606972
H -0.586934 -2.752904 2.472928
C 0.508365 -2.286743 5.134244
H -0.479378 -1.865719 5.356532
H 0.451883 -3.363356 5.340982
C 3.179654 0.478134 5.632736
H 2.917577 1.040339 6.536958
H 3.510652 1.205324 4.882349
H 4.032405 -0.162443 5.879155
C 0.789260 0.644923 4.899658
H -0.007990 0.207935 4.293555
H 1.124343 1.561147 4.400687
H 0.362264 0.955327 5.859255
C 1.212317 -1.288504 7.475252
H 1.912534 -0.588598 7.945890
H 1.245655 -2.212070 8.060121
H 0.206741 -0.860919 7.542903
h 2.324377 6.647484 1.064706
h 0.739862 4.616796 5.888886
h -1.407819 4.066468 4.365538
h -2.247926 2.706476 -0.635214
h -0.632057 2.123779 -2.860141
h 4.510497 2.200347 -3.719472
h 6.738905 2.997807 -2.416785
h 7.584613 3.625167 2.934167
h 6.041694 4.276656 5.087598

TS2a

Total QM energy at B2: -3306.196157 (a.u.)

Total QM/MM energy at B2: -3428.655942 (a.u.)

S 2.628441 5.713882 0.043359
O 2.760467 1.719902 1.683857
H 2.071103 1.595370 2.371093
O 2.014303 0.218147 0.716817
H 2.816330 0.122123 0.135357
Fe 2.679938 3.554467 1.026584
N 1.527020 3.972040 2.671649
N 1.031928 3.118519 -0.063445
N 3.853678 3.057302 -0.539395
N 4.318370 3.877936 2.197290
C 1.932006 4.296994 3.969331
C 0.775359 4.446611 4.841801
C -0.338667 4.229271 4.056560
C 0.140104 3.952567 2.709486
C -0.281917 3.298268 0.330641
C -1.198722 2.906590 -0.742519
C -0.426812 2.416353 -1.777602
C 0.971128 2.576371 -1.333613
C 3.436629 2.514135 -1.735811
C 4.572361 2.292682 -2.621961
C 5.699393 2.756225 -1.966410
C 5.239890 3.165982 -0.628472
C 5.630873 3.677805 1.798632
C 6.534472 3.801972 2.937799
C 5.758712 4.111324 4.035488
C 4.379683 4.157144 3.564568
C 3.262995 4.399136 4.357917
H 3.446896 4.652413 5.396361
C -0.672344 3.681916 1.609118
H -1.735978 3.734143 1.800452
C 2.108845 2.259934 -2.070964
H 1.955211 1.786592 -3.034716
C 6.034392 3.405629 0.490727
H 7.101061 3.261519 0.372215

C	1.710005 -1.528314 6.046563	O	1.822858 -0.056087 0.482101
C	2.960305 -2.371315 5.804123	H	2.663875 -0.214994 -0.035055
O	3.562722 -3.072765 6.638253	Fe	2.769429 3.459131 1.196532
C	3.356003 -2.183342 4.343936	N	1.594658 3.995210 2.770141
H	3.321567 -3.131663 3.797580	N	1.092370 3.079392 0.097353
H	4.382397 -1.806592 4.273345	N	3.956780 2.994198 -0.381947
C	2.032846 -0.278831 5.122390	N	4.423834 3.840949 2.313373
C	2.295428 -1.162264 3.844550	C	2.009270 4.292634 4.066004
H	2.569395 -0.629676 2.932958	C	0.860033 4.475592 4.941469
C	0.984546 -1.924917 3.745404	C	-0.262220 4.300443 4.157839
C	0.317576 -2.153288 2.612146	C	0.209375 4.006884 2.814045
H	0.713036 -1.790201 1.669005	C	-0.225225 3.288382 0.460018
H	-0.633932 -2.671015 2.580285	C	-1.132446 2.886322 -0.615243
C	0.594706 -2.264134 5.191911	C	-0.351080 2.366207 -1.628067
H	-0.389416 -1.862396 5.461982	C	1.043597 2.522480 -1.165997
H	0.567034 -3.343301 5.392241	C	3.525537 2.439422 -1.562841
C	3.256375 0.528927 5.590749	C	4.651459 2.193563 -2.458522
H	3.024774 1.098428 6.499217	C	5.788392 2.656910 -1.820325
H	3.552686 1.244813 4.815456	C	5.342913 3.087512 -0.486420
H	4.123343 -0.102701 5.809948	C	5.734997 3.632768 1.931369
C	0.835769 0.673446 4.964371	C	6.633151 3.766150 3.072182
H	0.020967 0.226698 4.390511	C	5.846718 4.079568 4.160991
H	1.143552 1.589909 4.449973	C	4.471545 4.120457 3.674863
H	0.444023 0.971420 5.943003	C	3.344349 4.358953 4.457823
C	1.379429 -1.275003 7.507889	H	3.523665 4.593891 5.501509
H	2.129924 -0.627511 7.976270	C	-0.613599 3.721453 1.722784
H	1.374221 -2.211930 8.073161	H	-1.676724 3.796598 1.912144
H	0.401106 -0.794278 7.612166	C	2.189064 2.197554 -1.889747
h	2.369886 6.677046 0.997198	H	2.035168 1.720782 -2.851968
h	0.791618 4.665575 5.909442	C	6.140643 3.333660 0.627586
h	-1.384945 4.208578 4.361420	H	7.206859 3.180847 0.512289
h	-2.278247 3.037938 -0.668760	C	1.717235 -1.497802 6.032872
h	-0.689283 1.972378 -2.737842	C	2.954688 -2.361442 5.797261
h	4.455269 1.829965 -3.601884	O	3.553777 -3.056985 6.639205
h	6.690834 2.809332 -2.416178	C	3.339360 -2.209536 4.329292
h	7.608766 3.623616 2.891456	H	3.290467 -3.169552 3.804588
h	6.085802 4.281649 5.061192	H	4.368581 -1.844248 4.241494
		C	2.045357 -0.274101 5.077165
IC2a		C	2.285455 -1.187326 3.817778
Total QM energy at B2: -3306.207004 (a.u.)		H	2.561830 -0.666060 2.901106
Total QM/MM energy at B2: -3428.664990 (a.u.)		C	0.965555 -1.937362 3.747384
S	2.731472 5.677797 0.054011	C	0.281987 -2.183725 2.627960
O	2.822278 1.682191 1.784943	H	0.670041 -1.847472 1.671966
H	1.911130 1.350462 1.930392	H	-0.678271 -2.685925 2.622883

C 0.587122 -2.241426 5.204817
H -0.390818 -1.825627 5.476119
H 0.551813 -3.315955 5.428156
C 3.284670 0.532338 5.504446
H 3.068342 1.138910 6.392617
H 3.577108 1.207491 4.693138
H 4.143664 -0.103732 5.742853
C 0.863627 0.692658 4.898911
H 0.012177 0.224171 4.400382
H 1.176187 1.545592 4.289242
H 0.525963 1.077240 5.866829
C 1.399391 -1.210790 7.490651
H 2.165864 -0.571436 7.944210
H 1.374316 -2.137114 8.073679
H 0.432367 -0.706396 7.588960
h 2.426630 6.659191 0.975033
h 0.882534 4.680751 6.011735
h -1.310605 4.315358 4.455720
h -2.211192 3.030035 -0.554250
h -0.605498 1.896843 -2.578349
h 4.524371 1.717437 -3.430746
h 6.777364 2.701979 -2.276361
h 7.708586 3.592982 3.033200
h 6.167957 4.275132 5.184039

TS2b

Total QM energy at B2: -3306.2068664 (a.u.)

Total QM/MM energy at B2: -3428.665088 (a.u.)

S 2.715597 5.682834 0.055818
O 2.903402 1.701297 1.808829
H 2.062306 1.188719 1.665327
O 1.808977 0.005841 0.494694
H 2.616053 -0.228419 -0.044832
Fe 2.773316 3.446843 1.195212
N 1.608681 3.995256 2.763010
N 1.097593 3.062609 0.092782
N 3.953461 3.014929 -0.391871
N 4.432414 3.834360 2.320512
C 2.023293 4.291629 4.060578
C 0.874080 4.472318 4.934841
C -0.248344 4.295286 4.150866
C 0.222500 4.001845 2.807496
C -0.218089 3.272722 0.457157
C -1.129477 2.874329 -0.617611
C -0.351457 2.359038 -1.634606
C 1.044955 2.518301 -1.176531
C 3.525058 2.458704 -1.574664
C 4.653506 2.209162 -2.463329
C 5.789922 2.669074 -1.819152
C 5.341387 3.100036 -0.487760
C 5.741268 3.626105 1.935375
C 6.644659 3.759303 3.074463
C 5.861545 4.072663 4.164475
C 4.484874 4.114311 3.679602
C 3.356651 4.355136 4.459093
H 3.532207 4.590562 5.503322
C -0.602571 3.710686 1.719855
H -1.665281 3.788135 1.911827
C 2.190229 2.209319 -1.904995
H 2.039323 1.737987 -2.870532
C 6.140737 3.333186 0.628964
H 7.205935 3.176275 0.509816
C 1.715790 -1.499119 6.036773
C 2.952248 -2.365487 5.805746
O 3.549129 -3.060073 6.649945
C 3.339412 -2.219057 4.337962
H 3.290268 -3.181162 3.817037
H 4.369053 -1.855073 4.250344
C 2.047159 -0.279003 5.077505
C 2.287839 -1.196802 3.822406
H 2.565686 -0.675548 2.907105
C 0.966861 -1.944273 3.751618
C 0.283314 -2.191769 2.632572
H 0.670859 -1.859542 1.674984
H -0.678598 -2.690492 2.627126
C 0.585944 -2.243926 5.209128
H -0.391762 -1.825820 5.477453
H 0.548716 -3.317771 5.435316
C 3.287307 0.526779 5.503296
H 3.070266 1.136555 6.389047
H 3.581218 1.198654 4.689921
H 4.145020 -0.109740 5.745478
C 0.868578 0.689561 4.890169
H 0.014712 0.218627 4.398258
H 1.184185 1.531572 4.267249
H 0.533573 1.085242 5.854616
C 1.396390 -1.206566 7.493003
H 2.163339 -0.566636 7.944896

H 1.369276 -2.130745 8.079369
H 0.430196 -0.700056 7.588098
h 2.420801 6.664717 0.979586
h 0.894732 4.677776 6.005087
h -1.296296 4.309173 4.450317
h -2.207649 3.021055 -0.553708
h -0.607526 1.891535 -2.585362
h 4.529933 1.731072 -3.435042
h 6.779775 2.712614 -2.273422
h 7.720288 3.588197 3.031894
h 6.183425 4.270843 5.186818

IC2b

Total QM energy at B2: -3306.257116 (a.u.)

Total QM/MM energy at B2: -3428.714904 (a.u.)

S 2.684635 5.700674 0.081309
O 2.804254 1.857236 1.823981
H 2.070223 0.494001 0.916173
O 1.800055 -0.275800 0.361305
H 2.550796 -0.529253 -0.225568
Fe 2.764326 3.419543 1.252708
N 1.606427 4.048474 2.798048
N 1.098022 3.069187 0.128397
N 3.932309 2.995801 -0.354217
N 4.416737 3.903577 2.335075
C 2.019992 4.343444 4.096014
C 0.867650 4.517014 4.968455
C -0.250706 4.338735 4.182571
C 0.225559 4.047073 2.838215
C -0.216111 3.295976 0.496430
C -1.130702 2.880659 -0.568011
C -0.359998 2.329720 -1.571834
C 1.036312 2.483631 -1.120342
C 3.507469 2.406619 -1.523715
C 4.632626 2.165803 -2.417163
C 5.762384 2.667579 -1.794558
C 5.316771 3.113933 -0.466790
C 5.726279 3.693447 1.939633
C 6.630544 3.821581 3.074570
C 5.851070 4.127535 4.170834
C 4.474491 4.174635 3.696382
C 3.351181 4.408637 4.488327
H 3.534358 4.636478 5.532664
C -0.598415 3.746183 1.752442
H -1.660930 3.818628 1.945273
C 2.176406 2.134959 -1.839930
H 2.022115 1.621388 -2.782112
C 6.121170 3.385348 0.636952
H 7.187227 3.240710 0.512112
C 1.702529 -1.494202 6.006890
C 2.934433 -2.367183 5.780100
O 3.532062 -3.055559 6.629476
C 3.320315 -2.230415 4.309913
H 3.256475 -3.193393 3.791578
H 4.355736 -1.882656 4.221197
C 2.046315 -0.275732 5.047571
C 2.278976 -1.197330 3.792884
H 2.558631 -0.686287 2.872395
C 0.947047 -1.926585 3.719912
C 0.250573 -2.134229 2.600116
H 0.634961 -1.778143 1.646868
H -0.722302 -2.614080 2.600434
C 0.570287 -2.234283 5.177267
H -0.407147 -1.819074 5.451156
H 0.535187 -3.309134 5.400546
C 3.291647 0.517736 5.482725
H 3.080346 1.110023 6.382067
H 3.583769 1.208808 4.684777
H 4.149770 -0.124644 5.707246
C 0.879037 0.705652 4.858505
H 0.007623 0.233247 4.400891
H 1.192343 1.520072 4.198547
H 0.574052 1.136350 5.818021
C 1.379144 -1.199296 7.461968
H 2.151886 -0.571265 7.920875
H 1.335264 -2.124363 8.046095
H 0.419216 -0.680001 7.551848
h 2.403222 6.696820 0.993913
h 0.888226 4.712304 6.040605
h -1.299707 4.344696 4.478592
h -2.208118 3.033548 -0.505833
h -0.621466 1.839804 -2.509748
h 4.509603 1.665311 -3.377600
h 6.746492 2.724433 -2.259708
h 7.705304 3.645882 3.028898
h 6.179466 4.313666 5.193369

TS2c

Total QM energy at B2: -3306.199531 (a.u.)

Total QM/MM energy at B2: -3428.657214 (a.u.)

S	2.716339	5.606104	0.077542
O	2.715244	1.569987	1.697152
H	1.784658	1.303007	1.847758
O	2.128778	0.241939	0.031578
H	3.035887	-0.135035	-0.147740
Fe	2.736226	3.443763	1.176982
N	1.592972	3.943268	2.774636
N	1.041248	3.052476	0.135364
N	3.873137	2.929505	-0.396734
N	4.396680	3.799120	2.238846
C	2.033487	4.192170	4.073924
C	0.899320	4.407911	4.960418
C	-0.234729	4.312207	4.177464
C	0.213480	4.034993	2.822279
C	-0.269973	3.393059	0.461874
C	-1.174353	2.973195	-0.603062
C	-0.410509	2.284809	-1.534941
C	0.964531	2.355743	-1.031011
C	3.440563	2.184502	-1.451580
C	4.511659	1.965532	-2.408882
C	5.624421	2.644096	-1.929121
C	5.232782	3.157927	-0.610132
C	5.703469	3.720974	1.784575
C	6.634616	3.878849	2.893453
C	5.875498	4.078073	4.031041
C	4.482245	4.039225	3.608016
C	3.376364	4.226905	4.437909
H	3.585322	4.429303	5.482990
C	-0.631969	3.842635	1.718944
H	-1.688133	3.974479	1.911432
C	2.110994	1.717160	-1.576516
H	1.938600	1.025961	-2.394559
C	6.067523	3.505855	0.448381
H	7.135440	3.473533	0.264623
C	1.680466	-1.584124	5.888564
C	2.963157	-2.395380	5.717787
O	3.528083	-3.095057	6.578945
C	3.447999	-2.172919	4.287732
H	3.459983	-3.112278	3.724488
H	4.470679	-1.781925	4.286080
C	2.047370	-0.307187	5.021800
C	2.408100	-1.151344	3.742592
H	2.745429	-0.571572	2.882195
C	1.122327	-1.933974	3.532078
C	0.536672	-2.161615	2.354244
H	0.972483	-1.773452	1.436852
H	-0.394047	-2.711581	2.258721
C	0.644929	-2.320104	4.940038
H	-0.365420	-1.949825	5.151090
H	0.629990	-3.404848	5.109385
C	3.230841	0.497967	5.587120
H	2.938293	1.032909	6.498771
H	3.559305	1.239809	4.851534
H	4.090235	-0.131962	5.839619
C	0.859112	0.642782	4.803039
H	0.031730	0.164977	4.272915
H	1.181335	1.504274	4.210675
H	0.482449	1.021146	5.759196
C	1.237038	-1.373453	7.325322
H	1.952102	-0.749200	7.873732
H	1.180842	-2.330189	7.852234
H	0.255970	-0.888599	7.367623
h	2.401192	6.589173	0.993295
h	0.938317	4.604876	6.031749
h	-1.280476	4.368105	4.479715
h	-2.240904	3.197459	-0.587542
h	-0.668039	1.765364	-2.457937
h	4.370226	1.377470	-3.315660
h	6.563377	2.766001	-2.469091
h	7.717255	3.783290	2.810826
h	6.224071	4.251312	5.049153

IC2c

Total QM energy at B2: -3306.283376 (a.u.)

Total QM/MM energy at B2: -3428.741912 (a.u.)

S	2.674243	5.615060	0.102531
O	2.800087	1.739474	2.003515
H	2.570623	1.097770	1.288850
O	2.167771	0.275637	-0.463144
H	2.867888	-0.364146	-0.770211
Fe	2.752603	3.423814	1.269771
N	1.624870	4.029577	2.820946
N	1.089665	2.957427	0.192048
N	3.860213	2.857683	-0.323137
N	4.410449	3.883367	2.307722
C	2.053589	4.269642	4.128977

C	0.905542 4.462934 5.001305	H	0.010466 0.156601 4.292930
C	-0.216358 4.359928 4.199735	H	1.192878 1.437856 4.036954
C	0.262965 4.093604 2.851759	H	0.558415 1.126309 5.672999
C	-0.223695 3.402702 0.492630	C	1.289053 -1.302990 7.320564
C	-1.127987 3.002616 -0.589632	H	2.023111 -0.676461 7.840729
C	-0.384161 2.246525 -1.478081	H	1.227365 -2.246145 7.872435
C	0.980469 2.249517 -0.930681	H	0.316682 -0.801321 7.368446
C	3.465004 2.135912 -1.374497	h	2.387131 6.624900 0.998152
C	4.505394 2.021685 -2.380261	h	0.930359 4.649157 6.074977
C	5.607236 2.718952 -1.898897	h	-1.267373 4.392998 4.486687
C	5.228700 3.179084 -0.553961	h	-2.181184 3.283066 -0.603431
C	5.698602 3.774618 1.848427	h	-0.645458 1.702396 -2.385668
C	6.646524 3.916755 2.944132	h	4.359977 1.465035 -3.306037
C	5.897701 4.127403 4.090592	h	6.533146 2.876485 -2.452016
C	4.505144 4.113441 3.673507	h	7.726599 3.802500 2.852207
C	3.390583 4.297267 4.497570	h	6.252577 4.299941 5.106643
H	3.594596 4.485474 5.547341		
C	-0.575122 3.884065 1.721424	**TS2d**	
H	-1.628687 4.059338 1.897310	Total QM energy at B2: -3306.196031 (a.u.)	
C	2.144225 1.432342 -1.393306	Total QM/MM energy at B2: -3428.653475 (a.u.)	
H	1.965217 1.052746 -2.403991	S	2.688754 5.623719 0.093305
C	6.045999 3.532359 0.494960	O	2.872824 1.711215 1.981869
H	7.113438 3.538903 0.301428	H	2.233090 1.081018 1.559294
C	1.703244 -1.549442 5.880214	O	1.310989 -0.438918 0.825025
C	2.976877 -2.373623 5.701912	H	2.006482 -0.818183 0.211588
O	3.553339 -3.061309 6.565757	Fe	2.799202 3.388263 1.256437
C	3.436393 -2.185397 4.256629	N	1.644415 4.004176 2.813417
H	3.437803 -3.136846 3.714081	N	1.125432 2.942904 0.162697
H	4.458901 -1.794593 4.229557	N	3.952146 2.918775 -0.343161
C	2.055894 -0.296376 4.972761	N	4.451970 3.823149 2.359827
C	2.388208 -1.173971 3.710406	C	2.055354 4.294301 4.108067
H	2.707570 -0.601689 2.840663	C	0.902588 4.473538 4.981639
C	1.097035 -1.955838 3.544803	C	-0.216364 4.307437 4.194056
C	0.485089 -2.213663 2.387301	C	0.260283 4.005995 2.850352
H	0.904797 -1.862863 1.448392	C	-0.182733 3.191880 0.522304
H	-0.453289 -2.753790 2.323735	C	-1.105845 2.786337 -0.541775
C	0.645136 -2.303326 4.971159	C	-0.342853 2.229301 -1.548234
H	-0.358419 -1.920844 5.191790	C	1.057008 2.369023 -1.096711
H	0.627099 -3.383610 5.167187	C	3.527837 2.359252 -1.526273
C	3.255044 0.522971 5.482003	C	4.650064 2.156929 -2.432306
H	2.981180 1.096783 6.375980	C	5.781951 2.637494 -1.793659
H	3.563137 1.226285 4.702222	C	5.336934 3.043759 -0.452343
H	4.117352 -0.099730 5.745117	C	5.755905 3.615318 1.962089
C	0.875046 0.657890 4.734856	C	6.670527 3.758379 3.093879

C	5.895613	4.068992 4.189814
C	4.513677	4.105077 3.716917
C	3.390251	4.346515 4.504178
H	3.571441	4.575389 5.549215
C	-0.560849	3.683939 1.770096
H	-1.623690	3.777306 1.957636
C	2.196203	2.067023 -1.836228
H	2.041143	1.592462 -2.799661
C	6.142105	3.304661 0.655547
H	7.207901	3.158611 0.526134
C	1.341550	-1.484190 5.730232
C	2.553895	-2.406991 5.850278
O	2.910731	-3.047232 6.854996
C	3.325841	-2.325332 4.535392
H	3.359312	-3.296219 4.028622
H	4.360119	-2.020967 4.718798
C	2.006771	-0.297821 4.909029
C	2.515227	-1.250202 3.756615
H	3.047981	-0.736222 2.958701
C	1.226084	-1.926492 3.336768
C	0.877020	-2.302597 2.086190
H	1.605826	-2.451547 1.300527
H	-0.114071	-2.692491 1.869015
C	0.419988	-2.121500 4.620545
H	-0.541755	-1.596648 4.600422
H	0.199980	-3.179313 4.816882
C	3.146569	0.420011 5.653535
H	2.747395	1.010074 6.486650
H	3.653660	1.105484 4.966168
H	3.891816	-0.265868 6.071370
C	1.000871	0.757044 4.423342
H	0.174300	0.330673 3.849002
H	1.525208	1.453575 3.763006
H	0.586763	1.314143 5.270424
C	0.637792	-1.170469 7.035256
H	1.332784	-0.771002 7.781746
H	0.192163	-2.081447 7.447459
H	-0.162649	-0.440757 6.879982
h	2.406021	6.624055 1.000904
h	0.921234	4.664284 6.054641
h	-1.266311	4.327279 4.486089
h	-2.180480	2.958511 -0.481915
h	-0.607226	1.752948 -2.492300
h	4.524066	1.717706 -3.421889
h	6.763840	2.712257 -2.260962
h	7.747362	3.597719 3.042110
h	6.223972	4.271107 5.209322

IC2d

Total QM energy at B2: -3306.239563 (a.u.)

Total QM/MM energy at B2: -3428.701897 (a.u.)

