Revealing the Nature of the Second Branch Point in the Catalytic Mechanism of the Fe(II)/2OG-Dependent Ethylene Forming Enzyme

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WT1 Snapshot	**B3LYP**	**PBE**	**B97D**	**B2-PLYP**
WT1-RC	0	0	0	0
WT1-TS1	8.332071141	-0.01883	3.838476	15.68209
WT1-EFI	-36.45830195	-24.2576	-23.5529	-42.82
WT1-TS2	-28.02206423	-29.5933	-29.0029	-19.3536
WT1-EFII	-51.02593499	-45.1455	-49.3179	-14.3091
WT1-TS4	-37.18872301	-38.7914	-40.7392	-51.8147
WT1-Ethylene	-86.60697866	-65.3595	-80.9381	-95.1706

Table S2 Single Point Energies obtained for the stationary points of the **WT2** snapshot using different functionals with the def2-TZVP basis set. The energies of the TSs and IMs are denoted relative to the **WT2-RC** using different functionals at kcal/mol.

WT2 Snapshot	**B3LYP**	**PBE**	**B97-D**	**B2-PLYP**
WT2-RC	0	0	0	0
WT2-TS1	7.936112647	-0.23908	3.207201	52.27531
WT2-EFI	-36.76829164	-24.0913	-23.777	-42.9254
WT2-TS2	-28.73868008	-29.4277	-29.1666	-21.0705
WT2-EFII	-52.99066724	-48.4306	-48.6734	-10.3169
WT2-TS3	-34.70064784	-35.79	-37.6882	-50.3758
WT2-EFIII	-47.63361864	-48.0057	-54.1647	-62.7114
WT2-TS4	-45.08467505	-41.6265	-55.5823	-42.4372
WT2-EFIV	-99.68302162	-80.9732	-89.3762	-109.361

Table S3 Single Point Energies obtained for the stationary points of the **WT-EFIV** snapshot using different functionals with the def2-TZVP basis set. The energies of the TSs and IMs are denoted relative to the **WT-EFIV-RC** using different functionals at kcal/mol.

WT-EFIV	**B3LYP**	**PBE**	**B97**	**B2-PLYP**
WT-EFIV-RC	0	0	0	0
WT-EFIV-TS1	6.239954468	6.177831	7.503759	6.245602
WT-EFIV-IM1	6.906369557	6.94402	9.004761	6.836716
WT-EFIV-TS2	33.48704447	29.84749	30.86468	41.14517
WT-EFIV-3HP	25.72663448	25.26981	22.35126	30.48065
WT-EFIV-TS2'	86.53920764	81.60134	78.17764	102.3876
WT-EFIV-Ethylene	36.1244669	36.19287	31.08745	41.55995

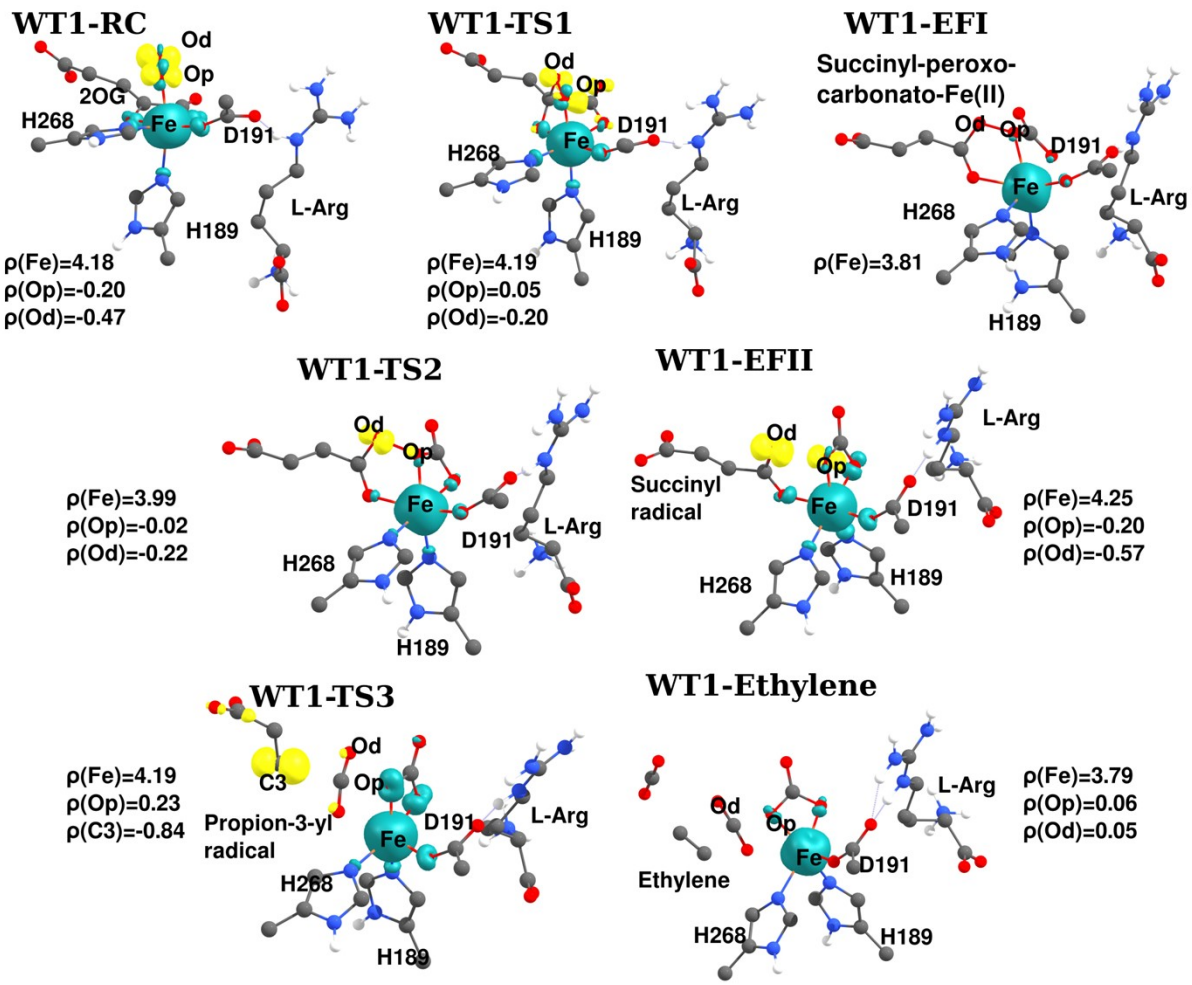

Figure S1. Spin density plots for RC, TSs, IMs, and PD complexes obtained for QM/MM simulations starting from WT1-RC.

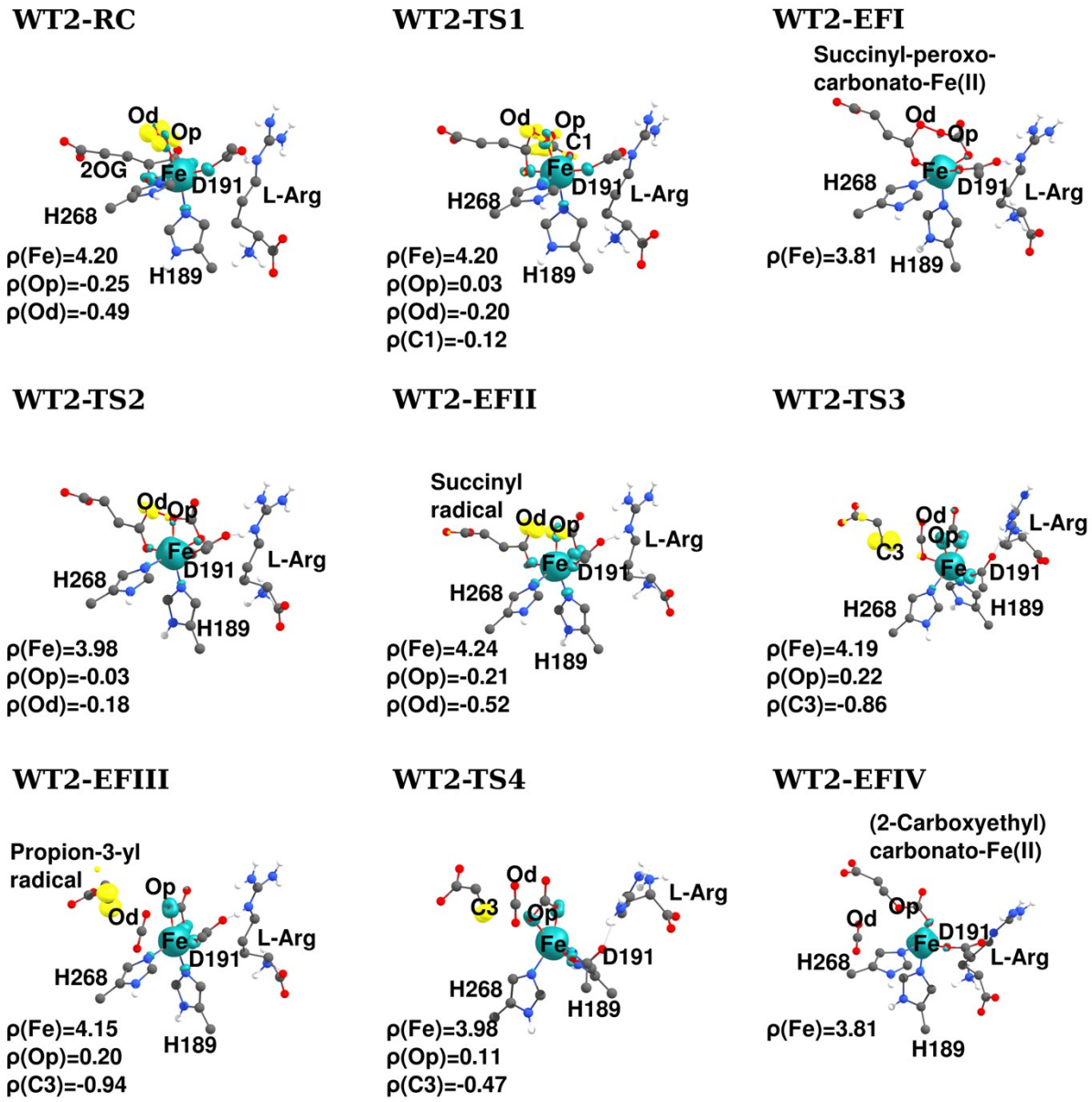

Figure S2. Spin density plots for RC, TSs, IMs, and PD complexes obtained for QM/MM simulations starting from WT2-RC.

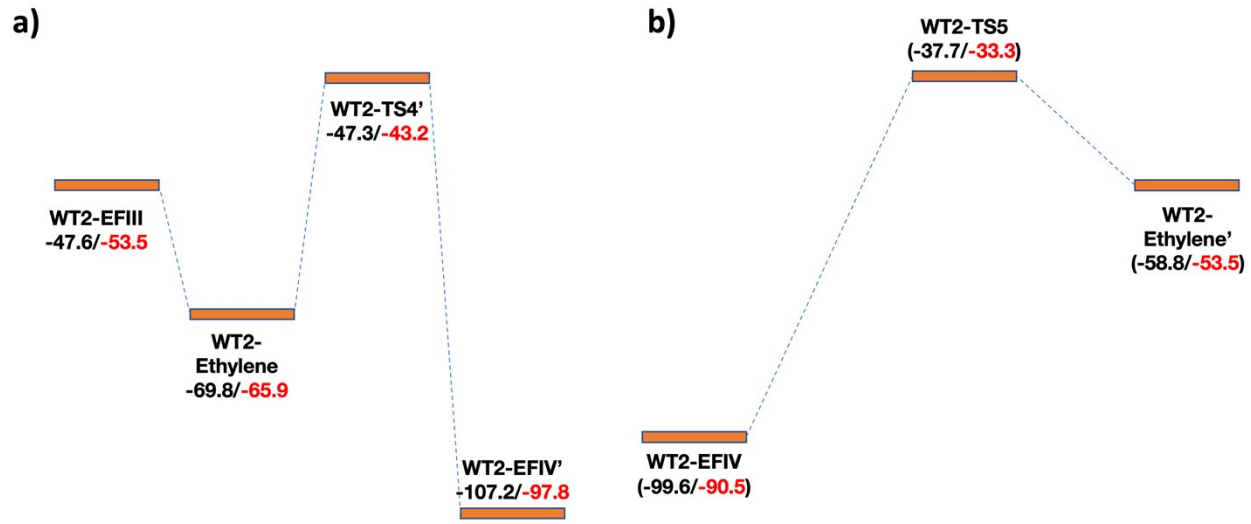

Figure S3. a) EFIV formation in WT2 EFE snapshot without additional restraints. b) Reaction profile of ethylene formation from EFIV in WT2 EFE snapshot. Relative energies were mentioned in kcal/mol at QM(B2)/MM (black) and QM(B3)/MM(red) levels. The profile was plotted at QM(B3)/MM levels.

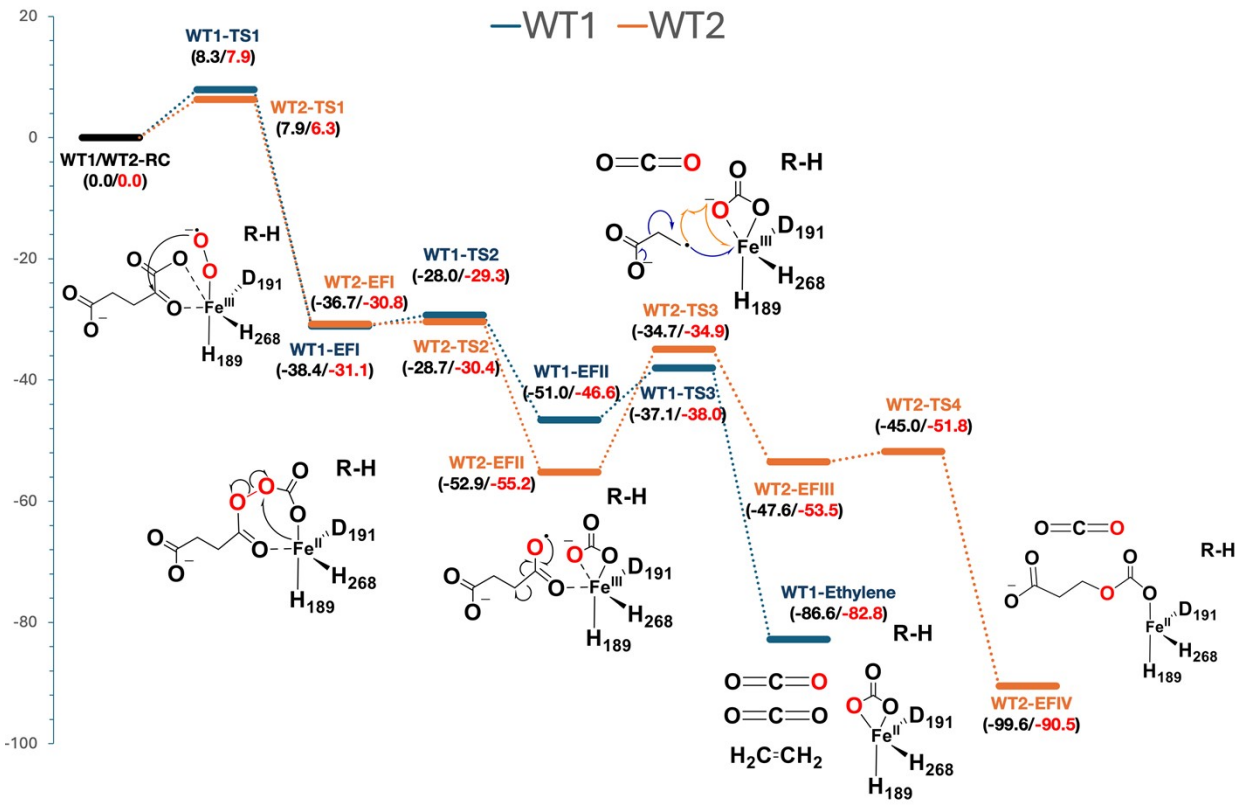

Figure S4. Overlaid Reaction profiles of O_2 activation reaction of WT1 and WT2 EFE snapshots. Relative energies were given in kcal/mol at QM(B2)/MM (black) and QM(B3)/MM (red) levels. The profile was plotted at QM(B3)/MM levels.

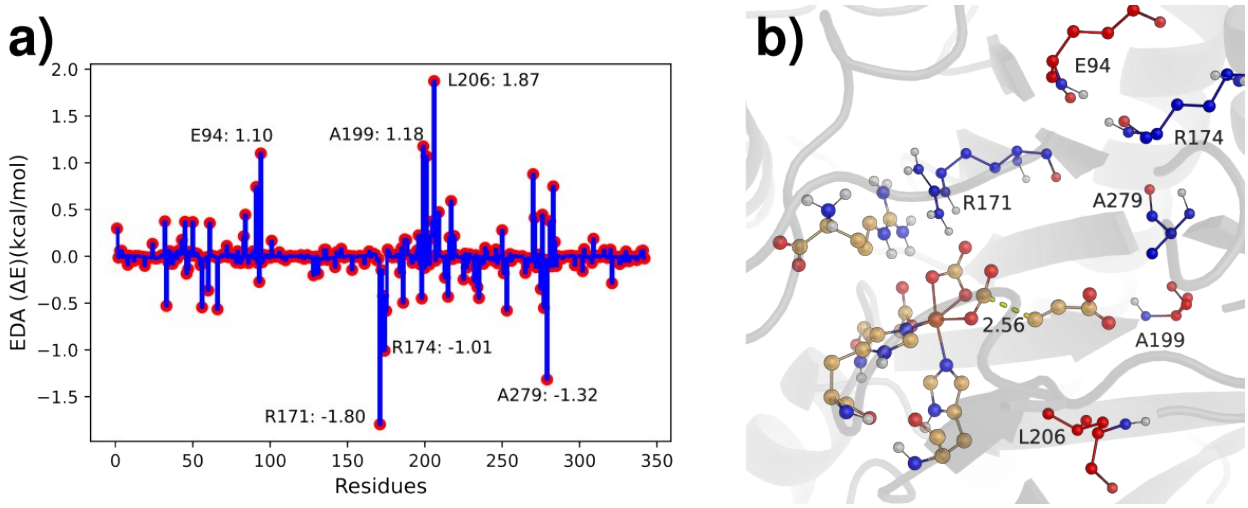

Figure S5. a) EDA plot of C2-C3 bond-breaking reaction in WT1 EFE. b) Residues stabilizing (blue) and destabilizing (red) the transition state were visualized around the active site of the WT1 EFE snapshot.

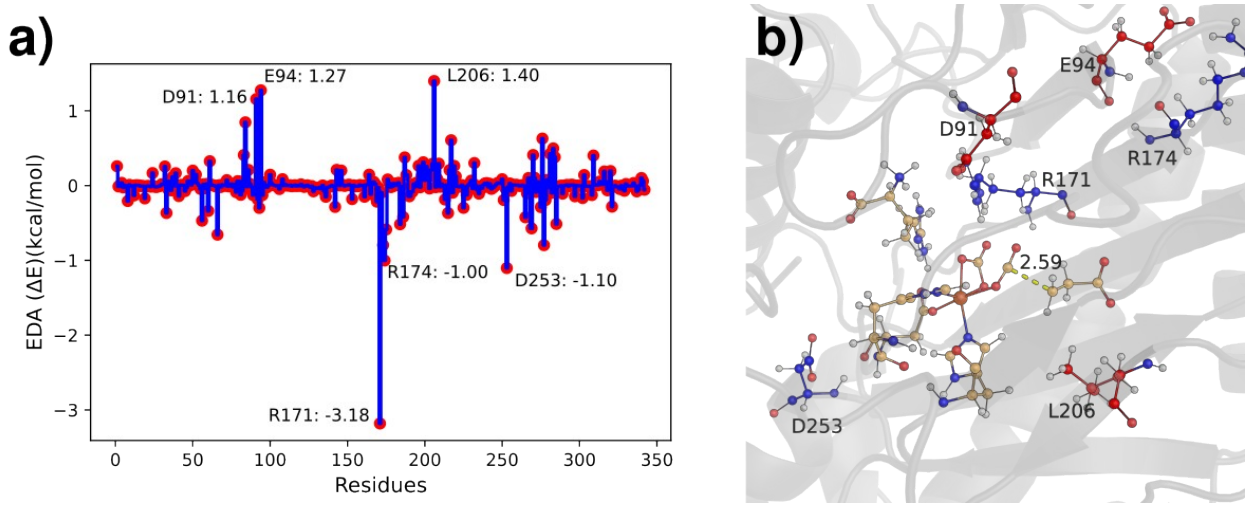

Figure S6. a) EDA plot of C2-C3 bond-breaking reaction in WT2 EFE. b) Residues stabilizing (blue) and destabilizing (red) the transition state were visualized around the active site of the WT2 EFE snapshot.

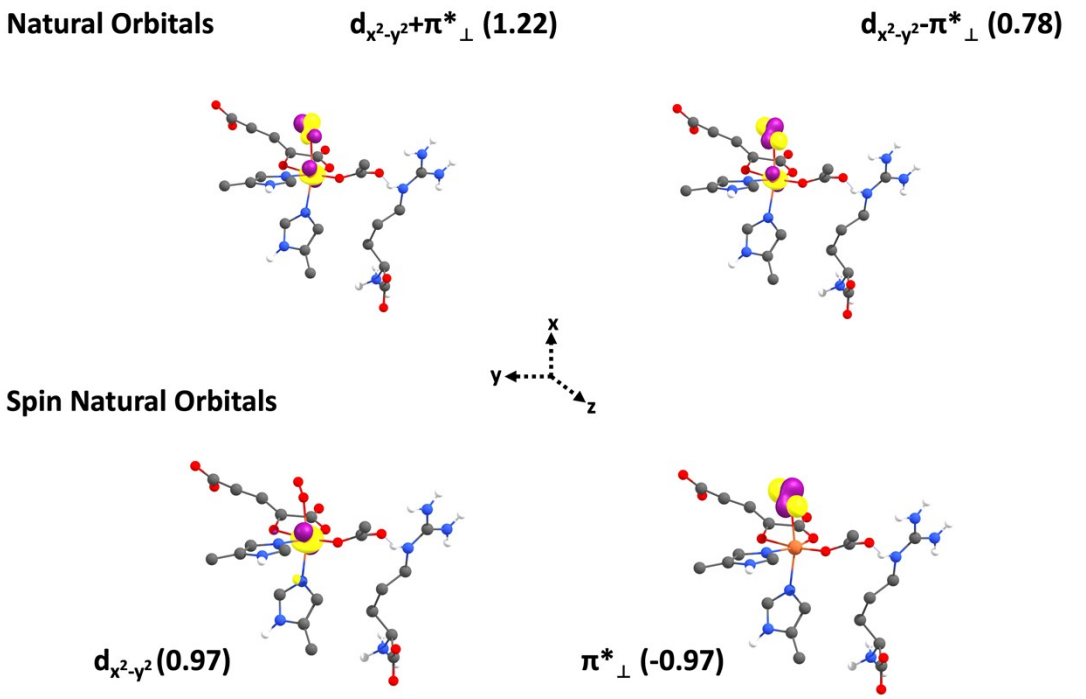

Figure S7. Orbital analysis showing Fe-O bond character in WT1-RC.

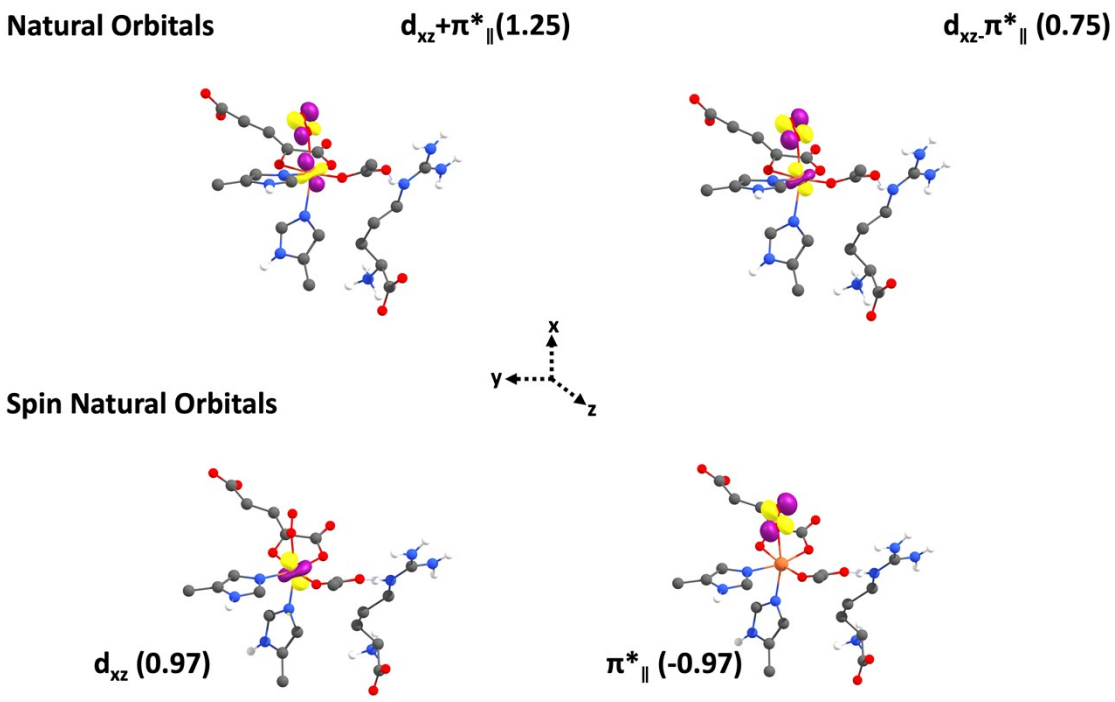

Figure S8. Orbital analysis showing Fe-O bond character in WT2-RC.

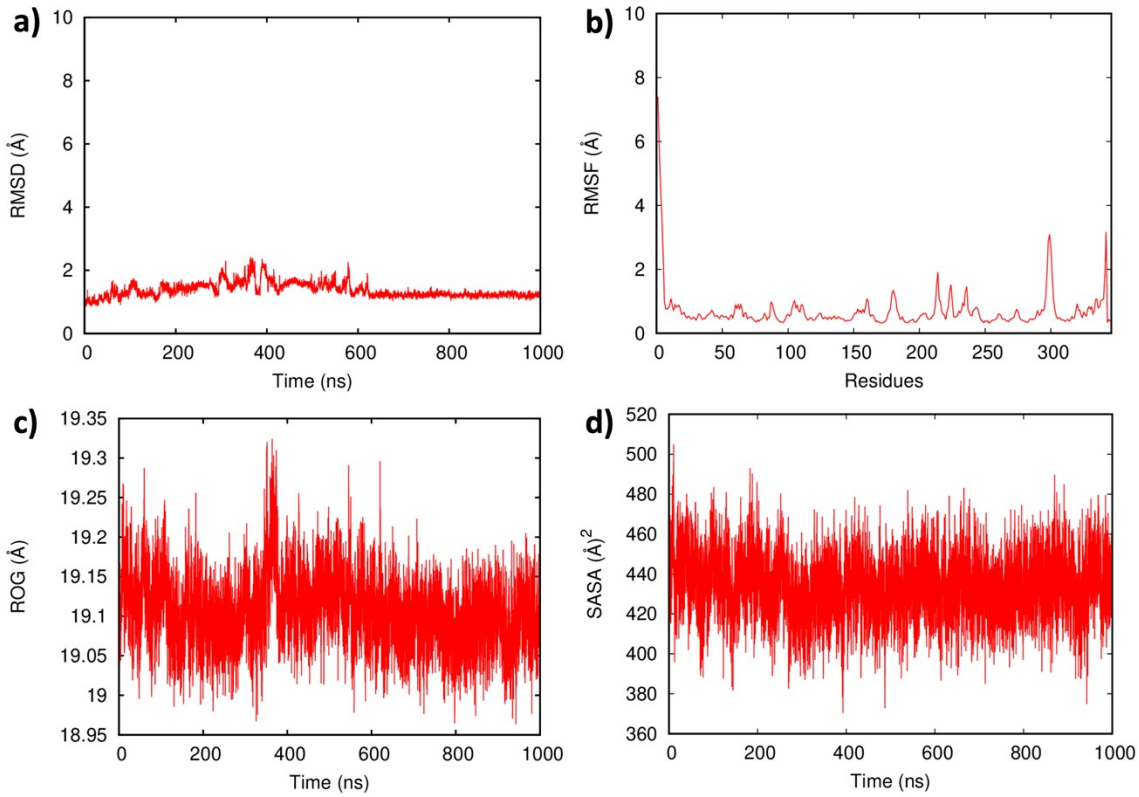

Figure S9. Molecular dynamics analysis of the A198L-EFE-Fe(III)-OO$^{\bullet-}$·L-Arg complex. a) The root mean square deviation (RMSD) of the dynamics suggests the system is equilibrated, b) the root mean square fluctuation (RMSF) of the system identifies flexible regions, c) Radius of gyration (ROG) shows the stability of the overall protein fold, and d) Solvent accessible surface area (SASA) implies that the system is equilibrated.

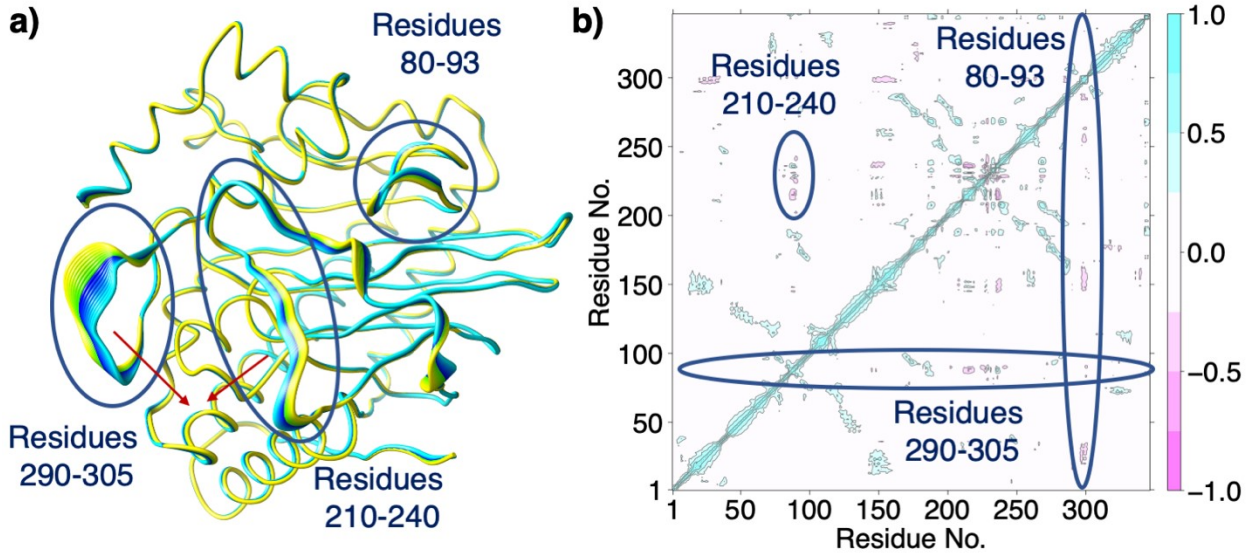

Figure S10. The overall protein dynamics of the WT-EFE-Fe(III)-$OO^{\bullet-}$·L-Arg. a) Principal component analysis shows the flexible regions of the EFE. b) Dynamic cross-correlation matrix shows the regions of correlated and anticorrelated motions. Reproduced from Chaturvedi et al.[1]

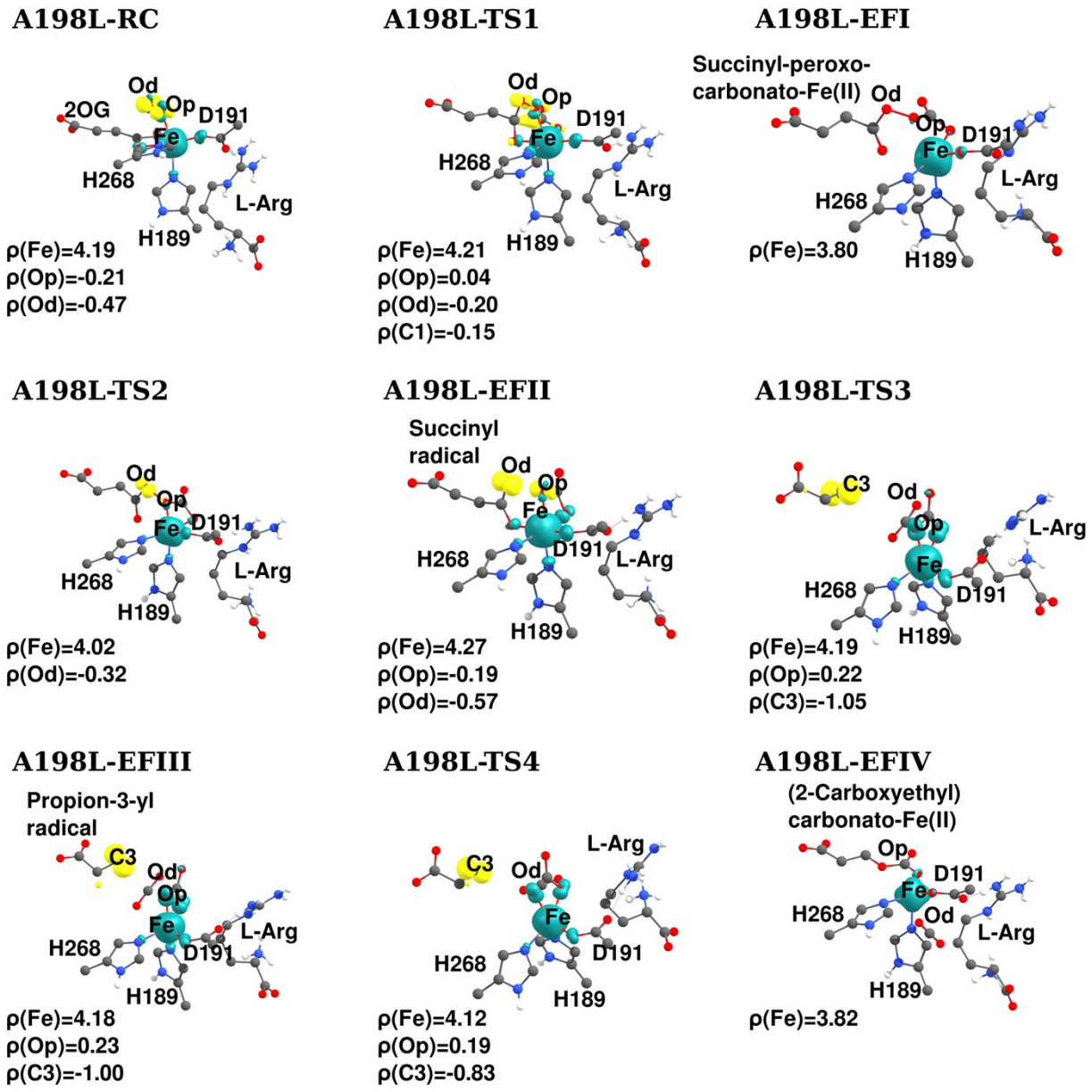

Figure S11. Spin density plots for RC, TSs, IMs, and PD complexes obtained for QM/MM simulations starting from A198L-RC.

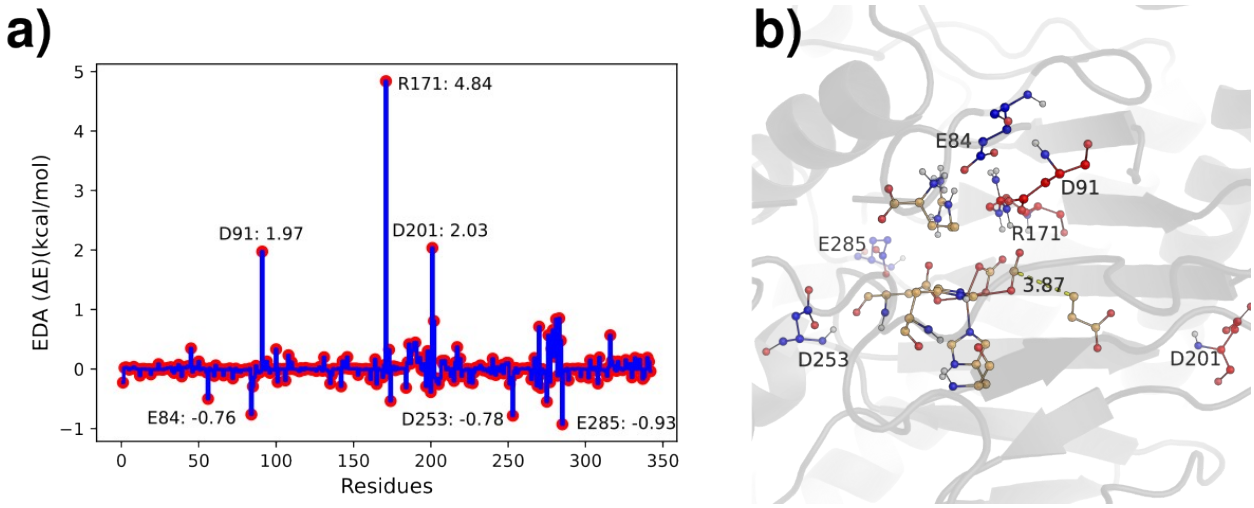

Figure S12. EDA analysis of C2-C3 bond-breaking reaction in A198L EFE. b) Residues stabilizing (blue) and destabilizing (red) the transition state are visualized around the active site of the A198L EFE snapshot.

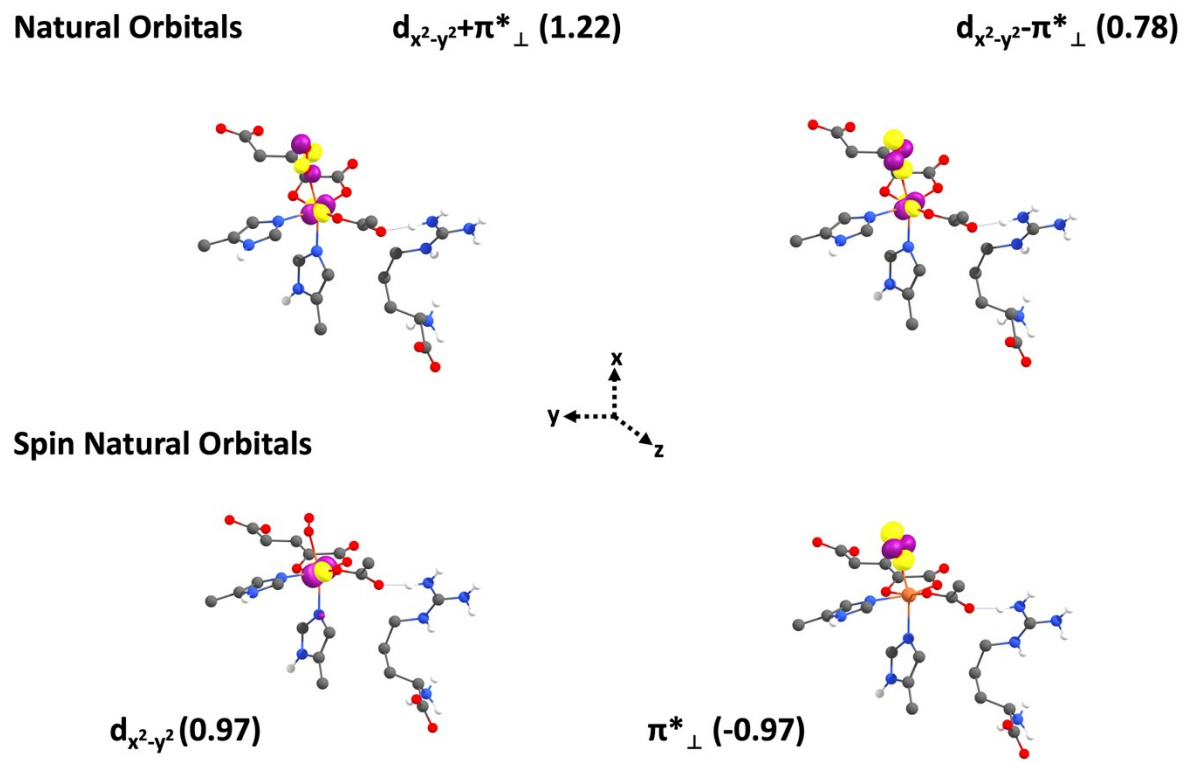

Figure S13. Orbital Analysis showing Fe-O bond character in A198L-RC.

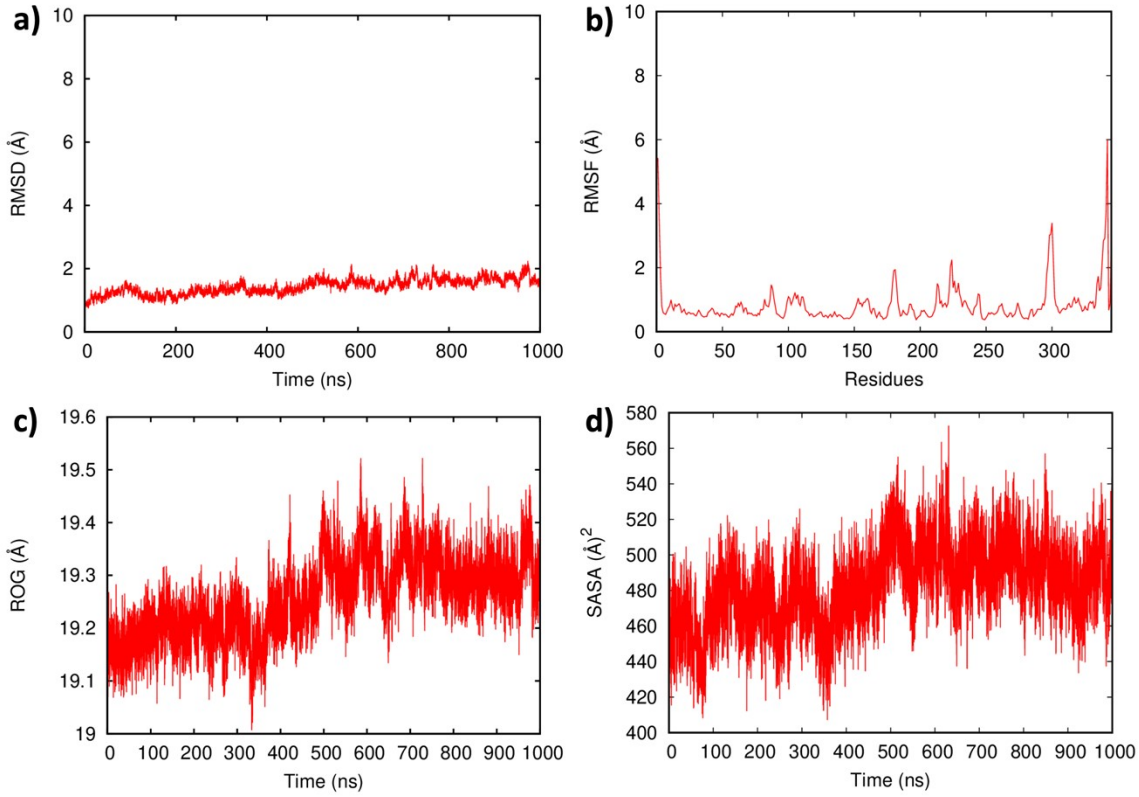

Figure S14. Molecular dynamics analysis of the WT-EFE-Carboxyethyl-carbonatoiron-(II) (EFIV) complex. a) RMSD of the dynamics suggests the system is equilibrated, b) RMSF of the system identifies flexible regions, c) ROG shows the stability of the overall protein fold, and d) SASA implies that the system is equilibrated.

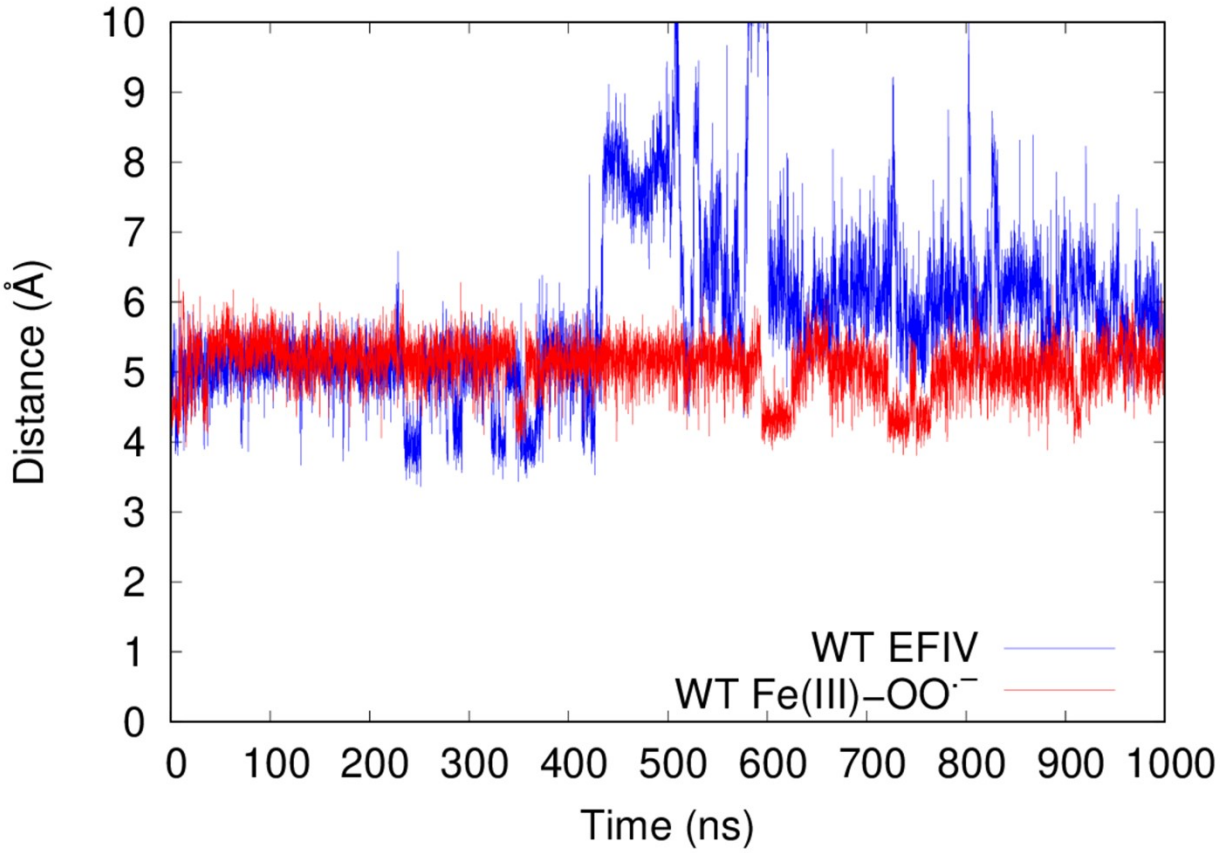

Figure S15. Plot depicting the distance between Fe and C5 of L-Arg in WT-EFIV and WT- Fe(III)-$OO^{\bullet-}$ dynamics.

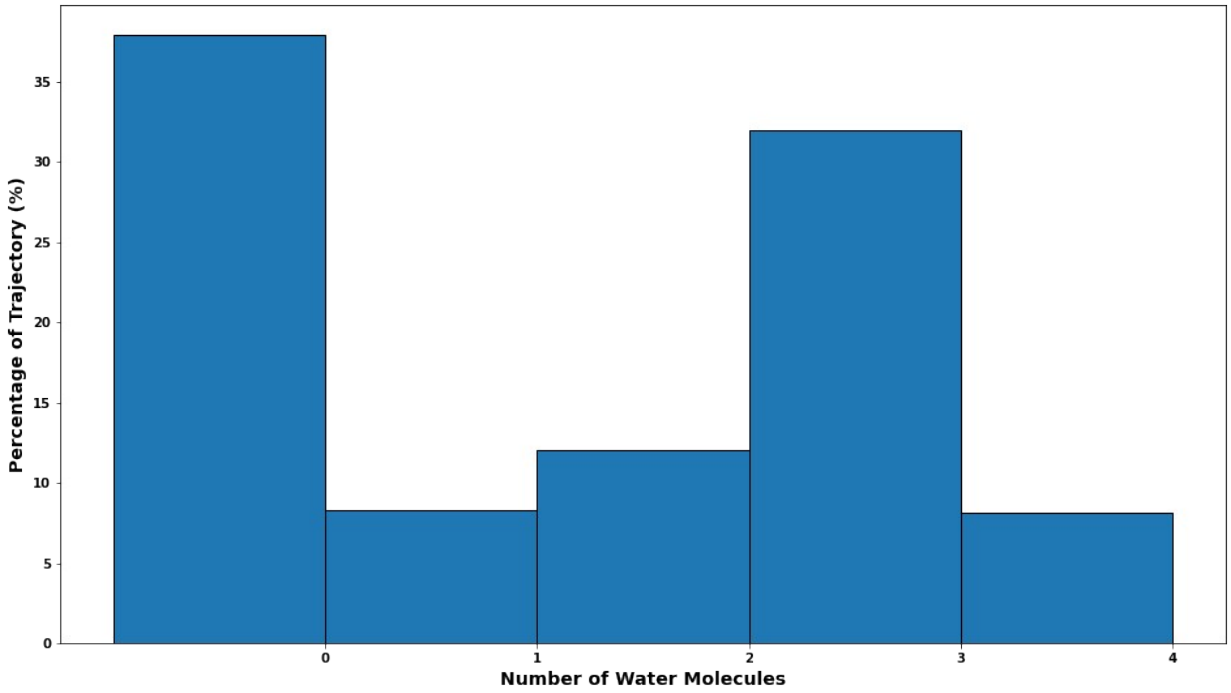

Figure S16. Histogram plot showing the number of water molecules approaching within 5Å of Fe(II) center during one μs simulation of WT-EFE-EFIV intermediate dynamics.

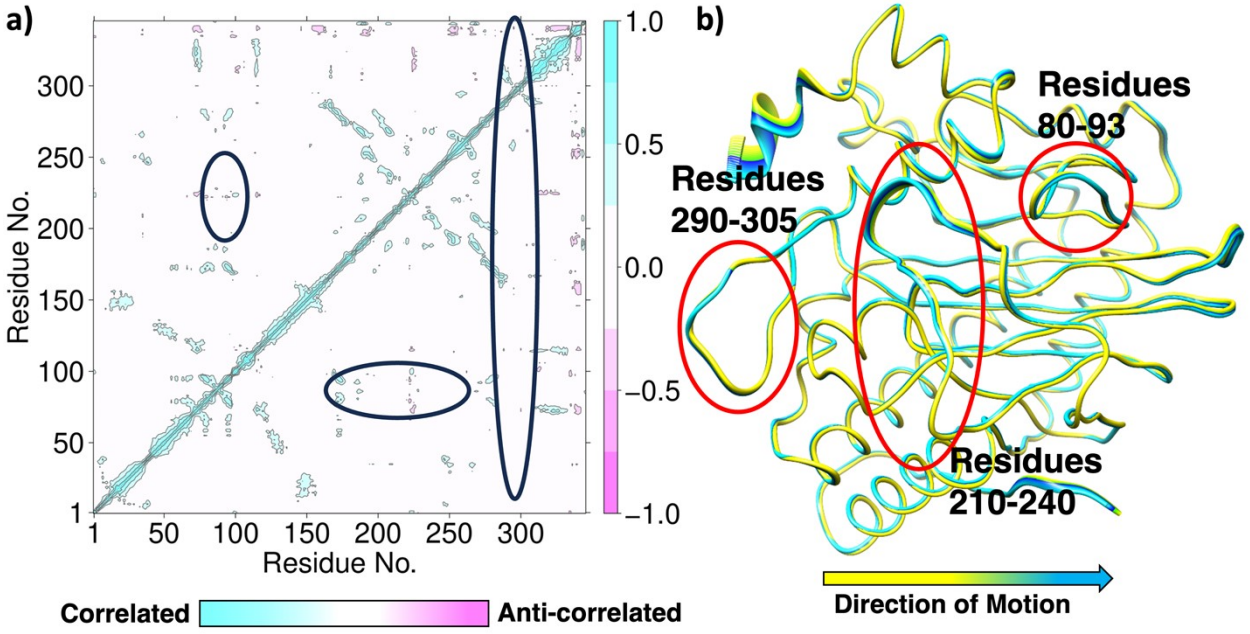

Figure S17. The overall protein dynamics of WT-EFIV intermediate complex. a) Dynamic cross-correlation matrix shows the regions of correlated and anticorrelated motions in the WT-EFIV

complex. b) Principal component analysis shows the flexible regions of the WT-EFIV complex. The circled regions show a loss of correlated/anticorrelated motion in (a) and flexibility in (b) compared to WT-EFE-Fe(III)-OO$^{\bullet-}$··L-Arg system.