S	2.722927	5.554476 0.095785
O	2.808041	1.584563 1.913118
H	1.915366	1.162672 1.862137
O	0.407681	-0.124789 1.658976
H	0.187171	0.009038 0.711626
Fe	2.763585	3.300566 1.290336
N	1.588329	3.919801 2.821497
N	1.093073	2.892162 0.190930
N	3.951355	2.827527 -0.284867
N	4.417127	3.724387 2.392604
C	1.996024	4.223065 4.113081
C	0.841760	4.442449 4.974963
C	-0.276449	4.283714 4.184055
C	0.201119	3.959664 2.848011
C	-0.220029	3.158985 0.519492
C	-1.123108	2.732319 -0.549085
C	-0.341653	2.141369 -1.527038
C	1.050292	2.277253 -1.049609
C	3.530880	2.218531 -1.442957
C	4.658156	1.976557 -2.338317
C	5.785327	2.487919 -1.721021
C	5.335933	2.944847 -0.395830
C	5.726792	3.531015 2.011399
C	6.627871	3.691666 3.150620
C	5.839819	4.006797 4.235502
C	4.461339	4.023170 3.749954
C	3.330910	4.271078 4.520624
H	3.501386	4.515622 5.563868
C	-0.613910	3.658724 1.759855
H	-1.677509	3.767055 1.932222
C	2.201336	1.924090 -1.752444
H	2.056340	1.395972 -2.688870
C	6.133750	3.222521 0.709883
H	7.202397	3.088435 0.591593
C	1.374846	-1.762165 5.694391
C	2.705607	-2.514203 5.655401
O	3.165289	-3.263375 6.537827

C	3.431158 -2.081844 4.379826	N	1.476933 3.990512 2.710798
H	3.565674 -2.921209 3.690027	N	0.979152 3.101711 -0.018027
H	4.427101 -1.698715 4.619707	N	3.799906 3.049688 -0.500761
C	1.878618 -0.357092 5.146551	N	4.266256 3.890766 2.236913
C	2.477586 -0.980252 3.817606	C	1.885774 4.313386 4.007658
H	2.949884 -0.261263 3.145914	C	0.727464 4.446696 4.881683
C	1.270415 -1.710509 3.276299	C	-0.386648 4.222401 4.099195
C	0.711051 -1.565648 1.915909	C	0.088977 3.951276 2.749264
H	1.411205 -1.911394 1.141673	C	-0.332982 3.275312 0.382852
H	-0.216489 -2.147115 1.822968	C	-1.250963 2.906359 -0.698109
C	0.543109 -2.298459 4.467519	C	-0.481455 2.450422 -1.751073
H	-0.495598 -1.941862 4.543342	C	0.918436 2.597714 -1.306803
H	0.490014 -3.398769 4.463109	C	3.376156 2.540297 -1.711748
C	2.923211 0.311685 6.060122	C	4.512745 2.333692 -2.601971
H	2.446802 0.684717 6.975239	C	5.642832 2.772613 -1.934536
H	3.374235 1.166398 5.543512	C	5.184722 3.157748 -0.586357
H	3.729117 -0.362828 6.369679	C	5.578008 3.691805 1.829902
C	0.747838 0.647256 4.882266	C	6.484419 3.823755 2.967662
H	0.021995 0.288615 4.149622	C	5.711774 4.128114 4.068349
H	1.174205 1.569051 4.478715	C	4.328957 4.171450 3.604456
H	0.222762 0.894547 5.812794	C	3.216208 4.411044 4.402378
C	0.633936 -1.807234 7.015724	H	3.399529 4.658035 5.442534
H	1.291365 -1.555151 7.855722	C	-0.725983 3.660983 1.659674
H	0.238140 -2.814730 7.190575	H	-1.789721 3.702796 1.852749
H	-0.210952 -1.109768 7.010518	C	2.051113 2.306679 -2.059865
h	2.413137 6.552711 0.996841	H	1.893324 1.878004 -3.043912
h	0.860896 4.649105 6.045007	C	5.983270 3.411230 0.526943
h	-1.326771 4.316951 4.473516	H	7.049713 3.265644 0.409991
h	-2.195024 2.927607 -0.518680	C	1.189971 -1.730611 5.716004
h	-0.592066 1.660557 -2.472649	C	2.428054 -2.621518 5.851401
h	4.535666 1.480532 -3.301137	O	2.730063 -3.339261 6.818890
h	6.770250 2.545650 -2.184335	C	3.342207 -2.330700 4.667162
h	7.705743 3.535409 3.107696	H	3.449020 -3.203711 4.013908
h	6.161426 4.230062 5.252747	H	4.340792 -2.066058 5.022763
		C	1.928861 -0.406397 5.222755
TS2e		C	2.611723 -1.140507 3.986288
Total QM energy at B2: -3306.168971 (a.u.)		H	3.228011 -0.511159 3.346520
Total QM/MM energy at B2: -3428.623204 (a.u.)		C	1.394751 -1.710995 3.298218
S	2.601773 5.697738 0.054989	C	1.150093 -1.709497 1.940555
O	2.755734 1.747411 1.823267	H	1.922060 -1.975231 1.224362
H	2.250845 1.792103 2.663459	H	0.140759 -1.940186 1.601667
O	1.744546 0.119061 1.464824	C	0.444366 -2.150206 4.397965
H	2.282943 -0.045744 0.643644	H	-0.529353 -1.645478 4.340192
Fe	2.623313 3.574938 1.065303	H	0.238902 -3.229003 4.358171

C	2.925561	0.163406 6.250295
H	2.384496	0.601852 7.097296
H	3.520631	0.962271 5.792529
H	3.613970	-0.582939 6.660570
C	0.953038	0.714438 4.823121
H	0.375287	0.490010 3.923389
H	1.503601	1.643049 4.641602
H	0.254586	0.925450 5.640428
C	0.306822	-1.672661 6.946346
H	0.887671	-1.429896 7.843009
H	-0.171493	-2.645637 7.111604
H	-0.483079	-0.924545 6.829150
h	2.349509	6.666972 1.004353
h	0.745707	4.656379 5.951153
h	-1.432642	4.197073 4.404679
h	-2.330005	3.038928 -0.619627
h	-0.744902	2.043142 -2.727180
h	4.391328	1.919543 -3.602873
h	6.631382	2.833581 -2.389639
h	7.560351	3.657220 2.915675
h	6.044816	4.301230 5.091667

IC2e

Total QM energy at B2: -3306.240064 (a.u.)

Total QM/MM energy at B2: -3428.702471 (a.u.)

S	2.601773	5.697738 0.054989
O	2.755734	1.747411 1.823267
H	2.250845	1.792103 2.663459
O	1.744546	0.119061 1.464824
H	2.282943	-0.045744 0.643644
Fe	2.623313	3.574938 1.065303
N	1.476933	3.990512 2.710798
N	0.979152	3.101711 -0.018027
N	3.799906	3.049688 -0.500761
N	4.266256	3.890766 2.236913
C	1.885774	4.313386 4.007658
C	0.727464	4.446696 4.881683
C	-0.386648	4.222401 4.099195
C	0.088977	3.951276 2.749264
C	-0.332982	3.275312 0.382852
C	-1.250963	2.906359 -0.698109
C	-0.481455	2.450422 -1.751073
C	0.918436	2.597714 -1.306803
C	3.376156	2.540297 -1.711748
C	4.512745	2.333692 -2.601971
C	5.642832	2.772613 -1.934536
C	5.184722	3.157748 -0.586357
C	5.578008	3.691805 1.829902
C	6.484419	3.823755 2.967662
C	5.711774	4.128114 4.068349
C	4.328957	4.171450 3.604456
C	3.216208	4.411044 4.402378
H	3.399529	4.658035 5.442534
C	-0.725983	3.660983 1.659674
H	-1.789721	3.702796 1.852749
C	2.051113	2.306679 -2.059865
H	1.893324	1.878004 -3.043912
C	5.983270	3.411230 0.526943
H	7.049713	3.265644 0.409991
C	1.189971	-1.730611 5.716004
C	2.428054	-2.621518 5.851401
O	2.730063	-3.339261 6.818890
C	3.342207	-2.330700 4.667162
H	3.449020	-3.203711 4.013908
H	4.340792	-2.066058 5.022763
C	1.928861	-0.406397 5.222755
C	2.611723	-1.140507 3.986288
H	3.228011	-0.511159 3.346520
C	1.394751	-1.710995 3.298218
C	1.150093	-1.709497 1.940555
H	1.922060	-1.975231 1.224362
H	0.140759	-1.940186 1.601667
C	0.444366	-2.150206 4.397965
H	-0.529353	-1.645478 4.340192
H	0.238902	-3.229003 4.358171
C	2.925561	0.163406 6.250295
H	2.384496	0.601852 7.097296
H	3.520631	0.962271 5.792529
H	3.613970	-0.582939 6.660570
C	0.953038	0.714438 4.823121
H	0.375287	0.490010 3.923389
H	1.503601	1.643049 4.641602
H	0.254586	0.925450 5.640428
C	0.306822	-1.672661 6.946346
H	0.887671	-1.429896 7.843009
H	-0.171493	-2.645637 7.111604
H	-0.483079	-0.924545 6.829150
h	2.349509	6.666972 1.004353

h 0.745707 4.656379 5.951153
h -1.432642 4.197073 4.404679
h -2.330005 3.038928 -0.619627
h -0.744902 2.043142 -2.727180
h 4.391328 1.919543 -3.602873
h 6.631382 2.833581 -2.389639
h 7.560351 3.657220 2.915675
h 6.044816 4.301230 5.091667

IC2f

Total QM energy at B2: -3306.241149 (a.u.)

Total QM/MM energy at B2: -3428.703872 (a.u.)

S 2.753400 5.576849 0.093659
O 2.710722 1.597371 1.725660
H 3.304309 1.089049 1.132313
O 0.373444 0.303992 1.911466
H 1.214667 0.860069 1.852912
Fe 2.756630 3.388414 1.168462
N 1.588471 3.903948 2.756739
N 1.093568 3.018965 0.052899
N 3.944976 2.871333 -0.404454
N 4.408262 3.760760 2.286590
C 1.994995 4.208482 4.044794
C 0.840166 4.409620 4.917933
C -0.276265 4.230087 4.131525
C 0.202973 3.921154 2.788545
C -0.212788 3.221976 0.420550
C -1.127745 2.814303 -0.647649
C -0.355662 2.276961 -1.658310
C 1.042827 2.427547 -1.205554
C 3.522874 2.308559 -1.580779
C 4.648659 2.071969 -2.476342
C 5.779714 2.566005 -1.848932
C 5.334905 2.999078 -0.516099
C 5.719916 3.575961 1.897247
C 6.619840 3.727656 3.033281
C 5.833007 4.028303 4.127520
C 4.455910 4.045357 3.651030
C 3.331509 4.274586 4.438689
H 3.511797 4.517316 5.480681
C -0.608207 3.645626 1.693601
H -1.673246 3.713726 1.875994
C 2.180819 2.065404 -1.911332
H 2.028320 1.564285 -2.861081
C 6.128368 3.277276 0.589678
H 7.198555 3.159205 0.470243
C 1.269918 -1.826234 5.714806
C 2.637147 -2.502625 5.673329
O 3.097109 -3.311305 6.501341
C 3.404612 -1.895435 4.495564
H 3.621235 -2.647433 3.729534
H 4.362616 -1.496708 4.840944
C 1.736095 -0.342687 5.370886
C 2.428143 -0.777175 4.010476
H 2.890762 0.034863 3.446415
C 1.284637 -1.480079 3.317095
C 0.736032 -1.113064 1.980771
H 1.440585 -1.355254 1.168654
H -0.186007 -1.671318 1.789353
C 0.534924 -2.241998 4.385360
H -0.523190 -1.942413 4.438641
H 0.536312 -3.334428 4.240609
C 2.701648 0.249384 6.418196
H 2.154370 0.516928 7.330618
H 3.158555 1.166095 6.026163
H 3.507021 -0.431401 6.715533
C 0.574258 0.638708 5.168952
H -0.032510 0.404100 4.292251
H 0.972394 1.644093 5.003735
H -0.062842 0.675464 6.062042
C 0.463361 -2.052720 6.974009
H 1.047336 -1.802611 7.867925
H 0.163523 -3.104603 7.055791
H -0.444773 -1.440795 6.969840
h 2.431802 6.568522 0.997819
h 0.860846 4.633567 5.984463
h -1.325974 4.246393 4.424630
h -2.205331 2.962377 -0.577306
h -0.615800 1.801640 -2.604071
h 4.526001 1.580751 -3.441602
h 6.763475 2.631376 -2.313698
h 7.697997 3.573376 2.990382
h 6.156847 4.229780 5.148598

TS2f

Total QM energy at B2: -3306.236796 (a.u.)

Total QM/MM energy at B2: -3428.696776 (a.u.)

S 2.793311 5.528557 0.116752

O	2.628510	1.506678 1.716056
H	3.238834	1.057248 1.095913
O	0.567401	0.276687 2.041633
H	1.570129	0.906645 1.854480
Fe	2.735776	3.385689 1.184153
N	1.573431	3.891528 2.779162
N	1.065937	3.016485 0.079202
N	3.926792	2.833876 -0.376206
N	4.392312	3.693900 2.314250
C	1.990724	4.197611 4.065265
C	0.838033	4.414071 4.938507
C	-0.282753	4.239999 4.155945
C	0.186414	3.920335 2.811700
C	-0.241440	3.220624 0.457005
C	-1.155765	2.833293 -0.619450
C	-0.383782	2.321061 -1.644183
C	1.017019	2.459128 -1.190173
C	3.486771	2.319573 -1.576638
C	4.611901	2.101772 -2.478756
C	5.750184	2.558186 -1.835504
C	5.314718	2.952463 -0.486717
C	5.706692	3.513241 1.918783
C	6.607151	3.684204 3.054121
C	5.822372	3.993246 4.145975
C	4.440642	3.998877 3.674970
C	3.325127	4.250866 4.464426
H	3.508588	4.505678 5.502928
C	-0.635055	3.644937 1.726341
H	-1.698476	3.721559 1.913366
C	2.149673	2.107548 -1.915760
H	1.988194	1.645792 -2.883853
C	6.119028	3.219365 0.616422
H	7.188084	3.093587 0.496681
C	1.234628	-1.781470 5.704986
C	2.576607	-2.509857 5.676880
O	3.007467	-3.323385 6.510998
C	3.367222	-1.941732 4.497629
H	3.551086	-2.700720 3.729873
H	4.341747	-1.575099 4.827444
C	1.761070	-0.310927 5.386341
C	2.457933	-0.754868 4.017653
H	2.964585	0.033779 3.460896
C	1.317705	-1.408059 3.318117
C	0.866330	-1.137683 1.929412
H	1.620124	-1.358953 1.162935
H	-0.040953	-1.699261 1.692278
C	0.514123	-2.132481 4.356043
H	-0.525131	-1.773832 4.370357
H	0.454988	-3.212446 4.144810
C	2.752169	0.236835 6.430393
H	2.216303	0.504807 7.348667
H	3.223477	1.149882 6.048999
H	3.541892	-0.467875 6.711639
C	0.635508	0.714331 5.196119
H	-0.007366	0.502849 4.341045
H	1.067808	1.700605 5.007371
H	0.029661	0.780724 6.107874
C	0.394049	-1.994003 6.944982
H	0.964818	-1.749798 7.848078
H	0.077508	-3.040970 7.023368
H	-0.502665	-1.366797 6.921682
h	2.453334	6.520779 1.013556
h	0.864161	4.642419 6.003984
h	-1.331343	4.271015 4.451856
h	-2.232772	2.986608 -0.551512
h	-0.645902	1.873096 -2.602664
h	4.480832	1.659756 -3.466435
h	6.732342	2.628939 -2.302864
h	7.687738	3.549501 3.006655
h	6.148309	4.208074 5.163659

PC2

Total QM energy at B2: -3306.307578 (a.u.)

Total QM/MM energy at B2: -3428.759975 (a.u.)

S	2.718509	5.482471 0.109900
O	2.655199	1.280188 1.499885
H	3.115966	0.796935 0.775438
O	0.537732	-0.552833 2.304123
H	1.783098	0.863811 1.713658
Fe	2.687636	3.340277 1.118254
N	1.542670	3.775085 2.743228
N	0.993708	2.957260 0.044151
N	3.857507	2.844462 -0.471573
N	4.349484	3.598062 2.244624
C	1.978488	4.113915 4.022796
C	0.837053	4.356779 4.901287
C	-0.293898	4.175707 4.134494
C	0.153418	3.825257 2.792150

C	-0.315999 3.160125 0.441774	C	0.229169 -1.873037 6.950909
C	-1.236925 2.834658 -0.646570	H	0.783895 -1.596304 7.854735
C	-0.473649 2.389562 -1.710299	H	-0.117366 -2.906249 7.073147
C	0.930502 2.498524 -1.263560	H	-0.648133 -1.224355 6.869066
C	3.393532 2.426414 -1.705439	h	2.396008 6.455664 1.033607
C	4.508150 2.263132 -2.630672	h	0.873973 4.600996 5.962918
C	5.662196 2.636860 -1.960347	h	-1.338247 4.226626 4.442406
C	5.244075 2.941852 -0.584022	h	-2.313584 2.982647 -0.563077
C	5.663748 3.415167 1.832226	h	-0.746619 2.012013 -2.695698
C	6.574992 3.589060 2.959375	h	4.358012 1.929513 -3.657425
C	5.803979 3.910391 4.057055	h	6.643409 2.711986 -2.429008
C	4.416413 3.914575 3.601058	h	7.654698 3.451067 2.902292
C	3.312981 4.176722 4.405055	h	6.136621 4.126166 5.072366
H	3.510710 4.447099 5.436600		
C	-0.690159 3.561048 1.719676	**RC2'**	
H	-1.749347 3.653762 1.922169	Total QM energy at B2: -3306.205616 (a.u.)	
C	2.056483 2.227501 -2.037170	Total QM/MM energy at B2: -3428.790420 (a.u.)	
H	1.880828 1.850744 -3.039469	S	2.907542 5.096715 0.229236
C	6.062485 3.144764 0.525776	O	2.601947 1.025638 1.993482
H	7.127490 3.000684 0.395157	H	1.856430 1.126695 2.633413
C	1.104399 -1.751501 5.721733	O	2.003195 -0.027422 1.059808
C	2.414181 -2.533510 5.764303	H	2.753160 -0.146585 0.407960
O	2.800336 -3.315165 6.650496	Fe	2.727070 3.043166 1.242513
C	3.253739 -2.057643 4.580110	N	1.440602 3.435217 2.774808
H	3.386432 -2.861082 3.845201	N	1.192805 2.644835 -0.000039
H	4.249893 -1.762703 4.918913	N	3.988026 2.316313 -0.135218
C	1.710234 -0.324498 5.350373	N	4.245300 3.283727 2.573908
C	2.420939 -0.858579 4.044674	C	1.740875 3.904271 4.058108
H	2.984337 -0.119090 3.474504	C	0.519369 4.052438 4.834249
C	1.236605 -1.458887 3.297032	C	-0.528188 3.701947 4.005147
C	1.184566 -1.843288 1.876152	C	0.049526 3.340002 2.719626
H	2.035047 -1.720726 1.217605	C	-0.152498 2.676945 0.320765
H	0.483650 -2.612670 1.565795	C	-0.964201 2.444408 -0.875460
C	0.387137 -2.140384 4.375825	C	-0.098309 2.354345 -1.949692
H	-0.637100 -1.755817 4.370096	C	1.255176 2.442471 -1.371758
H	0.334315 -3.226466 4.234103	C	3.713066 2.103499 -1.475741
C	2.685855 0.228839 6.408263	C	4.895926 1.597303 -2.157295
H	2.139802 0.516414 7.314532	C	5.880818 1.431966 -1.200533
H	3.177202 1.129572 6.022066	C	5.330652 1.989179 0.045693
H	3.463163 -0.481053 6.711013	C	5.576427 2.983869 2.331315
C	0.628321 0.732655 5.090779	C	6.405744 3.408805 3.459256
H	-0.053431 0.472334 4.281200	C	5.566053 4.000662 4.383461
H	1.094343 1.685395 4.828819	C	4.211692 3.872455 3.838169
H	0.037914 0.894144 6.000371	C	3.030412 4.163208 4.513570

H	3.116423 4.556453 5.521211	
C	-0.662135 2.969340 1.582632	**TS2a'**
H	-1.740419 2.971247 1.680787	Total QM energy at B2: -3306.178872 (a.u.)
C	2.455258 2.251828 -2.051908	Total QM/MM energy at B2: -3428.764237 (a.u.)
H	2.404109 2.117886 -3.126642	S 2.914293 5.122667 0.224825
C	6.049832 2.348860 1.183365	O 2.616417 1.198090 1.978946
H	7.124322 2.216457 1.137940	H 1.854688 1.134124 2.591187
C	1.196195 -1.997975 6.144948	O 1.811098 -0.226357 0.924303
C	2.487642 -2.801248 6.262543	H 2.605263 -0.301887 0.328709
O	2.875442 -3.442950 7.254425	Fe 2.723856 3.000143 1.278656
C	3.279645 -2.597641 4.970968	N 1.436356 3.507852 2.771510
H	3.416476 -3.539326 4.428264	N 1.191195 2.685230 0.002624
H	4.277849 -2.209648 5.202443	N 3.995158 2.330020 -0.117371
C	1.779738 -0.720882 5.388058	N 4.252084 3.320554 2.579988
C	2.383934 -1.577334 4.210532	C 1.736403 3.958629 4.055533
H	2.896943 -1.010737 3.434288	C 0.517308 4.092834 4.839390
C	1.166724 -2.362711 3.733253	C -0.529240 3.740990 4.010545
C	0.853252 -2.677145 2.474481	C 0.052785 3.395070 2.722021
H	1.458761 -2.354518 1.636567	C -0.152582 2.732023 0.314584
H	-0.035817 -3.246522 2.227399	C -0.963909 2.514235 -0.885654
C	0.376841 -2.702992 5.000871	C -0.093695 2.412297 -1.953936
H	-0.638185 -2.288944 4.977613	C 1.257232 2.477041 -1.363210
H	0.282436 -3.782586 5.177449	C 3.719543 2.095974 -1.446685
C	2.820035 0.051394 6.225960	C 4.892038 1.553148 -2.122701
H	3.606280 -0.584213 6.647188	C 5.872076 1.385273 -1.162905
H	2.327401 0.554871 7.066176	C 5.325737 1.970366 0.072201
H	3.300894 0.824915 5.616000	C 5.574622 2.992386 2.354107
C	0.696629 0.267709 4.930515	C 6.404717 3.405319 3.485051
H	1.158301 1.182433 4.543335	C 5.568470 4.016328 4.399776
H	0.074647 0.585583 5.775043	C 4.217555 3.911087 3.842936
H	0.044765 -0.147166 4.156470	C 3.031741 4.207642 4.508256
C	0.426600 -1.776324 7.435426	H 3.116690 4.600573 5.516490
H	1.092525 -1.504925 8.261697	C -0.656338 3.027657 1.578120
H	-0.123419 -2.678760 7.726831	H -1.734869 3.030056 1.675899
H	-0.309614 -0.978263 7.301096	C 2.462246 2.260762 -2.028888
h	2.591384 6.078096 1.146450	H 2.416912 2.117225 -3.103064
h	0.479442 4.329446 5.887691	C 6.041117 2.338781 1.208440
h	-1.589516 3.672698 4.251708	H 7.112984 2.181518 1.173420
h	-2.047166 2.328378 -0.833135	C 1.221833 -2.013063 6.142599
h	-0.267306 2.258490 -3.022221	C 2.534233 -2.787823 6.216944
h	4.892216 1.368851 -3.223064	O 2.961047 -3.434771 7.190509
h	6.825748 0.914215 -1.365179	C 3.282027 -2.556404 4.902694
h	7.476576 3.215757 3.523425	H 3.433193 -3.494644 4.357219
h	5.784019 4.467225 5.344126	H 4.274687 -2.138649 5.106772

C	1.747387 -0.725085 5.366223	N	4.310760 3.287260 2.650162
C	2.334507 -1.562675 4.168669	C	1.771834 3.947157 4.113136
H	2.793473 -0.982779 3.367438	C	0.560498 4.107352 4.905527
C	1.124540 -2.384006 3.734653	C	-0.497886 3.777920 4.082999
C	0.782563 -2.689213 2.481695	C	0.072720 3.419711 2.795082
H	1.341729 -2.297916 1.640634	C	-0.137276 2.757218 0.393123
H	-0.095604 -3.280524 2.249677	C	-0.933498 2.554283 -0.817799
C	0.386588 -2.745748 5.026282	C	-0.046916 2.455837 -1.872104
H	-0.640712 -2.360675 5.034299	C	1.297231 2.505896 -1.258456
H	0.324767 -3.826844 5.210527	C	3.768036 2.081058 -1.329457
C	2.793995 0.075521 6.169701	C	4.924615 1.509491 -2.015925
H	3.604681 -0.540279 6.573846	C	5.907208 1.318112 -1.063992
H	2.314036 0.576042 7.019369	C	5.379013 1.911407 0.174679
H	3.241926 0.849320 5.535297	C	5.628336 2.954925 2.443542
C	0.629177 0.235028 4.938736	C	6.455582 3.383754 3.569530
H	1.066188 1.136274 4.497065	C	5.613242 4.005358 4.472051
H	0.038967 0.564589 5.801649	C	4.265545 3.890541 3.907168
H	-0.042700 -0.208736 4.199035	C	3.075440 4.178874 4.565523
C	0.481923 -1.806414 7.452663	H	3.160216 4.568660 5.575033
H	1.162869 -1.531028 8.265394	C	-0.645415 3.058838 1.655474
H	-0.051738 -2.716308 7.750883	H	-1.723935 3.072631 1.752495
H	-0.265391 -1.014794 7.338402	C	2.507423 2.278918 -1.909664
h	2.593527 6.122257 1.120523	H	2.467915 2.148673 -2.985978
h	0.478890 4.357584 5.896035	C	6.095309 2.274974 1.306373
h	-1.589123 3.695269 4.260792	H	7.164085 2.095770 1.284503
h	-2.048580 2.414430 -0.845712	C	1.254523 -1.982660 6.088821
h	-0.256696 2.323859 -3.028029	C	2.568949 -2.752779 6.153158
h	4.880365 1.301685 -3.183218	O	3.007329 -3.400146 7.122033
h	6.808472 0.848870 -1.316202	C	3.301218 -2.515660 4.830559
h	7.471078 3.192015 3.558831	H	3.439322 -3.450465 4.275605
h	5.787228 4.481050 5.361153	H	4.299272 -2.107283 5.025186
		C	1.771529 -0.684628 5.323921
IC2a'		C	2.356677 -1.505229 4.114257
Total QM energy at B2: -3306.188455 (a.u.)		H	2.822845 -0.902445 3.332695
Total QM/MM energy at B2: -3428.772661 (a.u.)		C	1.134086 -2.300104 3.670206
S	3.044791 5.091421 0.267322	C	0.730613 -2.503677 2.413994
O	2.658952 1.137564 1.991865	H	1.256341 -2.056313 1.575902
H	1.726053 0.878208 2.140718	H	-0.174086 -3.057817 2.183623
O	1.667547 -0.243769 0.374101	C	0.425942 -2.715340 4.963819
H	2.567950 -0.448166 -0.010651	H	-0.613662 -2.367033 4.992751
Fe	2.756399 2.921533 1.391178	H	0.403058 -3.802203 5.123230
N	1.458881 3.510992 2.834116	C	2.823602 0.112349 6.122195
N	1.208279 2.703945 0.107763	H	3.650112 -0.503382 6.493602
N	4.053933 2.303318 -0.009113	H	2.359117 0.588889 6.994034

H	3.247073 0.902535 5.491785	C	5.627879 2.957729 2.454731
C	0.652698 0.277026 4.904309	C	6.456463 3.382955 3.582509
H	1.086490 1.106741 4.338367	C	5.615908 4.008268 4.482600
H	0.147558 0.700606 5.779314	C	4.267971 3.899236 3.915009
H	-0.095105 -0.204300 4.268575	C	3.077134 4.193595 4.569072
C	0.512628 -1.793037 7.400611	H	3.159209 4.581506 5.579465
H	1.192919 -1.520684 8.215165	C	-0.644497 3.064086 1.658782
H	-0.013511 -2.709795 7.691584	H	-1.722757 3.076404 1.758313
H	-0.239832 -1.004523 7.295001	C	2.503432 2.284672 -1.905053
h	2.656384 6.102453 1.122483	H	2.466174 2.154959 -2.981466
h	0.528483 4.372075 5.962392	C	6.092494 2.278360 1.318204
h	-1.558090 3.750383 4.334544	H	7.160169 2.092265 1.296023
h	-2.019305 2.463071 -0.790057	C	1.253104 -1.979477 6.088169
h	-0.195355 2.375180 -2.948917	C	2.566157 -2.752157 6.155157
h	4.899492 1.257277 -3.076031	O	3.003777 -3.395996 7.126712
h	6.834693 0.767837 -1.222218	C	3.298795 -2.523688 4.830799
h	7.523118 3.177814 3.647140	H	3.436330 -3.462284 4.282081
h	5.828582 4.486595 5.426046	H	4.296947 -2.114296 5.022934
		C	1.771551 -0.687796 5.313515
TS2b'		C	2.354090 -1.517212 4.108490
Total QM energy at B2: -3306.188505 (a.u.)		H	2.818268 -0.916912 3.324236
Total QM/MM energy at B2: -3428.773045 (a.u.)		C	1.132191 -2.318517 3.673475
S	3.014999 5.112002 0.244856	C	0.734614 -2.557208 2.421890
O	2.680782 1.154952 2.032148	H	1.258601 -2.133724 1.571653
H	1.786338 0.763968 1.900428	H	-0.166719 -3.120573 2.203837
O	1.684382 -0.261377 0.431600	C	0.420347 -2.715704 4.970347
H	2.548034 -0.502197 -0.014244	H	-0.616065 -2.357634 4.995002
Fe	2.758276 2.931010 1.400349	H	0.387985 -3.800893 5.138726
N	1.462363 3.534898 2.830300	C	2.826396 0.111344 6.106186
N	1.205838 2.694812 0.113705	H	3.651167 -0.504105 6.482288
N	4.052068 2.321883 -0.002426	H	2.362455 0.594416 6.974814
N	4.311685 3.295336 2.660285	H	3.251278 0.895858 5.470011
C	1.774315 3.965065 4.112089	C	0.657512 0.275158 4.884638
C	0.562874 4.118072 4.904643	H	1.096693 1.091830 4.304163
C	-0.494782 3.786267 4.081782	H	0.155018 0.709271 5.756310
C	0.075863 3.433942 2.792911	H	-0.092770 -0.209575 4.254298
C	-0.139145 2.755211 0.396940	C	0.513054 -1.780659 7.399657
C	-0.937515 2.558468 -0.814519	H	1.194097 -1.506035 8.212697
C	-0.051630 2.459787 -1.869034	H	-0.015858 -2.694436 7.695276
C	1.292487 2.502076 -1.254658	H	-0.236994 -0.990455 7.289430
C	3.764506 2.092855 -1.322287	h	2.645323 6.120536 1.111196
C	4.917681 1.514147 -2.004813	h	0.530342 4.379621 5.962283
C	5.899164 1.320516 -1.050418	h	-1.554198 3.753557 4.336015
C	5.375313 1.922119 0.184068	h	-2.023820 2.473210 -0.787348

h -0.199837 2.382621 -2.946135
h 4.892968 1.259046 -3.064237
h 6.823326 0.764532 -1.208132
h 7.523059 3.172422 3.660709
h 5.832146 4.489093 5.436599

IC2b'

Total QM energy at B2: -3306.241188 (a.u.)

Total QM/MM energy at B2: -3428.824102 (a.u.)

S 2.963573 5.143222 0.265373
O 2.600063 1.361245 2.077832
H 2.001768 0.139396 0.913291
O 1.764988 -0.517421 0.215688
H 2.573263 -0.760195 -0.295496
Fe 2.726258 2.909350 1.475889
N 1.444465 3.618592 2.866271
N 1.202247 2.702493 0.157689
N 4.018186 2.327328 0.054275
N 4.278646 3.369763 2.699138
C 1.749971 4.056832 4.144361
C 0.535203 4.191781 4.935495
C -0.515526 3.842719 4.113848
C 0.062938 3.485826 2.828131
C -0.140511 2.766812 0.445182
C -0.940142 2.574793 -0.765345
C -0.057630 2.481101 -1.823306
C 1.286498 2.516316 -1.214628
C 3.745140 2.092470 -1.267817
C 4.901263 1.502442 -1.933194
C 5.870731 1.307488 -0.967540
C 5.341674 1.924756 0.255910
C 5.589718 3.002825 2.504958
C 6.416424 3.425664 3.632047
C 5.582028 4.077004 4.519809
C 4.237159 3.987112 3.949982
C 3.049398 4.297273 4.600394
H 3.131787 4.695871 5.606368
C -0.650019 3.083855 1.703613
H -1.727995 3.081041 1.803470
C 2.493451 2.295087 -1.864858
H 2.461307 2.166929 -2.941112
C 6.054047 2.295554 1.385287
H 7.119181 2.096959 1.373503
C 1.268438 -1.926007 6.016737
C 2.575790 -2.704912 6.103947
O 3.014393 -3.319349 7.094285
C 3.298120 -2.533006 4.764771
H 3.420846 -3.493269 4.250950
H 4.302199 -2.127596 4.933672
C 1.786530 -0.666208 5.189170
C 2.354903 -1.546699 4.013373
H 2.816652 -0.985695 3.200695
C 1.120099 -2.344522 3.612903
C 0.694840 -2.580603 2.369617
H 1.202435 -2.167860 1.500443
H -0.225367 -3.123763 2.176712
C 0.424873 -2.703039 4.931184
H -0.613753 -2.351761 4.956983
H 0.402252 -3.782134 5.137661
C 2.853228 0.158635 5.938205
H 3.690582 -0.441976 6.310731
H 2.405636 0.663089 6.803153
H 3.257665 0.929183 5.272198
C 0.673091 0.284908 4.731911
H 1.097483 1.024648 4.046232
H 0.234190 0.815667 5.584588
H -0.124094 -0.233539 4.194025
C 0.541711 -1.672817 7.326732
H 1.232325 -1.366181 8.120114
H 0.017131 -2.573336 7.666912
H -0.209185 -0.886592 7.194344
h 2.620762 6.173990 1.116457
h 0.502858 4.435444 5.997403
h -1.574875 3.793905 4.365766
h -2.026224 2.487332 -0.736301
h -0.208175 2.411369 -2.900590
h 4.883349 1.229557 -2.988315
h 6.790205 0.739897 -1.110629
h 7.476215 3.187795 3.723311
h 5.805184 4.555928 5.473171

TS2c'

Total QM energy at B2: -3306.171648 (a.u.)

Total QM/MM energy at B2: -3428.754408 (a.u.)

S 2.971096 5.075653 0.244249
O 2.537612 1.096410 1.878880
H 1.587142 0.862573 1.834194
O 1.930341 0.004553 -0.172286

H	2.743967 -0.572756 -0.282343	H	-0.617910 -2.359558 4.741177
Fe	2.720204 2.932960 1.396236	H	0.417055 -3.783077 4.844958
N	1.448137 3.537047 2.866754	C	2.768062 0.088431 6.118437
N	1.109373 2.741520 0.154887	H	3.596060 -0.535281 6.472598
N	4.006390 2.286602 -0.030238	H	2.273770 0.503099 7.005432
N	4.308100 3.294479 2.621388	H	3.192890 0.922978 5.549381
C	1.794467 3.897378 4.167674	C	0.649560 0.308879 4.819110
C	0.599754 4.102107 4.971583	H	1.099229 1.117133 4.234917
C	-0.479965 3.882032 4.140791	H	0.160151 0.754957 5.691656
C	0.063335 3.553992 2.833677	H	-0.114737 -0.163105 4.196046
C	-0.227640 3.022717 0.413892	C	0.385938 -1.868507 7.210185
C	-1.029620 2.842555 -0.794480	H	1.013997 -1.577655 8.059794
C	-0.169087 2.410701 -1.787736	H	-0.104275 -2.816795 7.461872
C	1.151858 2.324914 -1.143547	H	-0.398977 -1.115126 7.083708
C	3.632147 1.802565 -1.248842	h	2.606760 6.087381 1.109125
C	4.771221 1.240063 -1.961003	h	0.588645 4.352722 6.032307
C	5.860752 1.330561 -1.112558	h	-1.538237 3.899580 4.401212
C	5.373686 2.040640 0.078660	h	-2.095543 3.066477 -0.836101
C	5.644787 3.109307 2.328020	h	-0.316865 2.191322 -2.845139
C	6.487599 3.551633 3.435782	h	4.675448 0.822993 -2.963474
C	5.640275 4.033613 4.415788	h	6.830964 0.873745 -1.307683
C	4.281986 3.834842 3.903458	h	7.571230 3.435207 3.451783
C	3.103988 4.068648 4.610194	h	5.856008 4.487350 5.383077
H	3.213454 4.401316 5.637827		
C	-0.695753 3.337174 1.677013	**IC2c'**	
H	-1.767814 3.423597 1.793241	Total QM energy at B2: -3306.262196 (a.u.)	
C	2.301112 1.723726 -1.688269	Total QM/MM energy at B2: -3428.842690 (a.u.)	
H	2.168143 1.251848 -2.657344	S	2.770387 5.082558 0.234367
C	6.115948 2.525041 1.146791	O	2.757078 1.250988 2.168544
H	7.194231 2.478959 1.051324	H	2.515293 0.629935 1.439633
C	1.197279 -2.001386 5.933191	O	2.182574 -0.099765 -0.425417
C	2.517448 -2.757735 6.039756	H	2.856197 -0.789003 -0.678804
O	2.934809 -3.397912 7.022896	Fe	2.780723 2.938360 1.427839
C	3.293955 -2.491953 4.746196	N	1.531980 3.566002 2.878666
H	3.432105 -3.413517 4.168149	N	1.193001 2.530984 0.215536
H	4.292703 -2.107806 4.981069	N	4.025897 2.303522 -0.056338
C	1.748379 -0.672549 5.245670	N	4.353339 3.486321 2.558985
C	2.387411 -1.444251 4.028520	C	1.871255 3.848088 4.202770
H	2.886694 -0.807909 3.295156	C	0.665020 4.052648 4.989022
C	1.180486 -2.205695 3.496144	C	-0.401790 3.909948 4.121246
C	0.805825 -2.339674 2.220644	C	0.168327 3.618901 2.815591
H	1.355033 -1.880517 1.403234	C	-0.116157 3.044056 0.398510
H	-0.096191 -2.880121 1.944380	C	-0.892424 2.835650 -0.826150
C	0.427967 -2.689536 4.740413	C	-0.076528 2.150132 -1.708718

C	1.185242	1.951999 -0.981054
C	3.684845	1.652670 -1.171206
C	4.811630	1.454633 -2.059965
C	5.926010	1.985657 -1.421899
C	5.428418	2.533140 -0.148621
C	5.656546	3.546567 2.148237
C	6.524442	3.994531 3.231581
C	5.705260	4.215378 4.330464
C	4.351758	3.887903 3.888519
C	3.180370	3.991505 4.644622
H	3.302013	4.241880 5.695553
C	-0.573769	3.460602 1.614308
H	-1.631372	3.675588 1.684330
C	2.323427	1.058175 -1.343360
H	2.213187	0.696986 -2.370131
C	6.107924	3.171673 0.855835
H	7.141404	3.425253 0.663492
C	1.218188	-2.076943 5.811795
C	2.545852	-2.794920 6.029019
O	2.919409	-3.376903 7.064651
C	3.386760	-2.585074 4.765844
H	3.589458	-3.535884 4.258377
H	4.355954	-2.148721 5.029490
C	1.768333	-0.782131 5.060419
C	2.489581	-1.616822 3.936162
H	3.015208	-1.007850 3.200564
C	1.338793	-2.454601 3.397883
C	1.061062	-2.726085 2.120333
H	1.669741	-2.346629 1.306082
H	0.203109	-3.323299 1.826973
C	0.523521	-2.859410 4.631268
H	-0.523843	-2.544475 4.551612
H	0.518751	-3.943207 4.810879
C	2.729012	0.066069 5.918789
H	3.567378	-0.502119 6.336819
H	2.187640	0.511213 6.761879
H	3.137502	0.877576 5.307093
C	0.677181	0.143357 4.503244
H	1.142559	0.821399 3.778272
H	0.223102	0.738109 5.304277
H	-0.116519	-0.402062 3.985009
C	0.347215	-1.883834 7.041735
H	0.932936	-1.525996 7.896071
H	-0.132428	-2.826099 7.334481
H	-0.445646	-1.155742 6.839216
h	2.499261	6.118522 1.104777
h	0.638517	4.294991 6.051394
h	-1.463946	3.937513 4.364415
h	-1.907024	3.216418 -0.943068
h	-0.208261	1.822452 -2.739901
h	4.694701	0.960440 -3.024416
h	6.934258	1.930278 -1.832308
h	7.609742	4.052837 3.149168
h	5.920644	4.597928 5.328127

TS2d'

Total QM energy at B2: -3306.17801 (a.u.)

Total QM/MM energy at B2: -3428.765307 (a.u.)

S	2.994658	5.109424 0.233286
O	2.722932	1.202209 2.082742
H	1.808049	0.880992 2.223086
O	1.691140	-0.620499 1.012085
H	2.396402	-0.704820 0.305460
Fe	2.777344	2.943233 1.419351
N	1.474724	3.546724 2.847199
N	1.219381	2.657666 0.142750
N	4.068214	2.308212 0.020688
N	4.329255	3.335604 2.662541
C	1.786748	3.987271 4.124268
C	0.575425	4.138130 4.919104
C	-0.482157	3.800529 4.099696
C	0.088158	3.443247 2.811399
C	-0.126490	2.734874 0.423844
C	-0.924608	2.532500 -0.785686
C	-0.038305	2.413654 -1.839068
C	1.305155	2.453010 -1.225331
C	3.780884	2.062861 -1.296062
C	4.936487	1.482234 -1.974850
C	5.917164	1.298927 -1.018827
C	5.391260	1.913907 0.210034
C	5.642741	2.981751 2.466392
C	6.467215	3.397584 3.600102
C	5.627095	4.031071 4.494915
C	4.281587	3.935375 3.920111
C	3.090228	4.225336 4.575537
H	3.173279	4.614353 5.585442
C	-0.631965	3.062222 1.681373
H	-1.710316	3.078460 1.780509

C	2.516894	2.233391 -1.876353
H	2.477116	2.090476 -2.951010
C	6.107931	2.287041 1.339137
H	7.174341	2.093341 1.324435
C	1.195047	-1.974818 6.024108
C	2.485654	-2.781469 6.141159
O	2.885012	-3.403411 7.143470
C	3.266433	-2.592840 4.839493
H	3.393133	-3.541680 4.306093
H	4.270117	-2.211620 5.059812
C	1.780730	-0.708371 5.255527
C	2.373528	-1.571320 4.075175
H	2.871942	-0.998341 3.293950
C	1.143399	-2.340850 3.608794
C	0.808034	-2.647455 2.352226
H	1.441073	-2.418637 1.512475
H	-0.113060	-3.177010 2.125582
C	0.358929	-2.670160 4.885033
H	-0.654158	-2.249697 4.874689
H	0.254645	-3.749490 5.060218
C	2.838245	0.066821 6.068552
H	3.628578	-0.569557 6.481663
H	2.365477	0.582439 6.913420
H	3.310402	0.823312 5.431756
C	0.705183	0.285311 4.796370
H	1.185029	1.114845 4.270735
H	0.166987	0.705994 5.653422
H	-0.019418	-0.167336 4.113915
C	0.431278	-1.747052 7.316906
H	1.098768	-1.455868 8.135425
H	-0.100376	-2.656288 7.622679
H	-0.317310	-0.960253 7.178121
h	2.631909	6.122279 1.097511
h	0.543519	4.393523 5.978266
h	-1.541497	3.764081 4.353736
h	-2.012056	2.462983 -0.759421
h	-0.186595	2.330801 -2.915735
h	4.914828	1.229573 -3.034925
h	6.840350	0.739048 -1.168263
h	7.529841	3.171633 3.688642
h	5.844631	4.507453 5.450847

IC2d'

Total QM energy at B2: -3306.22712 (a.u.)

Total QM/MM energy at B2: -3428.815133 (a.u.)

S	2.955706	5.025913 0.294173
O	2.617447	1.203653 2.303741
H	2.163959	0.519477 1.754363
O	1.451869	-1.201021 1.251633
H	2.093091	-1.439790 0.536425
Fe	2.745449	2.849551 1.510291
N	1.462057	3.556351 2.901856
N	1.218614	2.522055 0.208957
N	4.024405	2.182518 0.113697
N	4.287539	3.277448 2.761616
C	1.760702	4.019062 4.170051
C	0.540581	4.176446 4.953176
C	-0.505497	3.814476 4.132782
C	0.081331	3.428550 2.855929
C	-0.124197	2.618348 0.492440
C	-0.927243	2.417740 -0.716303
C	-0.044950	2.292541 -1.772949
C	1.298326	2.327760 -1.163252
C	3.770540	1.976694 -1.219669
C	4.949564	1.444092 -1.890843
C	5.912040	1.240372 -0.917995
C	5.350209	1.804175 0.320408
C	5.592713	2.889455 2.577479
C	6.425417	3.323033 3.702604
C	5.597636	4.000741 4.574163
C	4.251366	3.917221 3.995985
C	3.060877	4.253091 4.631614
H	3.140261	4.668164 5.631609
C	-0.628172	2.992487 1.740132
H	-1.707417	3.008194 1.836929
C	2.513421	2.138531 -1.814671
H	2.486639	2.025077 -2.893618
C	6.053055	2.173344 1.462871
H	7.119478	1.978410 1.456421
C	1.121315	-2.017199 5.897684
C	2.445811	-2.744278 6.120033
O	2.783319	-3.378022 7.138111
C	3.349774	-2.437291 4.922662
H	3.581159	-3.346656 4.354573
H	4.303589	-2.023747 5.270212
C	1.710486	-0.665725 5.288623
C	2.479799	-1.408167 4.124936
H	3.024608	-0.736838 3.461535

C	1.353526 -2.194560 3.493866	
C	1.075936 -2.384813 2.044103	
H	1.603951 -3.261322 1.630673	
H	0.000355 -2.563885 1.893792	
C	0.469259 -2.679910 4.622289	
H	-0.572986 -2.336122 4.518163	
H	0.416024 -3.776998 4.724962	
C	2.629089 0.103162 6.262254	
H	3.431645 -0.505964 6.692736	
H	2.042869 0.502703 7.099111	
H	3.086906 0.948418 5.736859	
C	0.650485 0.307605 4.759885	
H	1.150731 1.057273 4.139221	
H	0.130857 0.808732 5.584361	
H	-0.093973 -0.183851 4.126266	
C	0.200061 -1.927967 7.101830	
H	0.745484 -1.619821 8.001201	
H	-0.269042 -2.897919 7.309842	
H	-0.597985 -1.201426 6.915702	
h	2.619597 6.069908 1.131699	
h	0.506127 4.429858 6.012734	
h	-1.567033 3.770369 4.376221	
h	-2.015488 2.362650 -0.688830	
h	-0.193110 2.210112 -2.849667	
h	4.964755 1.262954 -2.965564	
h	6.850003 0.706538 -1.070679	
h	7.484549 3.083683 3.797568	
h	5.824090 4.496786 5.517944	

RC2”

Total QM energy at B2: -3306.226727 (a.u.)

Total QM/MM energy at B2: -3417.165054 (a.u.)

S	2.834004 5.648166 0.398932	
O	2.993067 1.433319 1.783441	
H	2.426175 1.460560 2.592135	
O	2.243877 0.376361 0.971310	
H	2.921409 0.167595 0.265916	
Fe	2.903354 3.496908 1.187768	
N	1.679473 3.688441 2.818458	
N	1.314580 3.071169 -0.004836	
N	4.151595 3.011616 -0.331377	
N	4.474419 3.735621 2.457321	
C	2.017504 4.028301 4.134513	
C	0.819786 4.119063 4.955864	
C	-0.251522 3.832338 4.133086	
C	0.287751 3.599547 2.800338	
C	-0.017275 3.134039 0.366207	
C	-0.883974 2.885710 -0.788838	
C	-0.061682 2.640253 -1.872327	
C	1.315095 2.770790 -1.359031	
C	3.789610 2.670442 -1.624100	
C	4.974465 2.388699 -2.424043	
C	6.075189 2.533129 -1.596602	
C	5.545387 2.978836 -0.298301	
C	5.811094 3.703106 2.081580	
C	6.669756 3.964189 3.232832	
C	5.841283 4.157394 4.319518	
C	4.474487 4.031510 3.825828	
C	3.321580 4.193892 4.584907	
H	3.446716 4.461287 5.627708	
C	-0.470755 3.353838 1.662361	
H	-1.540991 3.335180 1.810983	
C	2.483189 2.591849 -2.091656	
H	2.375314 2.331362 -3.139238	
C	6.281217 3.394097 0.807897	
H	7.352293 3.492495 0.685357	
C	1.815949 -1.639773 6.062921	
C	3.013610 -2.566992 5.864116	
O	3.631489 -3.192968 6.742136	
C	3.354667 -2.565630 4.377924	
H	3.233770 -3.563678 3.940084	
H	4.402765 -2.279952 4.232553	
C	2.184097 -0.505433 5.015315	
C	2.349983 -1.520034 3.821356	
H	2.630424 -1.071242 2.868971	
C	0.976471 -2.164441 3.823285	
C	0.212682 -2.354027 2.745228	
H	0.572621 -2.089685 1.755740	
H	-0.797168 -2.743448 2.798406	
C	0.641351 -2.393952 5.304184	
H	-0.323283 -1.958632 5.588833	
H	0.601561 -3.457774 5.574352	
C	3.468068 0.267513 5.370911	
H	3.737689 0.959748 4.564926	
H	4.327364 -0.387473 5.542535	
H	3.318878 0.861776 6.279581	
C	1.037313 0.497090 4.772729	
H	0.050593 0.087587 4.997875	

H 0.998743 0.805290 3.720330
H 1.168594 1.395720 5.374042
C 1.530503 -1.229672 7.499185
H 1.422330 -2.106758 8.146270
H 0.609869 -0.638875 7.559741
H 2.345679 -0.627579 7.916184
h 2.601877 6.518916 1.444043
h 0.783341 4.360795 6.018080
h -1.297623 3.735723 4.423613
h -1.971034 2.942598 -0.732868
h -0.276767 2.380245 -2.908763
h 4.901674 2.055606 -3.459329
h 7.094201 2.280177 -1.889339
h 7.758637 3.928800 3.198866
h 6.136728 4.332702 5.353948

TS2a"

Total QM energy at B2: -3306.199967 (a.u.)

Total QM/MM energy at B2: -3417.140405 (a.u.)

S 2.896405 5.642203 0.375554
O 2.954544 1.570065 1.793926
H 2.350665 1.459299 2.556085
O 2.005672 0.131582 0.910828
H 2.715720 0.014793 0.221801
Fe 2.922054 3.427219 1.226265
N 1.702150 3.758494 2.827636
N 1.322291 3.071096 0.018342
N 4.168590 2.957028 -0.306212
N 4.505766 3.753226 2.462572
C 2.045996 4.091124 4.138707
C 0.853736 4.186046 4.969494
C -0.220167 3.906908 4.149513
C 0.316539 3.667770 2.816620
C -0.005848 3.148796 0.386363
C -0.879007 2.874937 -0.759237
C -0.061834 2.593777 -1.836144
C 1.319505 2.727830 -1.322298
C 3.801912 2.589873 -1.585519
C 4.977963 2.279269 -2.389678
C 6.084135 2.439258 -1.574185
C 5.559696 2.910998 -0.280075
C 5.838774 3.690325 2.089131
C 6.705212 3.951996 3.233421
C 5.880485 4.166582 4.319214
C 4.512190 4.057430 3.826004
C 3.357284 4.243777 4.579456
H 3.490007 4.515694 5.620213
C -0.446860 3.401859 1.681788
H -1.515950 3.384570 1.844631
C 2.488944 2.512553 -2.044516
H 2.376659 2.219735 -3.083692
C 6.297781 3.345788 0.817170
H 7.369898 3.433497 0.690857
C 1.833756 -1.689247 6.052486
C 3.085286 -2.531125 5.810198
O 3.713756 -3.192790 6.656653
C 3.455879 -2.385989 4.339136
H 3.425611 -3.351727 3.821500
H 4.479566 -2.004989 4.243889
C 2.141172 -0.464363 5.092663
C 2.386238 -1.376818 3.832463
H 2.635584 -0.863833 2.903068
C 1.071690 -2.136719 3.772085
C 0.370448 -2.366619 2.659325
H 0.737759 -2.012807 1.701522
H -0.589926 -2.869148 2.658383
C 0.712501 -2.453522 5.231585
H -0.269969 -2.057161 5.514262
H 0.698539 -3.529421 5.450685
C 3.371518 0.350883 5.533659
H 3.683854 1.020923 4.725097
H 4.225964 -0.278451 5.803010
H 3.135025 0.968678 6.407841
C 0.941728 0.485490 4.937605
H 0.097188 0.017338 4.426988
H 1.218310 1.371728 4.358615
H 0.603775 0.834472 5.919997
C 1.517731 -1.386759 7.510929
H 1.518299 -2.297484 8.117336
H 0.538326 -0.905540 7.609270
H 2.268589 -0.716270 7.945589
h 2.639722 6.538558 1.392907
h 0.825367 4.414946 6.034795
h -1.272145 3.822037 4.421920
h -1.965911 2.934522 -0.703054
h -0.277390 2.305637 -2.865016
h 4.894147 1.912744 -3.412761
h 7.101674 2.183072 -1.869227

h 7.793546 3.905768 3.195244
h 6.178273 4.344007 5.352610’

IC2a”

Total QM energy at B2: -3306.207218 (a.u.)
Total QM/MM energy at B2: -3417.147190 (a.u.)