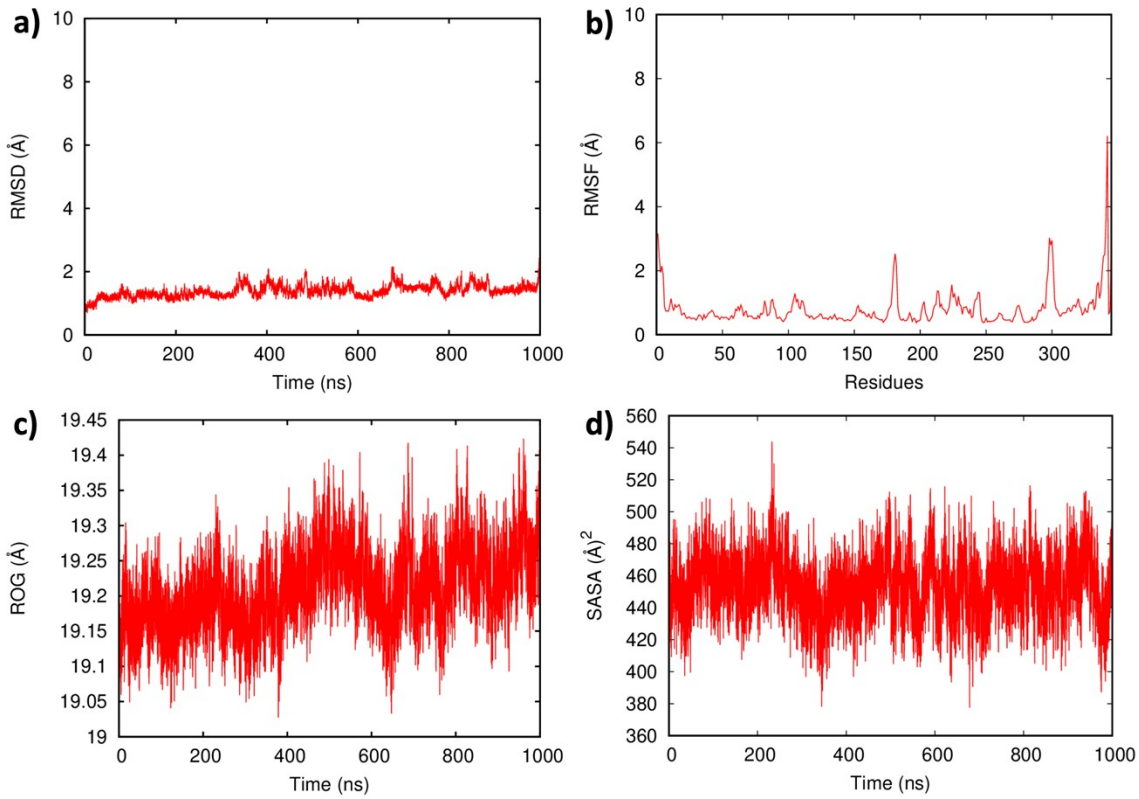

Figure S18. Molecular dynamics analysis of the A198L-EFE-EFIV complex. a) RMSD of the dynamics suggests the system is equilibrated, b) RMSF of the system identifies flexible regions, c) ROG shows the stability of the overall protein fold, and d) SASA implies that the system is equilibrated.

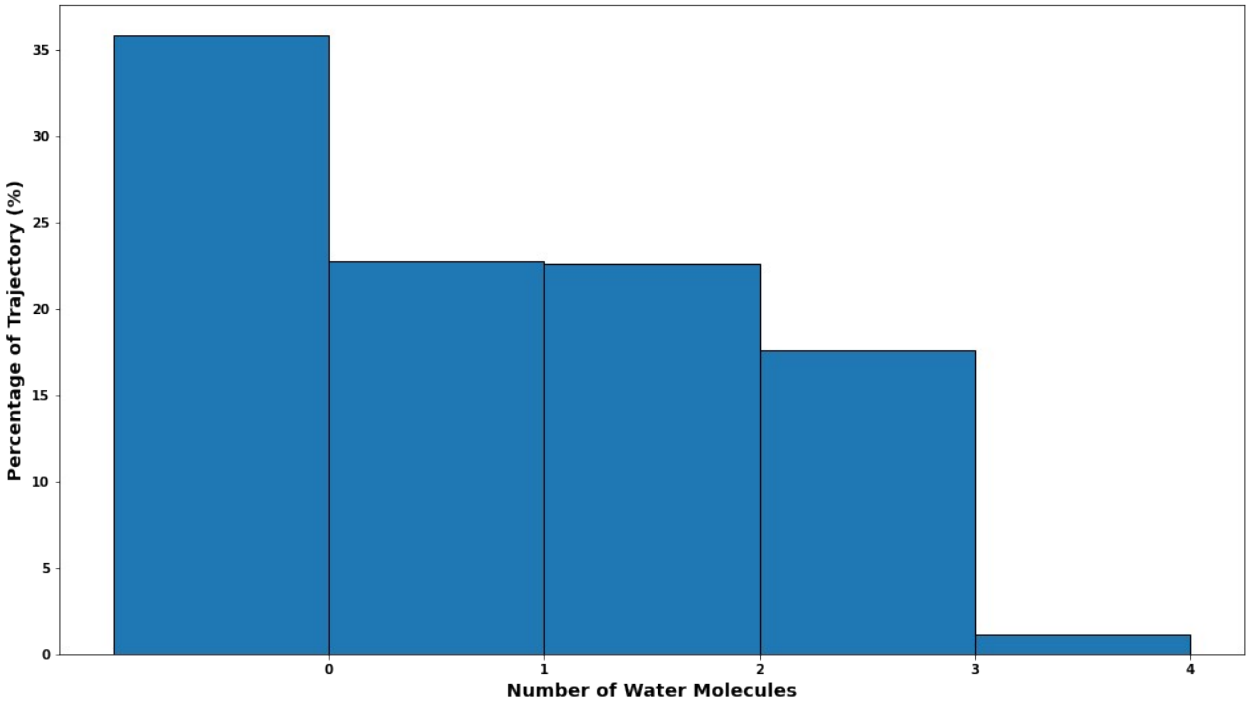

Figure S19. Histogram plot showing the number of water molecules approaching within 5Å of the Fe(II) center during one μs simulation of A198L-EFE-EFIV intermediate dynamics.

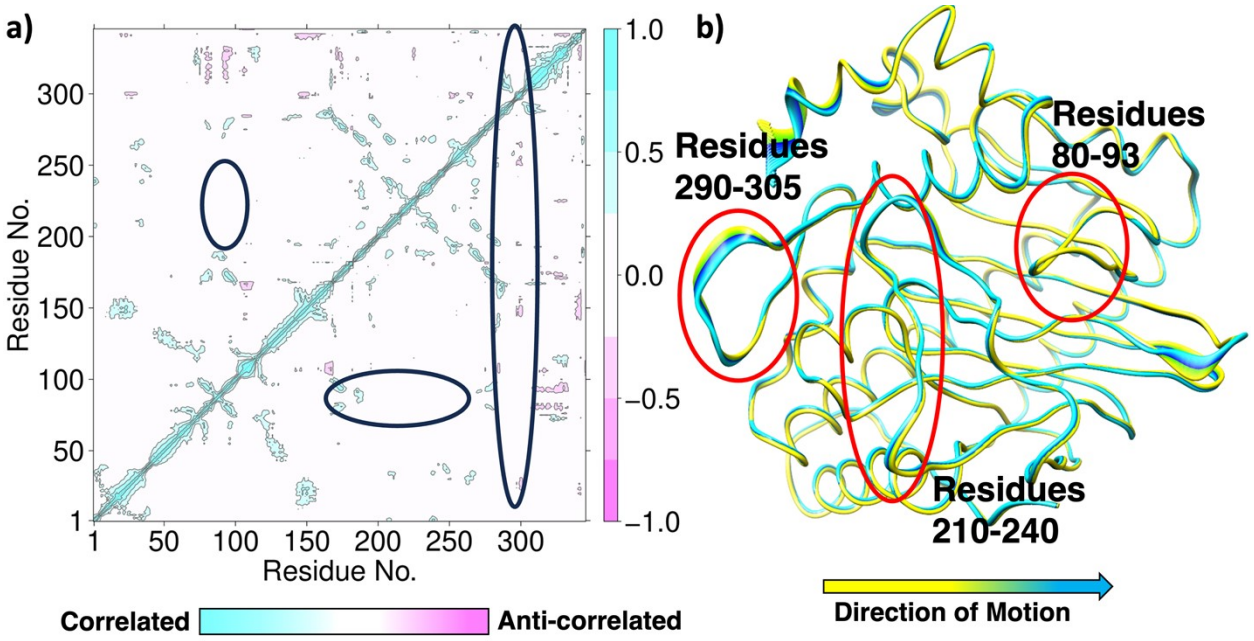

Figure S20. The overall protein dynamics of A198L-EFE-EFIV intermediate complex. a) Dynamic cross-correlation matrix shows the regions of correlated and anticorrelated motions in the A198L-EFE-EFIV complex. b) Principal component analysis shows the flexible regions of the A198L-EFE-EFIV complex. The circled regions show a loss of correlated/anticorrelated motion in (a) and flexibility in (b) compared to WT-EFE-Fe(III)-$OO^{\bullet-}$·L-Arg system.

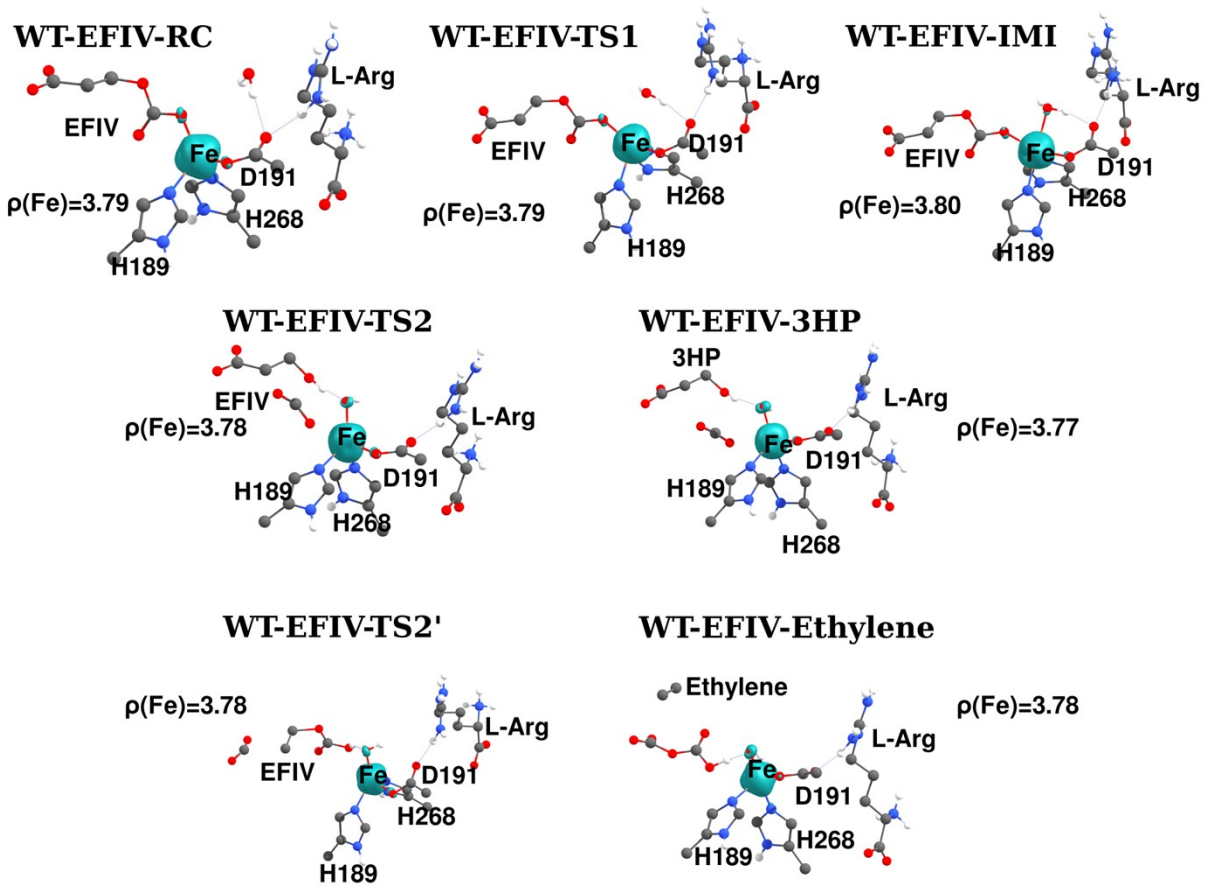

Figure S21. Spin density plots for RC, TSs, IMs, and PD complexes obtained for QM/MM simulations starting from WT-EFIV-RC.

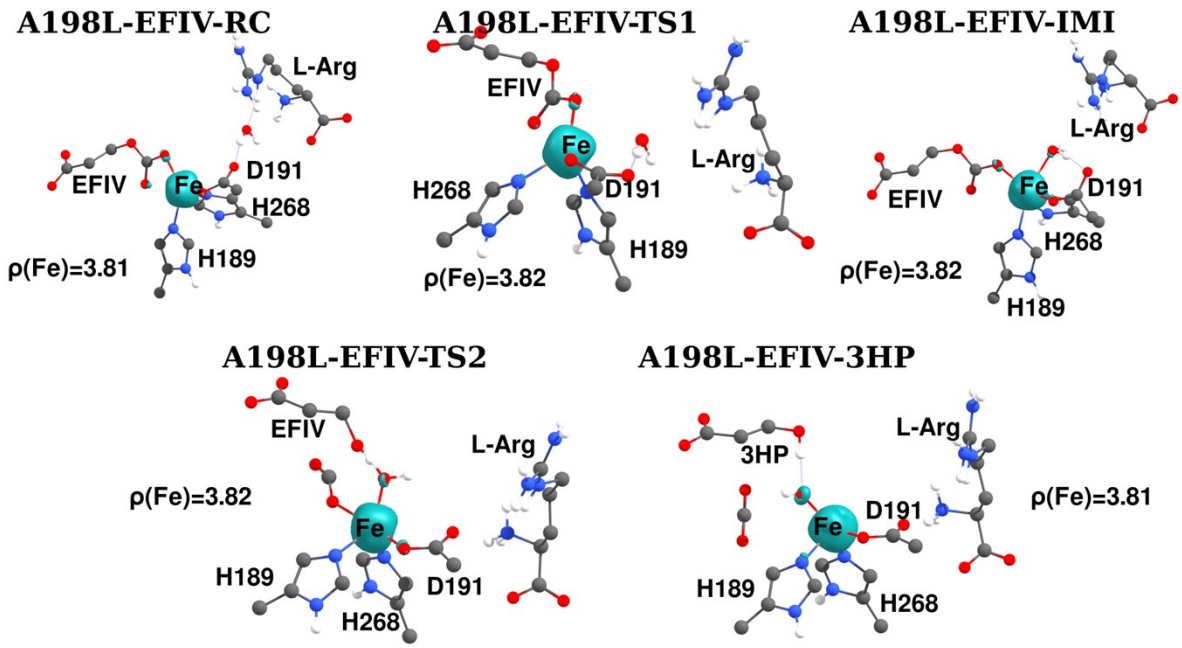

Figure S22. Spin density plots for RC, TSs, IMs, and PD complexes obtained for QM/MM simulations starting from A198L-EFIV-RC.

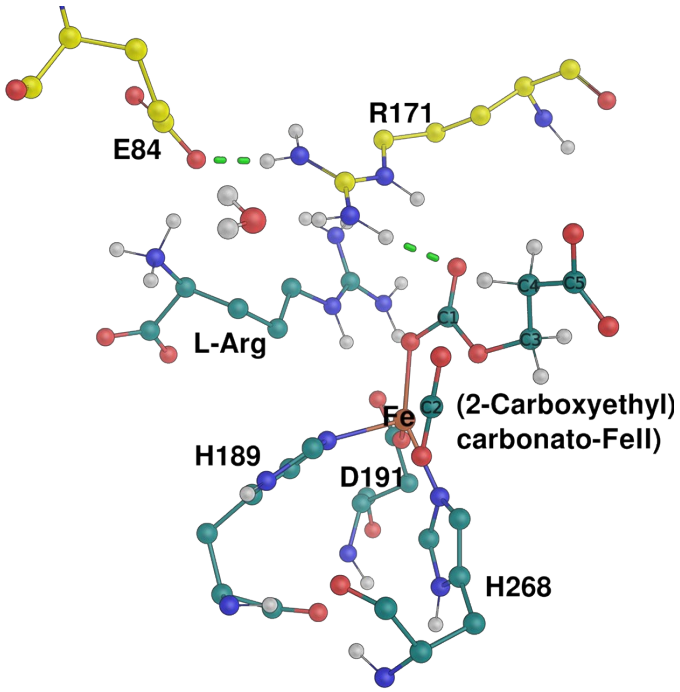

Figure S23. Residues considered for proton transfer to break down **EFIV**. Active site residues are shown in green, and SCS residues are shown in yellow.

QM/MM Optimized Coordinates

WT1 Snapshot

WT1-RC

QM(B1)/MM Energy = -3441.695045307911 a.u.
QM(B2)/MM Energy = -3444.272461000000 a.u.
QM(B3)/MM Energy = -3443.670768906480 a.u.

1 C	30.6727150	34.2455951	29.4403360
2 H	30.4298650	35.0441366	30.1568464
3 H	29.7466936	33.6653314	29.2988161
4 C	31.7688162	33.4037716	30.0183795
5 N	32.1476680	32.1556647	29.5594042
6 H	31.7128088	31.6219154	28.7978907
7 C	33.1952566	31.7250856	30.2852354
8 H	33.7080525	30.7820497	30.1097803
9 N	33.5180378	32.6214650	31.2074037
10 C	32.6320159	33.6661875	31.0564807
11 H	32.6974897	34.5450487	31.6857074
12 C	35.7417414	37.0934793	33.0248251
13 H	36.2740570	36.9945164	32.0702850
14 H	36.4826125	37.3691187	33.7919403
15 C	35.0950928	35.7791090	33.4657825
16 O	34.6400409	35.6973718	34.6152760
17 O	35.0570957	34.8432886	32.5886456
18 C	36.8078553	33.0452050	26.5250592
19 H	37.3210367	32.0731848	26.5246679
20 H	37.4868541	33.7746932	26.0548899
21 C	36.4973136	33.4568918	27.9248628
22 N	36.2319026	34.7598521	28.2987802
23 H	36.2466371	35.5789021	27.6805552
24 C	35.9559281	34.7780729	29.6151231
25 H	35.6785079	35.6668608	30.1745028
26 N	36.0493501	33.5573040	30.1233221
27 C	36.3941416	32.7220721	29.0833009
28 H	36.5491188	31.6571227	29.2376244
29 Fe	35.4334786	32.9962303	32.1032201
30 O	37.4298604	33.1081731	32.6385261
31 O	37.9930463	32.1408893	33.2306495
32 C	35.7293558	30.8881788	33.9880352
33 O	35.1444310	32.0226063	33.8511579
34 O	35.7323754	30.1803800	34.9958797
35 C	36.4235212	30.4044444	32.6886290
36 O	36.0735233	31.0017917	31.6538010
37 C	37.2892939	29.1917727	32.6954591
38 C	38.2684148	29.0777504	31.5336056
39 C	38.8737850	27.6636013	31.3283316
40 O	38.2522775	26.6863562	31.8187134
41 O	39.9159071	27.6354714	30.6330603
42 H	37.7503716	29.3360121	30.5937242
43 H	39.0914527	29.8018818	31.6352100
44 H	37.7882155	29.1398496	33.6738621
45 H	36.6293714	28.3004799	32.6795224
46 N	28.1655150	31.4261409	35.0152777
47 C	28.9496014	32.7038582	34.9862903
48 C	28.1849202	33.6998557	34.0650814
49 O	27.0111015	33.3765515	33.7879246
50 C	30.3993825	32.3774686	34.5891703
51 C	31.4696556	33.4254114	34.9191386
52 C	31.7707751	33.6323381	36.4093386
53 N	32.9931054	34.4224155	36.5402784
54 C	33.5239614	34.8931902	37.6737033
55 N	32.9863496	34.6538544	38.8762043
56 N	34.6367128	35.6387427	37.6031053
57 O	28.7917566	34.7430335	33.7153901
58 H	28.9130134	33.1012386	36.0138974
59 H	30.6828808	31.4293653	35.0792201
60 H	30.4325178	32.1757520	33.5058748
61 H	32.4039975	33.0960354	34.4340751
62 H	31.1872702	34.3878307	34.4715291
63 H	30.9366470	34.1408159	36.9248377
64 H	31.8948759	32.6531839	36.9047804
65 H	33.5183218	34.6532001	35.6846212
66 H	33.4253555	35.0891014	39.6850854
67 H	32.1815416	34.0347391	39.0252212
68 H	35.0982581	35.7525034	36.7027472
69 H	35.1594799	35.8285993	38.4566244
70 H	28.6044355	30.7122264	35.6282122
71 H	27.1906786	31.5711749	35.3298056
72 H	28.0924455	31.0214511	34.0612781
73 H	30.8939763	34.6870889	28.4686397
74 H	34.9825501	37.8689984	32.9235046
75 H	35.9516154	32.9855312	25.8532262

WT1-TS1

QM(B1)/MM Energy = -3442.504838 a.u.
QM(B2)/MM Energy = -3445.071778000000 a.u.
QM(B3)/MM Energy = -3444.479747817268 a.u.

1 C	30.6458872	34.2608240	29.4268870
2 H	30.3949914	35.0604129	30.1391226
3 H	29.7223133	33.6789971	29.2778855
4 C	31.7366343	33.4219260	30.0167454
5 N	32.1200271	32.1702152	29.5663349
6 H	31.6892396	31.6321044	28.8049927
7 C	33.1640830	31.7432964	30.2976723
8 H	33.6829013	30.8007374	30.1380324
9 N	33.4796289	32.6488826	31.2172034
10 C	32.5953750	33.6929023	31.0563782
11 H	32.6554405	34.5710687	31.6862578
12 C	35.7595914	37.0769849	33.0249471
13 H	36.3012737	36.9927355	32.0739735
14 H	36.4932474	37.3493046	33.8003546
15 C	35.1257920	35.7485864	33.4465402
16 O	34.6255720	35.6602350	34.5755063
17 O	35.1583520	34.8065987	32.5734330
18 C	36.8115928	33.0428242	26.5239243
19 H	37.3243717	32.0706228	26.5195666
20 H	37.4880354	33.7731141	26.0512499
21 C	36.5072007	33.4531124	27.9263399
22 N	36.2418760	34.7551900	28.3033501
23 H	36.2564298	35.5753201	27.6857254
24 C	35.9684512	34.7714656	29.6198623

25 H	35.6940405	35.6578929	30.1840897
26 N	36.0637318	33.5500259	30.1273910
27 C	36.4077577	32.7170971	29.0848869
28 H	36.5667088	31.6514431	29.2345447
29 Fe	35.3864709	32.9311904	32.0724840
30 O	37.5651980	32.9020472	32.7075774
31 O	37.9103055	31.7127300	33.0876137
32 C	35.7838691	30.9651435	34.0430728
33 O	35.1549923	32.0852128	33.9025671
34 O	35.7353344	30.2255372	35.0225831
35 C	36.6239264	30.6191678	32.7693070
36 O	36.0332354	31.0951522	31.7001787
37 C	37.3326333	29.2833307	32.7122754
38 C	38.2773339	29.1234773	31.5249161
39 C	38.8755766	27.7027022	31.3337892
40 O	38.2610294	26.7315411	31.8429206
41 O	39.9126112	27.6628662	30.6282671
42 H	37.7327461	29.3681838	30.5956571
43 H	39.1125846	29.8382780	31.5839180
44 H	37.8488329	29.1259727	33.6691856
45 H	36.5546487	28.4999737	32.6678474
46 N	28.1614416	31.4267898	35.0167938
47 C	28.9481962	32.7027901	34.9870844
48 C	28.1856267	33.6998323	34.0655116
49 O	27.0120052	33.3776000	33.7863696
50 C	30.3971178	32.3724485	34.5896841
51 C	31.4703142	33.4181546	34.9170076
52 C	31.7709603	33.6285207	36.4066726
53 N	32.9954146	34.4158607	36.5360923
54 C	33.5243197	34.8914684	37.6678712
55 N	32.9841218	34.6593006	38.8703035
56 N	34.6383859	35.6362228	37.5952875
57 O	28.7937192	34.7427916	33.7170159
58 H	28.9131214	33.1008335	36.0144682
59 H	30.6787259	31.4247400	35.0813597
60 H	30.4289527	32.1679920	33.5068699
61 H	32.4046324	33.0840027	34.4350941
62 H	31.1916179	34.3803457	34.4662070
63 H	30.9380577	34.1408838	36.9202787
64 H	31.8924604	32.6506602	36.9050802
65 H	33.5226985	34.6387710	35.6798969
66 H	33.4222732	35.0967275	39.6785113
67 H	32.1791562	34.0404513	39.0203323
68 H	35.1058990	35.7362370	36.6967829
69 H	35.1627120	35.8244729	38.4482885
70 H	28.5996764	30.7119668	35.6291976
71 H	27.1871816	31.5731755	35.3322587
72 H	28.0868783	31.0222683	34.0628366
73 H	30.8799670	34.6986075	28.4565162
74 H	34.9983954	37.8505755	32.9239257
75 H	35.9524955	32.9840951	25.8556655

WT1-EFI
QM(B1)/MM Energy = -3442.57373460442 a.u.
QM(B2)/MM Energy = -3445.136554000000 a.u.
QM(B3)/MM Energy = -3444.534848918557 a.u.

1 C	30.6037939	34.2689236	29.4265629
2 H	30.3573281	35.0708006	30.1379392
3 H	29.6719351	33.7036276	29.2637958
4 C	31.6752020	33.4102969	30.0239934
5 N	32.0643617	32.1750254	29.5437325
6 H	31.6529970	31.6576925	28.7592082
7 C	33.0899169	31.7227503	30.2879230
8 H	33.6021296	30.7806750	30.1055161
9 N	33.3858199	32.5901935	31.2432673
10 C	32.5075625	33.6413584	31.0954729
11 H	32.5518680	34.5055026	31.7490405
12 C	35.8316882	37.2018259	33.0792958
13 H	36.3878506	37.1634308	32.1337027
14 H	36.5375087	37.5126058	33.8667172
15 C	35.2798162	35.8299113	33.4803127
16 O	34.7660851	35.7082730	34.6082315
17 O	35.4099313	34.9141843	32.6045329
18 C	36.7922996	32.9674687	26.6112697
19 H	37.2872109	31.9857606	26.5939723
20 H	37.4898340	33.6923687	26.1612368
21 C	36.4860936	33.3600399	28.0187370
22 N	36.2800711	34.6657507	28.4164182
23 H	36.3106602	35.4919879	27.8083280
24 C	36.0310035	34.6712223	29.7415145
25 H	35.8049534	35.5594393	30.3241957
26 N	36.0803213	33.4414264	30.2368743
27 C	36.3666541	32.6140296	29.1711487
28 H	36.4681312	31.5373603	29.2910417
29 Fe	35.2168870	32.9747982	32.1963637
30 O	36.5727279	32.1712114	33.8161502
31 O	37.4014071	31.0403974	33.5574768
32 C	35.3839901	31.7393310	34.6324419
33 O	34.4433748	32.4628419	34.2944232
34 O	35.5564617	30.8002960	35.3846711
35 C	36.8430891	30.2693740	32.5912009
36 O	35.8618845	30.6397416	31.9678527
37 C	37.5941057	28.9863832	32.4581990
38 C	38.4795848	28.9291027	31.2135332
39 C	39.0778542	27.5138466	30.9959354
40 O	38.4453856	26.5456771	31.4821606
41 O	40.1265641	27.4904183	30.3165820
42 H	37.8777893	29.1793953	30.3225148
43 H	39.3044031	29.6559403	31.2629062
44 H	38.1971921	28.8331621	33.3634105
45 H	36.8672119	28.1620925	32.3948183
46 N	28.1145144	31.4717185	34.9981881
47 C	28.8581130	32.7728095	34.9832334
48 C	28.0576366	33.7553793	34.0794821
49 O	26.8842858	33.4124492	33.8225366
50 C	30.3112622	32.5095198	34.5594509
51 C	31.3399945	33.5942310	34.9041378
52 C	31.7598667	33.6734106	36.3772217
53 N	32.9717364	34.4807488	36.4883572
54 C	33.5213502	34.9369174	37.6186347
55 N	32.9900563	34.7009672	38.8258745

56 N	34.6440625	35.6659677	37.5354235
57 O	28.6416285	34.8066646	33.7160169
58 H	28.8184149	33.1551889	36.0166370
59 H	30.6422325	31.5591746	35.0143321
60 H	30.3327230	32.3413632	33.4701620
61 H	32.2461833	33.3706790	34.3225459
62 H	30.9612224	34.5726922	34.5808968
63 H	30.9639281	34.1123387	37.0036414
64 H	31.9433921	32.6560575	36.7665161
65 H	33.5287199	34.6429234	35.6367346
66 H	33.4226340	35.1524971	39.6298900
67 H	32.1701597	34.1025017	38.9758908
68 H	35.0778302	35.7868184	36.6190534
69 H	35.1897592	35.8353150	38.3772576
70 H	28.5443519	30.7766377	35.6380783
71 H	27.1213842	31.5967367	35.2604722
72 H	28.0965916	31.0490936	34.0493439
73 H	30.8582453	34.7053920	28.4607384
74 H	35.0234111	37.9255972	32.9748432
75 H	35.9444179	32.9364913	25.9270153

WT2-TS2
QM(B1)/MM Energy = -3442.556317293416 a.u.
QM(B2)/MM Energy = -3445.119950000000 a.u.
QM(B3)/MM Energy = -3444.531974942643 a.u.

1 C	30.5994196	34.2749015	29.4208735
2 H	30.3504721	35.0765567	30.1315544
3 H	29.6708491	33.7041467	29.2599077
4 C	31.6813925	33.4266154	30.0136148
5 N	32.0669109	32.1845614	29.5467196
6 H	31.6445642	31.6527985	28.7779029
7 C	33.1180522	31.7561992	30.2681174
8 H	33.6332708	30.8143543	30.0936027
9 N	33.4331456	32.6482991	31.1944601
10 C	32.5422384	33.6876379	31.0546507
11 H	32.6051733	34.5638941	31.6886112
12 C	35.8097010	37.1203947	33.0850945
13 H	36.3885334	37.0960022	32.1523820
14 H	36.4991786	37.3880717	33.9012419
15 C	35.2038938	35.7550611	33.4299597
16 O	34.7574443	35.5842669	34.5776379
17 O	35.2012640	34.8971960	32.4837214
18 C	36.8125873	32.9560121	26.6169144
19 H	37.3017941	31.9717096	26.5953445
20 H	37.5090008	33.6776012	26.1599249
21 C	36.5258037	33.3501548	28.0275893
22 N	36.3100957	34.6560127	28.4235431
23 H	36.3221499	35.4811842	27.8128755
24 C	36.0834492	34.6665404	29.7502591
25 H	35.8377838	35.5514857	30.3289262
26 N	36.1583234	33.4381209	30.2504281
27 C	36.4380114	32.6073766	29.1838363
28 H	36.5531089	31.5334884	29.3112272
29 Fe	35.2703483	32.9200759	32.1683900
30 O	36.3939714	32.3806446	33.7501313
31 O	37.4158454	31.0595566	33.5002399
32 C	35.3014306	31.8478212	34.5584496
33 O	34.2435576	32.3293708	34.1030492
34 O	35.5555349	31.0475515	35.4387659
35 C	36.8859390	30.3620588	32.5286532
36 O	35.9369905	30.7515975	31.8330292
37 C	37.5756955	29.0290978	32.3879101
38 C	38.4781377	28.9531875	31.1606205
39 C	39.0747265	27.5350297	30.9633343
40 O	38.4398126	26.5724976	31.4575078
41 O	40.1277403	27.5011354	30.2907348
42 H	37.8939678	29.2016810	30.2576571
43 H	39.3064420	29.6757688	31.2191163
44 H	38.1541819	28.8266488	33.2993956
45 H	36.7980898	28.2529379	32.3080746
46 N	28.0996085	31.4616604	35.0025829
47 C	28.8300137	32.7698790	34.9907328
48 C	28.0269281	33.7453074	34.0825266
49 O	26.8586513	33.3926001	33.8161465
50 C	30.2867997	32.5210815	34.5734267
51 C	31.3013555	33.6148148	34.9279139
52 C	31.7237706	33.6830047	36.4009978
53 N	32.9487385	34.4720742	36.5070222
54 C	33.5070480	34.9331379	37.6307100
55 N	32.9752388	34.7176808	38.8408082
56 N	34.6385555	35.6492703	37.5364062
57 O	28.6042566	34.8017080	33.7234533
58 H	28.7823409	33.1522498	36.0237703
59 H	30.6255872	31.5728990	35.0265932
60 H	30.3159024	32.3562172	33.4838122
61 H	32.2083569	33.4054138	34.3430008
62 H	30.9107324	34.5920896	34.6159434
63 H	30.9374867	34.1321574	37.0321187
64 H	31.8948907	32.6628475	36.7875357
65 H	33.4984572	34.6248755	35.6498009
66 H	33.4183769	35.1664567	39.6407987
67 H	32.1541580	34.1222566	38.9976400
68 H	35.0811900	35.7385175	36.6213101
69 H	35.1940287	35.8100581	38.3737599
70 H	28.5363736	30.7705105	35.6419722
71 H	27.1047451	31.5756028	35.2635584
72 H	28.0871878	31.0404176	34.0530687
73 H	30.8543149	34.7118928	28.4554025
74 H	35.0251095	37.8694746	32.9784995
75 H	35.9584272	32.9297462	25.9403143

WT1-EFII
QM(B1)/MM Energy = -3442.590503810633 a.u.
QM(B2)/MM Energy = -3445.156609000000 a.u.
QM(B3)/MM Energy = -3444.559635714044 a.u.

1 C	30.5780884	34.2943821	29.3704537
2 H	30.3236604	35.0948814	30.0804059
3 H	29.6537815	33.7175542	29.2085231
4 C	31.6667413	33.4536832	29.9606593
5 N	32.0508165	32.2080588	29.5011625

6 H	31.6188837	31.6662031	28.7447722
7 C	33.1190442	31.7929930	30.2023728
8 H	33.6393845	30.8537138	30.0317997
9 N	33.4460498	32.7033186	31.1064633
10 C	32.5479559	33.7356231	30.9773913
11 H	32.6155869	34.6138642	31.6062330
12 C	35.7982604	37.0829540	33.0501559
13 H	36.3796520	37.0587904	32.1193016
14 H	36.4893625	37.3340906	33.8699918
15 C	35.1778410	35.7241864	33.3854951
16 O	34.7320653	35.5399252	34.5244362
17 O	35.1630821	34.8665759	32.4276154
18 C	36.8087347	33.0020880	26.5725082
19 H	37.3176608	32.0274596	26.5628323
20 H	37.4910111	33.7305675	26.1058130
21 C	36.5120333	33.4081027	27.9775858
22 N	36.2914083	34.7153037	28.3680576
23 H	36.3169735	35.5391463	27.7555899
24 C	36.0403872	34.7294469	29.6891752
25 H	35.7928489	35.6178791	30.2612958
26 N	36.1047329	33.5008881	30.1906923
27 C	36.4025584	32.6677722	29.1313366
28 H	36.5089894	31.5950571	29.2641460
29 Fe	35.2596028	32.9204787	32.1299026
30 O	36.3791499	32.5815145	33.8015266
31 O	37.5196797	30.8633733	33.2076429
32 C	35.3458298	31.9831673	34.4469748
33 O	34.2466984	32.1851421	33.7892806
34 O	35.4803045	31.3268780	35.4694114
35 C	36.9208463	30.4452409	32.1779117
36 O	35.9576340	31.0403390	31.6081356
37 C	37.4244898	29.1286348	31.6262310
38 C	38.9152586	28.8652614	31.8187672
39 C	39.3006576	27.4702334	31.2821206
40 O	38.5345374	26.5205070	31.5856842
41 O	40.3389886	27.4200311	30.5849221
42 H	39.5266784	29.6273080	31.3128827
43 H	39.1591727	28.9047379	32.8933320
44 H	36.8622100	28.3211607	32.1278707
45 H	37.1392731	29.1111209	30.5636196
46 N	28.1046801	31.4607253	35.0246455
47 C	28.8435099	32.7655884	35.0001011
48 C	28.0491207	33.7371497	34.0816264
49 O	26.8776521	33.3916301	33.8190615
50 C	30.3006642	32.4885397	34.6009154
51 C	31.3392408	33.5751273	34.9002044
52 C	31.6566523	33.8119343	36.3820648
53 N	32.9164986	34.5483831	36.4851089
54 C	33.4825233	35.0141691	37.6028423
55 N	32.9257648	34.8601680	38.8092364
56 N	34.6491903	35.6750472	37.5088957
57 O	28.6314935	34.7893376	33.7174352
58 H	28.7913740	33.1596519	36.0284785
59 H	30.6221334	31.5606047	35.1043941
60 H	30.3339737	32.2661148	33.5214872
61 H	32.2721740	33.2535547	34.4104792
62 H	31.0210000	34.5212711	34.4434325
63 H	30.8525322	34.3727298	36.8903637
64 H	31.7423491	32.8448464	36.9065932
65 H	33.4664787	34.6798168	35.6268703
66 H	33.3852267	35.2990897	39.6057596
67 H	32.0556109	34.3368444	38.9613533
68 H	35.1318941	35.6844130	36.6114920
69 H	35.2011964	35.8181243	38.3520898
70 H	28.5181796	30.7867286	35.6970944
71 H	27.1021116	31.5886670	35.2451251
72 H	28.1201571	31.0163178	34.0856379
73 H	30.8380864	34.7305251	28.4059603
74 H	35.0240269	37.8435288	32.9493805
75 H	35.9521997	32.9530161	25.9001936

WT1-TS3

QM(B1)/MM Energy = -3442.576386131143 a.u.

QM(B2)/MM Energy = -3445.134558000000 a.u.

QM(B3)/MM Energy = -3444.545849966572 a.u.

1 C	30.4796509	34.4082673	29.3316753
2 H	30.2201349	35.2287339	30.0160775
3 H	29.5496293	33.8455336	29.1553221
4 C	31.5363420	33.5606890	29.9649797
5 N	31.9036238	32.3007915	29.5360983
6 H	31.4780399	31.7460450	28.7857115
7 C	32.9607706	31.8861195	30.2520653
8 H	33.4612703	30.9355891	30.0950134
9 N	33.3011465	32.8093734	31.1387859
10 C	32.4168454	33.8510616	30.9795713
11 H	32.4947815	34.7436190	31.5858352
12 C	35.7685249	37.1886449	33.0567930
13 H	36.3332104	37.1405052	32.1167078
14 H	36.4730331	37.4494875	33.8612824
15 C	35.1306765	35.8501931	33.4191993
16 O	34.7665431	35.6439160	34.5796404
17 O	34.9929540	35.0238328	32.4379838
18 C	36.7931335	32.9560115	26.6465370
19 H	37.2923358	31.9769749	26.6375089
20 H	37.4887255	33.6803969	26.1939314
21 C	36.4778366	33.3616992	28.0485869
22 N	36.2698528	34.6752645	28.4240833
23 H	36.3143005	35.4936325	27.8048592
24 C	35.9932894	34.7051325	29.7382727
25 H	35.7454993	35.6031428	30.2952408
26 N	36.0266916	33.4788871	30.2537314
27 C	36.3338720	32.6313707	29.2070192
28 H	36.4279366	31.5580283	29.3493639
29 Fe	35.1085242	33.1091024	32.1881448
30 O	36.3676071	32.5786073	33.5945642
31 O	35.4802279	29.3292494	33.4425028
32 C	35.4088131	32.1181917	34.3954142
33 O	34.2321230	32.2462086	33.8125046
34 O	35.5900733	31.5975704	35.4860524
35 C	35.5448389	29.9508492	32.4649850
36 O	35.3985434	30.6777630	31.5451374

37 C	37.6003454	28.8024947	31.4722561
38 C	38.7768753	28.5911802	32.3237300
39 C	39.3957092	27.1671432	31.9645448
40 O	38.6179946	26.1965923	32.1052777
41 O	40.5711451	27.1840767	31.5586977
42 H	39.5488336	29.3619008	32.1999754
43 H	38.4878638	28.5251014	33.3869127
44 H	36.8321062	28.0267542	31.5181244
45 H	37.6737383	29.3763402	30.5441613
46 N	28.1149908	31.4639878	35.0220078
47 C	28.8475962	32.7729676	35.0021581
48 C	28.0541578	33.7408495	34.0793780
49 O	26.8881605	33.3867304	33.8042973
50 C	30.3085788	32.5012261	34.6132166
51 C	31.3453061	33.5891433	34.9151147
52 C	31.6524120	33.8343909	36.3976662
53 N	32.9122726	34.5711495	36.5073792
54 C	33.4755675	35.0290447	37.6302299
55 N	32.9091282	34.8739899	38.8321093
56 N	34.6456997	35.6837779	37.5480460
57 O	28.6309903	34.7992030	33.7241949
58 H	28.7877296	33.1661441	36.0304233
59 H	30.6284126	31.5758759	35.1219779
60 H	30.3499564	32.2752357	33.5347595
61 H	32.2817838	33.2601170	34.4371424
62 H	31.0328394	34.5327493	34.4489124
63 H	30.8455589	34.3981746	36.8982864
64 H	31.7343924	32.8698808	36.9270921
65 H	33.4708089	34.6944965	35.6553671
66 H	33.3659263	35.3077183	39.6329756
67 H	32.0425214	34.3435767	38.9791047
68 H	35.1328945	35.7077716	36.6537156
69 H	35.1903999	35.8245712	38.3962910
70 H	28.5361925	30.7880133	35.6878390
71 H	27.1134056	31.5841642	35.2505754
72 H	28.1271077	31.0245652	34.0805813
73 H	30.7863960	34.8133465	28.3673697
74 H	34.9933017	37.9473222	32.9495322
75 H	35.9463925	32.9164837	25.9613111

WT1-Ethylene
QM(B1)/MM Energy = -3442.642698458781 a.u.
QM(B2)/MM Energy = -3445.213311000000 a.u.
QM(B3)/MM Energy = -3444.617316226098 a.u.

1 C	30.5177757	34.3835636	29.3406152
2 H	30.2752705	35.2092098	30.0259678
3 H	29.5744729	33.8371518	29.1762372
4 C	31.5553088	33.5163387	29.9821131
5 N	31.9280290	32.2645486	29.5340515
6 H	31.5423143	31.7417706	28.7424887
7 C	32.9212200	31.8057970	30.3230918
8 H	33.4188727	30.8515242	30.1682637
9 N	33.2108981	32.6814227	31.2685217
10 C	32.3652318	33.7467038	31.0725034
11 H	32.4194501	34.6236492	31.7075179
12 C	35.7536085	37.1583227	33.0027649
13 H	36.2832483	37.0652649	32.0453997
14 H	36.4929373	37.4479915	33.7666342
15 C	35.1169481	35.8316825	33.4436314
16 O	34.6671694	35.7781242	34.6106267
17 O	35.0864608	34.9111197	32.5799338
18 C	36.7523311	32.9930222	26.6451445
19 H	37.2663329	32.0201503	26.6385895
20 H	37.4499821	33.7322563	26.2185294
21 C	36.3950315	33.3681473	28.0458432
22 N	36.1860916	34.6682201	28.4595851
23 H	36.2303643	35.5014801	27.8643930
24 C	35.8948056	34.6440055	29.7808547
25 H	35.6505704	35.5202051	30.3745060
26 N	35.9176219	33.4074815	30.2531050
27 C	36.2248273	32.6028864	29.1796244
28 H	36.3104476	31.5233602	29.2814085
29 Fe	35.0767108	32.8797141	32.3278279
30 O	36.4369288	31.6434706	33.2116318
31 O	37.0364150	28.7603717	32.6051325
32 C	35.6545543	31.4051267	34.2601629
33 O	34.4497170	31.9100807	34.1055071
34 O	36.0055247	30.7604736	35.2575120
35 C	36.2982318	29.3544660	31.9292555
36 O	35.5326424	29.7943382	31.1671394
37 C	38.9109356	31.6638198	30.9522129
38 C	39.5903650	30.5709387	31.3020094
39 C	39.4937174	27.3355556	32.5893540
40 O	39.9621869	27.9570045	33.4428238
41 O	39.0487188	26.6584566	31.7428782
42 H	40.3232295	30.0965940	30.6403006
43 H	39.4456846	30.1303161	32.2910504
44 H	38.1790798	32.1007677	31.6385710
45 H	39.0453235	32.1387406	29.9748016
46 N	28.1675410	31.4650233	35.0040561
47 C	28.9319157	32.7572581	34.9645557
48 C	28.1341508	33.7376691	34.0585819
49 O	26.9577153	33.3956647	33.8029293
50 C	30.3800058	32.4447152	34.5511557
51 C	31.4621369	33.4910681	34.8417254
52 C	31.7351816	33.7833511	36.3216420
53 N	32.9725711	34.5503537	36.4327561
54 C	33.5247077	35.0154761	37.5542341
55 N	32.9866811	34.8141973	38.7659872
56 N	34.6638619	35.7209908	37.4671043
57 O	28.7131325	34.7915733	33.6997662
58 H	28.9007749	33.1535989	35.9927876
59 H	30.6719017	31.5087065	35.0572275
60 H	30.4016079	32.2185798	33.4723777
61 H	32.3994999	33.1025318	34.4100091
62 H	31.2145808	34.4309429	34.3294013
63 H	30.9036603	34.3394380	36.7917816
64 H	31.8276070	32.8331916	36.8762325
65 H	33.5262900	34.7263154	35.5761364
66 H	33.4326377	35.2637839	39.5628877
67 H	32.1286933	34.2723704	38.9150255

68 H	35.1035244	35.8079315	36.5487703
69 H	35.2234077	35.8578592	38.3046541
70 H	28.5809489	30.7815530	35.6665235
71 H	27.1732890	31.6135002	35.2436875
72 H	28.1571546	31.0251926	34.0632226
73 H	30.8027664	34.7857125	28.3684405
74 H	34.9808760	37.9201382	32.8998627
75 H	35.9251379	32.9483024	25.9367528

WT2 Snapshot

WT2-RC

QM(B1)/MM Energy = -3442.040471280877 a.u.
QM(B2)/MM Energy = -3444.607097000000 a.u.
QM(B3)/MM Energy = -3444.014542478170 a.u.

1 C	45.2049333	32.5719876	29.3558561
2 H	44.3184534	31.9371491	29.4884547
3 H	46.0677238	31.8932386	29.2609290
4 C	45.3316964	33.4780686	30.5420199
5 N	46.4702422	34.1900559	30.8740181
6 H	47.3727105	34.1762346	30.3857748
7 C	46.2066199	34.9544759	31.9467828
8 H	46.9175943	35.6437553	32.3953266
9 N	44.9551928	34.7727918	32.3451389
10 C	44.3981249	33.8522820	31.4806044
11 H	43.3612509	33.5423256	31.5686303
12 C	39.7969060	35.4470957	32.3303211
13 H	40.0966956	36.2754843	31.6789884
14 H	38.9693187	35.7885510	32.9709918
15 C	40.9333803	34.9810326	33.2344469
16 O	40.6783902	34.2185136	34.1712728
17 O	42.1055733	35.3955869	32.9101469
18 C	45.2812436	39.5032727	29.0120964
19 H	45.9356977	40.1962495	29.5584713
20 H	44.6005562	40.1131624	28.3964201
21 C	44.5170020	38.6541167	29.9700773
22 N	43.3329184	38.0230883	29.6451234
23 H	42.8311987	38.0991926	28.7526049
24 C	42.9606768	37.2571775	30.6853547
25 H	42.0854839	36.6151792	30.6933944
26 N	43.8253353	37.3791075	31.6827034
27 C	44.7993941	38.2536037	31.2564717
28 H	45.6342515	38.5312770	31.8958451
29 Fe	43.7894804	36.1657770	33.4590630
30 O	42.9639462	37.8563396	34.3549975
31 O	43.4617069	38.2669859	35.4481081
32 C	44.6870164	36.0459252	36.1480864
33 O	43.9348190	35.4052771	35.3254228
34 O	44.8416162	35.8017627	37.3451242
35 C	45.4750444	37.1879479	35.4590821
36 O	45.5276048	37.1149010	34.2112250
37 C	46.2954127	38.1385914	36.2660264
38 C	46.5373172	39.4864385	35.5984937
39 C	47.5992013	40.3962449	36.2665204
40 O	48.4631612	39.8639403	37.0129487
41 O	47.5123078	41.6008615	35.9401239
42 H	46.8807472	39.3202056	34.5622765
43 H	45.5983045	40.0546315	35.5162350
44 H	45.8302101	38.2310417	37.2585760
45 H	47.2744453	37.6599877	36.4578893
46 N	46.5695546	29.3410217	35.1516656
47 C	45.1687758	29.7488213	34.8538150
48 C	44.6867423	28.9913068	33.5953418
49 O	43.4968298	29.1884252	33.2665595
50 C	45.1385522	31.2755038	34.6954907
51 C	43.7527448	31.9153458	34.7140468
52 C	42.9866375	31.6446587	36.0056578
53 N	41.7982926	32.4786336	36.0547624
54 C	40.8355720	32.3826806	36.9647565
55 N	40.9319297	31.5478941	38.0139894
56 N	39.7402898	33.1453439	36.8334000
57 O	45.5456229	28.2821450	33.0180968
58 H	44.5645280	29.4222512	35.7128215
59 H	45.7453770	31.7144337	35.5061082
60 H	45.6540694	31.5439292	33.7573539
61 H	43.8818918	33.0030670	34.6054308
62 H	43.1611156	31.5493712	33.8617933
63 H	42.6943809	30.5834212	36.0664716
64 H	43.6302762	31.8527438	36.8786301
65 H	41.6479709	33.1781831	35.3142338
66 H	41.6815585	30.8501042	38.0919678
67 H	40.0996394	31.4311913	38.5875823
68 H	39.0950180	33.2133376	37.6189141
69 H	39.7392961	33.8881923	36.1382427
70 H	47.2476609	29.7480789	34.4796536
71 H	46.8738287	29.6101193	36.1087918
72 H	46.6779067	28.3188365	35.0674437
73 H	45.1213695	33.0982271	28.4049848
74 H	39.4803241	34.6068746	31.7123636
75 H	45.8804729	38.9360798	28.2998580

WT2-TS1

QM(B1)/MM Energy = -3442.027242732788 a.u.
QM(B2)/MM Energy = -3444.594450000000 a.u.
QM(B3)/MM Energy = -3444.002150066068 a.u.