S 2.889295 5.652475 0.399283
O 3.032534 1.595858 1.769489
H 2.423748 1.409297 2.511333
O 1.764167 -0.003255 0.761820
H 2.554194 -0.073252 0.161134
Fe 2.973898 3.404831 1.299222
N 1.737005 3.772569 2.886009
N 1.357166 3.079888 0.085224
N 4.221071 2.971888 -0.247574
N 4.551474 3.800604 2.513437
C 2.081248 4.094431 4.197165
C 0.890092 4.191615 5.030163
C -0.185775 3.922492 4.210584
C 0.354871 3.684410 2.878392
C 0.028406 3.154557 0.447255
C -0.841266 2.874507 -0.699086
C -0.018419 2.587242 -1.769869
C 1.358318 2.724336 -1.252206
C 3.852458 2.590803 -1.513014
C 5.025276 2.269030 -2.320871
C 6.134539 2.435955 -1.511047
C 5.612237 2.921161 -0.222783
C 5.880784 3.730516 2.144257
C 6.747626 3.986947 3.288422
C 5.920369 4.195570 4.375157
C 4.555474 4.089137 3.877090
C 3.395059 4.249570 4.633852
H 3.526207 4.506236 5.679413
C -0.410740 3.413000 1.743521
H -1.480333 3.397667 1.907673
C 2.532053 2.506894 -1.965525
H 2.421260 2.202660 -3.001296
C 6.342076 3.369600 0.872754
H 7.414665 3.454601 0.749945
C 1.827367 -1.675379 6.031790
C 3.079877 -2.514400 5.788157
O 3.717445 -3.162872 6.638275
C 3.437234 -2.386679 4.311738
H 3.408287 -3.359834 3.807988
H 4.458694 -2.002927 4.204494
C 2.122069 -0.461898 5.054004
C 2.356236 -1.391181 3.801816
H 2.594404 -0.885598 2.865403
C 1.043377 -2.154916 3.765918
C 0.327254 -2.391890 2.664410
H 0.680631 -2.038759 1.701398
H -0.635756 -2.888837 2.682463
C 0.698987 -2.452413 5.233314
H -0.283488 -2.055939 5.517084
H 0.693244 -3.525153 5.469066
C 3.354519 0.369349 5.462480
H 3.652254 1.023105 4.635196
H 4.219518 -0.245827 5.731738
H 3.123742 1.003675 6.326581
C 0.919212 0.480901 4.892808
H 0.076814 0.004022 4.387563
H 1.201360 1.356199 4.301277
H 0.580463 0.847035 5.866863
C 1.529707 -1.360394 7.488896
H 1.528963 -2.268260 8.100033
H 0.556982 -0.867999 7.594943
H 2.292023 -0.696221 7.912574
h 2.625243 6.562427 1.402582
h 0.863874 4.416631 6.096346
h -1.239369 3.848570 4.479924
h -1.928552 2.927002 -0.643234
h -0.231125 2.296381 -2.798568
h 4.937181 1.896527 -3.341433
h 7.151888 2.178328 -1.805486
h 7.836114 3.943450 3.251442
h 6.217720 4.374524 5.408416

TS2b”

Total QM energy at B2: -3306.208027 (a.u.)
Total QM/MM energy at B2: -3417.147894 (a.u.)

S 2.918351 5.630972 0.408113
O 3.030367 1.575208 1.848609
H 2.143128 1.244317 2.102080
O 1.784859 0.043172 0.705554
H 2.531190 -0.142821 0.072863
Fe 3.000469 3.391575 1.308363
N 1.763536 3.774562 2.891471

N	1.385246	3.054245 0.103712
N	4.247798	2.943450 -0.235999
N	4.583762	3.776277 2.515791
C	2.113917	4.076076 4.203983
C	0.925910	4.175849 5.042659
C	-0.154226	3.922806 4.224721
C	0.381458	3.690656 2.888265
C	0.055355	3.144857 0.462180
C	-0.813139	2.860298 -0.682204
C	0.009762	2.556198 -1.748859
C	1.385077	2.688205 -1.231694
C	3.877401	2.554021 -1.499782
C	5.048088	2.238200 -2.310619
C	6.159468	2.415877 -1.505590
C	5.638941	2.901390 -0.216725
C	5.913197	3.724078 2.142387
C	6.778789	3.992719 3.282789
C	5.952864	4.187760 4.372637
C	4.587795	4.063624 3.878556
C	3.429022	4.218270 4.638942
H	3.564002	4.465127 5.686189
C	-0.385643	3.419729 1.755372
H	-1.455525	3.411041 1.918706
C	2.556500	2.465092 -1.946605
H	2.443498	2.157062 -2.980894
C	6.371520	3.362910 0.872075
H	7.443048	3.454510 0.743522
C	1.816136	-1.676587 6.003505
C	3.072459	-2.515969 5.784307
O	3.699698	-3.156985 6.647846
C	3.448915	-2.399634 4.311182
H	3.424995	-3.376413 3.814189
H	4.471528	-2.017051 4.213393
C	2.127017	-0.469442 5.022871
C	2.376510	-1.404946 3.780641
H	2.633681	-0.897533 2.851250
C	1.064343	-2.168529 3.728472
C	0.365278	-2.414335 2.617747
H	0.731670	-2.064246 1.658268
H	-0.596802	-2.913988 2.622338
C	0.700434	-2.460023 5.192558
H	-0.286659	-2.064307 5.460820
H	0.692976	-3.531642 5.432972
C	3.357190	0.363654 5.433210
H	3.656299	1.004011 4.596221
H	4.218450	-0.250287 5.717853
H	3.119710	1.007786 6.288132
C	0.931560	0.476887 4.833817
H	0.072717	-0.014985 4.371717
H	1.221758	1.310076 4.188266
H	0.613606	0.897963 5.792621
C	1.494472	-1.352874 7.453742
H	1.484703	-2.257311 8.070198
H	0.519733	-0.860507 7.539957
H	2.249255	-0.684901 7.884830
h	2.648495	6.538212 1.412324
h	0.903232	4.399198 6.109274
h	-1.208371	3.854701 4.493436
h	-1.899894	2.925639 -0.629658
h	-0.203525	2.252977 -2.773862
h	4.957807	1.863133 -3.330050
h	7.177120	2.163344 -1.803378
h	7.867618	3.963526 3.241960
h	6.250897	4.367813 5.405509

IC2b”

Total QM energy at B2: -3306.262876 (a.u.)

Total QM/MM energy at B2: -3417.199537 (a.u.)

S	2.920372	5.658638 0.416023
O	3.038211	1.734186 1.892895
H	2.160823	0.463856 0.961529
O	1.813900	-0.266132 0.397307
H	2.499651	-0.508654 -0.268609
Fe	2.989773	3.326146 1.412068
N	1.770423	3.833123 2.948466
N	1.365027	3.047504 0.194495
N	4.231395	2.954032 -0.164932
N	4.592297	3.811383 2.566166
C	2.134467	4.133940 4.256812
C	0.954000	4.234418 5.103033
C	-0.133642	3.982541 4.296282
C	0.388361	3.741029 2.958539
C	0.037909	3.143681 0.555498
C	-0.836318	2.857236 -0.583360
C	-0.019411	2.555591 -1.654499
C	1.359439	2.686238 -1.144311
C	3.848868	2.553496 -1.422373
C	5.011524	2.215865 -2.233712

C	6.130453	2.397450 -1.438549
C	5.625500	2.904992 -0.156017
C	5.919529	3.755994 2.184686
C	6.793007	4.031949 3.318892
C	5.973199	4.228980 4.411635
C	4.604646	4.107110 3.925745
C	3.450460	4.267803 4.689187
H	3.589976	4.511502 5.736199
C	-0.392370	3.439672 1.846278
H	-1.459446	3.426286 2.023819
C	2.525811	2.464862 -1.864091
H	2.409090	2.154271 -2.896653
C	6.370641	3.375204 0.918941
H	7.441212	3.459038 0.780764
C	1.806232	-1.646083 5.926511
C	3.064581	-2.489174 5.734583
O	3.681069	-3.118818 6.614492
C	3.461819	-2.388861 4.263920
H	3.434348	-3.369437 3.774663
H	4.489450	-2.017134 4.176955
C	2.139128	-0.445151 4.943391
C	2.402890	-1.391059 3.711635
H	2.679046	-0.892344 2.783564
C	1.085635	-2.146798 3.642360
C	0.394605	-2.382949 2.524179
H	0.765898	-2.018982 1.569873
H	-0.570825	-2.878673 2.528364
C	0.703987	-2.434203 5.102621
H	-0.287964	-2.041129 5.356381
H	0.696992	-3.504823 5.348386
C	3.365352	0.382078 5.376999
H	3.666315	1.044360 4.558569
H	4.227581	-0.234764 5.652629
H	3.120798	1.006362 6.245007
C	0.958597	0.511021 4.714942
H	0.079419	0.003706 4.311298
H	1.254401	1.276387 3.992186
H	0.672120	1.011198 5.645688
C	1.457091	-1.316031 7.368749
H	1.404114	-2.222297 7.980749
H	0.494710	-0.796363 7.430271
H	2.219150	-0.672056 7.823057
h	2.651053	6.581621 1.405931
h	0.940551	4.444980 6.172402
h	-1.185931	3.916956 4.572781
h	-1.923311	2.911633 -0.523734
h	-0.238030	2.251044 -2.677985
h	4.913559	1.816778 -3.243266
h	7.144307	2.133052 -1.738983
h	7.881615	4.004620 3.271439
h	6.276274	4.408144 5.443193

TS2c”

Total QM energy at B2: -3306.195015 (a.u.)

Total QM/MM energy at B2: -3417.136430 (a.u.)

S	2.875833	5.621039 0.435919
O	2.935284	1.485551 1.726616
H	2.044154	1.209044 2.020917
O	2.188005	0.280707 0.040707
H	3.075988	-0.110577 -0.182347
Fe	2.939005	3.389112 1.301532
N	1.741490	3.752346 2.909343
N	1.299239	3.059270 0.157081
N	4.137370	2.990283 -0.263034
N	4.552785	3.758466 2.456866
C	2.133928	4.003266 4.227215
C	0.965382	4.145208 5.082881
C	-0.139389	3.984719 4.270937
C	0.363338	3.763823 2.922635
C	-0.033842	3.285377 0.502195
C	-0.905702	2.943663 -0.622837
C	-0.098025	2.417541 -1.615172
C	1.268722	2.491627 -1.076801
C	3.754435	2.300135 -1.383994
C	4.887391	2.084288 -2.271177
C	5.975386	2.726139 -1.698256
C	5.504598	3.209965 -0.390379
C	5.871141	3.780121 2.027033
C	6.768196	4.001231 3.155903
C	5.974941	4.121817 4.281525
C	4.596989	3.981847 3.827955
C	3.458858	4.098217 4.631782
H	3.626696	4.300333 5.683989
C	-0.444045	3.587515 1.785288
H	-1.509937	3.635436 1.962217
C	2.431707	1.941291 -1.657774
H	2.286940	1.311905 -2.529536
C	6.285619	3.581077 0.705322

H	7.360333	3.592212 0.564970
C	1.848894	-1.715697 5.824368
C	3.145029	-2.507170 5.665654
O	3.732302	-3.158793 6.548580
C	3.617092	-2.322635 4.225076
H	3.652442	-3.279380 3.691384
H	4.631941	-1.909880 4.207967
C	2.191933	-0.459705 4.919654
C	2.554578	-1.334953 3.660108
H	2.874786	-0.776039 2.779688
C	1.277379	-2.138632 3.482743
C	0.678275	-2.389460 2.315808
H	1.099721	-2.000159 1.392790
H	-0.250460	-2.944995 2.233761
C	0.820282	-2.496934 4.904969
H	-0.196060	-2.141883 5.113883
H	0.830099	-3.577021 5.102855
C	3.368654	0.380922 5.451673
H	3.704632	1.074662 4.674190
H	4.226444	-0.225027 5.762266
H	3.058463	0.973263 6.320359
C	0.985724	0.465065 4.692219
H	0.152923	-0.039009 4.195638
H	1.284131	1.311681 4.067827
H	0.625638	0.875599 5.640933
C	1.412539	-1.458339 7.257253
H	1.356413	-2.390609 7.826070
H	0.432219	-0.970404 7.289806
H	2.129493	-0.812846 7.777686
h	2.599158	6.523508 1.442571
h	0.967084	4.354645 6.152554
h	-1.193153	3.966250 4.548977
h	-1.982080	3.114080 -0.601944
h	-0.315539	2.011654 -2.603104
h	4.798534	1.531702 -3.206495
h	6.945933	2.845768 -2.179705
h	7.855692	4.002088 3.082295
h	6.296741	4.283125 5.310355

IC2c”

Total QM energy at B2: -3306.287469 (a.u.)

Total QM/MM energy at B2: -3417.225887 (a.u.)

S	2.866575	5.611781 0.388298
O	3.078430	1.640051 2.038679
H	2.867182	1.024415 1.296650
O	2.447510	0.298528 -0.497779
H	3.008340	-0.416658 -0.904271
Fe	2.993908	3.357752 1.392659
N	1.814200	3.846063 2.943798
N	1.367972	2.918954 0.246273
N	4.154559	2.885624 -0.201327
N	4.612279	3.828833 2.484489
C	2.207556	4.064666 4.267749
C	1.033849	4.185562 5.120644
C	-0.066548	4.047911 4.296620
C	0.450877	3.851340 2.950233
C	0.038120	3.314605 0.539021
C	-0.824626	2.990907 -0.599816
C	-0.038284	2.327715 -1.525774
C	1.305776	2.297492 -0.929619
C	3.806288	2.176294 -1.280235
C	4.888325	2.076386 -2.239744
C	5.961031	2.787119 -1.709830
C	5.523410	3.233613 -0.379497
C	5.912974	3.829716 2.039243
C	6.832382	4.030619 3.151028
C	6.054133	4.153236 4.291828
C	4.672276	4.037123 3.853868
C	3.533072	4.144973 4.663468
H	3.706327	4.324326 5.719794
C	-0.357205	3.684115 1.792712
H	-1.419994	3.807968 1.954189
C	2.480502	1.490925 -1.381252
H	2.336975	1.152953 -2.411970
C	6.298602	3.619354 0.692808
H	7.369704	3.677183 0.527000
C	1.796220	-1.713497 5.722188
C	3.090587	-2.521788 5.651508
O	3.643753	-3.128925 6.586739
C	3.616463	-2.420457 4.219273
H	3.667097	-3.405731 3.741334
H	4.631595	-2.009219 4.216099
C	2.180357	-0.512542 4.759254
C	2.578386	-1.461820 3.567480
H	2.927722	-0.943953 2.674852
C	1.309825	-2.279263 3.392797
C	0.775645	-2.654670 2.228364
H	1.246744	-2.378462 1.289158

H	-0.144617 -3.222897 2.151053	C	-0.867644 2.845717 -0.680773
C	0.790088 -2.533375 4.815084	C	-0.048432 2.551025 -1.753073
H	-0.225218 -2.145138 4.959224	C	1.330229 2.693442 -1.242212
H	0.767668 -3.598761 5.079999	C	3.824289 2.551932 -1.512172
C	3.345130 0.351808 5.279734	C	4.993684 2.219798 -2.321404
H	3.668195 1.024731 4.479732	C	6.104782 2.375731 -1.512044
H	4.207531 -0.235429 5.614861	C	5.587764 2.869214 -0.224173
H	3.015335 0.958312 6.131867	C	5.868498 3.698642 2.135041
C	1.006730 0.417823 4.409259	C	6.739725 3.968536 3.273516
H	0.130302 -0.121631 4.038459	C	5.917058 4.181606 4.362605
H	1.341903 1.102750 3.623895	C	4.549580 4.066594 3.870822
H	0.704990 1.009956 5.280124	C	3.391638 4.232991 4.630264
C	1.311321 -1.380683 7.123291	H	3.527971 4.494273 5.673872
H	1.183621 -2.287970 7.721857	C	-0.427716 3.398256 1.757784
H	0.355253 -0.846592 7.092078	H	-1.496596 3.384694 1.926751
H	2.034988 -0.749452 7.651593	C	2.502300 2.472559 -1.959301
h	2.589516 6.546331 1.365131	H	2.387204 2.169839 -2.995194
h	1.028292 4.374197 6.194168	C	6.324067 3.322787 0.865995
h	-1.123488 4.018256 4.561318	H	7.396910 3.400409 0.738178
h	-1.878588 3.267685 -0.624833	C	1.767994 -1.705150 5.956571
h	-0.261437 1.870738 -2.489849	C	3.032540 -2.550481 5.819385
h	4.788102 1.540232 -3.183439	O	3.583738 -3.216230 6.715037
h	6.902044 2.967126 -2.229598	C	3.544338 -2.382699 4.394546
h	7.918899 4.014905 3.065594	H	3.544881 -3.337534 3.856038
h	6.384591 4.310315 5.318566	H	4.578977 -2.022265 4.401513
		C	2.188713 -0.460345 5.070898
TS2d”		C	2.545222 -1.343764 3.814386
Total QM energy at B2: -3306.194205 (a.u.)		H	2.895622 -0.800977 2.939960
Total QM/MM energy at B2: -3417.135813 (a.u.)		C	1.233009 -2.078069 3.595517
S	2.903104 5.626933 0.401009	C	0.644885 -2.311756 2.422589
O	2.986847 1.569533 1.753111	H	1.112689 -2.046421 1.482277
H	2.423633 1.398451 2.533010	H	-0.322560 -2.798463 2.348362
O	1.545541 -0.209406 1.182904	C	0.716506 -2.413527 5.005325
H	2.172425 -0.260578 0.419240	H	-0.280351 -1.998867 5.198179
Fe	2.955482 3.373867 1.304340	H	0.656294 -3.493977 5.192519
N	1.725562 3.755422 2.890290	C	3.380725 0.326816 5.646844
N	1.333169 3.054794 0.093800	H	3.761332 1.030756 4.897835
N	4.197966 2.932098 -0.247473	H	4.212279 -0.314086 5.957827
N	4.540512 3.767666 2.509847	H	3.073849 0.908379 6.524501
C	2.075684 4.081346 4.198408	C	1.021351 0.511230 4.831800
C	0.888350 4.185035 5.036429	H	0.216273 0.067188 4.243024
C	-0.191590 3.918658 4.221695	H	1.370335 1.396102 4.293352
C	0.343005 3.671970 2.888351	H	0.610551 0.859029 5.785549
C	0.005691 3.133272 0.460343	C	1.319910 -1.439710 7.383462

H 1.270137 -2.368312 7.957935
H 0.336294 -0.958527 7.407332
H 2.028778 -0.786444 7.905738
h 2.633977 6.537132 1.402734
h 0.867148 4.411288 6.102462
h -1.244959 3.850659 4.493462
h -1.954604 2.900604 -0.621005
h -0.265266 2.247306 -2.777185
h 4.901661 1.852913 -3.343653
h 7.119516 2.105764 -1.804448
h 7.828206 3.929391 3.231779
h 6.217211 4.361931 5.394815

IC2d"

Total QM energy at B2: -3306.240318 (a.u.)

Total QM/MM energy at B2: -3417.182340 (a.u.)

S 2.886786 5.477373 0.414662
O 2.704131 1.449344 1.918585
H 2.812426 1.449219 2.891083
O 0.472165 -0.223595 1.825555
H 1.296224 0.339705 1.733328
Fe 2.798581 3.235211 1.363036
N 1.607651 3.728684 2.933228
N 1.178891 2.927877 0.157236
N 4.015882 2.702872 -0.173824
N 4.410479 3.589171 2.571637
C 1.968901 4.092300 4.228192
C 0.790033 4.194891 5.075346
C -0.293946 3.883567 4.282117
C 0.228187 3.609113 2.950695
C -0.140615 3.003882 0.540335
C -1.031067 2.729049 -0.591831
C -0.227645 2.465362 -1.683368
C 1.158128 2.590461 -1.187297
C 3.640438 2.353575 -1.444997
C 4.793205 1.925238 -2.230713
C 5.892971 1.971465 -1.393600
C 5.400064 2.525437 -0.121916
C 5.730836 3.443975 2.199054
C 6.619353 3.760203 3.311532
C 5.813483 4.079290 4.388288
C 4.439873 3.985499 3.909800
C 3.289509 4.238170 4.654643
H 3.433080 4.552090 5.682812
C -0.553961 3.278722 1.844016
H -1.618110 3.239409 2.034863
C 2.319662 2.348092 -1.909345
H 2.198683 2.058681 -2.947989
C 6.161324 2.963947 0.953872
H 7.237644 2.955857 0.827337
C 1.782692 -1.805336 5.782784
C 3.062020 -2.633012 5.679036
O 3.559303 -3.344396 6.572005
C 3.705750 -2.318085 4.331079
H 3.738407 -3.201756 3.685111
H 4.740558 -1.987873 4.467743
C 2.313872 -0.460401 5.124920
C 2.773695 -1.194841 3.788867
H 3.238268 -0.565561 3.028903
C 1.484195 -1.867231 3.372570
C 0.813328 -1.637262 2.061807
H 1.436443 -2.006739 1.232577
H -0.140201 -2.172217 2.013955
C 0.817209 -2.338086 4.651075
H -0.182259 -1.896937 4.787113
H 0.685034 -3.430218 4.712235
C 3.449622 0.197426 5.933731
H 3.926332 0.993094 5.347745
H 4.229094 -0.505013 6.245231
H 3.046727 0.657381 6.844362
C 1.192919 0.573272 4.919938
H 0.512451 0.312348 4.107018
H 1.621865 1.549694 4.681679
H 0.617834 0.706798 5.843565
C 1.167921 -1.735325 7.167818
H 0.716475 -2.699096 7.415143
H 0.378697 -0.976748 7.212692
H 1.914500 -1.508348 7.936077
h 2.620634 6.417853 1.388832
h 0.781684 4.419558 6.141893
h -1.343145 3.805254 4.566926
h -2.117430 2.761296 -0.509110
h -0.455910 2.191828 -2.713484
h 4.692983 1.569062 -3.255975
h 6.878899 1.585287 -1.652207
h 7.706313 3.695185 3.262996
h 6.125443 4.293414 5.410491

RC3

Total QM energy at B2: -3306.220833 (a.u.)

Total QM/MM energy at B2: -3413.894672 (a.u.)

S	5.053389	4.537999	-0.078068
O	4.536947	0.280229	1.175735
H	3.604338	0.079229	0.922622
O	5.318368	-0.622186	0.234002
H	5.643957	0.090170	-0.395618
Fe	4.789517	2.425903	0.701305
N	3.674962	2.704464	2.386399
N	3.093427	2.198323	-0.403713
N	5.889250	1.857086	-0.937734
N	6.446256	2.402674	1.837671
C	4.126684	2.889151	3.693826
C	3.000003	3.069546	4.609108
C	1.861176	3.011528	3.833857
C	2.290775	2.785491	2.456167
C	1.789417	2.409100	0.041695
C	0.850481	2.313024	-1.073153
C	1.585153	2.035912	-2.212445
C	2.992890	2.019324	-1.784202
C	5.434661	1.822178	-2.257157
C	6.539730	1.574368	-3.167760
C	7.678158	1.396172	-2.394319
C	7.281976	1.672341	-1.011089
C	7.743050	2.152215	1.398845
C	8.676802	2.227695	2.517708
C	7.935633	2.536642	3.639264
C	6.547061	2.642644	3.207830
C	5.467041	2.889633	4.050892
H	5.694536	3.066686	5.095923
C	1.436266	2.661352	1.364608
H	0.379363	2.763730	1.583841
C	4.096857	1.893642	-2.623208
H	3.904043	1.826107	-3.688487
C	8.111076	1.840843	0.090823
H	9.174780	1.726914	-0.069634
C	3.668736	-3.638681	4.497839
C	4.382966	-3.591537	5.856565
O	4.979579	-4.548179	6.382154
C	4.408009	-2.143878	6.338485
H	5.408514	-1.850752	6.663926
H	3.741746	-1.998160	7.197577
C	2.751333	-2.352266	4.573014
C	3.920548	-1.417898	5.055761
H	3.661545	-0.366338	5.189319
C	5.021780	-1.688461	4.024733
C	6.018738	-0.867247	3.698333
H	6.076506	0.145072	4.080324
H	6.808537	-1.163599	3.015803
C	4.829789	-3.135388	3.558377
H	4.499466	-3.194001	2.513676
H	5.733759	-3.747536	3.650506
C	1.593255	-2.505420	5.581162
H	0.777316	-3.086258	5.134154
H	1.188200	-1.526478	5.864036
H	1.889877	-3.020423	6.500398
C	2.166445	-1.894899	3.224615
H	2.943831	-1.641596	2.499720
H	1.554578	-0.997146	3.378442
H	1.521484	-2.666600	2.789041
C	3.053402	-4.981177	4.136718
H	3.769956	-5.788252	4.322308
H	2.760471	-5.018906	3.081633
H	2.163418	-5.186351	4.744998
h	4.751545	5.413517	0.945018
h	3.063566	3.240840	5.683671
h	0.818506	3.116257	4.133754
h	-0.217286	2.496732	-0.954031
h	1.284795	1.815998	-3.236891
h	6.400117	1.488056	-4.245316
h	8.628486	1.022641	-2.775657
h	9.735514	1.976984	2.451833
h	8.270608	2.646749	4.670639

TS3a

Total QM energy at B2: -3306.197656 (a.u.)