1 C	45.1830768	32.5868369	29.3946052
2 H	44.2976708	31.9483567	29.5162725
3 H	46.0491904	31.9106206	29.3097850
4 C	45.2932756	33.4862391	30.5885486
5 N	46.4327800	34.1811723	30.9564961
6 H	47.3416529	34.1682296	30.4789275
7 C	46.1556311	34.9190679	32.0465173
8 H	46.8564395	35.5920262	32.5349387
9 N	44.8951297	34.7394410	32.4181658
10 C	44.3469966	33.8454451	31.5214242
11 H	43.3075905	33.5383568	31.5879094
12 C	39.7773995	35.4690330	32.3286504
13 H	40.0597122	36.3020590	31.6752398
14 H	38.9458723	35.7954281	32.9724284
15 C	40.9259523	35.0277647	33.2314646
16 O	40.6913119	34.2395785	34.1545608

17 O	42.0800297	35.4935310	32.9225287
18 C	45.2857987	39.5126410	28.9806935
19 H	45.9369536	40.2104726	29.5250423
20 H	44.6037205	40.1170792	28.3611879
21 C	44.5248270	38.6632075	29.9408482
22 N	43.3369821	38.0361168	29.6216721
23 H	42.8297101	38.1158507	28.7326738
24 C	42.9718116	37.2631644	30.6589359
25 H	42.0956164	36.6224342	30.6762851
26 N	43.8477571	37.3750820	31.6475340
27 C	44.8203000	38.2495520	31.2197988
28 H	45.6647258	38.5168469	31.8510486
29 Fe	43.7868956	36.2504675	33.4567889
30 O	43.0944389	37.8060632	34.4877837
31 O	43.9192368	38.1181525	35.5259455
32 C	44.5143837	35.9579645	36.2861174
33 O	43.8423896	35.3301754	35.4538347
34 O	44.8016449	35.8097140	37.4600336
35 C	45.1606192	37.4185337	35.4544707
36 O	45.4627488	36.9895747	34.2634028
37 C	46.2022746	38.1421304	36.2908216
38 C	46.5902446	39.4626910	35.6245818
39 C	47.6607499	40.3389005	36.3211857
40 O	48.4879364	39.8086835	37.1040727
41 O	47.6098597	41.5384248	35.9639542
42 H	46.9722071	39.2541379	34.6094867
43 H	45.6973487	40.0907930	35.4878479
44 H	45.8042613	38.3014017	37.3029362
45 H	47.0742617	37.4808355	36.3872136
46 N	46.5686264	29.3378416	35.1438789
47 C	45.1684425	29.7482764	34.8478443
48 C	44.6826851	28.9891732	33.5916340
49 O	43.4923746	29.1867671	33.2653461
50 C	45.1401797	31.2746867	34.6866048
51 C	43.7542392	31.9139948	34.6988709
52 C	42.9852644	31.6499122	35.9898282
53 N	41.7991709	32.4875428	36.0362515
54 C	40.8358145	32.3921433	36.9460189
55 N	40.9343830	31.5616811	37.9987469
56 N	39.7393970	33.1521684	36.8108323
57 O	45.5395395	28.2778339	33.0139564
58 H	44.5647669	29.4238455	35.7080692
59 H	45.7446498	31.7156031	35.4983161
60 H	45.6578913	31.5410731	33.7491220
61 H	43.8832506	33.0002638	34.5811062
62 H	43.1647579	31.5438218	33.8471873
63 H	42.6898656	30.5896260	36.0520305
64 H	43.6285978	31.8560180	36.8640179
65 H	41.6478765	33.1846701	35.2925820
66 H	41.6830936	30.8628597	38.0765045
67 H	40.1013531	31.4433509	38.5711933
68 H	39.0935195	33.2233205	37.5955120
69 H	39.7396050	33.8919763	36.1119367
70 H	47.2474107	29.7461285	34.4733312
71 H	46.8743043	29.6027293	36.1016245
72 H	46.6753381	28.3157707	35.0559865
73 H	45.1075563	33.1075534	28.4400277
74 H	39.4717763	34.6241836	31.7114868
75 H	45.8874616	38.9413648	28.2737902

WT2-EFI
QM(B1)/MM Energy = -3442.102452181826 a.u.
QM(B2)/MM Energy = -3444.665691000000 a.u.
QM(B3)/MM Energy = -3444.063692531798 a.u.

1 C	45.1415034	32.5194163	29.2912975
2 H	44.2466226	31.8904166	29.3982546
3 H	45.9978091	31.8351772	29.1778677
4 C	45.2732037	33.3883823	30.5041900
5 N	46.4121624	34.0929602	30.8433162
6 H	47.3122798	34.0938781	30.3517239
7 C	46.1534921	34.8328871	31.9359903
8 H	46.8685080	35.5103494	32.3949555
9 N	44.9081415	34.6408154	32.3424032
10 C	44.3471840	33.7401049	31.4611908
11 H	43.3125339	33.4187690	31.5475946
12 C	39.6571516	35.5160146	32.3319183
13 H	39.9388598	36.3522685	31.6821327
14 H	38.7711414	35.8160027	32.9145101
15 C	40.7693825	35.1597091	33.3203550
16 O	40.5441566	34.2848215	34.1744456
17 O	41.8554100	35.8078713	33.1658482
18 C	45.2798465	39.4675667	29.1195455
19 H	45.9417597	40.1612054	29.6574567
20 H	44.5861207	40.0811553	28.5220737
21 C	44.5292263	38.6154728	30.0886881
22 N	43.3203352	38.0189808	29.7965393
23 H	42.8102764	38.0922996	28.9087385
24 C	42.9414385	37.2889375	30.8654742
25 H	42.0369663	36.6903492	30.9070802
26 N	43.8246260	37.3915294	31.8493359
27 C	44.8202548	38.2187083	31.3763608
28 H	45.6917180	38.4714628	31.9764736
29 Fe	43.7869786	35.9632415	33.5460543
30 O	43.6482168	36.8853857	35.7210866
31 O	44.6499405	37.8392757	36.0756016
32 C	43.9962220	35.5384952	36.2896661
33 O	43.7172830	34.7063638	35.4195432
34 O	44.4705079	35.5143771	37.4083096
35 C	45.7119005	37.7126138	35.2528594
36 O	45.7261233	36.8955079	34.3434829
37 C	46.8110521	38.6571854	35.6050197
38 C	46.3753997	40.0429383	36.0754416
39 C	47.5989298	40.9089242	36.4514047
40 O	48.5557295	40.3073548	37.0087963
41 O	47.5045957	42.1204921	36.1714427
42 H	45.7860020	40.5699554	35.3103810
43 H	45.7404110	39.9484047	36.9710949
44 H	47.4141158	38.2062705	36.4125615
45 H	47.4613624	38.7077700	34.7205478
46 N	46.5468568	29.3640405	35.0882457
47 C	45.1186057	29.6564977	34.7737159

48 C	44.6891037	28.7909513	33.5659400
49 O	43.4891711	28.8790562	33.2295701
50 C	44.9696747	31.1584825	34.4946251
51 C	43.5344814	31.6779958	34.5102921
52 C	42.8931031	31.5937603	35.8934421
53 N	41.6770832	32.3856309	35.9261285
54 C	40.7593329	32.3423096	36.8853258
55 N	40.8917319	31.5545919	37.9672685
56 N	39.6695943	33.1154954	36.7654399
57 O	45.5994012	28.1208091	33.0205287
58 H	44.5359792	29.3480316	35.6541094
59 H	45.5601033	31.7187026	35.2410466
60 H	45.4319615	31.3813604	33.5173636
61 H	43.5592791	32.7313174	34.2031655
62 H	42.9258736	31.1149805	33.7888125
63 H	42.6524507	30.5483680	36.1441529
64 H	43.6039410	31.9618853	36.6551283
65 H	41.5399915	33.1184771	35.2150167
66 H	41.6451652	30.8622058	38.0516193
67 H	40.0713608	31.4517192	38.5617020
68 H	39.0658318	33.2407799	37.5751513
69 H	39.6549969	33.8173912	36.0267630
70 H	47.2034842	29.8463229	34.4449626
71 H	46.8189678	29.6138980	36.0601073
72 H	46.7396005	28.3580251	34.9586373
73 H	45.0699560	33.0818157	28.3603545
74 H	39.4244185	34.6481569	31.7148888
75 H	45.8700408	38.9159232	28.3878164

WT2-TS2
QM(B1)/MM Energy = -3442.089257604097 a.u.
QM(B2)/MM Energy = -3444.652895000000 a.u.
QM(B3)/MM Energy = -3444.062369452164 a.u.

1 C	45.1560277	32.5141961	29.2712901
2 H	44.2609191	31.8857121	29.3799143
3 H	46.0115173	31.8296699	29.1542317
4 C	45.2918198	33.3833220	30.4833154
5 N	46.4331835	34.0882058	30.8160251
6 H	47.3337803	34.0837768	30.3259412
7 C	46.1751627	34.8438995	31.8967344
8 H	46.8908283	35.5252406	32.3490744
9 N	44.9280196	34.6599025	32.3010372
10 C	44.3645063	33.7505314	31.4327416
11 H	43.3262528	33.4446336	31.5207717
12 C	39.7619648	35.4830977	32.3621385
13 H	40.0388026	36.3240321	31.7158388
14 H	38.9144707	35.7927996	32.9934507
15 C	40.9098792	35.0545492	33.2775637
16 O	40.6585968	34.2726258	34.2086038
17 O	42.0585903	35.5165529	32.9724897
18 C	45.2780796	39.4794622	29.1183620
19 H	45.9395734	40.1776927	29.6506044
20 H	44.5820093	40.0886015	28.5188987
21 C	44.5309443	38.6341450	30.0959406
22 N	43.3307243	38.0175432	29.8052050
23 H	42.8238260	38.0751539	28.9141402
24 C	42.9560536	37.2942061	30.8777901
25 H	42.0708350	36.6683951	30.9174199
26 N	43.8342951	37.4213629	31.8657273
27 C	44.8229900	38.2568807	31.3880827
28 H	45.6880838	38.5226103	31.9903619
29 Fe	43.8920280	36.0007028	33.5503470
30 O	43.5695439	36.6953027	35.4661588
31 O	44.6284349	37.8846794	35.9461014
32 C	44.0220581	35.4753421	36.1501670
33 O	44.1327835	34.5923059	35.2733726
34 O	44.2296438	35.5036488	37.3466362
35 C	45.6605088	37.8207631	35.1401371
36 O	45.7384461	37.0448631	34.1781259
37 C	46.7572153	38.7771981	35.5143717
38 C	46.3301544	40.0845930	36.1741946
39 C	47.5699015	40.9403588	36.5168159
40 O	48.5508888	40.3184266	37.0073291
41 O	47.4735734	42.1601682	36.2734842
42 H	45.6576656	40.6685417	35.5284239
43 H	45.7913930	39.8663155	37.1107989
44 H	47.4343730	38.2534778	36.2120752
45 H	47.3319660	38.9508576	34.5922969
46 N	46.5490765	29.3608219	35.0759447
47 C	45.1178117	29.6327838	34.7558697
48 C	44.6991618	28.7537737	33.5543568
49 O	43.5000015	28.8305511	33.2121136
50 C	44.9464891	31.1287412	34.4586167
51 C	43.5036271	31.6236539	34.4966558
52 C	42.8947203	31.5401404	35.8954581
53 N	41.7074037	32.3730698	35.9659692
54 C	40.7828468	32.3229548	36.9183700
55 N	40.9004752	31.5168067	37.9870158
56 N	39.6992349	33.1064763	36.8031395
57 O	45.6166967	28.0879000	33.0158967
58 H	44.5381756	29.3248162	35.6384178
59 H	45.5401931	31.7117860	35.1841340
60 H	45.3858996	31.3434865	33.4690368
61 H	43.5048138	32.6743216	34.1805321
62 H	42.8903175	31.0435523	33.7931396
63 H	42.6270246	30.5000660	36.1414181
64 H	43.6347206	31.8754358	36.6434141
65 H	41.5633914	33.0923307	35.2416023
66 H	41.6586762	30.8300727	38.0759408
67 H	40.0814175	31.4190389	38.5834843
68 H	39.0949420	33.2293279	37.6134179
69 H	39.6931822	33.8216046	36.0780836
70 H	47.2019320	29.8487977	34.4330883
71 H	46.8151951	29.6188386	36.0474502
72 H	46.7555769	28.3567690	34.9507765
73 H	45.0824362	33.0802827	28.3427442
74 H	39.4796278	34.6382149	31.7340255
75 H	45.8673404	38.9245709	28.3883384

WT2-EFII
QM(B1)/MM Energy = -3442.120332545037 a.u.

QM(B2)/MM Energy = -3444.654580000000 a.u.
QM(B3)/MM Energy = -3444.058197310041 a.u.

1 C	45.2012007	32.5555230	29.3048261
2 H	44.3126093	31.9226213	29.4375236
3 H	46.0622165	31.8763964	29.1996227
4 C	45.3367834	33.4621656	30.4895085
5 N	46.4802369	34.1687840	30.8112366
6 H	47.3840964	34.1435216	30.3276122
7 C	46.2181215	34.9660449	31.8599843
8 H	46.9362036	35.6524486	32.3009158
9 N	44.9624810	34.8091040	32.2470746
10 C	44.3992241	33.8720628	31.4099914
11 H	43.3587201	33.5770877	31.5014634
12 C	39.8310676	35.4949990	32.4004719
13 H	40.0882464	36.3440773	31.7570978
14 H	39.0039872	35.7973175	33.0612449
15 C	40.9991386	35.0571953	33.2831659
16 O	40.7757407	34.3002079	34.2319459
17 O	42.1554305	35.4924038	32.9269041
18 C	45.2746049	39.4972239	29.0989663
19 H	45.9347377	40.1943524	29.6338955
20 H	44.5848999	40.1064896	28.4921189
21 C	44.5187943	38.6577821	30.0745714
22 N	43.3336867	38.0173256	29.7685048
23 H	42.8362308	38.0641310	28.8713605
24 C	42.9525703	37.2969608	30.8386958
25 H	42.0807575	36.6523104	30.8640457
26 N	43.8097050	37.4533463	31.8414573
27 C	44.7912759	38.3048030	31.3771861
28 H	45.6305857	38.5945025	32.0034153
29 Fe	43.9122484	36.0713367	33.5696429
30 O	43.1719666	36.4243717	35.4674842
31 O	44.9112918	37.4978893	36.2968319
32 C	43.7242455	35.2839993	35.9541808
33 O	44.3907454	34.6748475	35.0201320
34 O	43.6013918	34.9164493	37.1134846
35 C	45.6528148	37.7258602	35.3076800
36 O	45.4631608	37.2975323	34.1313856
37 C	46.8481184	38.6199479	35.5971927
38 C	46.4253281	40.0386722	35.9621721
39 C	47.6354447	40.9122862	36.3763787
40 O	48.5840279	40.3259088	36.9575322
41 O	47.5255185	42.1257430	36.1075481
42 H	45.8924034	40.5383954	35.1395381
43 H	45.7369682	40.0081171	36.8231565
44 H	47.4257541	38.2130444	36.4392934
45 H	47.4774158	38.5954682	34.6964610
46 N	46.5562724	29.3752215	35.0731536
47 C	45.1214093	29.6354593	34.7560601
48 C	44.7056533	28.7587398	33.5523124
49 O	43.5078626	28.8398765	33.2057485
50 C	44.9369071	31.1305425	34.4647432
51 C	43.4934062	31.6206194	34.5172403
52 C	42.8745811	31.4883152	35.9078568
53 N	41.6752089	32.3026779	35.9818078
54 C	40.7793283	32.2762635	36.9607935
55 N	40.9020064	31.4597805	38.0186853
56 N	39.7074790	33.0827406	36.8733021
57 O	45.6230639	28.0910537	33.0155958
58 H	44.5472100	29.3193010	35.6391583
59 H	45.5350556	31.7159375	35.1827611
60 H	45.3658121	31.3517447	33.4718277
61 H	43.5022778	32.6845903	34.2438269
62 H	42.8819333	31.0679429	33.7901742
63 H	42.6209245	30.4390347	36.1283083
64 H	43.5968009	31.8225380	36.6712394
65 H	41.5419306	33.0342370	35.2726989
66 H	41.6611493	30.7732975	38.1019321
67 H	40.1037410	31.3885647	38.6458330
68 H	39.1265286	33.2054170	37.7011139
69 H	39.7353755	33.8510182	36.2064631
70 H	47.2037113	29.8808078	34.4383386
71 H	46.8176765	29.6221505	36.0487871
72 H	46.7747152	28.3758276	34.9309538
73 H	45.1149224	33.0977635	28.3632326
74 H	39.5278268	34.6590838	31.7701087
75 H	45.8672203	38.9381467	28.3748759

WT2-TS3

QM(B1)/MM Energy = -3442.105788563047 a.u.
QM(B2)/MM Energy = -3444.662396000000 a.u.
QM(B3)/MM Energy = -3444.070239212831 a.u.

1 C	45.0975660	32.4245086	29.1109325
2 H	44.1899841	31.8090098	29.1854383
3 H	45.9425411	31.7326241	28.9680608
4 C	45.2443572	33.2380177	30.3577026
5 N	46.4063203	33.8845855	30.7301730
6 H	47.3151338	33.8715497	30.2561775
7 C	46.1631259	34.6222015	31.8233427
8 H	46.9059727	35.2537048	32.2980611
9 N	44.8986912	34.4888342	32.1953282
10 C	44.3143762	33.6222849	31.2958786
11 H	43.2640355	33.3606742	31.3642371
12 C	39.7792959	35.4193927	32.3034984
13 H	40.1141244	36.2460849	31.6670248
14 H	38.9478411	35.7706118	32.9329340
15 C	40.8880408	34.9021464	33.2121117
16 O	40.6022827	34.2171884	34.1936635
17 O	42.0865824	35.1748984	32.8171410
18 C	45.2665644	39.4455646	29.2164885
19 H	45.9251140	40.1326338	29.7665979
20 H	44.5603459	40.0662920	28.6417185
21 C	44.5322162	38.5559425	30.1663141
22 N	43.3389827	37.9385275	29.8444326
23 H	42.8333205	38.0293660	28.9549062
24 C	42.9730902	37.1578776	30.8752892
25 H	42.1009593	36.5134192	30.8738657
26 N	43.8491104	37.2489409	31.8728482
27 C	44.8273397	38.1238226	31.4410492
28 H	45.6826867	38.3768674	32.0619497
29 Fe	43.7874333	35.7629479	33.4804519

30 O	43.2955511	36.4951640	35.2466901
31 O	46.5651247	36.2816625	36.2057489
32 C	43.7490227	35.4351743	35.9116026
33 O	44.3082520	34.5855795	35.0678439
34 O	43.7068239	35.2749201	37.1241377
35 C	46.3047229	36.5452120	35.1092620
36 O	45.9933551	36.6316402	33.9733895
37 C	47.0971855	39.0083452	35.1813204
38 C	46.6590011	39.5528066	36.4686687
39 C	47.7776709	40.5900456	36.8988765
40 O	48.7796778	40.0827121	37.4515535
41 O	47.5585034	41.7711895	36.5735983
42 H	45.6909063	40.0660937	36.3974424
43 H	46.6329765	38.7738634	37.2471882
44 H	48.0485082	38.4695398	35.1536479
45 H	46.7438231	39.4283858	34.2371960
46 N	46.5466157	29.3802100	35.0529338
47 C	45.1078920	29.6247172	34.7397946
48 C	44.6980447	28.7379064	33.5413276
49 O	43.4983867	28.8032945	33.1977126
50 C	44.9039794	31.1158054	34.4399121
51 C	43.4543061	31.5875722	34.5005733
52 C	42.8630239	31.4909557	35.9057271
53 N	41.6652466	32.3085035	35.9878039
54 C	40.7670789	32.2754108	36.9658280
55 N	40.8989906	31.4655695	38.0279641
56 N	39.6885141	33.0701318	36.8767283
57 O	45.6215272	28.0792296	33.0038255
58 H	44.5394357	29.3070080	35.6260677
59 H	45.4979796	31.7156360	35.1496028
60 H	45.3215314	31.3338025	33.4414836
61 H	43.4434446	32.6425754	34.1983352
62 H	42.8393890	31.0050217	33.8003246
63 H	42.6129227	30.4475597	36.1556539
64 H	43.6029652	31.8411781	36.6447137
65 H	41.5062554	33.0161609	35.2611429
66 H	41.6614062	30.7825423	38.1110478
67 H	40.1014124	31.3900568	38.6554024
68 H	39.0993410	33.1833444	37.7000549
69 H	39.6869630	33.8192399	36.1884503
70 H	47.1889416	29.8935476	34.4190962
71 H	46.8080557	29.6250377	36.0291506
72 H	46.7751387	28.3835848	34.9064771
73 H	45.0411218	33.0448548	28.2164764
74 H	39.4602987	34.5948524	31.6659709
75 H	45.8572474	38.9195030	28.4665418

WT2-EFIII
QM(B1)/MM Energy = -3442.120892480834 a.u.
QM(B2)/MM Energy = -3444.683006000000 a.u.
QM(B3)/MM Energy = -3444.099940278030 a.u.

1 C	45.1365754	32.4967345	29.1891899
2 H	44.2386405	31.8707267	29.2847715
3 H	45.9907047	31.8119531	29.0678752
4 C	45.2702814	33.3553485	30.4082960
5 N	46.4286925	34.0068346	30.7863074
6 H	47.3436101	33.9723421	30.3245990
7 C	46.1668444	34.7760730	31.8560006
8 H	46.9000890	35.4171654	32.3376741
9 N	44.8931785	34.6587094	32.2013855
10 C	44.3228719	33.7714131	31.3146572
11 H	43.2718851	33.5096900	31.3723160
12 C	39.8184206	35.4049709	32.2968424
13 H	40.1667500	36.2237055	31.6575670
14 H	38.9906779	35.7779582	32.9195972
15 C	40.9126332	34.8836441	33.2237529
16 O	40.6093452	34.1241454	34.1464084
17 O	42.1092530	35.2498534	32.9238931
18 C	45.2837023	39.4794520	29.1498914
19 H	45.9518382	40.1726744	29.6789714
20 H	44.5821762	40.0915224	28.5601181
21 C	44.5452344	38.6274993	30.1283610
22 N	43.3565153	37.9919115	29.8240995
23 H	42.8528501	38.0498570	28.9304142
24 C	42.9857028	37.2537327	30.8821719
25 H	42.1162998	36.6053160	30.9004927
26 N	43.8555938	37.3932809	31.8812835
27 C	44.8346298	38.2544197	31.4224521
28 H	45.6850604	38.5363786	32.0392196
29 Fe	43.8048803	35.9649560	33.4715620
30 O	43.3501637	36.7169394	35.2478450
31 O	46.9354143	37.1486312	36.1515619
32 C	44.1421999	35.8604557	35.8827598
33 O	44.8869409	35.2047821	34.9989038
34 O	44.1778470	35.6651758	37.0909186
35 C	46.9641248	37.2342705	34.9981974
36 O	47.0180979	37.3101104	33.8321515
37 C	45.3677605	39.9960417	35.6136934
38 C	46.1542144	40.1465375	36.8515873
39 C	47.6122876	40.6761076	36.6093665
40 O	48.5113951	40.1650083	37.3153548
41 O	47.7168483	41.5842722	35.7564593
42 H	45.7030740	40.9384412	37.4947582
43 H	46.1780044	39.2243442	37.4469384
44 H	45.4328104	40.7814008	34.8559987
45 H	44.6712090	39.1642184	35.4667585
46 N	46.5658456	29.3431829	35.1145185
47 C	45.1559329	29.7220858	34.8198348
48 C	44.6765599	28.9406230	33.5757089
49 O	43.4820183	29.1174690	33.2513588
50 C	45.0949295	31.2447111	34.6365927
51 C	43.6977843	31.8582861	34.6691481
52 C	42.9470962	31.5659822	35.9652566
53 N	41.7521577	32.3912035	36.0384746
54 C	40.8148056	32.2975914	36.9764446
55 N	40.9432776	31.4712851	38.0269472
56 N	39.7110399	33.0519416	36.8668033
57 O	45.5419569	28.2374855	33.0005243
58 H	44.5646914	29.3969375	35.6882957
59 H	45.7051521	31.7132565	35.4262231
60 H	45.5880583	31.5086046	33.6852735

61 H	43.8193402	32.9471320	34.5631765
62 H	43.1051266	31.4875077	33.8195690
63 H	42.6655750	30.5013569	36.0171272
64 H	43.5964098	31.7712485	36.8335768
65 H	41.5508582	33.0474892	35.2719701
66 H	41.7074479	30.7887029	38.1012198
67 H	40.1353360	31.3658906	38.6357352
68 H	39.0849761	33.1184213	37.6683855
69 H	39.6971060	33.8089235	36.1876916
70 H	47.2362605	29.7630727	34.4427194
71 H	46.8673829	29.6200069	36.0705817
72 H	46.6939845	28.3232721	35.0301905
73 H	45.0668218	33.0807955	28.2715439
74 H	39.4815933	34.5836594	31.6643377
75 H	45.8665404	38.9268685	28.4129936

WT2-TS4
QM(B1)/MM Energy = -3442.109477787044 a.u.
QM(B2)/MM Energy = -3444.678841000000 a.u.
QM(B3)/MM Energy = -3444.098635713044 a.u.

1 C	45.0776640	32.5386315	29.2675082
2 H	44.1620948	31.9380278	29.3580818
3 H	45.9150533	31.8296663	29.1665514
4 C	45.2243150	33.4058611	30.4798953
5 N	46.4059109	34.0138667	30.8537482
6 H	47.3160142	33.9546753	30.3863451
7 C	46.1716578	34.7844236	31.9314409
8 H	46.9335902	35.3966402	32.4039846
9 N	44.9000984	34.7105574	32.2908206
10 C	44.2974686	33.8506620	31.3985221
11 H	43.2390181	33.6160722	31.4593607
12 C	39.8889265	35.4912708	32.2995187
13 H	40.2502789	36.2967021	31.6504240
14 H	39.0482275	35.8882342	32.8911580
15 C	40.9627737	35.0181608	33.2857188
16 O	40.6531476	34.1409538	34.1092702
17 O	42.1010465	35.5809036	33.1824117
18 C	45.3109818	39.5135642	29.1007413
19 H	45.9774403	40.2271362	29.6044372
20 H	44.5986009	40.1017178	28.4996998
21 C	44.5948278	38.6840422	30.1121212
22 N	43.4038529	38.0368368	29.8549686
23 H	42.8827270	38.0634279	28.9712433
24 C	43.0632787	37.3310432	30.9503392
25 H	42.1914181	36.6890725	31.0165012
26 N	43.9548446	37.5002975	31.9200144
27 C	44.9166014	38.3455318	31.4084564
28 H	45.7899028	38.6412309	31.9863264
29 Fe	43.9405904	36.1337055	33.6177005
30 O	43.8917808	37.2539599	35.3921378
31 O	47.3203464	37.1152149	36.0269698
32 C	44.4290130	36.2228289	36.0372139
33 O	44.9433827	35.3444180	35.1843176
34 O	44.4560766	36.0702137	37.2593793
35 C	47.3421153	37.1597313	34.8707908
36 O	47.3855904	37.2284183	33.7056168
37 C	45.3318979	39.5823723	35.6415064
38 C	46.0399536	39.7891546	36.8772285
39 C	47.4218966	40.5182756	36.6442355
40 O	48.3747599	39.9961150	37.2455534
41 O	47.3741298	41.5343042	35.9346198
42 H	45.5418306	40.5549169	37.5053993
43 H	46.1976532	38.8629189	37.4366964
44 H	44.9996036	40.4650664	35.0824616
45 H	45.1062072	38.5945497	35.2376219
46 N	46.5666446	29.3535002	35.1276512
47 C	45.1676426	29.7697492	34.8320155
48 C	44.6736428	28.9977355	33.5887702
49 O	43.4817572	29.1934702	33.2677897
50 C	45.1493990	31.2947825	34.6570232
51 C	43.7731499	31.9555244	34.6841103
52 C	42.9786455	31.6281873	35.9448147
53 N	41.7951505	32.4694411	36.0130951
54 C	40.8465606	32.3735121	36.9378539
55 N	40.9634113	31.5507971	37.9945575
56 N	39.7437203	33.1265635	36.8141052
57 O	45.5260818	28.2778137	33.0137014
58 H	44.5676699	29.4579375	35.6991568
59 H	45.7663515	31.7345850	35.4574451
60 H	45.6606891	31.5522478	33.7136641
61 H	43.9315385	33.0442718	34.6341644
62 H	43.1898600	31.6463902	33.8036935
63 H	42.6799151	30.5667189	35.9481422
64 H	43.6046301	31.7895186	36.8398560
65 H	41.5948957	33.1227761	35.2382388
66 H	41.7210969	30.8618782	38.0724494
67 H	40.1435106	31.4382448	38.5856457
68 H	39.1056239	33.1968189	37.6050712
69 H	39.7287473	33.8600142	36.1092123
70 H	47.2448010	29.7539210	34.4521503
71 H	46.8750279	29.6251302	36.0824235
72 H	46.6666539	28.3305915	35.0464387
73 H	45.0372373	33.1039502	28.3364617
74 H	39.5501704	34.6608808	31.6800320
75 H	45.8924146	38.9429536	28.3765821

WT2-EFIV
QM(B1)/MM Energy = -3442.193657207740 a.u.
QM(B2)/MM Energy = -3444.765968000000 a.u.
QM(B3)/MM Energy = -3444.158692085099 a.u.

1 C	45.0952351	32.4604350	29.1278671
2 H	44.1847229	31.8511546	29.2112117
3 H	45.9364732	31.7606369	29.0006987
4 C	45.2447025	33.2962826	30.3602996
5 N	46.4081916	33.9519668	30.7129854
6 H	47.3143299	33.9320005	30.2345234
7 C	46.1678833	34.7059304	31.7967914
8 H	46.9140940	35.3556314	32.2422659
9 N	44.9107056	34.5711115	32.1875900
10 C	44.3233597	33.6891569	31.3048626

11 H	43.2753041	33.4164370	31.3872040
12 C	39.7261296	35.4100513	32.2060341
13 H	40.0762996	36.2192215	31.5549650
14 H	38.8675685	35.7849219	32.7861664
15 C	40.8076766	34.9551251	33.1868475
16 O	40.5066421	34.0991000	34.0423471
17 O	41.9451520	35.4919307	33.0337645
18 C	45.2409270	39.4975748	29.0731430
19 H	45.8909102	40.1929436	29.6223671
20 H	44.5581779	40.1073809	28.4590798
21 C	44.4764127	38.6459579	30.0309213
22 N	43.3049260	37.9912831	29.7068294
23 H	42.8099718	38.0471834	28.8088322
24 C	42.9285369	37.2461523	30.7615271
25 H	42.0614348	36.5933610	30.7735794
26 N	43.7786251	37.3982375	31.7718183
27 C	44.7435116	38.2782622	31.3299657
28 H	45.5807897	38.5765243	31.9521406
29 Fe	43.8363235	35.9521870	33.3346956
30 O	45.3164383	37.6036821	35.1944514
31 O	48.6163135	37.6952728	34.3759217
32 C	44.9442393	36.5123780	35.9279796
33 O	44.3777417	35.6313333	35.1758234
34 O	45.1432522	36.3885941	37.1311734
35 C	48.2048517	37.7336559	33.2943242
36 O	47.8073208	37.7609999	32.1989832
37 C	45.8154720	38.8341298	35.7866092
38 C	46.9358121	38.6737752	36.7935316
39 C	47.8880426	39.8882827	36.9301909
40 O	48.7921398	39.7336438	37.7862220
41 O	47.7079558	40.8856271	36.1864907
42 H	46.5338990	38.4204870	37.7791323
43 H	47.5649223	37.8189884	36.5089805
44 H	44.9585118	39.3849981	36.2044042
45 H	46.1764880	39.4228195	34.9320712
46 N	46.5641180	29.3814635	35.1430106
47 C	45.1653261	29.7978441	34.8460498
48 C	44.6777584	29.0363387	33.5921768
49 O	43.4853906	29.2292800	33.2704398
50 C	45.1434476	31.3256185	34.6918136
51 C	43.7612294	31.9757059	34.6779055
52 C	42.9429377	31.6661818	35.9267848
53 N	41.7370907	32.4765433	35.9445273
54 C	40.7962909	32.4076791	36.8805931
55 N	40.9384912	31.6380791	37.9752320
56 N	39.6829634	33.1374858	36.7313132
57 O	45.5341138	28.3242211	33.0141183
58 H	44.5615181	29.4747108	35.7064154
59 H	45.7298551	31.7570142	35.5207964
60 H	45.6848637	31.5968738	33.7692813
61 H	43.9036658	33.0654572	34.6098369
62 H	43.2007763	31.6438690	33.7912100
63 H	42.6735244	30.5973716	35.9540324
64 H	43.5435931	31.8696870	36.8314665
65 H	41.5219207	33.0995886	35.1476913
66 H	41.6882891	30.9410999	38.0569460
67 H	40.1188209	31.5336646	38.5696738
68 H	39.0482235	33.2339223	37.5217080
69 H	39.6454768	33.8197188	35.9761223
70 H	47.2431913	29.7774074	34.4655019
71 H	46.8725837	29.6546802	36.0974475
72 H	46.6629713	28.3578034	35.0664991
73 H	45.0439572	33.0597060	28.2188501
74 H	39.4268601	34.5615486	31.5907715
75 H	45.8476568	38.9428321	28.3574568

A198L Snapshot

A198L-RC

QM(B1)/MM Energy = -3441.532826025984 a.u.

QM(B2)/MM Energy = -3444.101723000000 a.u.

QM(B3)/MM Energy = -3443.512906603785 a.u.

1 C	40.0879197	29.0371523	29.6694732
2 H	40.7734258	28.9524679	30.5270392
3 H	40.6918698	28.8819896	28.7613738
4 C	39.4567497	30.3957244	29.6931263
5 N	38.8136309	30.9837808	28.6192404
6 H	38.7160394	30.5942870	27.6728960
7 C	38.2976250	32.1595030	29.0231684
8 H	37.7030495	32.8122213	28.3897939
9 N	38.5848605	32.3810479	30.2999761
10 C	39.3131008	31.2911607	30.7295683
11 H	39.7008472	31.2229140	31.7422009
12 C	38.9684755	32.4506852	35.5414815
13 H	37.9162820	32.4874690	35.8434415
14 H	39.5401644	33.1773433	36.1412976
15 C	39.1368982	32.8553313	34.0690546
16 O	40.2493680	33.1179179	33.6220888
17 O	38.0360528	32.9171974	33.3809185
18 C	33.3372821	30.5652288	29.4936747
19 H	32.9123606	31.3618466	28.8640238
20 H	32.4998309	30.1115602	30.0498972
21 C	34.3396616	31.1527826	30.4304534
22 N	34.7503270	30.5567342	31.6095364
23 H	34.4295692	29.6580827	31.9864360
24 C	35.6899865	31.3380231	32.1765856
25 H	36.2097269	31.1107639	33.1038547
26 N	35.9000649	32.4154526	31.4363093
27 C	35.0587421	32.3218119	30.3507004
28 H	35.0302510	33.0959194	29.5877656
29 Fe	37.5829873	33.7345118	31.6499567
30 O	36.1966066	35.0710462	32.4452766
31 O	36.0661972	36.2466743	31.9977481
32 C	38.4345207	36.2691110	30.6257434
33 O	38.7909453	35.3281474	31.4232448
34 O	39.0430695	37.3176743	30.4136477
35 C	37.1432327	35.9456603	29.8326460
36 O	36.8135799	34.7504721	29.8282941
37 C	36.4762882	37.0058331	29.0163520
38 C	35.1207101	36.6233841	28.4375851
39 C	34.4585473	37.6872918	27.5179613
40 O	35.2111994	38.5175338	26.9500450

41 O	33.2164363	37.5832386	27.3837608
42 H	35.2229800	35.7017909	27.8372802
43 H	34.4217913	36.3670901	29.2443990
44 H	36.4209118	37.9101435	29.6448822
45 H	37.1705614	37.3043571	28.2093957
46 N	45.3992999	32.0859658	29.0209605
47 C	44.6077452	31.4940726	30.1417412
48 C	45.1325431	30.0632498	30.4730026
49 O	44.5052250	29.5010586	31.3999059
50 C	43.1069901	31.5295987	29.8478057
51 C	42.4517781	32.9104195	29.6643907
52 C	42.2197503	33.7198863	30.9431109
53 N	43.4378531	34.3678133	31.4356134
54 C	43.5724008	34.8582055	32.6729092
55 N	44.7111091	35.5256710	32.9738135
56 N	42.6050017	34.7494857	33.5821807
57 O	46.1262721	29.6443184	29.8360542
58 H	44.8237795	32.1068097	31.0281982
59 H	42.9185717	30.9283375	28.9414329
60 H	42.6232051	30.9977378	30.6797837
61 H	42.9893804	33.5224617	28.9195271
62 H	41.4560931	32.7421966	29.2260854
63 H	41.4431790	34.4832161	30.7614001
64 H	41.8222273	33.0597851	31.7280423
65 H	44.1547023	34.6148191	30.7339800
66 H	44.9191181	35.7871969	33.9306124
67 H	45.4961315	35.4587444	32.3347866
68 H	41.7624465	34.1840023	33.4264382
69 H	42.7433768	35.0356906	34.5593068
70 H	44.9478082	31.9435553	28.0964087
71 H	45.5276192	33.1116995	29.1445562
72 H	46.3091328	31.5911591	28.9458094
73 H	39.3670157	28.2201183	29.6981068
74 H	39.3334655	31.4434690	35.7423921
75 H	33.7143390	29.7730994	28.8468159

A198L-TS1
QM(B1)/MM Energy = -3441.516747858313 a.u.
QM(B2)/MM Energy = -3444.086030000000 a.u.
QM(B3)/MM Energy = -3443.497264647648 a.u.

1 C	40.0824982	29.0503517	29.6772471
2 H	40.7735314	28.9542379	30.5292967
3 H	40.6803502	28.9054149	28.7634159
4 C	39.4555899	30.4104478	29.7207799
5 N	38.8249706	31.0208797	28.6507883
6 H	38.7305853	30.6427485	27.6996030
7 C	38.3213227	32.1977593	29.0685108
8 H	37.7443115	32.8791092	28.4494276
9 N	38.6015169	32.3947538	30.3513915
10 C	39.3139528	31.2912998	30.7701480
11 H	39.6965097	31.2066561	31.7831451
12 C	38.9320124	32.4709192	35.5204659
13 H	37.8788248	32.4940715	35.8194451
14 H	39.4931277	33.2005384	36.1268460
15 C	39.0984996	32.8846601	34.0499119
16 O	40.2132862	33.1412364	33.6034995
17 O	37.9975990	32.9568703	33.3641072
18 C	33.3183641	30.5591634	29.4854224
19 H	32.8981185	31.3567636	28.8539483
20 H	32.4774558	30.1016617	30.0332637
21 C	34.3136990	31.1440748	30.4305409
22 N	34.7198664	30.5430917	31.6086689
23 H	34.3985079	29.6434416	31.9820474
24 C	35.6621164	31.3176076	32.1797576
25 H	36.1792606	31.0848723	33.1068080
26 N	35.8760878	32.3956965	31.4429720
27 C	35.0378222	32.3098503	30.3555250
28 H	35.0191287	33.0857916	29.5939599
29 Fe	37.5077358	33.7520169	31.6244903
30 O	36.3470525	35.2193220	32.2808922
31 O	36.3018356	36.2831461	31.4226589
32 C	38.5669801	36.3235723	30.7367966
33 O	38.9420112	35.3626403	31.4279479
34 O	39.0589291	37.3830771	30.3993384
35 C	36.8978752	35.9695694	30.1578931
36 O	36.9349020	34.7044955	29.8886064
37 C	36.4426826	36.9914866	29.1229318
38 C	35.0997255	36.6113949	28.4943680
39 C	34.4636066	37.6698951	27.5494802
40 O	35.2185856	38.5103579	27.0046535
41 O	33.2265156	37.5473548	27.3787354
42 H	35.2262832	35.6885995	27.9009993
43 H	34.3707892	36.3613105	29.2754325
44 H	36.3902346	37.9700537	29.6214078
45 H	37.2165724	37.0866705	28.3495728
46 N	45.3999371	32.0887792	29.0152305
47 C	44.6091633	31.4941756	30.1348906
48 C	45.1365537	30.0640470	30.4645015
49 O	44.5115608	29.5006078	31.3922543
50 C	43.1084044	31.5264894	29.8405793
51 C	42.4513946	32.9058868	29.6545434
52 C	42.2151395	33.7152306	30.9322659
53 N	43.4308045	34.3639684	31.4300619
54 C	43.5606217	34.8513861	32.6689476
55 N	44.6986096	35.5181097	32.9758443
56 N	42.5893965	34.7426291	33.5744107
57 O	46.1296863	29.6471317	29.8256598
58 H	44.8242799	32.1064417	31.0218470
59 H	42.9212847	30.9237632	28.9350378
60 H	42.6248615	30.9951286	30.6729941
61 H	42.9902543	33.5184665	28.9109198
62 H	41.4569205	32.7366195	29.2137960
63 H	41.4386835	34.4775598	30.7471817
64 H	41.8141356	33.0553962	31.7156980
65 H	44.1510577	34.6109293	30.7318957
66 H	44.9030398	35.7751463	33.9346564
67 H	45.4875502	35.4480599	32.3418918
68 H	41.7450845	34.1799445	33.4153362
69 H	42.7268565	35.0259620	34.5526133
70 H	44.9485159	31.9470240	28.0905698
71 H	45.5276398	33.1142717	29.1404684

72 H	46.3100727	31.5945218	28.9388520
73 H	39.3633412	28.2316304	29.7012422
74 H	39.3063796	31.4665075	35.7181360
75 H	33.7049271	29.7698160	28.8407776

A198L-EFI
QM(B1)/MM Energy = -3441.590936912901 a.u.
QM(B2)/MM Energy = -3444.158916000000 a.u.
QM(B3)/MM Energy = -3443.557405633113 a.u.

1 C	40.1439077	28.9210950	29.6926310
2 H	40.8306318	28.7986741	30.5445730
3 H	40.7323213	28.7371410	28.7798054
4 C	39.5815322	30.3084053	29.7276290
5 N	38.9558498	30.9369521	28.6667289
6 H	38.8365109	30.5661209	27.7157287
7 C	38.4996689	32.1326721	29.0889885
8 H	37.9430988	32.8313865	28.4692535
9 N	38.8103924	32.3234032	30.3641374
10 C	39.4931312	31.1970228	30.7752208
11 H	39.8839653	31.0994632	31.7861933
12 C	39.0126592	32.3151627	35.7476611
13 H	37.9776441	32.3455366	36.1051617
14 H	39.6120640	33.0334214	36.3312685
15 C	39.1176711	32.7316761	34.2777116
16 O	40.2235561	32.8707447	33.7551513
17 O	37.9831588	32.9324853	33.6844591
18 C	33.4484699	30.7114269	29.5268415
19 H	33.0492011	31.5185738	28.8932709
20 H	32.5965361	30.2983473	30.0927999
21 C	34.4710902	31.2688926	30.4643408
22 N	34.8079449	30.6860021	31.6720980
23 H	34.4472402	29.8007929	32.0455681
24 C	35.7557126	31.4457567	32.2603061
25 H	36.2227062	31.2213860	33.2165132
26 N	36.0460517	32.4991724	31.5105597
27 C	35.2472284	32.4048744	30.3912951
28 H	35.2833285	33.1473722	29.5964468
29 Fe	37.9175128	33.5682728	31.8054567
30 O	37.4797558	35.7948473	31.6848899
31 O	36.6364606	36.6239968	30.8937904
32 C	38.9042287	36.0826615	31.4280721
33 O	39.5306727	35.0939593	31.8360969
34 O	39.1888039	37.1361744	30.8906377
35 C	36.6549697	36.2234645	29.5821279
36 O	37.1847500	35.1980330	29.2250019
37 C	35.9123360	37.2247278	28.7591394
38 C	34.6295071	36.6408856	28.1745451
39 C	33.9000863	37.6654088	27.2704406
40 O	34.6370757	38.4907759	26.6737876
41 O	32.6583057	37.5571117	27.2041035
42 H	34.8770086	35.7515088	27.5713375
43 H	33.9566705	36.2919085	28.9672315
44 H	35.6981170	38.1121928	29.3701092
45 H	36.5590534	37.5463087	27.9290542
46 N	45.4870146	32.0284179	29.0595469
47 C	44.6954771	31.4346020	30.1807191
48 C	45.2370323	30.0204082	30.5374256
49 O	44.6197395	29.4735076	31.4794281
50 C	43.2004151	31.4339533	29.8635473
51 C	42.5371297	32.8019734	29.6400849
52 C	42.2639247	33.6246150	30.8996088
53 N	43.4599482	34.2788399	31.4390510
54 C	43.5420145	34.7578090	32.6853942
55 N	44.6637583	35.4356018	33.0350875
56 N	42.5482486	34.6314556	33.5627538
57 O	46.2276465	29.5936660	29.9000531
58 H	44.8841309	32.0635561	31.0617307
59 H	43.0368941	30.8087571	28.9689759
60 H	42.7108010	30.9150142	30.6999224
61 H	43.0873992	33.4086739	28.9006598
62 H	41.5548179	32.6203510	29.1781341
63 H	41.4994486	34.3856385	30.6840458
64 H	41.8365869	32.9737844	31.6774024
65 H	44.1924639	34.5463357	30.7618040
66 H	44.8312300	35.6749024	34.0057283
67 H	45.4828822	35.3465517	32.4429242
68 H	41.7039562	34.0797297	33.3732751
69 H	42.6619482	34.9123227	34.5443928
70 H	45.0342713	31.8929428	28.1342342
71 H	45.6122132	33.0545341	29.1844852
72 H	46.3970916	31.5353187	28.9832268
73 H	39.3795102	28.1448435	29.7272294
74 H	39.3889668	31.3038462	35.9016042
75 H	33.7812721	29.8965525	28.8839655

A198L-TS2
QM(B1)/MM Energy = -3441.573577093435 a.u.
QM(B2)/MM Energy = -3444.144387000000 a.u.
QM(B3)/MM Energy = -3443.554999645384 a.u.

1 C	40.1407247	28.9212865	29.6991289
2 H	40.8329921	28.7925952	30.5454779
3 H	40.7201247	28.7385980	28.7806105
4 C	39.5866351	30.3109744	29.7450581
5 N	38.9632657	30.9594853	28.6941551
6 H	38.8435797	30.6025210	27.7374844
7 C	38.5155822	32.1528560	29.1318303
8 H	37.9605533	32.8697856	28.5307602
9 N	38.8294074	32.3184956	30.4109892
10 C	39.5050042	31.1831347	30.8053129
11 H	39.8969836	31.0681037	31.8129627
12 C	38.9993594	32.2723228	35.7777880
13 H	37.9431885	32.2801597	36.0680630
14 H	39.5472805	32.9943372	36.4044155
15 C	39.1974867	32.7013346	34.3259830
16 O	40.3196616	32.8956462	33.8771336
17 O	38.0860596	32.8432005	33.6573462
18 C	33.4706334	30.7784144	29.5451435
19 H	33.0952624	31.5955685	28.9096893
20 H	32.6047558	30.3861109	30.1049391
21 C	34.4983501	31.3111859	30.4920406

22 N	34.8174116	30.7081768	31.6966772
23 H	34.4393533	29.8258396	32.0592944
24 C	35.7764031	31.4373823	32.2984584
25 H	36.2353317	31.1894297	33.2523333
26 N	36.0905130	32.4926648	31.5595473
27 C	35.2963489	32.4318276	30.4335900
28 H	35.3583582	33.1876060	29.6533626
29 Fe	37.9350649	33.5469691	31.8555048
30 O	37.5310220	35.4891492	31.7273822
31 O	36.5107276	36.5409675	30.8242577
32 C	38.8716733	35.9251624	31.5163205
33 O	39.6081484	34.9437022	31.8025256
34 O	39.1205788	37.0465070	31.1137801
35 C	36.5659970	36.1430197	29.5664594
36 O	37.0470256	35.0966897	29.1614429
37 C	35.8960005	37.1788678	28.6869360
38 C	34.5765088	36.6382924	28.1485834
39 C	33.8533318	37.6657581	27.2495240
40 O	34.5920552	38.4859317	26.6472863
41 O	32.6096191	37.5687303	27.1919634
42 H	34.7694728	35.7251130	27.5603274
43 H	33.9178117	36.3332825	28.9707813
44 H	35.7366365	38.1114950	29.2450716
45 H	36.5727184	37.4054023	27.8494381
46 N	45.5257017	31.9960176	29.0741161
47 C	44.7273651	31.4110049	30.1949826
48 C	45.2607403	29.9974062	30.5617559
49 O	44.6330124	29.4571366	31.5005759
50 C	43.2333633	31.4157936	29.8754842
51 C	42.5736966	32.7873943	29.6708207
52 C	42.3313564	33.6040477	30.9400677
53 N	43.5341768	34.2736195	31.4447599
54 C	43.6217162	34.7950377	32.6727746
55 N	44.7505411	35.4694648	33.0018993
56 N	42.6221607	34.7073187	33.5494790
57 O	46.2561901	29.5645998	29.9357266
58 H	44.9153923	32.0422301	31.0745580
59 H	43.0685866	30.8014890	28.9737839
60 H	42.7438504	30.8884645	30.7067447
61 H	43.1116341	33.3939495	28.9224406
62 H	41.5813410	32.6131243	29.2277736
63 H	41.5492054	34.3533984	30.7530175
64 H	41.9412052	32.9445114	31.7310876
65 H	44.2546561	34.5323654	30.7513717
66 H	44.9144994	35.7577319	33.9597205
67 H	45.5708353	35.3443412	32.4179781
68 H	41.7703169	34.1729387	33.3560517
69 H	42.7342971	34.9873700	34.5315136
70 H	45.0731750	31.8658610	28.1478343
71 H	45.6593848	33.0212728	29.1971081
72 H	46.4320367	31.4962833	29.0016163
73 H	39.3727846	28.1488130	29.7393784
74 H	39.3815553	31.2641905	35.9379835
75 H	33.7896602	29.9561759	28.9046649

A198L-EFII

QM(B1)/MM Energy = -3441.605526634069 a.u.
QM(B2)/MM Energy = -3444.174011000000 a.u.
QM(B3)/MM Energy = -3443.578277505414 a.u.

1 C	40.1489018	28.8763623	29.6714382
2 H	40.8183512	28.7651234	30.5384432
3 H	40.7563092	28.6903362	28.7719914
4 C	39.5725133	30.2579121	29.6819691
5 N	38.9574968	30.8635954	28.6006978
6 H	38.8567656	30.4838448	27.6511827
7 C	38.4621347	32.0479923	28.9966844
8 H	37.8980671	32.7263829	28.3635389
9 N	38.7354558	32.2532668	30.2786232
10 C	39.4345326	31.1513304	30.7193672
11 H	39.8029464	31.0739227	31.7376457
12 C	38.8872249	32.3795085	35.4955608
13 H	37.8120992	32.3698043	35.7050905
14 H	39.3738156	33.1223068	36.1482560
15 C	39.1829060	32.8048975	34.0477179
16 O	40.3271672	33.0887737	33.7200140
17 O	38.1480865	32.8482296	33.2537361
18 C	33.4150227	30.6537310	29.5291203
19 H	32.9864328	31.4482235	28.8989254
20 H	32.5826873	30.2207759	30.1091214
21 C	34.4391627	31.2462778	30.4417002
22 N	34.8481957	30.6807230	31.6380627
23 H	34.5275292	29.7879060	32.0309553
24 C	35.7875435	31.4771052	32.1851631
25 H	36.3144880	31.2704651	33.1126870
26 N	36.0048767	32.5386739	31.4176525
27 C	35.1639044	32.4087375	30.3317903
28 H	35.1455331	33.1458033	29.5344960
29 Fe	37.8440084	33.7166181	31.5091311
30 O	37.6271632	35.6369615	32.1873149
31 O	36.4591328	36.5784836	30.6316008
32 C	38.8201569	36.0063913	31.6575779
33 O	39.4697610	34.9500593	31.2709427
34 O	39.1773766	37.1670507	31.5304397
35 C	36.5945945	35.7941059	29.6462864
36 O	37.0627427	34.6238235	29.7087241
37 C	36.0951474	36.3749722	28.3299083
38 C	34.5873195	36.6068687	28.3946022
39 C	33.9981035	37.5762927	27.3397789
40 O	34.7850214	38.3685569	26.7677289
41 O	32.7579078	37.4943885	27.1987940
42 H	34.0352763	35.6567943	28.3532003
43 H	34.3610640	37.0553418	29.3715890
44 H	36.5782028	37.3485649	28.1539129
45 H	36.3902745	35.6824292	27.5278293
46 N	45.5190165	31.9871730	29.0382731
47 C	44.7134785	31.3973223	30.1497485
48 C	45.2355669	29.9741366	30.4975577
49 O	44.5983815	29.4206085	31.4224007
50 C	43.2189320	31.4251404	29.8336547
51 C	42.5705304	32.8082682	29.6709840
52 C	42.3537567	33.5979011	30.9630343

53 N	43.5614123	34.2829697	31.4382185
54 C	43.6698552	34.8100508	32.6607785
55 N	44.8016921	35.4899028	32.9700046
56 N	42.6825988	34.7245470	33.5517235
57 O	46.2357466	29.5488159	29.8743107
58 H	44.9105930	32.0154664	31.0366818
59 H	43.0453127	30.8371679	28.9160031
60 H	42.7262506	30.8801616	30.6516571
61 H	43.1036602	33.4259058	28.9283707
62 H	41.5705257	32.6538806	29.2379282
63 H	41.5486250	34.3319419	30.8128217
64 H	42.0043919	32.9159580	31.7539331
65 H	44.2806143	34.5213335	30.7366854
66 H	44.9879036	35.7623947	33.9285737
67 H	45.6101902	35.3668906	32.3696390
68 H	41.8358903	34.1730843	33.3789926
69 H	42.8000584	35.0241078	34.5271436
70 H	45.0663219	31.8697261	28.1106919
71 H	45.6630878	33.0094139	29.1725323
72 H	46.4206679	31.4786023	28.9623803
73 H	39.3854672	28.0987651	29.6954686
74 H	39.2761361	31.3851041	35.7145931
75 H	33.7615849	29.8479860	28.8820216

A198L-TS3
QM(B1)/MM Energy = -3441.579214 a.u.
QM(B2)/MM Energy = -3444.143641000000 a.u.
QM(B3)/MM Energy = -3443.554488835027 a.u.