Total QM/MM energy at B2: -3413.870815 (a.u.)

S	5.069025	4.611279	-0.054350
O	4.587634	0.519529	1.130360
H	4.938753	0.228197	2.005797
O	5.393887	-0.913317	0.183005
H	5.077827	-0.490161	-0.646453
Fe	4.792787	2.398244	0.694024
N	3.683169	2.741345	2.383403
N	3.108251	2.299900	-0.438930
N	5.896603	1.950783	-0.945925
N	6.448499	2.461485	1.854160
C	4.122094	2.955814	3.692719

C	2.985987 3.106761 4.600530	H	2.917357 -1.413901 2.415037
C	1.854189 3.005277 3.819061	H	1.533100 -0.854634 3.346129
C	2.298997 2.783318 2.445834	H	1.538936 -2.497779 2.690143
C	1.808433 2.446293 0.013121	C	3.144431 -4.819723 3.911376
C	0.862170 2.335794 -1.098944	H	3.874784 -5.619260 4.071535
C	1.600401 2.098684 -2.242918	H	2.864886 -4.814334 2.852431
C	3.009680 2.121944 -1.811808	H	2.252156 -5.071442 4.498111
C	5.459158 1.898351 -2.254932	h	4.761633 5.487388 0.966576
C	6.559217 1.564049 -3.152941	h	3.038456 3.281770 5.675092
C	7.665260 1.319108 -2.357476	h	0.806385 3.083985 4.108853
C	7.253144 1.643464 -0.981871	h	-0.210752 2.478078 -0.969866
C	7.735512 2.169413 1.425281	h	1.309272 1.877713 -3.269798
C	8.673295 2.267191 2.537607	h	6.429859 1.477306 -4.231741
C	7.937957 2.622326 3.650860	h	8.596389 0.883979 -2.720418
C	6.554079 2.742142 3.214044	h	9.730641 2.010433 2.473098
C	5.463989 3.001311 4.047075	h	8.267796 2.725859 4.684569
H	5.686662 3.210257 5.087905	**IC3a**	
C	1.455294 2.658508 1.344638	Total QM energy at B2: -3306.220509 (a.u.)	
H	0.395738 2.738109 1.562207	Total QM/MM energy at B2: -3413.887630 (a.u.)	
C	4.123368 1.997297 -2.638502	S	5.029602 4.612244 -0.054509
H	3.941045 1.913885 -3.704851	O	4.452528 0.549408 1.084344
C	8.082161 1.792845 0.126492	H	4.516124 0.349009 2.040950
H	9.138502 1.615767 -0.024666	O	6.113408 -0.989869 -0.139034
C	3.725607 -3.483042 4.342782	H	5.415553 -0.351338 0.293576
C	4.414165 -3.487262 5.717212	Fe	4.675398 2.369809 0.728591
O	4.974331 -4.464102 6.246893	N	3.580963 2.804428 2.402508
C	4.429033 -2.056331 6.247226	N	2.996330 2.344531 -0.419843
H	5.428653 -1.763755 6.576407	N	5.789420 1.910041 -0.916543
H	3.773211 -1.945996 7.118805	N	6.346339 2.443872 1.879127
C	2.773288 -2.224783 4.474170	C	4.021788 3.004194 3.707333
C	3.918151 -1.283694 5.001436	C	2.892340 3.164471 4.618708
H	3.632590 -0.247230 5.186344	C	1.756511 3.074878 3.838921
C	5.028132 -1.477588 3.965872	C	2.199868 2.853091 2.466487
C	6.023679 -0.623787 3.700483	C	1.698754 2.493502 0.029018
H	6.080071 0.345327 4.183871	C	0.751859 2.369752 -1.083307
H	6.838118 -0.873586 3.027246	C	1.491917 2.118606 -2.222171
C	4.871257 -2.901384 3.428664	C	2.900817 2.142184 -1.784048
H	4.545375 -2.901624 2.381696	C	5.354092 1.858212 -2.218768
H	5.795634 -3.486282 3.488132	C	6.445967 1.505764 -3.121147
C	1.625496 -2.452399 5.481606	C	7.553380 1.253731 -2.330952
H	0.824702 -3.037387 5.013244	C	7.143216 1.578270 -0.954055
H	1.193665 -1.497120 5.803436	C	7.621988 2.115447 1.459565
H	1.939473 -2.995148 6.379466	C	8.565260 2.199564 2.569305
C	2.169361 -1.726123 3.148110	C	7.839337 2.583156 3.678836

C 6.457657 2.728323 3.239202
C 5.369433 3.011068 4.064202
H 5.592082 3.210973 5.107039
C 1.353605 2.715194 1.362766
H 0.294550 2.791589 1.584240
C 4.018703 1.990224 -2.602487
H 3.837532 1.906133 -3.668945
C 7.965105 1.718557 0.160235
H 9.018408 1.520371 0.021571
C 3.679038 -3.569975 4.405486
C 4.423555 -3.548577 5.748854
O 4.994797 -4.519358 6.277623
C 4.480422 -2.106038 6.240050
H 5.497751 -1.823049 6.518692
H 3.863477 -1.963127 7.135182
C 2.752580 -2.291819 4.538659
C 3.933484 -1.357047 4.997303
H 3.667626 -0.312828 5.172480
C 4.986608 -1.590116 3.910111
C 5.958596 -0.750601 3.539856
H 6.051343 0.237792 3.977462
H 6.699639 -1.014510 2.791791
C 4.796073 -3.032710 3.432190
H 4.426851 -3.081799 2.400671
H 5.716547 -3.624744 3.481130
C 1.635959 -2.472670 5.588566
H 0.818679 -3.071407 5.168390
H 1.217543 -1.503323 5.885235
H 1.976782 -2.980659 6.496317
C 2.109735 -1.816827 3.222315
H 2.837304 -1.522001 2.461968
H 1.481955 -0.939548 3.421299
H 1.463927 -2.593830 2.797400
C 3.064478 -4.908772 4.029688
H 3.796834 -5.712398 4.159629
H 2.727507 -4.917739 2.987426
H 2.204276 -5.144108 4.668699
h 4.733170 5.508828 0.951776
h 2.952669 3.328148 5.694643
h 0.710501 3.152949 4.135289
h -0.322325 2.505693 -0.957946
h 1.205338 1.886290 -3.247826
h 6.306333 1.408359 -4.197754
h 8.486648 0.831361 -2.703351
h 9.614676 1.913193 2.500135
h 8.174873 2.697120 4.709609

TS3b

Total QM energy at B2: -3306.190212 (a.u.)

Total QM/MM energy at B2: -3413.861129 (a.u.)

S 5.044261 4.575158 -0.056550
O 4.385830 0.435244 0.704131
H 4.849445 -0.005108 -0.039970
O 5.184252 -0.543488 2.192466
H 4.777695 0.279865 2.560184
Fe 4.708488 2.364731 0.573525
N 3.595873 2.630304 2.287479
N 3.041560 2.341288 -0.573684
N 5.827376 1.924304 -1.063419
N 6.360193 2.322604 1.771462
C 4.027721 2.798152 3.605014
C 2.885827 2.974365 4.504396
C 1.760614 2.926625 3.706308
C 2.214096 2.723010 2.330623
C 1.744582 2.492290 -0.116765
C 0.802465 2.412870 -1.238864
C 1.540971 2.175091 -2.381598
C 2.952643 2.173409 -1.947047
C 5.392314 1.887835 -2.375679
C 6.499947 1.560644 -3.268522
C 7.609420 1.327066 -2.473127
C 7.191806 1.632496 -1.093062
C 7.654595 2.076141 1.333416
C 8.590067 2.158925 2.453198
C 7.847123 2.468733 3.576528
C 6.456735 2.562706 3.142247
C 5.366446 2.791103 3.982159
H 5.581282 2.964790 5.031293
C 1.379743 2.666351 1.216123
H 0.320272 2.769807 1.422833
C 4.064869 2.023116 -2.770207
H 3.886048 1.950206 -3.837684
C 8.015710 1.760841 0.022157
H 9.076531 1.617795 -0.131700
C 3.608380 -3.567254 4.560901
C 4.369868 -3.538652 5.894456
O 4.903775 -4.518775 6.438772
C 4.549852 -2.082238 6.310503
H 5.584013 -1.873752 6.591962

H	3.938164 -1.824670 7.182122	N	5.779120 1.819023 -0.847490
C	2.800156 -2.208062 4.619557	N	6.310180 2.300035 1.922128
C	4.064226 -1.351359 5.018959	C	3.976094 2.917784 3.733394
H	3.912044 -0.276729 5.129475	C	2.847947 3.121280 4.643879
C	5.109724 -1.771873 4.004854	C	1.713288 3.110342 3.862634
C	6.239995 -1.061100 3.626387	C	2.146128 2.900359 2.482689
H	6.507247 -0.121149 4.098956	C	1.645631 2.528437 0.070636
H	7.049394 -1.572455 3.118211	C	0.718566 2.425637 -1.054765
C	4.781825 -3.187366 3.579424	C	1.457824 2.074673 -2.169986
H	4.420664 -3.210399 2.544203	C	2.859902 2.021869 -1.715648
H	5.639632 -3.867501 3.645327	C	5.304161 1.683975 -2.138142
C	1.693005 -2.225505 5.694936	C	6.397214 1.365689 -3.052606
H	0.830653 -2.794234 5.328495	C	7.551872 1.264551 -2.294170
H	1.345754 -1.209919 5.915569	C	7.155456 1.598093 -0.915838
H	2.006043 -2.682473 6.639080	C	7.613832 2.071543 1.492234
C	2.174344 -1.757129 3.286422	C	8.539199 2.160019 2.616285
H	2.902778 -1.599776 2.488086	C	7.783570 2.459566 3.732987
H	1.657794 -0.800656 3.433928	C	6.396232 2.553095 3.290449
H	1.428072 -2.483761 2.945270	C	5.309557 2.836676 4.114542
C	2.882712 -4.864640 4.245917	H	5.523324 2.997810 5.165243
H	3.548279 -5.721578 4.395324	C	1.291429 2.809338 1.387744
H	2.529363 -4.883322 3.209566	H	0.237648 2.949148 1.598994
H	2.017059 -5.000172 4.905138	C	3.969105 1.778984 -2.519733
h	4.735190 5.427351 0.983924	H	3.782260 1.638011 -3.579308
h	2.938682 3.164002 5.576456	C	7.989185 1.773995 0.184256
h	0.714031 3.034814 3.990959	H	9.054289 1.680053 0.031712
h	-0.267215 2.578292 -1.110464	C	3.829425 -3.670700 4.252672
h	1.250422 1.966375 -3.411202	C	4.414926 -3.226365 5.596048
h	6.371743 1.476890 -4.347696	O	4.729944 -3.982699 6.527738
h	8.551002 0.919402 -2.840959	C	4.665542 -1.722648 5.516236
h	9.654506 1.934651 2.384365	H	5.703151 -1.482786 5.767007
h	8.181712 2.593143 4.606401	H	4.030686 -1.194581 6.233850
		C	3.050855 -2.364976 3.808925
PC3		C	4.281960 -1.417741 4.041975
Total QM energy at B2: -3306.312297 (a.u.)		H	4.135107 -0.362899 3.806449
Total QM/MM energy at B2: -3413.977080 (a.u.)		C	5.384484 -2.103005 3.234794
S	5.068313 4.507320 -0.047391	C	6.704646 -1.487738 3.032016
O	4.234622 0.409363 1.141443	H	6.889112 -0.469103 3.362047
H	3.487159 0.133541 0.584612	H	7.578472 -2.120226 2.924619
O	5.756006 -1.587266 1.858429	C	5.114576 -3.608488 3.338027
H	4.905651 -0.308451 1.321313	H	4.892535 -4.032811 2.354641
Fe	4.652138 2.362701 0.774203	H	5.956469 -4.170503 3.757136
N	3.527511 2.785976 2.422910	C	1.847557 -2.042683 4.716971
N	2.942151 2.263096 -0.348106	H	1.008087 -2.709903 4.488155

H	1.513609 -1.014264 4.540095	C	7.487157 2.057415 1.480270
H	2.062799 -2.137434 5.785927	C	8.421129 2.149607 2.596860
C	2.572011 -2.374111 2.346052	C	7.683046 2.523384 3.701444
H	3.377178 -2.540544 1.626052	C	6.301812 2.658088 3.249845
H	2.106121 -1.409896 2.110938	C	5.211447 2.947606 4.066416
H	1.820107 -3.153133 2.193058	H	5.428316 3.117449 5.115539
C	3.105833 -5.007022 4.264366	C	1.194484 2.869734 1.350200
H	3.743004 -5.784305 4.701407	H	0.137034 2.972365 1.562516
H	2.831506 -5.320349 3.251069	C	3.889716 1.946489 -2.557720
H	2.192207 -4.953655 4.867742	H	3.708526 1.839480 -3.622417
h	4.739938 5.414893 0.938930	C	7.839644 1.648373 0.188661
h	2.916305 3.271663 5.721273	H	8.892675 1.446879 0.054966
h	0.670745 3.218305 4.161826	C	3.835189 -3.723598 4.313444
h	-0.343017 2.653351 -0.958565	C	4.274362 -3.419813 5.748584
h	1.165334 1.823551 -3.189522	O	4.692103 -4.263346 6.560244
h	6.230633 1.196640 -4.116439	C	4.288209 -1.907194 5.938366
h	8.512287 0.945698 -2.699144	H	5.226385 -1.566799 6.383327
h	9.605240 1.942706 2.549964	H	3.487945 -1.588671 6.617134
h	8.119024 2.599293 4.760612	C	2.966650 -2.450667 3.966083
TS3c		C	4.059338 -1.435614 4.471640
Total QM energy at B2: -3306.224476 (a.u.)		H	3.817205 -0.375740 4.367729
Total QM/MM energy at B2: -3413.886503 (a.u.)		C	5.321707 -1.898420 3.747643
S	5.061288 4.577454 -0.064639	C	6.418342 -1.161721 3.482011
O	4.176413 0.597287 1.117232	H	6.448109 -0.095122 3.676971
H	3.367435 0.488497 1.653432	H	7.321292 -1.617870 3.114939
O	5.912333 -1.277370 1.083041	C	5.170190 -3.403504 3.538935
H	5.225552 -0.514032 1.106113	H	5.050170 -3.638558 2.476568
Fe	4.536732 2.372742 0.744664	H	6.020513 -3.986034 3.910416
N	3.418976 2.858748 2.394890	C	1.645541 -2.398433 4.760089
N	2.851239 2.437080 -0.402367	H	0.896549 -3.051734 4.297757
N	5.665574 1.837563 -0.873046	H	1.243530 -1.379050 4.757101
N	6.207498 2.383031 1.885822	H	1.749301 -2.710850 5.804521
C	3.864807 3.003590 3.702039	C	2.651588 -2.288949 2.466842
C	2.742194 3.188804 4.617011	H	3.542521 -2.112944 1.858182
C	1.602789 3.157938 3.837329	H	1.974576 -1.435764 2.323631
C	2.037710 2.959413 2.460872	H	2.137169 -3.176054 2.078857
C	1.549342 2.638545 0.021103	C	3.250980 -5.109399 4.095099
C	0.619237 2.514978 -1.100772	H	3.906208 -5.869746 4.534704
C	1.368478 2.202169 -2.219642	H	3.133682 -5.332590 3.029048
C	2.769853 2.188075 -1.758688	H	2.268511 -5.205412 4.574266
C	5.216017 1.765999 -2.171713	h	4.742930 5.488504 0.921760
C	6.295658 1.374289 -3.076310	h	2.812020 3.338162 5.694454
C	7.411669 1.141872 -2.293516	h	0.559595 3.248936 4.139869
C	7.012793 1.495795 -0.919173	h	-0.452031 2.687721 -0.997764

h 1.086028 1.946283 -3.240823
h 6.143547 1.252822 -4.148772
h 8.345063 0.725445 -2.672236
h 9.475667 1.881491 2.532588
h 8.020648 2.655051 4.729431

IC3b

Total QM energy at B2: -3306.265762 (a.u.)
Total QM/MM energy at B2: -3413.928453 (a.u.)

S 5.062313 4.530851 -0.058869
O 4.395944 0.488085 1.154440
H 3.463118 0.272337 1.343271
O 6.299328 -1.207390 1.429089
H 5.539431 -0.560447 1.246090
Fe 4.641497 2.287412 0.763520
N 3.512995 2.770102 2.404088
N 2.935738 2.283269 -0.368139
N 5.781488 1.817604 -0.863668
N 6.321124 2.352154 1.890943
C 3.960477 2.912514 3.709598
C 2.840889 3.127145 4.622786
C 1.701322 3.116986 3.843536
C 2.131885 2.897280 2.469249
C 1.639108 2.532952 0.042038
C 0.709562 2.419043 -1.080522
C 1.453726 2.064851 -2.190803
C 2.852870 2.022051 -1.725047
C 5.312929 1.691473 -2.150935
C 6.402018 1.375760 -3.071943
C 7.551704 1.253454 -2.312212
C 7.152285 1.578620 -0.932092
C 7.612459 2.095608 1.477054
C 8.541760 2.181429 2.599349
C 7.788373 2.491487 3.712349
C 6.403020 2.590276 3.261964
C 5.306238 2.848240 4.078669
H 5.516758 3.002222 5.131323
C 1.285566 2.807520 1.364371
H 0.230532 2.946063 1.572088
C 3.972399 1.789168 -2.523336
H 3.786391 1.652282 -3.583967
C 7.979871 1.760296 0.169619
H 9.042064 1.631852 0.023568
C 3.792526 -3.770293 4.287553
C 4.268753 -3.360679 5.686204
O 4.624752 -4.150051 6.577890
C 4.378526 -1.840831 5.735021
H 5.348230 -1.523859 6.127280
H 3.621322 -1.413649 6.404759
C 2.978769 -2.489556 3.841985
C 4.139809 -1.490185 4.233306
H 3.948342 -0.433513 4.035991
C 5.319811 -2.087845 3.496648
C 6.454979 -1.362183 2.883723
H 6.594549 -0.378374 3.350960
H 7.380582 -1.934100 3.004893
C 5.123882 -3.587018 3.459488
H 4.980163 -3.974786 2.439983
H 5.963287 -4.154946 3.887755
C 1.674632 -2.300000 4.638170
H 0.901347 -2.987691 4.275077
H 1.299858 -1.278806 4.504543
H 1.787567 -2.474415 5.713188
C 2.654054 -2.441457 2.335709
H 3.547808 -2.325380 1.716717
H 1.990881 -1.591510 2.126740
H 2.130579 -3.348972 2.015333
C 3.140574 -5.140841 4.201261
H 3.782962 -5.895836 4.668771
H 2.969310 -5.436820 3.160252
H 2.177254 -5.157514 4.725804
h 4.744224 5.438589 0.930665
h 2.909717 3.285346 5.699030
h 0.659863 3.233436 4.143320
h -0.353662 2.638777 -0.983888
h 1.167005 1.804703 -3.209714
h 6.238129 1.225609 -4.139024
h 8.511878 0.930966 -2.714869
h 9.604158 1.947116 2.532468
h 8.120498 2.624122 4.741994

TS3f

Total QM energy at B2: -3306.258506 (a.u.)
Total QM/MM energy at B2: -3413.926510 (a.u.)

S 5.004646 4.499507 -0.016677
O 4.279909 0.401205 1.090853
H 3.793176 0.066844 0.314188
O 6.000997 -1.153183 1.734567
H 5.174390 -0.347689 1.404697
Fe 4.605410 2.297054 0.741351

N	3.514340	2.739051	2.409101
N	2.919990	2.256220	-0.414303
N	5.700746	1.782637	-0.900502
N	6.263545	2.278744	1.907432
C	3.956741	2.912523	3.713740
C	2.825350	3.097977	4.622036
C	1.691372	3.040748	3.838371
C	2.133050	2.818974	2.462374
C	1.629472	2.475778	0.031323
C	0.685415	2.399610	-1.085939
C	1.415913	2.112244	-2.224418
C	2.822426	2.066697	-1.786680
C	5.258218	1.711069	-2.205398
C	6.348190	1.330927	-3.097418
C	7.457611	1.091306	-2.303936
C	7.051535	1.440307	-0.930046
C	7.537966	1.963100	1.477842
C	8.488595	2.069820	2.582682
C	7.767518	2.460303	3.693193
C	6.377354	2.582055	3.262978
C	5.298691	2.886238	4.087406
H	5.519875	3.089188	5.129885
C	1.283697	2.714224	1.362497
H	0.227755	2.832683	1.578943
C	3.931402	1.863252	-2.602497
H	3.750361	1.764501	-3.667887
C	7.879787	1.568342	0.180078
H	8.932535	1.373221	0.036542
C	3.606671	-3.534541	4.416368
C	4.360668	-3.379399	5.741317
O	4.811070	-4.303796	6.435580
C	4.606872	-1.892409	5.972321
H	5.660029	-1.689472	6.176740
H	4.045428	-1.514730	6.834216
C	2.789550	-2.176855	4.367119
C	4.053297	-1.274833	4.627047
H	3.905634	-0.195482	4.649792
C	5.078120	-1.793964	3.670280
C	6.265613	-1.085121	3.160440
H	6.341683	-0.057114	3.528163
H	7.199389	-1.614349	3.387222
C	4.769458	-3.236771	3.393926
H	4.406592	-3.374501	2.367823
H	5.645403	-3.891052	3.502495
C	1.720206	-2.095166	5.475844
H	0.843507	-2.688850	5.191863
H	1.386751	-1.061815	5.620453
H	2.064758	-2.468945	6.445835
C	2.134211	-1.850833	3.013565
H	2.858234	-1.730003	2.203753
H	1.598198	-0.897902	3.091229
H	1.409384	-2.622088	2.733470
C	2.882987	-4.856155	4.223490
H	3.556438	-5.695305	4.428335
H	2.509925	-4.960894	3.199302
H	2.031811	-4.941311	4.909285
h	4.717673	5.407344	0.982235
h	2.888983	3.266830	5.696980
h	0.646979	3.145720	4.132124
h	-0.379222	2.600927	-0.967254
h	1.119316	1.897393	-3.251032
h	6.208336	1.216398	-4.172309
h	8.387336	0.664900	-2.680574
h	9.544163	1.809545	2.504576
h	8.111883	2.604929	4.717186

TS3e

Total QM energy at B2: -3306.206837 (a.u.)

Total QM/MM energy at B2: -3413.875160 (a.u.)

S	5.072951	4.569102	-0.043549
O	4.293027	0.559619	1.204070
H	4.943328	0.068414	1.772866
O	5.628989	-1.092261	0.695233
H	5.086686	-1.041607	-0.121930
Fe	4.650136	2.358892	0.740671
N	3.549396	2.828174	2.407931
N	2.971540	2.339055	-0.398990
N	5.760235	1.858823	-0.895090
N	6.312861	2.403257	1.880949
C	3.996863	3.029680	3.707949
C	2.871227	3.189423	4.627437
C	1.732975	3.090091	3.855566
C	2.171589	2.866928	2.480292
C	1.672035	2.491969	0.048548
C	0.728837	2.371450	-1.062777
C	1.470284	2.122760	-2.203723
C	2.875892	2.139233	-1.765096
C	5.322931	1.815203	-2.200923
C	6.408290	1.438219	-3.102171

C 7.508474 1.164791 -2.309068
C 7.102667 1.504040 -0.934168
C 7.591106 2.068062 1.464183
C 8.533112 2.178000 2.569467
C 7.807974 2.585702 3.672472
C 6.427314 2.723371 3.231524
C 5.344316 3.035621 4.055496
H 5.575363 3.253320 5.092973
C 1.323922 2.718789 1.380874
H 0.264727 2.789942 1.602222
C 3.993027 1.972725 -2.584732
H 3.810601 1.896797 -3.651901
C 7.932129 1.649847 0.174096
H 8.983826 1.442530 0.033469
C 3.761636 -3.513121 4.353790
C 4.400800 -3.551125 5.750376
O 4.996093 -4.523917 6.250004
C 4.331466 -2.146494 6.346573
H 5.300024 -1.827223 6.738537
H 3.627094 -2.106767 7.186310
C 2.761955 -2.294659 4.494692
C 3.850249 -1.340224 5.110800
H 3.520646 -0.322140 5.323433
C 5.010839 -1.455277 4.118847
C 5.983815 -0.560331 3.930386
H 5.976181 0.394534 4.442907
H 6.822240 -0.749434 3.267546
C 4.924368 -2.857047 3.514978
H 4.657729 -2.809485 2.452715
H 5.862559 -3.417405 3.592222
C 1.579567 -2.600451 5.440100
H 0.811426 -3.175037 4.908299
H 1.114391 -1.672045 5.793591
H 1.868185 -3.186236 6.319557
C 2.199046 -1.763853 3.163018
H 2.964142 -1.375477 2.486298
H 1.506434 -0.937748 3.366603
H 1.634867 -2.545432 2.639150
C 3.245053 -4.849760 3.846906
H 3.995577 -5.629456 4.010913
H 3.013166 -4.811807 2.777259
H 2.336390 -5.154240 4.381438
h 4.759971 5.483795 0.941199
h 2.936840 3.351971 5.703234
h 0.687473 3.159655 4.155821
h -0.345587 2.507301 -0.939395
h 1.181747 1.896015 -3.230075
h 6.271097 1.350832 -4.179950
h 8.433122 0.718965 -2.675582
h 9.584317 1.897726 2.502524
h 8.144748 2.705756 4.702150

IC3d

Total QM energy at B2: -3306.262988 (a.u.)