1 C	40.2089690	28.6819609	29.7446241
2 H	40.8919918	28.5359004	30.5956392
3 H	40.7875899	28.4785908	28.8309170
4 C	39.6741902	30.0783274	29.7777271
5 N	39.0468430	30.6999673	28.7160069
6 H	38.9448411	30.3491458	27.7550892
7 C	38.5302438	31.8628305	29.1447185
8 H	37.9559552	32.5274668	28.5088823
9 N	38.8034285	32.0464251	30.4322785
10 C	39.5253351	30.9438852	30.8366799
11 H	39.8884290	30.8363706	31.8540605
12 C	39.0245409	32.2057175	35.8073564
13 H	37.9510325	32.1758241	36.0256682
14 H	39.5142573	32.9324484	36.4729176
15 C	39.3013710	32.6550147	34.3781042
16 O	40.3676370	33.1600567	34.0703457
17 O	38.3094399	32.4572160	33.5415499
18 C	33.4685651	30.7554415	29.5586360
19 H	33.0820079	31.5741516	28.9325235
20 H	32.6122720	30.3562958	30.1276158
21 C	34.5071324	31.2842953	30.4957693
22 N	34.8448908	30.6641729	31.6870139
23 H	34.4615874	29.7825739	32.0490163
24 C	35.8119083	31.3809702	32.2849965
25 H	36.2941100	31.1115611	33.2213534
26 N	36.1171286	32.4487498	31.5547190
27 C	35.3049830	32.4052605	30.4393880
28 H	35.3452452	33.1746993	29.6710739
29 Fe	38.0013959	33.3913336	31.9053865
30 O	37.5573263	35.2527218	32.4322499
31 O	39.5241885	36.0790341	28.9666061
32 C	38.6770649	35.7375424	31.9225971
33 O	39.4002957	34.7332501	31.4180598
34 O	39.0029886	36.9093358	31.8380478
35 C	38.6521831	35.3416717	29.1641956
36 O	37.6956660	34.6738713	29.2225871
37 C	36.0037966	37.3638376	27.1991184
38 C	34.7289603	37.2736215	27.9230979
39 C	33.6492089	38.1072403	27.1694911
40 O	34.0924248	39.1292540	26.5933919
41 O	32.4758233	37.6870084	27.1854936
42 H	34.3836306	36.2371212	28.0595165
43 H	34.8110498	37.7170006	28.9374325
44 H	36.3818583	38.3501140	26.9357445
45 H	36.5348405	36.4724229	26.8548711
46 N	45.4749076	32.0574954	29.0764790
47 C	44.6949018	31.4613033	30.2045156
48 C	45.2125132	30.0296387	30.5323949
49 O	44.5837458	29.4730196	31.4621411
50 C	43.1944409	31.5049757	29.9205956
51 C	42.5492575	32.8952386	29.8046784
52 C	42.3798592	33.6621862	31.1181603
53 N	43.6042222	34.3330831	31.5647902
54 C	43.7384766	34.8556096	32.7881373
55 N	44.8791481	35.5190009	33.0840412
56 N	42.7610485	34.7731155	33.6914967
57 O	46.2009149	29.6029341	29.8929618
58 H	44.9173494	32.0690274	31.0931688
59 H	42.9981567	30.9400819	28.9923558
60 H	42.7148857	30.9436404	30.7350165
61 H	43.0614533	33.5259314	29.0571841
62 H	41.5337211	32.7508021	29.4050477
63 H	41.5697900	34.3992405	31.0087993
64 H	42.0547058	32.9645166	31.9066288
65 H	44.3052357	34.5765358	30.8457911
66 H	45.0712986	35.8343243	34.0280117
67 H	45.6702765	35.4301411	32.4556281
68 H	41.9099177	34.2311522	33.5270237
69 H	42.8897230	35.0541936	34.6716189
70 H	45.0126749	31.9187931	28.1560830
71 H	45.6030429	33.0839482	29.2006411
72 H	46.3850203	31.5667963	28.9881750
73 H	39.4030178	27.9490701	29.7817867
74 H	39.4161543	31.2022694	35.9740835
75 H	33.7857767	29.9379646	28.9111984

A198L-EFIII
QM(B1)/MM Energy = -3441.602576489275 a.u.
QM(B2)/MM Energy = -3444.167260000000 a.u.
QM(B3)/MM Energy = -3443.576987750989 a.u.

1 C	40.1880754	28.7150706	29.7165030
2 H	40.8739777	28.5731794	30.5660957

3 H	40.7667070	28.5152620	28.8020521
4 C	39.6478311	30.1095419	29.7503576
5 N	39.0832495	30.7659944	28.6737143
6 H	39.0093096	30.4251642	27.7067969
7 C	38.5700745	31.9327772	29.1035675
8 H	38.0529813	32.6391891	28.4611461
9 N	38.7779936	32.0740159	30.4074471
10 C	39.4585784	30.9512040	30.8209006
11 H	39.7699708	30.8168019	31.8513778
12 C	39.0020593	32.2731655	35.7431794
13 H	37.9332173	32.2500471	35.9867212
14 H	39.5096823	32.9998888	36.3951096
15 C	39.2362604	32.7256943	34.3048555
16 O	40.2733193	33.2826257	33.9775135
17 O	38.2483120	32.4889479	33.4802311
18 C	33.4426508	30.7014671	29.5087104
19 H	33.0512514	31.5056720	28.8670769
20 H	32.5882428	30.2989133	30.0779143
21 C	34.4703497	31.2552150	30.4415051
22 N	34.8066602	30.6598292	31.6457467
23 H	34.4302260	29.7807229	32.0207589
24 C	35.7678705	31.3925581	32.2326620
25 H	36.2490268	31.1455298	33.1756310
26 N	36.0695017	32.4470759	31.4811023
27 C	35.2624765	32.3783007	30.3634995
28 H	35.3054029	33.1300186	29.5776956
29 Fe	37.9221982	33.4186013	31.8273183
30 O	37.4643843	35.2504808	32.3853966
31 O	38.7415272	36.5881636	28.8397272
32 C	38.4977370	35.7835295	31.7459590
33 O	39.1412755	34.8277422	31.0791431
34 O	38.8107866	36.9612105	31.7330067
35 C	38.0008228	35.6989489	28.7578135
36 O	37.3139990	34.7641643	28.6157311
37 C	35.7935182	37.4580255	29.1315555
38 C	34.7401682	36.7792031	28.3471691
39 C	33.9786314	37.7356053	27.3686965
40 O	34.6969178	38.5447830	26.7338046
41 O	32.7428775	37.5743460	27.2825241
42 H	35.1910625	36.0171564	27.6747833
43 H	34.0309245	36.2277447	28.9787618
44 H	36.4060092	38.2045188	28.6244855
45 H	35.9098996	37.3199055	30.2099092
46 N	45.4304840	32.0297410	29.0735777
47 C	44.6410441	31.4487059	30.2019142
48 C	45.1658577	30.0244883	30.5517288
49 O	44.5373298	29.4769949	31.4865306
50 C	43.1409087	31.4763998	29.9088039
51 C	42.4769296	32.8552601	29.7587257
52 C	42.2785809	33.6503976	31.0524255
53 N	43.4940613	34.3458409	31.4866021
54 C	43.6488630	34.8734373	32.7049208
55 N	44.7974904	35.5348486	32.9756654
56 N	42.6888232	34.8004877	33.6265521
57 O	46.1588749	29.5940315	29.9210145
58 H	44.8540625	32.0707340	31.0828274
59 H	42.9554044	30.8914786	28.9910049
60 H	42.6626622	30.9253933	30.7311067
61 H	42.9909837	33.4777729	29.0060895
62 H	41.4705434	32.6900090	29.3454675
63 H	41.4584271	34.3734002	30.9117626
64 H	41.9583890	32.9679044	31.8560180
65 H	44.1949669	34.5759539	30.7636387
66 H	45.0080710	35.8461240	33.9168562
67 H	45.5795798	35.4281100	32.3387096
68 H	41.8284082	34.2668821	33.4818908
69 H	42.8365962	35.0865801	34.6023894
70 H	44.9741150	31.8846403	28.1516498
71 H	45.5621514	33.0563307	29.1882067
72 H	46.3392181	31.5342396	28.9996726
73 H	39.3882405	27.9756186	29.7557722
74 H	39.3901831	31.2691419	35.9145380
75 H	33.7770369	29.8791354	28.8762361

A198L-TS4

QM(B1)/MM Energy = -3441.583226884309 a.u.

QM(B2)/MM Energy = -3444.153649000000 a.u.

QM(B3)/MM Energy = -3443.575344660928 a.u.

1 C	40.1400694	28.8740864	29.7091181
2 H	40.8198257	28.7732339	30.5691516
3 H	40.7371716	28.6884675	28.8028339
4 C	39.5456702	30.2476529	29.7225242
5 N	38.8816143	30.8257763	28.6578437
6 H	38.7714839	30.4427026	27.7103259
7 C	38.3610827	31.9967992	29.0670912
8 H	37.7607117	32.6376695	28.4283047
9 N	38.6711159	32.2290901	30.3379083
10 C	39.4146825	31.1465108	30.7577571
11 H	39.8184150	31.0811284	31.7649204
12 C	38.9845978	32.3366773	35.6928352
13 H	37.9216385	32.3416388	35.9592495
14 H	39.5194746	33.0573459	36.3321547
15 C	39.2124902	32.7785371	34.2439346
16 O	40.3374140	33.0585876	33.8500551
17 O	38.1347677	32.8440371	33.5137126
18 C	33.4546036	30.7575494	29.5298277
19 H	33.0515325	31.5530607	28.8842873
20 H	32.6048028	30.3536540	30.1060349
21 C	34.4754338	31.3376805	30.4559883
22 N	34.8603762	30.7454511	31.6464638
23 H	34.5292454	29.8469747	32.0171168
24 C	35.7842624	31.5331015	32.2335797
25 H	36.2891213	31.3034003	33.1688006
26 N	36.0165695	32.6137016	31.4991644
27 C	35.1989285	32.5089114	30.3931305
28 H	35.1714290	33.2784777	29.6233198
29 Fe	37.9213123	33.6722717	31.7624410
30 O	37.3950663	35.5738554	31.8258788
31 O	40.7284589	34.8175748	28.6739962
32 C	38.6062811	36.0078579	31.4975253
33 O	39.4174320	34.9725154	31.3083854

34 O	38.9448755	37.1772404	31.3668598
35 C	39.5744189	34.9175559	28.7542779
36 O	38.4143886	35.0289080	28.7090627
37 C	35.3038445	37.4717284	29.5616641
38 C	34.7803305	36.7647604	28.4111768
39 C	34.0097324	37.7344610	27.4090728
40 O	34.7106493	38.6292357	26.8938556
41 O	32.8021910	37.4838810	27.2416613
42 H	35.6206436	36.3875171	27.7898015
43 H	34.1342352	35.9183063	28.6837430
44 H	35.9415808	38.3434122	29.4048742
45 H	35.1780549	37.1097504	30.5837047
46 N	45.4757920	32.0895107	29.0708556
47 C	44.7710743	31.4506915	30.2246414
48 C	45.3573595	30.0427443	30.5210460
49 O	44.8137452	29.4731972	31.4971743
50 C	43.2633364	31.4180726	29.9887283
51 C	42.5582548	32.7746538	29.8719998
52 C	42.3722225	33.5492549	31.1775373
53 N	43.5608877	34.3083361	31.5830638
54 C	43.6808175	34.8508423	32.7975038
55 N	44.7947986	35.5680324	33.0786468
56 N	42.7131649	34.7347405	33.7072775
57 O	46.3016465	29.6375754	29.8086702
58 H	44.9899891	32.0679685	31.1068552
59 H	43.0682695	30.8330319	29.0724252
60 H	42.8328971	30.8464259	30.8238144
61 H	43.0240588	33.4197181	29.1074423
62 H	41.5482745	32.5801241	29.4883690
63 H	41.5188497	34.2375651	31.0811297
64 H	42.1174443	32.8455552	31.9849592
65 H	44.2426020	34.5708918	30.8525717
66 H	44.9770748	35.8944300	34.0205703
67 H	45.5939011	35.4807465	32.4599154
68 H	41.8708837	34.1759192	33.5397750
69 H	42.8362814	35.0280725	34.6839754
70 H	44.9778185	31.9388671	28.1713520
71 H	45.5662755	33.1194533	29.1986734
72 H	46.3997132	31.6369387	28.9268820
73 H	39.3800259	28.0937925	29.7483905
74 H	39.3643785	31.3297419	35.8657940
75 H	33.7827306	29.9319171	28.8983761

A198L-EFIV
QM(B1)/MM Energy = -3441.695045307911 a.u.
QM(B2)/MM Energy = -3444.272461000000 a.u.
QM(B3)/MM Energy = -3443.670768906480 a.u.

1 C	40.1421005	28.9512887	29.6764768
2 H	40.8323785	28.8461646	30.5278199
3 H	40.7300435	28.7743068	28.7623485
4 C	39.5455985	30.3243547	29.7091599
5 N	38.8974155	30.9318398	28.6501213
6 H	38.7921791	30.5611284	27.6968771
7 C	38.3900529	32.1034639	29.0814424
8 H	37.7973960	32.7674798	28.4574365
9 N	38.6903637	32.3043646	30.3570893
10 C	39.4177956	31.2050651	30.7598121
11 H	39.8106092	31.1172841	31.7697722
12 C	39.0870049	32.4306866	35.6859158
13 H	38.0846276	32.4989724	36.1247436
14 H	39.7550858	33.1333673	36.2096934
15 C	39.0541434	32.8350514	34.2094553
16 O	40.0953240	33.1451732	33.6139057
17 O	37.8898996	32.8616157	33.6636561
18 C	33.4047397	30.7410448	29.4985243
19 H	32.9993056	31.5332341	28.8503824
20 H	32.5529920	30.3189071	30.0581371
21 C	34.4006025	31.3288172	30.4455104
22 N	34.7507103	30.7451392	31.6495085
23 H	34.4159512	29.8464939	32.0154762
24 C	35.6589165	31.5359038	32.2571991
25 H	36.1331195	31.3165923	33.2109526
26 N	35.9143200	32.6101358	31.5215494
27 C	35.1283429	32.4980469	30.3935942
28 H	35.1253898	33.2629644	29.6184480
29 Fe	37.8153860	33.6034807	31.7832420
30 O	37.0258244	36.1518666	29.9805504
31 O	43.4616007	34.5544904	26.6230384
32 C	38.1936932	36.3554925	30.6373108
33 O	38.4925364	35.3979359	31.4419435
34 O	38.8729453	37.3677851	30.4559616
35 C	42.3981424	34.7268386	27.0528426
36 O	41.3373094	34.9042778	27.5003103
37 C	36.5136504	37.1986868	29.1199524
38 C	35.2287507	36.7072277	28.4804014
39 C	34.5141923	37.7354638	27.5552723
40 O	35.2301669	38.6126885	27.0114791
41 O	33.2827571	37.5659607	27.3959866
42 H	35.4499984	35.8146720	27.8651996
43 H	34.5216803	36.3746978	29.2530403
44 H	37.2630166	37.4611721	28.3615531
45 H	36.3416695	38.1016229	29.7276737
46 N	45.3092998	32.0284728	28.9608571
47 C	44.6371898	31.4488993	30.1674548
48 C	45.2293183	30.0495636	30.5094399
49 O	44.7062747	29.5221735	31.5195388
50 C	43.1187477	31.4162874	29.9934612
51 C	42.4268381	32.7682094	29.7616644
52 C	42.1661139	33.6364115	30.9937131
53 N	43.3699114	34.3133663	31.4800712
54 C	43.4937486	34.8055588	32.7186897
55 N	44.6259019	35.4872648	33.0209205
56 N	42.5276157	34.6885008	33.6269499
57 O	46.1585002	29.6176755	29.7942562
58 H	44.8937881	32.1049144	31.0104351
59 H	42.8842132	30.7532966	29.1427199
60 H	42.7124413	30.9268728	30.8900596
61 H	42.9823650	33.3507914	29.0109800
62 H	41.4428387	32.5736379	29.3125401
63 H	41.3918697	34.3859639	30.7517949
64 H	41.7552149	33.0116177	31.7995053

65 H 44.0809360 34.5684536 30.7763535
66 H 44.8227637 35.7455325 33.9814009
67 H 45.4297214 35.3785368 32.4110865
68 H 41.6717238 34.1379176 33.4744068
69 H 42.6696140 34.9799434 34.6024340
70 H 44.7946479 31.8383242 28.0773226
71 H 45.4084238 33.0615503 29.0405548
72 H 46.2331590 31.5713470 28.8168282
73 H 39.3896566 28.1638304 29.7189592
74 H 39.4367305 31.4098174 35.8394907
75 H 33.7581852 29.9239507 28.8696359

WT-EFIV Snapshot

WT-EFIV-RC

QM(B1)/MM Energy = -3330.325061289574 a.u.
QM(B2)/MM Energy = -3332.771315000000 a.u.
QM(B3)/MM Energy = -3332.149926259021 a.u.

1 C 31.9272067 49.5304678 36.8057964
2 H 32.3852376 49.1744429 35.8728335
3 H 32.1645902 50.6013551 36.8710753
4 C 32.4905213 48.7375827 37.9440979
5 N 32.3379343 49.0449326 39.2850657
6 H 31.8694587 49.8627148 39.6893922
7 C 32.8911324 48.0607655 40.0167430
8 H 32.9000490 48.0266695 41.1047089
9 N 33.4094997 47.1300448 39.2280652
10 C 33.1751425 47.5425983 37.9335133
11 H 33.5033746 46.9598054 37.0752815
12 C 34.1754842 42.9678019 36.2576211
13 H 33.4210128 42.2136033 36.5217164
14 H 35.1226117 42.4676301 36.0052133
15 C 34.4550691 43.8877868 37.4393183
16 O 35.4528327 44.6430529 37.4302986
17 O 33.6426045 43.8100750 38.4188679
18 C 28.3294440 45.8394819 41.5641231
19 H 28.4987497 45.9556413 42.6430542
20 H 27.5357263 45.0879025 41.4422126
21 C 29.5769989 45.3613533 40.9012079
22 N 29.5870404 44.6269242 39.7284536
23 H 28.7810513 44.3375987 39.1668826
24 C 30.8634356 44.3350610 39.4143840
25 H 31.1690087 43.7770310 38.5320798
26 N 31.6844882 44.8327949 40.3283038
27 C 30.8991465 45.4688799 41.2663208
28 H 31.3422986 45.9522912 42.1351524
29 Fe 33.7065709 45.1637162 39.8897831
30 O 35.7708474 45.3798172 43.3505649
31 C 34.8036722 45.6963183 42.4554539
32 O 35.1114580 45.2678829 41.2698689
33 O 33.7944816 46.3197303 42.7627175
34 C 35.5264952 45.6903931 44.7408009
35 C 34.6666056 44.6399459 45.4180178
36 C 34.3246168 44.9669354 46.8876407
37 O 34.8563317 45.9806779 47.4022741
38 O 33.5205231 44.1831166 47.4500338
39 H 33.7138566 44.5292156 44.8758041
40 H 35.1588291 43.6515800 45.3863438
41 H 36.5202747 45.7486064 45.2030642
42 H 35.0493116 46.6755029 44.8042521
43 N 38.1963503 51.7341226 35.2814595
44 C 37.1628868 50.6923715 34.9780361
45 C 35.7857255 51.3999562 34.7511447
46 O 34.7868967 50.6584336 34.7525340
47 C 37.1607926 49.5826521 36.0346717
48 C 38.2912045 48.5472790 35.8899421
49 C 38.2537712 47.4806308 36.9976000
50 N 39.3012005 46.4656744 36.8821030
51 C 39.1515412 45.2000062 36.4483504
52 N 40.2244078 44.4017115 36.3621361
53 N 37.9617440 44.7415859 36.0390017
54 O 35.8061848 52.6425092 34.5341405
55 H 37.4454794 50.2760766 33.9957935
56 H 37.1783912 50.0425834 37.0385444
57 H 36.1854786 49.0814564 35.9523612
58 H 38.2058485 48.0492934 34.9093546
59 H 39.2807493 49.0385106 35.9094787
60 H 38.3639531 47.9603801 37.9831582
61 H 37.2727276 46.9873903 37.0268127
62 H 40.2428547 46.7652839 37.1309942
63 H 41.1620727 44.7039963 36.6421937
64 H 40.0825560 43.3968329 36.2356104
65 H 37.9056277 43.8010432 35.6374272
66 H 37.0765800 45.0373811 36.4635140
67 H 38.2043601 52.4706083 34.5536502
68 H 38.0300419 52.2223598 36.1825772
69 H 39.1706718 51.3783700 35.3661175
70 O 37.7283929 44.5263350 39.1862082
71 H 36.9637435 44.2933195 38.6285819
72 H 37.4720180 45.4542054 39.4280227
73 H 30.8420682 49.4748450 36.7194970
74 H 33.8062856 43.5233178 35.3955528
75 H 27.8844813 46.7517260 41.1667743

WT-EFIV-TS1

QM(B1)/MM Energy = -3330.319177161306 a.u.
QM(B2)/MM Energy = -3332.761371000000 a.u.
QM(B3)/MM Energy = -3332.139727878517 a.u.

1 C 31.9601773 49.4783372 36.7949025
2 H 32.4043849 49.1188297 35.8562184
3 H 32.2078135 50.5475683 36.8576801
4 C 32.5377454 48.6828201 37.9250167
5 N 32.3912015 48.9739996 39.2702092
6 H 31.9058961 49.7763483 39.6857947
7 C 32.9872641 47.9995661 39.9852104
8 H 32.9998080 47.9555183 41.0736816
9 N 33.5276767 47.0936087 39.1826184
10 C 33.2617012 47.5106765 37.8954633
11 H 33.6025504 46.9474470 37.0290171
12 C 34.0701089 42.9959515 36.0905453
13 H 33.3094734 42.2782784 36.4267758
14 H 34.9993978 42.4527562 35.8567375

15 C	34.4180057	43.9932346	37.1831970
16 O	35.3249403	44.8378025	36.9821317
17 O	33.7876378	43.8769881	38.2813203
18 C	28.4941557	45.7887532	41.5389490
19 H	28.6728112	45.9044697	42.6170057
20 H	27.7231384	45.0117676	41.4250961
21 C	29.7452864	45.3439816	40.8534903
22 N	29.7507618	44.6278696	39.6685056
23 H	28.9405769	44.3456691	39.1093442
24 C	31.0284299	44.3385810	39.3488026
25 H	31.3256464	43.7958898	38.4546774
26 N	31.8561140	44.8183006	40.2657784
27 C	31.0710156	45.4425893	41.2146869
28 H	31.5166302	45.9144988	42.0896378
29 Fe	33.9434605	45.1116212	39.8525613
30 O	35.7435015	45.4981838	43.5085778
31 C	34.7360758	45.8707414	42.6684072
32 O	35.0026058	45.4895634	41.4625605
33 O	33.7585857	46.4969404	43.0504023
34 C	35.5417894	45.7275434	44.9171310
35 C	34.6492462	44.6764688	45.5476997
36 C	34.2806631	44.9737390	47.0148289
37 O	34.7552711	46.0117440	47.5408286
38 O	33.5089121	44.1511886	47.5649276
39 H	33.7038091	44.6102967	44.9858951
40 H	35.1131773	43.6756927	45.4955541
41 H	36.5462140	45.7179980	45.3608645
42 H	35.1078723	46.7233815	45.0563522
43 N	38.1936169	51.7306237	35.2843386
44 C	37.1619576	50.6889136	34.9742438
45 C	35.7865782	51.3979271	34.7380273
46 O	34.7887261	50.6556661	34.7292749
47 C	37.1489697	49.5804139	36.0322589
48 C	38.2696176	48.5335701	35.8922989
49 C	38.2201650	47.4716803	37.0044674
50 N	39.2753110	46.4584779	36.9112388
51 C	39.1450614	45.1892938	36.4731013
52 N	40.2214454	44.3888453	36.4418244
53 N	37.9726591	44.7111583	36.0534896
54 O	35.8093366	52.6409535	34.5251647
55 H	37.4506480	50.2723060	33.9939746
56 H	37.1716655	50.0426990	37.0345367
57 H	36.1687783	49.0884140	35.9522557
58 H	38.1833489	48.0342821	34.9123226
59 H	39.2637209	49.0156483	35.9139420
60 H	38.3158873	47.9574371	37.9887585
61 H	37.2400535	46.9740738	37.0263190
62 H	40.2182384	46.7780447	37.1308703
63 H	41.1545435	44.6915532	36.7355218
64 H	40.0938553	43.3912375	36.2551490
65 H	37.9098857	43.7659919	35.6634843
66 H	37.0566386	45.1094710	36.2797874
67 H	38.2044223	52.4670166	34.5562164
68 H	38.0212392	52.2200179	36.1837126
69 H	39.1679272	51.3761626	35.3737880
70 O	36.6582635	44.5033127	39.3210912
71 H	36.3146134	44.5962315	38.4084798
72 H	36.7765298	45.4512927	39.5855938
73 H	30.8740788	49.4362302	36.7131455
74 H	33.6971631	43.5141485	35.2071143
75 H	28.0100286	46.6896665	41.1620628

WT1-EFIV-IM1

QM(B1)/MM Energy = -3330.320953294473 a.u.

QM(B2)/MM Energy = -3332.760309000000 a.u.

QM(B3)/MM Energy = -3332.139735150667 a.u.