Total QM/MM energy at B2: -3413.927087 (a.u.)

S 5.043384 4.640310 -0.064826
O 4.337826 0.693645 1.103904
H 5.322896 -0.581115 0.599729
O 5.917560 -1.225166 0.132672
H 5.828787 -1.090401 -0.826587
Fe 4.588167 2.303907 0.765109
N 3.508375 2.864260 2.394410
N 2.914875 2.384421 -0.395058
N 5.717270 1.910366 -0.886313
N 6.279409 2.435457 1.874000
C 3.961637 3.052098 3.693363
C 2.840632 3.208835 4.615832
C 1.697816 3.116673 3.848860
C 2.125875 2.899759 2.471688
C 1.616292 2.525819 0.048454
C 0.676074 2.410377 -1.067079
C 1.421536 2.182800 -2.207973
C 2.827569 2.202779 -1.764127
C 5.274121 1.877294 -2.192631
C 6.351366 1.483789 -3.092769
C 7.451436 1.191408 -2.301659
C 7.058143 1.536443 -0.928225
C 7.555059 2.086008 1.463486
C 8.496076 2.184593 2.574408
C 7.772022 2.593960 3.673201
C 6.390778 2.743378 3.227074
C 5.308444 3.047232 4.047890
H 5.533873 3.251575 5.088821
C 1.270669 2.745767 1.382314
H 0.212892 2.807842 1.610661
C 3.946385 2.047262 -2.579412
H 3.768540 1.983459 -3.647890
C 7.892639 1.660881 0.178462
H 8.939271 1.430115 0.038968

C	3.762303 -3.577399 4.344412	O	6.644752 -0.618240 0.005201
C	4.432721 -3.578882 5.725833	H	5.757342 -0.215274 0.348195
O	5.019600 -4.545360 6.246782	Fe	4.619287 2.363544 0.666292
C	4.398581 -2.154459 6.275554	N	3.529892 2.749045 2.354918
H	5.382643 -1.839836 6.630661	N	2.942880 2.385686 -0.475805
H	3.715992 -2.080263 7.131261	N	5.710458 1.946980 -0.995439
C	2.780971 -2.340783 4.470069	N	6.281035 2.391663 1.815576
C	3.897218 -1.381195 5.027836	C	3.988784 2.965204 3.664443
H	3.581700 -0.354140 5.219882	C	2.862743 3.121297 4.581588
C	5.020933 -1.537569 3.998292	C	1.723425 3.015141 3.808324
C	5.974121 -0.649956 3.713533	C	2.161874 2.790311 2.434132
H	5.978360 0.335256 4.163903	C	1.633001 2.481552 -0.001631
H	6.772368 -0.862493 3.009405	C	0.685184 2.377386 -1.117925
C	4.910060 -2.964538 3.455723	C	1.426926 2.201055 -2.267306
H	4.604788 -2.973514 2.402502	C	2.841014 2.254265 -1.831837
H	5.844988 -3.530678 3.531483	C	5.279299 1.999316 -2.313245
C	1.615040 -2.606345 5.446956	C	6.367618 1.615231 -3.217784
H	0.833458 -3.193213 4.948815	C	7.414960 1.189371 -2.426387
H	1.161830 -1.663954 5.778211	C	6.990209 1.460519 -1.032327
H	1.917219 -3.164549 6.339672	C	7.535822 1.980938 1.393008
C	2.198746 -1.836855 3.136297	C	8.499001 2.090800 2.480037
H	2.960016 -1.446360 2.456437	C	7.798583 2.541116 3.585804
H	1.497989 -1.016358 3.334281	C	6.416280 2.702392 3.159071
H	1.641722 -2.630311 2.623524	C	5.331340 2.990867 4.000994
C	3.220462 -4.923119 3.890215	H	5.570223 3.199467 5.038845
H	3.975691 -5.702393 4.035596	C	1.297765 2.656310 1.326506
H	2.941915 -4.906301 2.830955	H	0.240837 2.715696 1.561866
H	2.335479 -5.213669 4.470195	C	3.963186 2.176613 -2.683413
h	4.742884 5.544165 0.933719	H	3.770187 2.165071 -3.750396
h	2.910063 3.365150 5.692313	C	7.804472 1.436358 0.130289
h	0.654748 3.185584 4.157610	H	8.821455 1.096779 0.007716
h	-0.399938 2.532947 -0.943623	C	3.623981 -3.546250 4.460890
h	1.138357 1.966089 -3.237978	C	4.425387 -3.510657 5.769288
h	6.213818 1.402376 -4.170971	O	4.959241 -4.489111 6.322394
h	8.365997 0.729822 -2.673928	C	4.588384 -2.054207 6.188561
h	9.544311 1.893076 2.508943	H	5.635622 -1.823602 6.393797
h	8.106413 2.711863 4.703904	H	4.034545 -1.837200 7.109707
		C	2.771309 -2.215657 4.581408
TS3d		C	4.019674 -1.327632 4.942806
Total QM energy at B2: -3306.2217 (a.u.)		H	3.818075 -0.264165 5.085537
Total QM/MM energy at B2: -3413.885314 (a.u.)		C	5.004013 -1.657366 3.817527
S	5.022142 4.615638 -0.049567	C	5.988044 -0.876832 3.361856
O	4.475057 0.514494 0.944426	H	6.140119 0.126838 3.745351
H	4.405483 0.294895 1.896605	H	6.673120 -1.194162 2.582419

C 4.724861 -3.109855 3.419685
H 4.313132 -3.194495 2.406584
H 5.617153 -3.744474 3.464113
C 1.701001 -2.290106 5.690187
H 0.851254 -2.896924 5.354233
H 1.317898 -1.291200 5.930637
H 2.072585 -2.734422 6.618815
C 2.088894 -1.762799 3.277731
H 2.789105 -1.593575 2.455557
H 1.564213 -0.814749 3.452785
H 1.343189 -2.495897 2.949004
C 2.924309 -4.863433 4.165664
H 3.622208 -5.699945 4.279260
H 2.529377 -4.885641 3.144071
H 2.091592 -5.034778 4.859066
h 4.718387 5.499091 0.966105
h 2.927296 3.292024 5.656182
h 0.678605 3.092755 4.108981
h -0.391521 2.474628 -0.978935
h 1.143675 1.996540 -3.299783
h 6.250900 1.623300 -4.301471
h 8.312766 0.706127 -2.811725
h 9.554907 1.830574 2.406478
h 8.146122 2.663921 4.611573

IC3c

Total QM energy at B2: -3306.284896 (a.u.)

Total QM/MM energy at B2: -3413.945498 (a.u.)

S 5.008845 4.625437 -0.027257
O 4.424393 0.522622 0.944860
H 4.247615 0.329787 1.889163
O 6.846816 -0.281334 0.507351
H 5.838737 -0.084841 0.630303
Fe 4.561876 2.387659 0.664602
N 3.492726 2.780842 2.358287
N 2.893332 2.426954 -0.480804
N 5.650645 1.965900 -1.014790
N 6.210350 2.369842 1.806853
C 3.946038 3.015609 3.645968
C 2.836310 3.154279 4.573234
C 1.683866 3.024595 3.809821
C 2.109916 2.799787 2.440688
C 1.584159 2.490696 0.000626
C 0.638792 2.381107 -1.106814
C 1.384039 2.236410 -2.266842
C 2.787620 2.314834 -1.835155
C 5.227107 2.128604 -2.354956
C 6.334630 1.794153 -3.253226
C 7.361599 1.306691 -2.458826
C 6.888229 1.468251 -1.072112
C 7.395011 1.887644 1.409783
C 8.411074 2.049720 2.438715
C 7.772294 2.597676 3.540773
C 6.376915 2.782908 3.155970
C 5.316877 3.075958 3.979702
H 5.553132 3.315362 5.012373
C 1.256215 2.651747 1.338131
H 0.197888 2.690460 1.574812
C 3.919857 2.286243 -2.701232
H 3.713853 2.314322 -3.765560
C 7.512998 1.001997 0.200747
H 8.566876 0.789995 0.067710
C 3.592633 -3.538529 4.493019
C 4.358466 -3.520258 5.823264
O 4.932492 -4.495956 6.340034
C 4.443851 -2.076162 6.305915
H 5.471051 -1.806071 6.561403
H 3.847035 -1.919384 7.212383
C 2.687802 -2.245858 4.629289
C 3.886457 -1.327157 5.066859
H 3.640267 -0.277849 5.237339
C 4.921809 -1.579157 3.968866
C 5.892735 -0.746630 3.585216
H 5.980257 0.250119 4.006345
H 6.625358 -1.011032 2.830661
C 4.712875 -3.025586 3.507175
H 4.342379 -3.086674 2.476683
H 5.625362 -3.629589 3.563049
C 1.581886 -2.397326 5.693817
H 0.760380 -3.008761 5.301356
H 1.166212 -1.419649 5.965544
H 1.933678 -2.875724 6.613000
C 2.037358 -1.769938 3.317602
H 2.758934 -1.568001 2.522069
H 1.490139 -0.836463 3.500789
H 1.316422 -2.507129 2.946001
C 2.950578 -4.868617 4.132604
H 3.670054 -5.685091 4.254404

H 2.598767 -4.875319 3.095227
H 2.095658 -5.085441 4.785309
h 4.698071 5.519957 0.976537
h 2.905397 3.323741 5.647746
h 0.641753 3.094619 4.121530
h -0.439205 2.457757 -0.964992
h 1.098973 2.038554 -3.300117
h 6.241866 1.867017 -4.336809
h 8.270339 0.853579 -2.854992
h 9.453206 1.749322 2.330143
h 8.142266 2.718276 4.558930

RC4

Total QM energy at B2: -3268.161624 (a.u.)

Total QM/MM energy at B2: -3409.590633 (a.u.)

S 5.071955 5.384721 0.425814
O 3.976998 1.278723 1.819505
H 3.157784 1.483936 2.331477
O 3.452875 0.254535 0.822053
H 4.316296 -0.140792 0.498677
Fe 4.507651 3.282615 1.192744
N 3.253685 3.685600 2.756595
N 2.930055 3.184127 -0.076284
N 5.706128 2.550112 -0.259394
N 6.027279 3.239541 2.529126
C 3.590690 4.010671 4.075383
C 2.385750 4.220698 4.864332
C 1.313441 4.009725 4.021578
C 1.857722 3.731367 2.701766
C 1.599944 3.413115 0.241760
C 0.769627 3.374490 -0.962310
C 1.606781 3.087512 -2.025521
C 2.959961 2.978749 -1.449205
C 5.380311 2.409758 -1.598212
C 6.529588 1.922549 -2.352809
C 7.563171 1.731381 -1.451316
C 7.050016 2.190827 -0.150565
C 7.335688 2.891602 2.232959
C 8.191789 3.106929 3.393341
C 7.392698 3.617146 4.397398
C 6.037766 3.681870 3.854423
C 4.895971 4.062559 4.552602
H 5.020686 4.386760 5.579914
C 1.115660 3.613172 1.531459
H 0.043123 3.719137 1.637977
C 4.123424 2.654997 -2.140215
H 4.045066 2.533789 -3.215244
C 7.786743 2.405273 1.008311
H 8.854736 2.241061 0.953988
O 4.775952 -3.674177 6.649997
C 4.133021 -2.704855 6.211117
C 3.785295 -1.428133 6.990084
H 4.680102 -0.994844 7.451951
H 3.087083 -1.665681 7.802377
C 3.631046 -2.526328 4.784346
C 2.370864 -1.600890 5.015038
C 4.338643 -0.148242 4.939861
H 5.187924 0.246677 5.508749
H 4.054503 0.628265 4.228576
C 4.683399 -1.489336 4.210823
H 4.554802 -1.409958 3.126988
H 5.710567 -1.826006 4.388478
C 3.163743 -0.547309 5.877291
H 2.566012 0.290922 6.245303
C 1.232690 -2.305433 5.782322
H 0.772621 -3.080688 5.160969
H 0.443833 -1.576279 6.015208
H 1.563614 -2.798318 6.704914
C 1.773150 -1.024184 3.718024
H 1.193832 -1.787633 3.186724
H 2.526613 -0.656800 3.020331
H 1.091090 -0.198044 3.954044
C 3.482090 -3.811125 3.986187
H 4.411262 -4.388690 4.022313
H 3.243791 -3.601634 2.937835
H 2.689691 -4.449233 4.394787
h 4.745252 6.305381 1.400492
h 2.366056 4.502941 5.916956
h 0.253776 4.000681 4.276713
h -0.293630 3.613656 -0.943590
h 1.409752 2.935883 -3.086772
h 6.492736 1.761555 -3.430209
h 8.523837 1.286822 -1.711231
h 9.247168 2.835262 3.414276
h 7.703316 3.897711 5.403810

TS4a

Total QM energy at B2: -3268.134866 (a.u.)

Total QM/MM energy at B2: -3409.564395 (a.u.)

S	5.072617	5.403753	0.425609
O	4.070738	1.445501	1.845197
H	3.270106	1.501076	2.409483
O	3.318472	0.077162	0.836958
H	4.206655	-0.263472	0.529932
Fe	4.508543	3.253145	1.231911
N	3.275003	3.760651	2.779618
N	2.936442	3.204355	-0.048253
N	5.712851	2.561540	-0.233413
N	6.046190	3.274531	2.552495
C	3.614189	4.078184	4.095187
C	2.410310	4.271589	4.893515
C	1.337518	4.051191	4.055292
C	1.882519	3.779365	2.733706
C	1.610205	3.427416	0.273013
C	0.771513	3.376424	-0.925657
C	1.604707	3.087413	-1.990563
C	2.960948	2.988644	-1.416406
C	5.388361	2.421717	-1.568049
C	6.532781	1.925059	-2.325398
C	7.561375	1.717418	-1.422582
C	7.048717	2.180362	-0.122379
C	7.344775	2.897144	2.262376
C	8.205236	3.103439	3.420531
C	7.414395	3.633714	4.420467
C	6.063478	3.721829	3.875647
C	4.923685	4.123208	4.566814
H	5.052398	4.447923	5.593862
C	1.137859	3.642193	1.565865
H	0.065005	3.739362	1.678300
C	4.126719	2.666697	-2.105951
H	4.047256	2.539976	-3.180486
C	7.783297	2.390593	1.038574
H	8.848050	2.205208	0.988559
O	4.789146	-3.673317	6.624811
C	4.148066	-2.704891	6.179984
C	3.815479	-1.419825	6.953149
H	4.717167	-0.987303	7.402140
H	3.124660	-1.649270	7.774211
C	3.629556	-2.536362	4.757792
C	2.377262	-1.601297	4.995852
C	4.357171	-0.163875	4.888330
H	5.218351	0.217412	5.450082
H	4.082299	0.613243	4.175049
C	4.675793	-1.509861	4.156294
H	4.518817	-1.425492	3.076501
H	5.704412	-1.853698	4.310564
C	3.187207	-0.545633	5.839507
H	2.597495	0.299289	6.206078
C	1.245856	-2.293999	5.784825
H	0.776866	-3.073882	5.176010
H	0.461652	-1.559166	6.016616
H	1.583995	-2.778441	6.709557
C	1.764802	-1.030407	3.703193
H	1.173490	-1.796245	3.188166
H	2.500198	-0.666582	2.983761
H	1.085931	-0.203429	3.947356
C	3.462201	-3.827255	3.972819
H	4.389965	-4.407881	3.997082
H	3.206744	-3.623452	2.927572
H	2.674572	-4.459322	4.399899
h	4.745532	6.346621	1.378690
h	2.392945	4.542407	5.949178
h	0.278975	4.026856	4.314059
h	-0.293797	3.605757	-0.901427
h	1.405463	2.928705	-3.050365
h	6.491975	1.764823	-3.402768
h	8.515995	1.258268	-1.679385
h	9.256753	2.817254	3.442346
h	7.728393	3.912890	5.426217

IC4a

Total QM energy at B2: -3268.142807 (a.u.)

Total QM/MM energy at B2: -3409.570487 (a.u.)

S	5.135821	5.421411	0.405117
O	4.297512	1.465061	1.824369
H	3.400677	1.358156	2.200014
O	3.195421	-0.048752	0.708974
H	4.111287	-0.362163	0.469292
Fe	4.572152	3.215575	1.271945
N	3.335550	3.790310	2.788007
N	2.979831	3.199696	0.002695
N	5.799549	2.567433	-0.209097
N	6.151811	3.330361	2.534289
C	3.688230	4.103308	4.090971
C	2.497554	4.299831	4.911381
C	1.412875	4.079122	4.089128
C	1.945603	3.801225	2.764302
C	1.654697	3.418422	0.310661

C	0.817408	3.352146	-0.885774
C	1.657135	3.061302	-1.945707
C	3.011583	2.971225	-1.363422
C	5.458814	2.416635	-1.528045
C	6.587898	1.902274	-2.303043
C	7.623807	1.684139	-1.411947
C	7.131547	2.165591	-0.110393
C	7.440722	2.936075	2.259847
C	8.299466	3.139179	3.420560
C	7.504420	3.669595	4.417088
C	6.157530	3.767514	3.860766
C	5.009650	4.147772	4.549613
H	5.138882	4.462250	5.580154
C	1.188812	3.648469	1.606666
H	0.116120	3.740275	1.727449
C	4.181083	2.653249	-2.049819
H	4.095169	2.514769	-3.122710
C	7.871329	2.393272	1.041012
H	8.932658	2.185535	0.996747
O	4.787928	-3.717115	6.598322
C	4.162431	-2.749832	6.127806
C	3.891959	-1.425413	6.854399
H	4.817275	-1.007006	7.266858
H	3.213029	-1.598871	7.699149
C	3.606980	-2.624186	4.714419
C	2.395414	-1.634109	4.945635
C	4.418495	-0.276275	4.721519
H	5.309386	0.099222	5.239704
H	4.144513	0.478031	3.983988
C	4.669479	-1.662041	4.039956
H	4.485333	-1.613827	2.962059
H	5.689587	-2.036030	4.180827
C	3.265684	-0.575121	5.721672
H	2.718917	0.306174	6.069211
C	1.262852	-2.254336	5.791430
H	0.743903	-3.031316	5.220787
H	0.518648	-1.479056	6.023789
H	1.610457	-2.725215	6.719878
C	1.768014	-1.093438	3.647750
H	1.149478	-1.862370	3.171010
H	2.491146	-0.765008	2.898847
H	1.111406	-0.244653	3.879609
C	3.366991	-3.940009	3.992387
H	4.273570	-4.553422	4.007404
H	3.079459	-3.771283	2.949162
H	2.573958	-4.524050	4.474484
h	4.783434	6.380393	1.332760
h	2.490980	4.573647	5.966392
h	0.356726	4.056730	4.357667
h	-0.250108	3.571277	-0.864398
h	1.461249	2.898331	-3.005488
h	6.528723	1.742032	-3.379559
h	8.568217	1.206079	-1.671977
h	9.349775	2.848955	3.446800
h	7.811674	3.942513	5.426631

TS4b

Total QM energy at B2: -3268.140412 (a.u.)

Total QM/MM energy at B2: -3409.568343 (a.u.)

S	5.134779	5.468187	0.418294
O	4.372925	1.481817	1.798511
H	3.426822	1.261449	1.921816
O	3.159201	-0.183769	0.932494
H	4.036122	-0.554091	0.631016
Fe	4.580064	3.239558	1.280130
N	3.345612	3.801230	2.787241
N	2.984520	3.200743	0.011555
N	5.813717	2.623331	-0.209960
N	6.168014	3.358826	2.534882
C	3.701138	4.111825	4.090062
C	2.511394	4.300984	4.913681
C	1.425347	4.076343	4.094565
C	1.954507	3.800777	2.768620
C	1.657850	3.409344	0.318687
C	0.821465	3.348622	-0.878357
C	1.663538	3.074560	-1.941150
C	3.019387	2.993919	-1.360249
C	5.472090	2.470870	-1.528360
C	6.590510	1.926035	-2.296936
C	7.615281	1.680014	-1.399090
C	7.134695	2.188243	-0.104253
C	7.455981	2.963468	2.260498
C	8.316445	3.168243	3.420144
C	7.521809	3.697781	4.416986
C	6.173304	3.793324	3.860446
C	5.022293	4.162887	4.549758
H	5.148846	4.474547	5.581450
C	1.193589	3.636366	1.616433
H	0.120525	3.717780	1.740367

C 4.193539 2.705680 -2.050664
H 4.111103 2.582629 -3.125759
C 7.880104 2.409433 1.045046
H 8.937803 2.183034 0.999723
O 4.815898 -3.682377 6.614066
C 4.168027 -2.725456 6.152698
C 3.875588 -1.408235 6.886805
H 4.800182 -0.966326 7.276354
H 3.223284 -1.600140 7.748384
C 3.594490 -2.608672 4.747541
C 2.354897 -1.659607 5.002696
C 4.328062 -0.234011 4.749842
H 5.213329 0.168382 5.257392
H 4.021872 0.511745 4.014906
C 4.614337 -1.609631 4.062153
H 4.405570 -1.563444 2.989326
H 5.648667 -1.950020 4.183142
C 3.202157 -0.575011 5.768204
H 2.632790 0.287863 6.125408
C 1.255940 -2.322129 5.858949
H 0.770260 -3.127211 5.297656
H 0.475123 -1.580421 6.082671
H 1.625578 -2.766897 6.791636
C 1.691443 -1.134271 3.719038
H 1.123629 -1.931588 3.226554
H 2.393662 -0.745064 2.981676
H 0.983452 -0.334461 3.969395
C 3.386941 -3.926870 4.019120
H 4.312366 -4.511877 4.020371
H 3.083326 -3.759590 2.980281
H 2.617673 -4.538746 4.505220
h 4.787701 6.421881 1.353361
h 2.505255 4.573084 5.969139
h 0.370109 4.050610 4.366368
h -0.247760 3.559005 -0.854624
h 1.469454 2.915679 -3.001884
h 6.531670 1.765440 -3.373418
h 8.538903 1.157398 -1.647812
h 9.367094 2.879072 3.444289
h 7.827383 3.967999 5.427765

IC4b

Total QM energy at B2: -3268.200791 (a.u.)

Total QM/MM energy at B2: -3409.623719 (a.u.)

S 5.134071 5.481682 0.407893
O 4.317929 1.639840 1.856941
H 3.328810 0.505775 1.090176
O 3.059583 -0.276758 0.553556
H 3.878277 -0.786633 0.340442
Fe 4.566154 3.194168 1.328691
N 3.364102 3.873646 2.810681
N 2.988746 3.201576 0.036390
N 5.786381 2.610274 -0.182569
N 6.166553 3.399271 2.555327
C 3.722015 4.187660 4.111567
C 2.532345 4.363277 4.937713
C 1.448228 4.117791 4.123198
C 1.977187 3.842151 2.796413
C 1.664699 3.404344 0.357930
C 0.816261 3.331922 -0.831387
C 1.648070 3.060998 -1.901611
C 3.009735 2.991392 -1.335483
C 5.451083 2.466391 -1.505812
C 6.569883 1.919235 -2.268697
C 7.588362 1.662075 -1.366442
C 7.108866 2.171122 -0.073039
C 7.447930 2.979107 2.277221
C 8.315015 3.183909 3.430395
C 7.531406 3.730419 4.427203
C 6.183495 3.843705 3.877618
C 5.041025 4.232979 4.569605
H 5.173244 4.545448 5.599866
C 1.210000 3.646093 1.653963
H 0.137408 3.717965 1.784878
C 4.177244 2.705145 -2.032809
H 4.092977 2.579075 -3.106875
C 7.858831 2.398279 1.070524
H 8.912349 2.154835 1.024686
O 4.794838 -3.649161 6.595991
C 4.177178 -2.693374 6.092451
C 3.910040 -1.343737 6.774835
H 4.838604 -0.912349 7.166239
H 3.235734 -1.485837 7.629164
C 3.621560 -2.612724 4.675906
C 2.406040 -1.620461 4.882932
C 4.422484 -0.260166 4.599501
H 5.314609 0.126874 5.108551
H 4.148166 0.478312 3.842830
C 4.673412 -1.667620 3.962944

H	4.474247 -1.663451 2.886404	C	0.716947 3.489063 -0.853584
H	5.696798 -2.032603 4.104755	C	1.510764 2.940055 -1.849878
C	3.277007 -0.533101 5.616471	C	2.832293 2.767052 -1.237007
H	2.727759 0.357149 5.936059	C	5.292905 2.172832 -1.457581
C	1.283467 -2.218464 5.758244	C	6.403603 1.816336 -2.324416
H	0.742078 -2.993221 5.205843	C	7.562707 1.939103 -1.565455
H	0.555518 -1.429605 5.996826	C	7.120382 2.408316 -0.245764
H	1.644381 -2.682975 6.684756	C	7.420140 3.023903 2.162190
C	1.766029 -1.126129 3.575186	C	8.288019 3.202178 3.317249
H	1.207586 -1.932504 3.087571	C	7.478740 3.591736 4.368286
H	2.478439 -0.752564 2.840670	C	6.117568 3.627956 3.844965
H	1.055807 -0.318596 3.792693	C	4.975069 3.964840 4.570613
C	3.384384 -3.951016 3.994534	H	5.121237 4.223503 5.614315
H	4.292556 -4.562005 4.025349	C	1.123152 3.884299 1.614533
H	3.094346 -3.813974 2.947545	H	0.065229 4.074486 1.746265
H	2.593712 -4.521913 4.495827	C	3.916209 2.016966 -1.764171
h	4.799306 6.442833 1.339809	H	3.710103 1.504839 -2.698327
h	2.526100 4.625211 5.995738	C	7.874223 2.667108 0.884521
h	0.394577 4.072947 4.398653	H	8.948314 2.587678 0.802494
h	-0.254275 3.534283 -0.798708	O	4.764105 -3.734249 6.572512
h	1.444732 2.894716 -2.959473	C	4.395926 -2.824997 5.806921
h	6.516052 1.760935 -3.345781	C	4.552753 -1.323544 6.070624
h	8.508717 1.133041 -1.613700	H	5.594791 -1.079637 6.299855
h	9.361383 2.879617 3.454615	H	3.951436 -1.029652 6.940168
h	7.844122 3.996483 5.436899	C	3.763091 -2.988687 4.427683
		C	2.863579 -1.684077 4.364378
TS4c		C	5.129832 -1.057860 3.666954
Total QM energy at B2: -3268.126371 (a.u.)		H	6.134028 -0.807490 4.029782
Total QM/MM energy at B2: -3409.551405 (a.u.)		H	4.971618 -0.489922 2.747642
S	5.068970 5.389432 0.415658	C	4.948800 -2.596402 3.458009
O	4.113341 1.363939 1.615686	H	4.658208 -2.835512 2.429363
H	3.155788 1.269239 1.811032	H	5.853950 -3.173279 3.678219
O	3.536524 0.493680 -0.324238	C	4.051656 -0.719341 4.737835
H	4.387699 -0.018058 -0.204228	H	3.788129 0.340337 4.790468
Fe	4.497319 3.202328 1.252896	C	1.713515 -1.699978 5.401608
N	3.279214 3.759234 2.797638	H	0.901481 -2.349916 5.054105
N	2.867102 3.227287 0.041452	H	1.306766 -0.687605 5.526684
N	5.727241 2.571770 -0.234844	H	2.030752 -2.070893 6.384684
N	6.104948 3.268210 2.498932	C	2.249141 -1.397542 2.982291
C	3.658563 3.995752 4.118688	H	1.574708 -2.204341 2.675782
C	2.487020 4.257996 4.944781	H	2.991501 -1.267762 2.192613
C	1.390115 4.157048 4.113277	H	1.651157 -0.476840 3.029525
C	1.902831 3.900037 2.779081	C	3.130963 -4.347098 4.164893
C	1.557799 3.616548 0.331119	H	3.855703 -5.148574 4.345059

H 2.785754 -4.426654 3.128299
H 2.275862 -4.527628 4.828005
h 4.729582 6.343711 1.352948
h 2.501050 4.529525 6.000310
h 0.333496 4.182056 4.379727
h -0.323648 3.813155 -0.867482
h 1.307994 2.671274 -2.886559
h 6.289241 1.577257 -3.381690
h 8.552010 1.688230 -1.948090
h 9.354705 2.978080 3.312055
h 7.795881 3.838440 5.381511

IC4c

Total QM energy at B2: -3268.115012 (a.u.)

Total QM/MM energy at B2: -3409.542687 (a.u.)

S 5.055332 5.409660 0.415692
O 4.209679 1.388321 1.555618
H 3.496188 1.269405 2.214440
O 3.724791 0.567597 -0.965351
H 3.933604 0.746183 0.014234
Fe 4.559604 3.209612 1.258501
N 3.332679 3.751145 2.797708
N 2.935057 3.218318 0.013568
N 5.779247 2.583866 -0.258584
N 6.157772 3.322258 2.488710
C 3.700977 3.978704 4.129380
C 2.522865 4.229350 4.943557
C 1.434877 4.135140 4.094089
C 1.968280 3.890533 2.768449
C 1.619297 3.659601 0.309114
C 0.789307 3.559571 -0.894869
C 1.577401 2.988106 -1.876936
C 2.885804 2.761985 -1.239369
C 5.373920 2.206412 -1.467587
C 6.488474 1.943173 -2.370754
C 7.646621 2.069734 -1.622144
C 7.203092 2.486368 -0.273815
C 7.463399 3.080510 2.152023
C 8.330648 3.227914 3.305716
C 7.520248 3.599244 4.369522
C 6.165568 3.648398 3.849577
C 5.015820 3.952372 4.577618
H 5.157868 4.191375 5.627237
C 1.191631 3.906469 1.579415
H 0.138623 4.126050 1.712086
C 3.951229 1.819101 -1.704157
H 3.809912 1.567137 -2.754698
C 7.930479 2.747879 0.849458
H 9.007843 2.695458 0.774557
O 4.733444 -3.793708 6.647042
C 4.294621 -2.863390 5.947438
C 4.325500 -1.378114 6.325703
H 5.325989 -1.079856 6.655422
H 3.639833 -1.191620 7.162004
C 3.724891 -2.972408 4.537639
C 2.760700 -1.717511 4.500335
C 5.027740 -0.930231 3.984236
H 5.993183 -0.659955 4.429657
H 4.909528 -0.315414 3.087982
C 4.938099 -2.459173 3.663639
H 4.710867 -2.641589 2.608860
H 5.858500 -3.005534 3.897725
C 3.868784 -0.716692 5.004370
H 3.538994 0.320900 5.111899
C 1.556894 -1.859329 5.463230
H 0.793097 -2.508543 5.020411
H 1.101266 -0.875242 5.639171
H 1.833827 -2.299434 6.430244
C 2.216252 -1.373106 3.102002
H 1.581415 -2.177235 2.715254
H 3.000756 -1.196544 2.363789
H 1.595606 -0.467972 3.159360
C 3.186796 -4.342598 4.154483
H 3.945060 -5.113820 4.328625
H 2.905293 -4.372379 3.096548
H 2.307376 -4.610710 4.753267
h 4.729686 6.361101 1.360711
h 2.523929 4.496627 6.000264
h 0.374701 4.160895 4.345942
h -0.246664 3.897852 -0.914782
h 1.384517 2.712585 -2.913734
h 6.333189 1.698320 -3.421468
h 8.640935 1.849061 -2.010356
h 9.394067 2.988755 3.302816
h 7.838288 3.835681 5.384911

TS4d

Total QM energy at B2: -3268.115012 (a.u.)

Total QM/MM energy at B2: -3409.542687 (a.u.)

S	5.121116	5.439360	0.396138
O	4.503952	1.466230	1.797698
H	4.078325	1.381669	2.666235
O	3.378554	-0.279970	1.317744
H	4.110598	-0.430588	0.653792
Fe	4.664134	3.234904	1.237005
N	3.423198	3.756842	2.779499
N	3.078928	3.165971	-0.039650
N	5.873044	2.606153	-0.247291
N	6.220382	3.382941	2.524618
C	3.757968	4.095649	4.082449
C	2.557938	4.268192	4.892175
C	1.485676	4.009492	4.063842
C	2.035884	3.731350	2.745475
C	1.753677	3.364135	0.283009
C	0.910568	3.321574	-0.911950
C	1.746407	3.062976	-1.983895
C	3.104068	2.974182	-1.412603
C	5.550017	2.450473	-1.571088
C	6.685787	1.924481	-2.327108
C	7.704655	1.696441	-1.419874
C	7.202183	2.195788	-0.127205
C	7.506626	2.984207	2.245161
C	8.366805	3.177889	3.406590
C	7.574328	3.703749	4.408436
C	6.228327	3.810269	3.855251
C	5.076276	4.173595	4.546674
H	5.198351	4.491305	5.576960
C	1.286956	3.564030	1.583619
H	0.211869	3.631212	1.703272
C	4.276191	2.678680	-2.104466
H	4.195077	2.544561	-3.178372
C	7.934540	2.432901	1.026489
H	8.994652	2.217855	0.985799
O	4.911397	-3.773342	6.610264
C	4.438196	-2.896857	5.863943
C	4.737063	-1.393975	5.944144
H	5.805237	-1.205277	5.788052
H	4.478784	-1.014563	6.941643
C	3.465866	-3.109378	4.715108
C	2.602951	-1.784355	4.843491
C	4.532915	-1.237391	3.453426
H	5.592517	-0.950299	3.449936
H	4.018173	-0.781152	2.519502
C	4.351903	-2.792450	3.444237
H	3.814706	-3.136989	2.550986
H	5.297139	-3.347817	3.479413
C	3.856344	-0.836998	4.795822
H	3.617856	0.228245	4.897842
C	1.810778	-1.709032	6.167589
H	1.012568	-2.465339	6.163022
H	1.351976	-0.714274	6.255897
H	2.430344	-1.884278	7.054637
C	1.609199	-1.550027	3.695979
H	0.720999	-2.173635	3.835141
H	2.022490	-1.755065	2.709164
H	1.281357	-0.502341	3.696149
C	2.763283	-4.458100	4.691800
H	3.495797	-5.273277	4.698131
H	2.151380	-4.558178	3.788471
H	2.113741	-4.596776	5.564726
h	4.788205	6.383225	1.346209
h	2.537056	4.552236	5.944292
h	0.428200	3.969652	4.325040
h	-0.157467	3.536805	-0.879635
h	1.547506	2.919660	-3.045952
h	6.638538	1.763075	-3.404039
h	8.640304	1.192776	-1.662668
h	9.414826	2.879701	3.434911
h	7.879934	3.965590	5.421408

IC4d

Total QM energy at B2: -3268.167873 (a.u.)

Total QM/MM energy at B2: -3409.596589 (a.u.)

S	5.127574	5.477477	0.381258
O	4.441541	1.485107	1.752718
H	4.435304	1.435200	2.731457
O	2.322873	-0.049373	1.439674
H	3.046006	0.624556	1.303337
Fe	4.680428	3.253683	1.250888
N	3.466813	3.805450	2.787843
N	3.090216	3.182515	-0.028960
N	5.873533	2.626939	-0.248552
N	6.249059	3.379875	2.528714
C	3.810469	4.145542	4.089903
C	2.614061	4.314651	4.906011
C	1.538946	4.049058	4.083718
C	2.081635	3.768537	2.762701

C	1.768243	3.375000 0.305663
C	0.912722	3.329340 -0.882728
C	1.738635	3.079338 -1.962427
C	3.103923	2.999300 -1.403723
C	5.547708	2.480148 -1.570958
C	6.664465	1.909961 -2.323628
C	7.664665	1.629594 -1.410019
C	7.185097	2.160566 -0.121602
C	7.528438	2.963248 2.241250
C	8.401679	3.163019 3.390917
C	7.622617	3.706368 4.395798
C	6.275072	3.824750 3.852185
C	5.129992	4.210221 4.547605
H	5.261793	4.531032 5.575946
C	1.319193	3.582885 1.610235
H	0.245467	3.641384 1.745204
C	4.273765	2.721144 -2.103583
H	4.190803	2.594865 -3.178317
C	7.931290	2.383510 1.025421
H	8.983859	2.132885 0.979409
O	5.003983	-3.953401 6.500496
C	4.490436	-3.131705 5.722973
C	4.849235	-1.640512 5.635337
H	5.886065	-1.507495 5.306111
H	4.751912	-1.166199 6.620142
C	3.362174	-3.397675 4.730539
C	2.552470	-2.037544 4.900627
C	4.261182	-1.701690 3.260091
H	4.850735	-1.178621 2.516207
H	2.747447	-0.788123 1.920334
C	4.039569	-3.192814 3.314096
H	3.369443	-3.560416 2.522276
H	4.966875	-3.775664 3.218666
C	3.809074	-1.132711 4.582116
H	3.627567	-0.055677 4.610227
C	1.989219	-1.833750 6.321593
H	1.206836	-2.583594 6.507237
H	1.549770	-0.828881 6.392581
H	2.734288	-1.936620 7.116989
C	1.395056	-1.858144 3.904703
H	0.485439	-2.324405 4.299673
H	1.587317	-2.301381 2.924879
H	1.186990	-0.796265 3.737408
C	2.629034	-4.717358 4.901253
H	3.333732	-5.556161 4.896110
H	1.915195	-4.865504 4.084202
H	2.077360	-4.758835 5.847098
h	4.799132	6.423124 1.331113
h	2.597053	4.592830 5.959763
h	0.482119	4.003635 4.346625
h	-0.156429	3.536140 -0.835652
h	1.533078	2.934077 -3.022952
h	6.620955	1.755825 -3.401782
h	8.565678	1.061547 -1.641458
h	9.450923	2.868395 3.409619
h	7.933099	3.965903 5.407880

RC5

Total QM energy at B2: -3229.806844 (a.u.)

Total QM/MM energy at B2: -3341.002776 (a.u.)

S	2.816907	5.823075 0.327302
O	2.872916	1.930912 2.016038
Fe	2.818251	3.488341 1.452523
N	1.648861	4.114194 2.985572
N	1.154810	3.156241 0.317772
N	3.986617	3.069254 -0.144289
N	4.454968	4.003616 2.534452
C	2.048585	4.395301 4.284092
C	0.889460	4.625930 5.133750
C	-0.222300	4.509919 4.327608
C	0.263738	4.186009 2.994776
C	-0.152940	3.440534 0.649038
C	-1.060349	3.048098 -0.429792
C	-0.289746	2.453998 -1.411826
C	1.101823	2.549121 -0.926404
C	3.574801	2.437446 -1.292133
C	4.703457	2.198851 -2.184367
C	5.819309	2.752438 -1.585161
C	5.368443	3.230111 -0.267145
C	5.764101	3.902783 2.118136
C	6.676295	4.119721 3.236394
C	5.895619	4.346817 4.350483
C	4.509354	4.279161 3.899942
C	3.381734	4.457885 4.692023
H	3.553186	4.681261 5.739470
C	-0.546942	3.926254 1.894012
H	-1.608696	4.066762 2.056736
C	2.245069	2.152992 -1.614011

H	2.096980 1.626236 -2.549725	S	2.771436 5.763107 0.377579
C	6.163706 3.586982 0.814401	O	2.404519 1.822432 2.076905
H	7.236574 3.518446 0.682737	Fe	2.665921 3.433222 1.504045
C	1.549241 -1.623589 5.477622	N	1.500780 4.110427 3.019928
C	2.921320 -2.290017 5.566605	N	1.001430 3.155099 0.344997
O	3.390640 -2.918873 6.532703	N	3.851404 2.943077 -0.058925
C	3.650115 -1.995069 4.250137	N	4.313619 3.847788 2.609892
H	3.870921 -2.921766 3.706235	C	1.903131 4.401385 4.316694
H	4.609322 -1.504349 4.453652	C	0.742418 4.661020 5.159542
C	1.958549 -0.294313 4.708620	C	-0.367770 4.536713 4.353595
C	2.631755 -1.069162 3.512811	C	0.119397 4.192374 3.024140
H	3.056166 -0.429288 2.738484	C	-0.305739 3.439654 0.678639
C	1.496331 -1.977182 3.058898	C	-1.213930 3.044720 -0.402022
C	1.155640 -2.285229 1.804699	C	-0.443515 2.452855 -1.383838
H	1.685706 -1.871608 0.951150	C	0.949535 2.543571 -0.894667
H	0.332200 -2.955681 1.574402	C	3.425711 2.358025 -1.231268
C	0.800330 -2.430036 4.346883	C	4.552448 2.115035 -2.124956
H	-0.263274 -2.162795 4.354008	C	5.679848 2.625872 -1.507877
H	0.858527 -3.514002 4.513038	C	5.236548 3.079819 -0.181643
C	2.931897 0.595994 5.507510	C	5.630921 3.737514 2.203193
H	3.275969 1.420690 4.874865	C	6.535807 3.986046 3.318919
H	3.813117 0.058941 5.875406	C	5.748699 4.264304 4.417502
H	2.423841 1.024258 6.380059	C	4.363819 4.186277 3.960719
C	0.764920 0.570913 4.270792	C	3.232247 4.431161 4.734087
H	0.313338 1.075286 5.133671	H	3.402282 4.691292 5.773689
H	-0.011205 -0.002883 3.756628	C	-0.693571 3.925488 1.923601
H	1.123514 1.334474 3.573805	H	-1.754578 4.061485 2.090489
C	0.775039 -1.491032 6.776898	C	2.091800 2.125952 -1.573084
H	0.347815 -2.456584 7.069151	H	1.940410 1.618530 -2.519328
H	-0.054134 -0.783584 6.661950	C	6.035641 3.414519 0.905609
H	1.414372 -1.144372 7.596219	H	7.108546 3.339583 0.777013
h	2.522994 6.773311 1.283865	C	2.054393 -1.643843 5.123689
h	0.905675 4.827031 6.204900	C	3.355772 -2.169089 5.720091
h	-1.276215 4.595425 4.592218	O	3.515920 -3.202230 6.398611
h	-2.129162 3.259947 -0.401076	C	4.429950 -1.105559 5.484160
h	-0.548363 1.988769 -2.363007	H	5.204343 -1.466207 4.797204
h	4.577957 1.712489 -3.151718	H	4.924454 -0.871398 6.432822
h	6.796058 2.830641 -2.062563	C	2.191391 -0.122245 5.601253
h	7.762056 4.065368 3.157431	C	3.593030 0.069931 4.889600
h	6.229625 4.522466 5.373056	H	4.047886 1.056753 4.997071
		C	3.275150 -0.329498 3.463646
TS5		C	3.679614 0.319715 2.332360
Total QM energy at B2: -3229.776096 (a.u.)		H	4.494705 1.033764 2.378645
Total QM/MM energy at B2: -3340.972264 (a.u.)		H	3.456203 -0.080096 1.348764

C 2.298903 -1.499157 3.571478
H 1.346492 -1.283134 3.069716
H 2.682311 -2.431278 3.133439
C 2.236016 0.042206 7.136477
H 2.570224 1.053180 7.399241
H 2.896310 -0.669054 7.643501
H 1.232249 -0.085169 7.559566
C 1.086399 0.788126 5.043128
H 0.107907 0.476519 5.428658
H 1.060583 0.813567 3.951980
H 1.254307 1.818011 5.372980
C 0.804673 -2.417984 5.511185
H 0.892023 -3.472670 5.224930
H -0.079257 -2.000657 5.016803
H 0.636066 -2.384621 6.593025
h 2.472539 6.726278 1.319550
h 0.762691 4.876537 6.227816
h -1.421323 4.631530 4.616468
h -2.284107 3.249680 -0.374106
h -0.699686 1.988456 -2.336086
h 4.422143 1.658136 -3.105941
h 6.659235 2.696236 -1.981076
h 7.621633 3.926711 3.244576
h 6.082750 4.481954 5.431950

IC5

Total QM energy at B2: -3229.800346 (a.u.)

Total QM/MM energy at B2: -3340.997565 (a.u.)

S 2.836558 5.660794 0.428364
O 2.509937 1.693385 2.281394
Fe 2.717775 3.428081 1.541041
N 1.543047 4.054695 3.062342
N 1.051416 3.076186 0.412126
N 3.904377 2.849628 0.000777
N 4.368039 3.820461 2.639334
C 1.950340 4.358535 4.353725
C 0.790757 4.635473 5.196077
C -0.320709 4.514881 4.392462
C 0.164357 4.150116 3.066806
C -0.257323 3.383067 0.731324
C -1.159561 3.003164 -0.357412
C -0.388839 2.397728 -1.331615
C 1.000723 2.463909 -0.828966
C 3.474510 2.252959 -1.165579
C 4.597594 2.011101 -2.064950
C 5.724097 2.541109 -1.462388
C 5.286591 3.006475 -0.137777
C 5.685846 3.717757 2.229002
C 6.588280 3.984773 3.341359
C 5.798768 4.259246 4.440244
C 4.413826 4.164479 3.987245
C 3.280496 4.398562 4.765297
H 3.452496 4.665787 5.802827
C -0.650102 3.884622 1.967264
H -1.710142 4.040213 2.126042
C 2.139463 2.028158 -1.503852
H 1.982660 1.515080 -2.446265
C 6.089385 3.380417 0.935016
H 7.162630 3.319908 0.801648
C 2.064235 -1.613453 5.012213
C 3.397278 -2.091369 5.579907
O 3.608759 -3.123470 6.244211
C 4.417325 -0.974319 5.348820
H 5.194263 -1.282763 4.639384
H 4.921499 -0.741059 6.291968
C 2.133763 -0.104255 5.542531
C 3.511128 0.186968 4.805908
H 3.920258 1.189488 4.938150
C 3.199452 -0.199137 3.385727
C 3.502361 0.629353 2.189773
H 4.522360 1.036562 2.234011
H 3.390520 0.068511 1.252138
C 2.281065 -1.399828 3.463206
H 1.316032 -1.202319 2.974027
H 2.690002 -2.299712 2.978217
C 2.212714 0.013901 7.080822
H 2.484563 1.037486 7.362100
H 2.933926 -0.662762 7.550307
H 1.231860 -0.193546 7.525178
C 0.968569 0.765557 5.047581
H 0.022652 0.395560 5.460673
H 0.905468 0.820305 3.959575
H 1.100795 1.793958 5.396923
C 0.859041 -2.461282 5.385303
H 0.993846 -3.499181 5.059072
H -0.051199 -2.070028 4.918545
H 0.704548 -2.475512 6.469444
h 2.507613 6.638915 1.344563

h 0.811505 4.857529 6.263001
h -1.374227 4.620740 4.651230
h -2.225981 3.227953 -0.340545
h -0.645582 1.941686 -2.287741
h 4.463504 1.549208 -3.043082
h 6.697672 2.618404 -1.946375
h 7.674735 3.942141 3.264773
h 6.131068 4.483907 5.453738

PC5

Total QM energy at B2: -3229.850203 (a.u.)

Total QM/MM energy at B2: -3341.048807 (a.u.)

S 2.721482 5.819433 0.349995
O 2.316396 0.865353 2.505375
Fe 2.698631 3.768366 1.427135
N 1.551933 4.145032 3.028036
N 1.066768 3.170250 0.385949
N 3.870095 3.037624 -0.052187
N 4.325328 3.978544 2.593942
C 1.949565 4.426000 4.337918
C 0.786683 4.663544 5.178527
C -0.322128 4.546846 4.369333
C 0.164201 4.224336 3.036334
C -0.248663 3.473252 0.708375
C -1.152026 3.068005 -0.367573
C -0.385077 2.447015 -1.334969
C 1.004914 2.538871 -0.851322
C 3.457396 2.376509 -1.200362
C 4.590812 2.106530 -2.073899
C 5.702262 2.692139 -1.496412
C 5.252021 3.210441 -0.194578
C 5.647703 3.912225 2.165394
C 6.555519 4.135242 3.282068
C 5.776347 4.353180 4.400570
C 4.390607 4.271192 3.962111
C 3.271796 4.474833 4.758627
H 3.444234 4.714467 5.802081
C -0.649902 3.969747 1.939698
H -1.710937 4.106543 2.102973
C 2.136605 2.109395 -1.534573
H 1.984022 1.560352 -2.457038
C 6.053790 3.615451 0.865874
H 7.126919 3.577468 0.728300
C 1.957861 -1.654946 5.102616
C 3.335946 -2.095072 5.584324
O 3.614729 -3.103615 6.258490
C 4.311776 -0.968864 5.225164
H 5.008502 -1.288615 4.439108
H 4.917943 -0.713089 6.098063
C 2.037707 -0.131162 5.590151
C 3.347220 0.164568 4.760842
H 3.745527 1.177824 4.838653
C 2.906038 -0.216850 3.353286
C 3.600029 0.199888 2.115200
H 4.470153 0.847321 2.174316
H 3.519705 -0.388045 1.206333
C 2.076693 -1.498125 3.534675
H 1.084672 -1.374674 3.090313
H 2.537834 -2.378449 3.070784
C 2.230847 0.022910 7.115467
H 2.486879 1.060925 7.357274
H 3.014885 -0.616019 7.533849
H 1.299253 -0.212816 7.642722
C 0.816754 0.705674 5.171453
H -0.051510 0.429086 5.781412
H 0.557088 0.599762 4.117133
H 1.014849 1.768865 5.341903
C 0.789562 -2.504923 5.575091
H 0.936026 -3.558537 5.310265
H -0.146908 -2.164230 5.120487
H 0.674687 -2.450857 6.662649
h 2.466075 6.766398 1.320753
h 0.802896 4.873762 6.247925
h -1.376078 4.631720 4.634005
h -2.220224 3.284050 -0.349014
h -0.647197 1.964252 -2.276403
h 4.474500 1.573964 -3.017780
h 6.673936 2.763327 -1.985133
h 7.641859 4.101999 3.199444
h 6.118201 4.539688 5.418616

RC5'

Total QM energy at B2: -3229.797041 (a.u.)

Total QM/MM energy at B2: -3340.786610 (a.u.)

S 2.747636 5.556518 0.308459
O 2.667300 1.638907 2.021980
Fe 2.665574 3.186757 1.433700
N 1.462920 3.875165 2.901637

N	1.041760 2.898145 0.232523	H	1.914052 0.759607 6.689906
N	3.882686 2.747424 -0.130391	H	2.820615 1.230846 5.239714
N	4.272418 3.718519 2.546285	H	3.337288 -0.163643 6.205147
C	1.826927 4.180385 4.209079	C	0.344412 0.375706 4.508084
C	0.642265 4.452260 5.011816	H	-0.390161 -0.177515 3.916502
C	-0.443412 4.338567 4.172840	H	0.718818 1.193436 3.883834
C	0.080027 3.970393 2.864843	H	-0.163843 0.810903 5.376828
C	-0.272383 3.214462 0.516273	C	0.325629 -1.812334 6.951488
C	-1.146348 2.861497 -0.602422	H	0.910613 -1.365315 7.762890
C	-0.355046 2.257552 -1.560833	H	0.045394 -2.824255 7.265429
C	1.018202 2.302783 -1.018338	H	-0.591677 -1.226620 6.823269
C	3.493690 2.128024 -1.297283	h	2.417882 6.536851 1.221998
C	4.646217 1.873904 -2.152255	h	0.631776 4.675646 6.078613
C	5.756561 2.398508 -1.508626	h	-1.503520 4.456885 4.396980
C	5.266480 2.884324 -0.208623	h	-2.208628 3.105534 -0.610971
C	5.596152 3.616579 2.162988	h	-0.588082 1.819400 -2.531288
C	6.478808 3.894053 3.290874	h	4.549685 1.392518 -3.125402
C	5.669434 4.154761 4.375506	h	6.755120 2.430815 -1.944404
C	4.293650 4.045818 3.898054	h	7.566750 3.872395 3.227782
C	3.144000 4.244157 4.656181	h	5.986655 4.401327 5.388740
H	3.287265 4.498852 5.700675		
C	-0.699860 3.709588 1.743189	**TS5'**	
H	-1.762551 3.875073 1.868555	Total QM energy at B2: -3229.764484 (a.u.)	
C	2.172718 1.879962 -1.668836	Total QM/MM energy at B2: -3340.752160 (a.u.)	
H	2.044466 1.357838 -2.610333	S	2.658975 5.390436 0.377405
C	6.032962 3.262402 0.888513	O	2.018884 1.549139 2.304236
H	7.108043 3.187879 0.791441	Fe	2.312924 2.984247 1.542512
C	1.117522 -1.861789 5.655473	N	1.157591 3.874185 2.943466
C	2.498327 -2.502691 5.753972	N	0.727618 2.807794 0.289478
O	2.950031 -3.154073 6.713503	N	3.551152 2.415125 0.031105
C	3.263330 -2.141675 4.478556	N	3.954129 3.444119 2.685171
H	3.523120 -3.042906 3.909999	C	1.526422 4.248579 4.231540
H	4.200886 -1.635703 4.733500	C	0.342761 4.581392 5.014506
C	1.530549 -0.493824 4.951629	C	-0.743702 4.420770 4.185843
C	2.249382 -1.210351 3.745681	C	-0.223045 3.977913 2.898901
H	2.680393 -0.536474 3.003622	C	-0.579766 3.157088 0.568450
C	1.152051 -2.132343 3.227654	C	-1.451734 2.844702 -0.564465
C	0.899572 -2.444251 1.953201	C	-0.665759 2.247388 -1.531372
H	1.473250 -2.008449 1.139048	C	0.699689 2.235507 -0.972755
H	0.108605 -3.135154 1.671880	C	3.161656 1.909732 -1.195575
C	0.408407 -2.626245 4.473417	C	4.320116 1.649180 -2.039290
H	-0.653419 -2.352181 4.454273	C	5.439995 2.049965 -1.329037
H	0.454888 -3.715674 4.601515	C	4.946488 2.464573 -0.009436
C	2.463283 0.374570 5.821813	C	5.274046 3.187057 2.358190

C	6.152527	3.489752 3.481835
C	5.350114	3.951974 4.502374
C	3.979500	3.915823 3.995902
C	2.837509	4.281316 4.697998
H	2.981374	4.628787 5.715555
C	-1.002474	3.670953 1.789739
H	-2.064378	3.838582 1.912404
C	1.842775	1.773644 -1.616120
H	1.711088	1.309596 -2.587006
C	5.712500	2.742831 1.116160
H	6.776926	2.555474 1.049699
C	1.146321	-1.688698 5.411503
C	2.507031	-2.296330 5.734809
O	2.749011	-3.197684 6.562004
C	3.563465	-1.468696 5.001811
H	4.085466	-2.068279 4.246374
H	4.314761	-1.122649 5.721574
C	1.574669	-0.150046 5.485676
C	2.711684	-0.314711 4.396431
H	3.266941	0.590066 4.156522
C	1.937476	-0.900523 3.223041
C	2.133577	-0.679897 1.915064
H	2.967235	-0.121581 1.519171
H	1.490610	-1.147900 1.169515
C	0.910972	-1.851468 3.859657
H	-0.125345	-1.574855 3.624986
H	1.041062	-2.893275 3.536858
C	2.092373	0.287572 6.874655
H	1.255227	0.390271 7.575813
H	2.573665	1.269984 6.795234
H	2.813964	-0.402312 7.325340
C	0.448199	0.806092 5.074862
H	0.070498	0.614080 4.069235
H	0.820339	1.832609 5.076844
H	-0.379233	0.746759 5.794298
C	0.009659	-2.178482 6.295602
H	0.239133	-2.022489 7.356009
H	-0.161580	-3.252374 6.152944
H	-0.920827	-1.648916 6.064379
h	2.349510	6.419136 1.243635
h	0.343015	4.822741 6.077435
h	-1.802978	4.547876 4.409101
h	-2.508667	3.110350 -0.584229
h	-0.895473	1.848244 -2.519289
h	4.228945	1.266214 -3.055701
h	6.449728	2.072262 -1.738925
h	7.234384	3.359683 3.454748
h	5.675872	4.274302 5.491340

IC5'

Total QM energy at B2: -3229.803359 (a.u.)

Total QM/MM energy at B2: -3340.787883 (a.u.)

S	2.731276	5.333887 0.394646
O	2.511913	1.427042 2.065902
Fe	2.611068	3.162793 1.490665
N	1.417529	3.796226 2.975415
N	0.976589	2.819763 0.307313
N	3.827816	2.638547 -0.059676
N	4.217573	3.585002 2.621380
C	1.789796	4.101337 4.281798
C	0.604226	4.379388 5.079207
C	-0.482559	4.272671 4.239645
C	0.033400	3.903917 2.929580
C	-0.330250	3.163367 0.591509
C	-1.203112	2.829635 -0.533694
C	-0.417021	2.219050 -1.493654
C	0.956214	2.235947 -0.948780
C	3.417818	2.026253 -1.229465
C	4.568797	1.760117 -2.082158
C	5.688410	2.269463 -1.440625
C	5.212081	2.767753 -0.140724
C	5.545485	3.511496 2.214923
C	6.424755	3.819146 3.332983
C	5.620055	4.085233 4.422984
C	4.241705	3.950992 3.969239
C	3.103116	4.165124 4.735042
H	3.252024	4.437321 5.773671
C	-0.756459	3.662607 1.814354
H	-1.815921	3.841769 1.942374
C	2.100036	1.802569 -1.609406
H	1.963737	1.290063 -2.554853
C	5.987069	3.162927 0.943882
H	7.061615	3.103619 0.844953
C	1.676684	-1.988111 4.891340
C	2.685281	-1.873831 6.032257
O	3.110624	-2.807565 6.738951
C	3.092546	-0.403418 6.152358
H	4.175637	-0.291671 6.036008

H 2.824399 -0.012416 7.142059
C 0.928594 -0.591952 5.037525
C 2.273290 0.243631 4.990579
H 2.161153 1.325646 5.058148
C 2.909737 -0.266497 3.712984
C 3.539815 0.569601 2.661613
H 4.331912 1.209773 3.075677
H 3.977510 -0.042749 1.861648
C 2.550387 -1.733484 3.600853
H 1.950765 -1.953745 2.703865
H 3.423011 -2.405251 3.567411
C 0.137319 -0.471224 6.355057
H -0.750471 -1.114832 6.322287
H -0.220131 0.554579 6.494911
H 0.711258 -0.753637 7.244428
C -0.012549 -0.255814 3.869251
H 0.491490 -0.240379 2.900950
H -0.427857 0.748256 4.017785
H -0.850950 -0.962855 3.829828
C 0.862830 -3.271729 4.883379
H 0.252001 -3.362643 5.788828
H 1.519581 -4.148312 4.843172
H 0.195137 -3.304260 4.015439
h 2.412176 6.344440 1.278559
h 0.595910 4.616607 6.143033
h -1.540843 4.409230 4.462025
h -2.261368 3.090425 -0.545843
h -0.655186 1.791781 -2.467710
h 4.467444 1.277310 -3.054110
h 6.686616 2.274495 -1.878376
h 7.512538 3.812241 3.264072
h 5.947741 4.349380 5.428427

PC5'

Total QM energy at B2: -3229.851118 (a.u.)

Total QM/MM energy at B2: -3340.837630 (a.u.)

S 2.704537 5.556498 0.263207
O 2.984929 0.278682 2.417091
Fe 2.688480 3.502023 1.306121
N 1.505147 3.831961 2.892057
N 1.079422 2.907184 0.228032
N 3.896671 2.803182 -0.160945
N 4.286868 3.737531 2.503253
C 1.873267 4.105194 4.213555
C 0.689915 4.336112 5.029336
C -0.399392 4.240769 4.191146
C 0.116552 3.923264 2.868067
C -0.240684 3.226225 0.514825
C -1.115179 2.873553 -0.602332
C -0.326422 2.269357 -1.563954
C 1.048049 2.315486 -1.030546
C 3.508831 2.145847 -1.316757
C 4.662374 1.880298 -2.166554
C 5.766239 2.451875 -1.554267
C 5.278953 2.975026 -0.265713
C 5.614602 3.715385 2.090407
C 6.501795 3.986616 3.213008
C 5.703129 4.173436 4.323343
C 4.325006 4.033444 3.871122
C 3.188326 4.183198 4.655621
H 3.340383 4.415344 5.704053
C -0.671305 3.700987 1.745784
H -1.733800 3.863271 1.877535
C 2.195076 1.890373 -1.689181
H 2.064102 1.361738 -2.626958
C 6.050063 3.409411 0.804838
H 7.125253 3.394888 0.690151
C 1.736409 -2.171243 4.871780
C 2.606102 -1.938670 6.101557
O 3.021477 -2.813463 6.882600
C 2.930142 -0.442674 6.163042
H 4.013608 -0.279005 6.148930
H 2.547797 -0.003735 7.091428
C 0.915259 -0.810696 4.836565
C 2.204740 0.090025 4.896717
H 2.039436 1.168077 4.874616
C 3.026829 -0.440838 3.721765
C 4.250949 0.218324 3.218694
H 4.560712 1.176246 3.624871
H 5.043670 -0.374907 2.770693
C 2.762356 -1.955349 3.690941
H 2.296742 -2.241913 2.742629
H 3.669561 -2.559336 3.813765
C -0.019619 -0.643204 6.051529
H -0.894405 -1.296621 5.954366
H -0.390064 0.386220 6.109165
H 0.455971 -0.878943 7.010197
C 0.093083 -0.602717 3.550867

H 0.693403 -0.647799 2.639907
H -0.372102 0.390088 3.575352
H -0.710725 -1.346352 3.481263
C 0.992353 -3.497303 4.849516
H 0.269159 -3.559387 5.671127
H 1.690459 -4.334274 4.965389
H 0.452490 -3.629953 3.905857
h 2.405605 6.505002 1.219934
h 0.683184 4.562048 6.095626
h -1.458182 4.363269 4.419235
h -2.177404 3.117887 -0.609044
h -0.564479 1.830499 -2.532870
h 4.570288 1.348769 -3.113689
h 6.758550 2.483220 -2.004161
h 7.588679 4.007498 3.133559
h 6.031086 4.397757 5.338326

PC5'

Total QM energy at B2: -3229.851118 (a.u.)

Total QM/MM energy at B2: -3340.837630 (a.u.)

S 2.704537 5.556498 0.263207
O 2.984929 0.278682 2.417091
Fe 2.688480 3.502023 1.306121
N 1.505147 3.831961 2.892057
N 1.079422 2.907184 0.228032
N 3.896671 2.803182 -0.160945
N 4.286868 3.737531 2.503253
C 1.873267 4.105194 4.213555
C 0.689915 4.336112 5.029336
C -0.399392 4.240769 4.191146
C 0.116552 3.923264 2.868067
C -0.240684 3.226225 0.514825
C -1.115179 2.873553 -0.602332
C -0.326422 2.269357 -1.563954
C 1.048049 2.315486 -1.030546
C 3.508831 2.145847 -1.316757
C 4.662374 1.880298 -2.166554
C 5.766239 2.451875 -1.554267
C 5.278953 2.975026 -0.265713
C 5.614602 3.715385 2.090407
C 6.501795 3.986616 3.213008
C 5.703129 4.173436 4.323343
C 4.325006 4.033444 3.871122
C 3.188326 4.183198 4.655621
H 3.340383 4.415344 5.704053
C -0.671305 3.700987 1.745784
H -1.733800 3.863271 1.877535
C 2.195076 1.890373 -1.689181
H 2.064102 1.361738 -2.626958
C 6.050063 3.409411 0.804838
H 7.125253 3.394888 0.690151
C 1.736409 -2.171243 4.871780
C 2.606102 -1.938670 6.101557
O 3.021477 -2.813463 6.882600
C 2.930142 -0.442674 6.163042
H 4.013608 -0.279005 6.148930
H 2.547797 -0.003735 7.091428
C 0.915259 -0.810696 4.836565
C 2.204740 0.090025 4.896717
H 2.039436 1.168077 4.874616
C 3.026829 -0.440838 3.721765
C 4.250949 0.218324 3.218694
H 4.560712 1.176246 3.624871
H 5.043670 -0.374907 2.770693
C 2.762356 -1.955349 3.690941
H 2.296742 -2.241913 2.742629
H 3.669561 -2.559336 3.813765
C -0.019619 -0.643204 6.051529
H -0.894405 -1.296621 5.954366
H -0.390064 0.386220 6.109165
H 0.455971 -0.878943 7.010197
C 0.093083 -0.602717 3.550867
H 0.693403 -0.647799 2.639907
H -0.372102 0.390088 3.575352
H -0.710725 -1.346352 3.481263
C 0.992353 -3.497303 4.849516
H 0.269159 -3.559387 5.671127
H 1.690459 -4.334274 4.965389
H 0.452490 -3.629953 3.905857
h 2.405605 6.505002 1.219934
h 0.683184 4.562048 6.095626
h -1.458182 4.363269 4.419235
h -2.177404 3.117887 -0.609044
h -0.564479 1.830499 -2.532870
h 4.570288 1.348769 -3.113689
h 6.758550 2.483220 -2.004161
h 7.588679 4.007498 3.133559
h 6.031086 4.397757 5.338326

RC5”

Total QM energy at B2: -3229.806779 (a.u.)

Total QM/MM energy at B2: -3341.221112 (a.u.)

S	2.897583	5.794005	0.260603
O	3.050755	1.923723	1.962853
Fe	2.989675	3.486413	1.421129
N	1.810194	4.100204	2.954484
N	1.340016	3.144791	0.280851
N	4.179738	3.081189	-0.171985
N	4.626176	3.989134	2.523750
C	2.201703	4.375576	4.259719
C	1.035065	4.568344	5.110583
C	-0.070158	4.447415	4.296330
C	0.426016	4.149675	2.960822
C	0.027799	3.419787	0.606861
C	-0.869917	3.034991	-0.483772
C	-0.090609	2.452040	-1.463673
C	1.298300	2.553796	-0.970185
C	3.774890	2.476231	-1.336638
C	4.912440	2.244407	-2.220019
C	6.030532	2.760666	-1.589461
C	5.566725	3.212607	-0.268516
C	5.940183	3.818083	2.137929
C	6.837853	3.996150	3.273059
C	6.045351	4.296024	4.362045
C	4.667178	4.277758	3.885317
C	3.530918	4.461410	4.668151
H	3.696363	4.684915	5.716269
C	-0.377543	3.891557	1.851701
H	-1.442051	4.021438	2.008385
C	2.447064	2.187069	-1.664793
H	2.305197	1.663337	-2.603870
C	6.353231	3.506108	0.838592
H	7.423560	3.386190	0.726662
C	1.655566	-1.623142	5.332913
C	3.033095	-2.281837	5.358500
O	3.511870	-2.982757	6.269280
C	3.753171	-1.868203	4.073344
H	3.986048	-2.736295	3.447485
H	4.703797	-1.380731	4.317231
C	2.048173	-0.232298	4.673622
C	2.722763	-0.900747	3.418269
H	3.137090	-0.196474	2.697308
C	1.599977	-1.787125	2.898667
C	1.282128	-2.023781	1.624936
H	1.822812	-1.563173	0.803896
H	0.480028	-2.699623	1.344235
C	0.907653	-2.342789	4.146832
H	-0.157704	-2.082801	4.179764
H	0.971834	-3.436000	4.227781
C	3.017186	0.601179	5.538265
H	3.884019	0.033956	5.896057
H	2.498528	0.992556	6.421526
H	3.385657	1.453334	4.957497
C	0.843327	0.649516	4.309588
H	0.391983	1.084873	5.209336
H	0.069516	0.105001	3.761417
H	1.185785	1.466032	3.667428
C	0.892058	-1.608234	6.642414
H	1.521500	-1.261246	7.470165
H	0.533833	-2.613655	6.891482
H	0.018244	-0.950245	6.574498
h	2.584006	6.768473	1.186036
h	1.041180	4.775543	6.180675
h	-1.126162	4.521651	4.555967
h	-1.937868	3.251961	-0.462070
h	-0.339184	1.998767	-2.423267
h	4.801899	1.762277	-3.191306
h	7.018807	2.823006	-2.044975
h	7.917203	3.850441	3.230165
h	6.369560	4.532600	5.375448

TS5”

Total QM energy at B2: -3229.770994 (a.u.)

Total QM/MM energy at B2: -3341.193491 (a.u.)

S	2.725870	5.627638	0.395654
O	3.027266	1.761276	2.034969
Fe	2.813350	3.376562	1.440589
N	1.657196	3.924843	3.004600
N	1.166789	3.018247	0.327265
N	3.997512	3.002345	-0.174315
N	4.465045	3.848827	2.541540
C	2.072971	4.212488	4.302866
C	0.913619	4.422777	5.159333
C	-0.202552	4.296014	4.360426
C	0.270688	3.980511	3.021560
C	-0.148619	3.297661	0.674704
C	-1.044778	2.959577	-0.426255

C	-0.271131	2.420950 -1.439534
C	1.120262	2.499876 -0.962566
C	3.575862	2.428030 -1.356697
C	4.711824	2.216478 -2.245687
C	5.833613	2.717966 -1.609343
C	5.380795	3.139612 -0.273258
C	5.778452	3.714839 2.122544
C	6.686043	3.911703 3.248071
C	5.906021	4.189988 4.350914
C	4.517949	4.137051 3.902327
C	3.399119	4.310452 4.705636
H	3.574845	4.545081 5.748926
C	-0.550874	3.739346 1.927055
H	-1.612637	3.872747 2.095258
C	2.254273	2.161890 -1.692790
H	2.098480	1.693040 -2.657648
C	6.184860	3.439145 0.820783
H	7.254503	3.338530 0.694705
C	1.052230	-0.970606 5.068510
C	0.710098	-2.382519 4.567678
O	-0.174415	-3.122388 5.012137
C	1.699317	-2.722660 3.443421
H	1.191822	-2.911847 2.491671
H	2.261508	-3.631494 3.685718
C	2.632999	-1.024136 4.942519
C	2.598758	-1.442986 3.420876
H	3.571067	-1.575655 2.944884
C	1.720097	-0.367128 2.819034
C	1.846050	0.222573 1.571237
H	2.543861	-0.177119 0.843649
H	1.039690	0.819909 1.170057
C	0.676720	-0.028158 3.868029
H	0.740981	1.024601 4.173303
H	-0.350522	-0.192239 3.516633
C	3.252737	-2.087140 5.871817
H	2.831298	-3.088351 5.742265
H	3.064491	-1.779793 6.909944
H	4.336222	-2.146439 5.699920
C	3.341572	0.318945 5.189665
H	3.163126	0.668454 6.214575
H	3.033738	1.100332 4.491686
H	4.424873	0.194175 5.063072
C	0.427693	-0.602651 6.403629
H	0.829643	-1.222117 7.214041
H	-0.654969	-0.765551 6.382690
H	0.605699	0.448064 6.652874
h	2.426488	6.596423 1.331695
h	0.935565	4.661196 6.222696
h	-1.254051	4.405374 4.625864
h	-2.111103	3.183400 -0.395919
h	-0.532730	2.008810 -2.414097
h	4.599416	1.754534 -3.226522
h	6.815324	2.789830 -2.077473
h	7.767807	3.792789 3.187135
h	6.242658	4.434465 5.358373

IC5”

Total QM energy at B2: -3229.794824 (a.u.)

Total QM/MM energy at B2: -3341.216883 (a.u.)

S	2.695953	5.616679 0.389935
O	2.881080	1.701884 2.008415
Fe	2.750182	3.423672 1.451201
N	1.594831	3.959695 3.013397
N	1.099263	3.047849 0.337784
N	3.935305	3.006331 -0.161452
N	4.394288	3.855520 2.555083
C	2.009386	4.266443 4.309103
C	0.849552	4.476699 5.163869
C	-0.266444	4.329720 4.369550
C	0.205711	4.005825 3.032962
C	-0.216221	3.309854 0.692649
C	-1.113744	2.972996 -0.405645
C	-0.339688	2.451265 -1.428209
C	1.051762	2.537903 -0.958007
C	3.507562	2.450036 -1.350534
C	4.643377	2.221687 -2.234090
C	5.773004	2.693200 -1.587418
C	5.321254	3.117979 -0.252942
C	5.709354	3.695137 2.142053
C	6.614817	3.892898 3.267449
C	5.835369	4.202862 4.362954
C	4.449669	4.165850 3.911471
C	3.333434	4.367011 4.712400
H	3.509202	4.620028 5.751221
C	-0.618129	3.747251 1.947035
H	-1.679965	3.866540 2.120957
C	2.183446	2.204220 -1.692404
H	2.024866	1.748679 -2.662767

C 6.122525 3.404273 0.846385
H 7.191031 3.285134 0.728538
C 1.091708 -0.927375 4.991165
C 0.834561 -2.355586 4.487512
O -0.037136 -3.129581 4.900613
C 1.893513 -2.665348 3.418229
H 1.439118 -2.885748 2.446231
H 2.475236 -3.550029 3.702502
C 2.678297 -0.920394 4.946585
C 2.735031 -1.345123 3.423874
H 3.737471 -1.438649 3.001337
C 1.853093 -0.298652 2.782587
C 2.144846 0.492726 1.569431
H 2.785383 -0.034788 0.853833
H 1.229723 0.805431 1.058190
C 0.737084 -0.005899 3.763350
H 0.717427 1.049356 4.070460
H -0.262857 -0.230580 3.361441
C 3.291977 -1.953905 5.912276
H 2.895035 -2.965763 5.787401
H 3.071701 -1.631921 6.939946
H 4.381163 -1.991222 5.770854
C 3.317936 0.449414 5.225349
H 3.082074 0.786152 6.242885
H 2.999154 1.217639 4.518711
H 4.410277 0.374218 5.142782
C 0.389219 -0.578729 6.292681
H 0.788928 -1.161560 7.131343
H -0.679472 -0.806975 6.227678
H 0.494160 0.484359 6.531403
h 2.408715 6.591765 1.323233
h 0.871830 4.711556 6.228018
h -1.318159 4.424407 4.639728
h -2.181997 3.186533 -0.369525
h -0.602936 2.044208 -2.404463
h 4.527923 1.763793 -3.216469
h 6.759465 2.740003 -2.048689
h 7.693578 3.745670 3.215834
h 6.174113 4.449534 5.369170

PC5”

Total QM energy at B2: -3229.844661 (a.u.)

Total QM/MM energy at B2: -3341.269826 (a.u.)

S 2.661504 5.701289 0.340306
O 2.883101 0.530190 2.071207
Fe 2.830011 3.628727 1.375844
N 1.683590 3.927408 3.003030
N 1.198411 3.028226 0.331966
N 4.008850 3.015575 -0.153184
N 4.460039 3.853339 2.541695
C 2.083962 4.219509 4.311676
C 0.922902 4.429944 5.162237
C -0.188122 4.303258 4.356748
C 0.292475 3.990146 3.020852
C -0.122625 3.293711 0.675540
C -1.023281 2.934145 -0.416489
C -0.248447 2.394403 -1.427332
C 1.142505 2.494122 -0.953273
C 3.596286 2.442528 -1.345771
C 4.729163 2.247095 -2.240593
C 5.847366 2.759654 -1.607888
C 5.392897 3.173219 -0.270687
C 5.782571 3.739761 2.126476
C 6.689551 3.929419 3.250997
C 5.909869 4.196939 4.357083
C 4.525000 4.141614 3.910389
C 3.408372 4.316072 4.715862
H 3.584717 4.549079 5.759867
C -0.525063 3.743896 1.925055
H -1.587592 3.873084 2.092903
C 2.278342 2.166908 -1.683541
H 2.126827 1.696663 -2.648500
C 6.193362 3.478440 0.822781
H 7.264465 3.392141 0.696916
C 1.179776 -0.805836 5.066682
C 0.441404 -2.052016 4.558370
O -0.634558 -2.491223 4.979163
C 1.288588 -2.647047 3.423236
H 0.734216 -2.675504 2.479598
H 1.567770 -3.680663 3.654686
C 2.683896 -1.283031 4.894989
C 2.496168 -1.673848 3.384187
H 3.378958 -2.054844 2.869140
C 1.938021 -0.380572 2.787527
C 1.767076 -0.170370 1.337737
H 2.101923 -0.927724 0.633482
H 0.995966 0.500658 0.977376
C 1.034431 0.216947 3.875441

H 1.386744 1.208741 4.172803
H -0.007402 0.322098 3.553859
C 3.033693 -2.476915 5.807141
H 2.397937 -3.352789 5.648798
H 2.905756 -2.174084 6.856126
H 4.074784 -2.786958 5.636020
C 3.726633 -0.173724 5.124235
H 3.734198 0.132849 6.178202
H 3.556151 0.712695 4.511104
H 4.726955 -0.548960 4.874177
C 0.713656 -0.294768 6.419527
H 0.901442 -1.031018 7.210235
H -0.363706 -0.100649 6.412089
H 1.223281 0.636145 6.689016
h 2.404405 6.641448 1.317213
h 0.940165 4.670870 6.225121
h -1.240785 4.408515 4.619213
h -2.091911 3.146406 -0.384209
h -0.507580 1.972285 -2.398276
h 4.621826 1.786214 -3.222496
h 6.826692 2.839250 -2.079747
h 7.771395 3.811241 3.190051
h 6.248537 4.438601 5.364540