1 C	31.9664259	49.4516695	36.7828593
2 H	32.4079498	49.0913130	35.8431647
3 H	32.2203603	50.5194180	36.8476929
4 C	32.5407607	48.6509951	37.9110082
5 N	32.4054527	48.9461955	39.2564565
6 H	31.9259608	49.7514047	39.6731630
7 C	33.0005823	47.9683870	39.9693925
8 H	33.0164191	47.9276732	41.0584423
9 N	33.5278826	47.0566175	39.1651605
10 C	33.2545836	47.4724119	37.8799478
11 H	33.5809489	46.9046247	37.0106295
12 C	34.0293840	42.9572642	36.0364904
13 H	33.2504817	42.2560974	36.3658782
14 H	34.9473964	42.3976493	35.7970740
15 C	34.3997900	43.9350502	37.1395285
16 O	35.3834176	44.7047350	36.9603923
17 O	33.7250493	43.8811388	38.2094093
18 C	28.5285435	45.7755118	41.5468678
19 H	28.7151216	45.9000819	42.6225656
20 H	27.7586589	44.9956919	41.4459134
21 C	29.7752118	45.3267807	40.8555303
22 N	29.7714417	44.6165029	39.6666982
23 H	28.9580893	44.3430804	39.1084450
24 C	31.0457308	44.3186242	39.3412024
25 H	31.3368627	43.7823939	38.4408911
26 N	31.8801660	44.7856679	40.2583273
27 C	31.1028712	45.4117706	41.2134192
28 H	31.5521844	45.8797183	42.0897517
29 Fe	33.9857819	45.0766962	39.8645808
30 O	35.6798388	45.5757628	43.5791046
31 C	34.6459729	45.9788005	42.7751728
32 O	34.8853304	45.6636388	41.5501833
33 O	33.6736608	46.5743412	43.2148561
34 C	35.5137080	45.7561728	44.9993014
35 C	34.6207238	44.6994566	45.6204507
36 C	34.2443132	44.9763934	47.0912567
37 O	34.6659647	46.0384500	47.6201319
38 O	33.5150366	44.1177617	47.6412497
39 H	33.6749029	44.6468915	45.0578588
40 H	35.0776121	43.6965357	45.5548490
41 H	36.5300928	45.7195249	45.4161681
42 H	35.0962622	46.7508389	45.1852030
43 N	38.2106950	51.7368191	35.2731481
44 C	37.1863473	50.6914966	34.9503986
45 C	35.8070801	51.3958152	34.7185401

46 O	34.8125303	50.6494168	34.7049115
47 C	37.1744147	49.5724567	35.9973066
48 C	38.3062122	48.5363386	35.8635858
49 C	38.2357869	47.4512314	36.9524836
50 N	39.3094169	46.4551419	36.8711905
51 C	39.2019097	45.1724757	36.4653834
52 N	40.2939087	44.3917656	36.4444921
53 N	38.0352346	44.6550812	36.0785463
54 O	35.8247171	52.6402345	34.5143504
55 H	37.4797593	50.2868563	33.9665350
56 H	37.1805046	50.0253215	37.0038037
57 H	36.1995926	49.0727593	35.9005530
58 H	38.2483343	48.0550245	34.8728107
59 H	39.2955127	49.0252725	35.9198965
60 H	38.2887002	47.9184637	37.9493930
61 H	37.2629726	46.9398926	36.9253648
62 H	40.2468494	46.7987196	37.0805326
63 H	41.2211883	44.7086305	36.7402718
64 H	40.1799266	43.3905273	36.2674519
65 H	37.9864809	43.7079658	35.6916670
66 H	37.1092902	45.0421369	36.2825114
67 H	38.2209086	52.4778246	34.5495299
68 H	38.0305221	52.2196720	36.1745324
69 H	39.1863461	51.3868670	35.3653372
70 O	36.2160591	44.5755735	39.4458412
71 H	36.0932223	44.6360736	38.4630812
72 H	36.5255547	45.4889728	39.6865074
73 H	30.8801294	49.4159648	36.7006875
74 H	33.6672295	43.4897921	35.1571012
75 H	28.0377469	46.6719036	41.1678329

WT-EFIV-TS2
QM(B1)/MM Energy = -3330.272325550502 a.u.
QM(B2)/MM Energy = -3332.717950000000 a.u.
QM(B3)/MM Energy = -3332.104301466555 a.u.

1 C	31.9309668	49.4963295	36.7828395
2 H	32.3685729	49.1025950	35.8549446
3 H	32.1980563	50.5621499	36.8178381
4 C	32.4803685	48.7242294	37.9428790
5 N	32.3088238	49.0820694	39.2677779
6 H	31.8346730	49.9083733	39.6443941
7 C	32.8516254	48.1309924	40.0439869
8 H	32.8461683	48.1630221	41.1280892
9 N	33.3836843	47.1668199	39.3053246
10 C	33.1638230	47.5281999	37.9896977
11 H	33.5221039	46.9157664	37.1658590
12 C	34.2564332	43.1989667	36.2242727
13 H	33.5800670	42.3897111	36.5336564
14 H	35.2443649	42.7750976	35.9896547
15 C	34.4428056	44.2012548	37.3642410
16 O	35.3364620	45.0731783	37.2902082
17 O	33.6526142	44.0573864	38.3488570
18 C	28.3582731	45.8257925	41.5917992
19 H	28.4932780	45.9273167	42.6771574
20 H	27.5750914	45.0692590	41.4365541
21 C	29.6311159	45.3647538	40.9651410
22 N	29.6959466	44.6396412	39.7870562
23 H	28.9136857	44.3519148	39.1914735
24 C	30.9881973	44.3611000	39.5247621
25 H	31.3399606	43.8265065	38.6441951
26 N	31.7693432	44.8576939	40.4753646
27 C	30.9371437	45.4791687	41.3806832
28 H	31.3235197	45.9742655	42.2693486
29 Fe	33.8094017	45.1989574	40.0287269
30 O	35.7242235	45.2813065	43.3012279
31 C	34.6610910	46.8137722	43.4022110
32 O	34.1714576	46.8848263	42.3072873
33 O	34.8034520	47.2482021	44.4856948
34 C	35.9229101	44.5755870	44.5353510
35 C	34.6544259	44.0437177	45.2029642
36 C	34.4139809	44.5576845	46.6515592
37 O	35.2082025	45.3975498	47.1271773
38 O	33.4027479	44.0716454	47.2231567
39 H	33.7655747	44.3317726	44.6157637
40 H	34.6278015	42.9419143	45.2402908
41 H	36.6528832	43.7690809	44.3395748
42 H	36.3760130	45.2956668	45.2328907
43 N	38.1851214	51.7491864	35.2465366
44 C	37.1405096	50.7151910	34.9535049
45 C	35.7697335	51.4328841	34.7241820
46 O	34.7661144	50.6983869	34.7270764
47 C	37.1223474	49.6229745	36.0271827
48 C	38.2143799	48.5478251	35.8886175
49 C	38.1419416	47.5001925	37.0132088
50 N	39.1782473	46.4681333	36.9277844
51 C	39.0206352	45.1999576	36.4904482
52 N	40.1071593	44.4203886	36.3610449
53 N	37.8228802	44.7078516	36.1781398
54 O	35.7987329	52.6753659	34.5079262
55 H	37.4180061	50.2847487	33.9760905
56 H	37.1765931	50.1043212	37.0189265
57 H	36.1308238	49.1509934	35.9741131
58 H	38.1060749	48.0399061	34.9151196
59 H	39.2203669	49.0054125	35.8961673
60 H	38.2501825	48.0002643	37.9887964
61 H	37.1528354	47.0214370	37.0390382
62 H	40.1336923	46.7813932	37.0959184
63 H	41.0523515	44.7536768	36.5718660
64 H	39.9898075	43.4160716	36.2112143
65 H	37.7733007	43.7853985	35.7342887
66 H	36.9089852	45.0487478	36.5438925
67 H	38.2007953	52.4810858	34.5143321
68 H	38.0250806	52.2448763	36.1447972
69 H	39.1555305	51.3841343	35.3349199
70 O	35.3816253	44.5066437	40.9922987
71 H	35.9778768	45.2510099	40.7398682
72 H	35.4607221	44.7716300	42.3886137
73 H	30.8438072	49.4700103	36.7089585
74 H	33.8302893	43.6749357	35.3411408
75 H	27.9182089	46.7411654	41.1961945

WT-EFIV-TS2’
QM(B1)/MM Energy = -3330.187675690165 a.u.
QM(B2)/MM Energy = -3332.630105000000 a.u.
QM(B3)/MM Energy = -3332.016741996543 a.u.

1 C	31.9592973	49.4655056	36.7779764
2 H	32.4003518	49.1098725	35.8362122
3 H	32.2168759	50.5317228	36.8515156
4 C	32.5255089	48.6542471	37.9020847
5 N	32.4592249	48.9868046	39.2446128
6 H	32.0336297	49.8222575	39.6593267
7 C	33.0252045	47.9930929	39.9588098
8 H	33.1185213	47.9984165	41.0436815
9 N	33.4546243	47.0289449	39.1573005
10 C	33.1581671	47.4318246	37.8734123
11 H	33.4273499	46.8264922	37.0107683
12 C	34.1565315	43.0141251	35.9891198
13 H	33.4534087	42.2101302	36.2489707
14 H	35.1429044	42.5811326	35.7674815
15 C	34.3233570	43.9748550	37.1597552
16 O	35.2623382	44.8023011	37.1669287
17 O	33.4691159	43.8539813	38.0917486
18 C	28.4355450	45.8013278	41.5724279
19 H	28.6062093	45.9304741	42.6501067
20 H	27.6535302	45.0353112	41.4636893
21 C	29.6847525	45.3277275	40.9053146
22 N	29.6858352	44.5885394	39.7345143
23 H	28.8757355	44.3134342	39.1715920
24 C	30.9584093	44.2798707	39.4205363
25 H	31.2611222	43.7315676	38.5298110
26 N	31.7910897	44.7684558	40.3311685
27 C	31.0107451	45.4184746	41.2652153
28 H	31.4462588	45.9110458	42.1335559
29 Fe	33.8250578	45.0094700	39.7337898
30 O	35.9867542	45.6208368	43.5544865
31 C	35.0912261	46.4202502	43.0037421
32 O	35.1027192	46.3375928	41.6635536
33 O	34.3201113	47.1629097	43.5740281
34 C	35.6138212	45.1502790	45.0450456
35 C	34.6799531	44.0564251	45.0879707
36 C	33.8858794	44.7929545	47.6712295
37 O	34.2890764	45.9168391	47.7735751
38 O	33.2483749	43.8943440	48.1277204
39 H	33.6727295	44.2328031	44.6949408
40 H	35.0431037	43.0274146	45.0279971
41 H	36.6157227	44.9115543	45.4205517
42 H	35.2494012	46.0919180	45.4697197
43 N	38.2367160	51.8103412	35.1706383
44 C	37.2052758	50.7678886	34.8570869
45 C	35.8235932	51.4696386	34.6472561
46 O	34.8315031	50.7199255	34.6319088
47 C	37.2060928	49.6549254	35.9090335
48 C	38.2805930	48.5672668	35.7320949
49 C	38.1968302	47.5134380	36.8482217
50 N	39.2122826	46.4635205	36.7655792
51 C	39.0265739	45.1767448	36.4063556
52 N	40.0986108	44.3715943	36.3169081
53 N	37.8214426	44.6839651	36.1185193
54 O	35.8312970	52.7178153	34.4622087
55 H	37.4863199	50.3629743	33.8700493
56 H	37.2914840	50.1178739	36.9069314
57 H	36.2084258	49.1942442	35.8762224
58 H	38.1478297	48.0731413	34.7550892
59 H	39.2936018	49.0089447	35.7321658
60 H	38.3105837	48.0064889	37.8262635
61 H	37.2010311	47.0500700	36.8682226
62 H	40.1678015	46.7527441	36.9710616
63 H	41.0480657	44.7029271	36.5090754
64 H	39.9628522	43.3629109	36.2195852
65 H	37.7631693	43.7487381	35.7032779
66 H	36.9114366	45.0204488	36.4815032
67 H	38.2669408	52.5432155	34.4403803
68 H	38.0537316	52.3031452	36.0659884
69 H	39.2051287	51.4462493	35.2828948
70 O	35.5877099	44.3302900	40.2805450
71 H	36.1029015	44.6400114	39.5118311
72 H	35.5016804	45.5006018	41.3201690
73 H	30.8728907	49.4285633	36.6978316
74 H	33.7602899	43.5386758	35.1196910
75 H	27.9677642	46.7020711	41.1750492

WT-EFIV-3HP
QM(B1)/MM Energy = -3330.277091333256 a.u.
QM(B2)/MM Energy = -3332.730317000000 a.u.
QM(B3)/MM Energy = -3332.115705923827 a.u.

1 C	31.9545165	49.4550575	36.7925960
2 H	32.3934689	49.0616002	35.8652231
3 H	32.2252982	50.5197671	36.8298036
4 C	32.4960317	48.6771983	37.9531807
5 N	32.3079244	49.0226831	39.2786149
6 H	31.8341536	49.8490146	39.6557623
7 C	32.8319823	48.0565078	40.0510926
8 H	32.7841164	48.0747198	41.1347165
9 N	33.3713574	47.0979622	39.3112192
10 C	33.1751632	47.4779360	37.9970773
11 H	33.5447050	46.8720994	37.1730678
12 C	34.2168779	43.1412271	36.1476743
13 H	33.5373495	42.3317738	36.4493086
14 H	35.2057268	42.7153630	35.9200106
15 C	34.3976288	44.1417931	37.2897394
16 O	35.2653128	45.0392028	37.2008109
17 O	33.6330265	43.9714442	38.2892903
18 C	28.3733367	45.7860256	41.5853105
19 H	28.5156382	45.8804469	42.6705579
20 H	27.5803075	45.0393224	41.4318366
21 C	29.6357717	45.3111370	40.9464689
22 N	29.6836223	44.6049107	39.7565761
23 H	28.8944302	44.3363924	39.1613484
24 C	30.9697849	44.3050096	39.4857390
25 H	31.3077919	43.7776153	38.5952048
26 N	31.7637075	44.7700212	40.4408507

27 C	30.9453975	45.3909666	41.3593515
28 H	31.3427940	45.8570936	42.2585487
29 Fe	33.8170591	45.0920670	39.9829840
30 O	35.9180903	45.1633188	43.5656214
31 C	34.3471533	47.0726373	43.6960539
32 O	33.8821851	46.8239678	42.6494436
33 O	34.7065693	47.4659046	44.7223240
34 C	36.1688203	44.2982508	44.6676235
35 C	34.9325684	43.7524717	45.3800013
36 C	34.4767662	44.5382533	46.6397075
37 O	35.2100308	45.4584384	47.0652458
38 O	33.3977917	44.1417261	47.1577869
39 H	34.0769260	43.6720751	44.6870550
40 H	35.1182522	42.7177220	45.7225011
41 H	36.8269132	43.4663067	44.3442996
42 H	36.7127148	44.9033860	45.4077515
43 N	38.1646494	51.7341491	35.2671513
44 C	37.1188722	50.7046732	34.9638270
45 C	35.7518305	51.4261841	34.7263933
46 O	34.7471984	50.6926721	34.7183436
47 C	37.0871685	49.6066968	36.0311712
48 C	38.1840790	48.5359194	35.9020302
49 C	38.0822819	47.4658917	37.0027657
50 N	39.1178694	46.4341256	36.9178476
51 C	38.9631015	45.1688762	36.4703414
52 N	40.0511101	44.3913712	36.3457484
53 N	37.7690984	44.6790038	36.1424358
54 O	35.7838612	52.6693116	34.5152989
55 H	37.4020532	50.2767846	33.9868736
56 H	37.1221304	50.0803569	37.0276105
57 H	36.0983213	49.1319693	35.9565767
58 H	38.1026662	48.0464003	34.9165101
59 H	39.1888636	48.9942633	35.9449708
60 H	38.1649134	47.9440532	37.9919983
61 H	37.0925285	46.9879268	36.9921073
62 H	40.0713565	46.7402646	37.1059492
63 H	40.9943365	44.7313327	36.5547310
64 H	39.9375097	43.3868506	36.1943461
65 H	37.7263952	43.7582233	35.6941809
66 H	36.8495793	45.0168104	36.4975585
67 H	38.1831165	52.4699848	34.5387537
68 H	38.0046972	52.2259768	36.1675614
69 H	39.1348528	51.3681353	35.3542046
70 O	35.3443486	44.5589215	41.0227250
71 H	35.8837283	45.3778711	40.9212164
72 H	35.5239593	44.6989121	42.7757043
73 H	30.8675573	49.4324993	36.7146356
74 H	33.7990901	43.6227728	35.2635735
75 H	27.9389520	46.7077996	41.1983870

WT-EFIV-Ethylene
QM(B1)/MM Energy = -3330.267432058443 a.u.
QM(B2)/MM Energy = -3332.713747000000 a.u.
QM(B3)/MM Energy = -3332.097851544466 a.u.

1 C	31.9480219	49.4877576	36.8374737
2 H	32.4134467	49.1238812	35.9106953
3 H	32.1983309	50.5559497	36.9045789
4 C	32.4876639	48.6897650	37.9846532
5 N	32.3138827	48.9924377	39.3236473
6 H	31.8350785	49.8061667	39.7230776
7 C	32.8615993	48.0017801	40.0567486
8 H	32.8397769	47.9702127	41.1446424
9 N	33.3953182	47.0774090	39.2740655
10 C	33.1793967	47.4977619	37.9800500
11 H	33.5398175	46.9240398	37.1286921
12 C	34.2158987	43.0825656	36.0967181
13 H	33.5189664	42.2873613	36.3958008
14 H	35.1929521	42.6346248	35.8603514
15 C	34.4327155	44.0674243	37.2409418
16 O	35.2932248	44.9659446	37.1515204
17 O	33.6967640	43.8774160	38.2660260
18 C	28.4012005	45.8016275	41.5507846
19 H	28.5695703	45.9225607	42.6293220
20 H	27.6153191	45.0403002	41.4328303
21 C	29.6519939	45.3287785	40.8867051
22 N	29.6648850	44.6472810	39.6819080
23 H	28.8602342	44.3907107	39.1032381
24 C	30.9399466	44.3306554	39.3811702
25 H	31.2462878	43.8088825	38.4766471
26 N	31.7584263	44.7608248	40.3305315
27 C	30.9706473	45.3752396	41.2823337
28 H	31.4040268	45.7862322	42.1936812
29 Fe	33.8126727	45.0619861	39.8675296
30 O	35.7336412	45.7959120	44.4732958
31 C	34.5219407	45.7016341	44.3268891
32 O	33.9032544	45.8942148	43.1746758
33 O	33.6347687	45.3445710	45.2542029
34 C	36.3035779	43.1134163	46.0432888
35 C	35.2027646	42.3657377	46.1232826
36 C	33.8117656	45.3095411	46.7135591
37 O	34.5221865	46.1780801	47.2216690
38 O	33.1227030	44.4178174	47.2104908
39 H	34.2618912	42.6926628	45.6740116
40 H	35.1885160	41.4120932	46.6584591
41 H	37.2423559	42.8056806	46.5127138
42 H	36.3114235	44.0778694	45.5290610
43 N	38.2306356	51.7760145	35.1975447
44 C	37.1929215	50.7333309	34.9091420
45 C	35.8143235	51.4416698	34.6938419
46 O	34.8174642	50.6981165	34.6949805
47 C	37.1901698	49.6463169	35.9886771
48 C	38.2554968	48.5459578	35.8382365
49 C	38.1639324	47.5017971	36.9663300
50 N	39.1963890	46.4638133	36.9039358
51 C	39.0451125	45.1898651	36.4822259
52 N	40.1286622	44.3996413	36.4036099
53 N	37.8556296	44.6995009	36.1340007
54 O	35.8308457	52.6867586	34.4920385
55 H	37.4659736	50.3050115	33.9297883
56 H	37.2905448	50.1397795	36.9699821
57 H	36.1881038	49.1944256	35.9763716

58 H	38.1273961	48.0384975	34.8671003
59 H	39.2716936	48.9797852	35.8388827
60 H	38.2598795	48.0041417	37.9426997
61 H	37.1717057	47.0287020	36.9782091
62 H	40.1467725	46.7717461	37.1063923
63 H	41.0686669	44.7233645	36.6492254
64 H	40.0062958	43.3948597	36.2577651
65 H	37.8101239	43.7703744	35.7035250
66 H	36.9352461	45.0490126	36.4581193
67 H	38.2533702	52.5003718	34.4583674
68 H	38.0564573	52.2802693	36.0883623
69 H	39.1996143	51.4126165	35.3053664
70 O	35.2181767	45.1619873	41.1842755
71 H	35.6764032	46.0244098	40.9674915
72 H	34.5303673	45.6147219	42.3743545
73 H	30.8638597	49.4485196	36.7320228
74 H	33.8050239	43.5837072	35.2203014
75 H	27.9387000	46.7078294	41.1596855

A198L-EFIV Snapshot

A198L-EFIV-RC

QM(B1)/MM Energy = -3330.510763971405 a.u.

QM(B2)/MM Energy = -3332.957082000000 a.u.

QM(B3)/MM Energy = -3332.334967387384 a.u.

1 C	30.1289996	31.4772100	41.9113133
2 H	30.0216006	32.4798526	42.3502815
3 H	30.1063343	30.7628338	42.7480893
4 C	31.4253680	31.4281290	41.1564209
5 N	32.0193577	30.2744629	40.6798719
6 H	31.6927486	29.3141935	40.8250075
7 C	33.1259218	30.6053445	39.9941132
8 H	33.7752374	29.8907427	39.4937302
9 N	33.2999155	31.9209797	40.0030371
10 C	32.2535948	32.4435048	40.7346530
11 H	32.1784741	33.5105773	40.9090877
12 C	32.4717475	36.8856400	38.8420379
13 H	32.1880345	36.8667528	37.7824347
14 H	33.2122966	37.6967604	38.9610151
15 C	33.1838891	35.6006597	39.2548208
16 O	33.4688927	35.3859329	40.4510715
17 O	33.5260696	34.8387501	38.2940850
18 C	30.9808405	29.8800926	35.2043470
19 H	31.7342227	29.1922521	34.7965318
20 H	30.3656496	30.2278639	34.3588958
21 C	31.6581081	31.0338719	35.8567859
22 N	31.0690615	32.2735999	36.0137741
23 H	30.1147403	32.5367742	35.7424971
24 C	31.9388987	33.0779134	36.6524334
25 H	31.7348655	34.1064463	36.9359915
26 N	33.0689078	32.4312363	36.9071608
27 C	32.9120586	31.1572205	36.4099483
28 H	33.7061318	30.4183428	36.4986984
29 Fe	34.3265366	32.9985752	38.5164240
30 O	37.9044990	31.5150356	38.8165844
31 C	36.6257800	31.8459701	38.6160410
32 O	36.3088719	33.0211024	39.0505177
33 O	35.7973539	31.0806808	38.0957432
34 C	38.3394078	30.2135650	38.3631621
35 C	38.5381610	30.1626002	36.8604971
36 C	39.0950000	28.8119612	36.3798971
37 O	39.6922725	28.1064952	37.2258081
38 O	38.8984070	28.5284023	35.1701980
39 H	37.5845659	30.3376230	36.3443156
40 H	39.2378807	30.9589564	36.5465706
41 H	39.2837485	30.0245382	38.8866322
42 H	37.6037967	29.4611393	38.6847095
43 N	34.3890516	32.1438048	47.1255961
44 C	33.8180469	33.4498358	47.5880381
45 C	32.2779795	33.3247864	47.4496388
46 O	31.5589719	33.9393017	48.2739929
47 C	34.3736403	34.6091299	46.7448996
48 C	35.8955749	34.5313414	46.5692860
49 C	36.5722573	35.7543435	45.9663372
50 N	36.1577446	36.0021983	44.5870879
51 C	36.7082694	36.9592953	43.8370072
52 N	37.9415917	37.4222957	44.0992445
53 N	36.0366821	37.4682252	42.8026544
54 O	31.8828195	32.6298679	46.4891417
55 H	34.0958810	33.5686250	48.6447632
56 H	33.8745869	34.6137964	45.7622726
57 H	34.0849091	35.5452648	47.2457972
58 H	36.3721552	34.3530680	47.5484241
59 H	36.1598697	33.6711124	45.9327210
60 H	36.3634075	36.6507680	46.5795984
61 H	37.6574257	35.5737945	46.0114539
62 H	35.4087233	35.4472078	44.1265333
63 H	38.5858655	36.9649968	44.7500070
64 H	38.1685088	38.3499308	43.7403011
65 H	35.0247757	37.3284125	42.7007445
66 H	36.5145593	38.0578889	42.1265370
67 H	34.1616260	31.3930138	47.8017013
68 H	33.9294605	31.8542033	46.2448431
69 H	35.4271445	32.1239200	47.0475449
70 O	34.5120311	34.4541252	42.9631572
71 H	34.2526388	34.7244329	42.0603229
72 H	33.7343233	33.9443496	43.2946779
73 H	29.2388653	31.2520614	41.3239156
74 H	31.5805017	37.1065218	39.4293702
75 H	30.2873445	29.3261058	35.8369836

A198L-EFIV-TS1

QM(B1)/MM Energy = -3330.487382 a.u.

QM(B2)/MM Energy = -3332.934200000000 a.u.

QM(B3)/MM Energy = -3332.312153924226 a.u.

1 C	29.9170202	31.5003331	41.9864967
2 H	29.7761467	32.5037459	42.4156055
3 H	29.8533328	30.7876232	42.8235091
4 C	31.2498887	31.4622619	41.2988679
5 N	31.8843785	30.3208812	40.8452676
6 H	31.5706528	29.3527266	40.9599917

7 C	33.0166979	30.6731542	40.2115017
8 H	33.7031780	29.9735741	39.7404994
9 N	33.1661487	31.9889785	40.2369514
10 C	32.0787912	32.4906690	40.9163819
11 H	31.9663463	33.5561849	41.0771286
12 C	32.2138786	36.8954296	38.6606081
13 H	31.8654728	36.7083529	37.6359560
14 H	32.9158600	37.7471295	38.5941499
15 C	33.0176558	35.7311560	39.2184315
16 O	33.1231280	35.6006388	40.4596853
17 O	33.6090726	34.9714764	38.3956381
18 C	31.1736109	29.9742356	35.3404663
19 H	31.9480225	29.2895887	34.9648624
20 H	30.6263614	30.3522129	34.4618128
21 C	31.8004847	31.1100543	36.0779930
22 N	31.1854939	32.3398520	36.2190282
23 H	30.2457706	32.5943902	35.8955737
24 C	32.0040387	33.1380686	36.9338010
25 H	31.7617930	34.1606494	37.2031310
26 N	33.1219999	32.5040446	37.2587589
27 C	33.0119214	31.2383902	36.7239866
28 H	33.8118481	30.5110574	36.8467282
29 Fe	34.3693286	33.1467404	38.9726906
30 O	37.9565483	31.5073153	38.8616218
31 C	36.6500314	31.8099976	38.7883021
32 O	36.3757478	32.9892318	39.2357279
33 O	35.7941807	31.0133017	38.3811405
34 C	38.3676541	30.2073940	38.3987384
35 C	38.4995011	30.1536706	36.8887299
36 C	39.0698797	28.8181409	36.3854689
37 O	39.6967156	28.1179020	37.2153253
38 O	38.8595174	28.5384777	35.1770390
39 H	37.5204478	30.3122868	36.4141494
40 H	39.1671278	30.9653332	36.5454272
41 H	39.3360734	30.0164060	38.8756889
42 H	37.6485631	29.4544311	38.7541673
43 N	34.4348968	32.2249866	47.1769886
44 C	33.9962675	33.6221845	47.5242847
45 C	32.4416705	33.6112748	47.4241015
46 O	31.7843613	33.7462811	48.4751994
47 C	34.6457171	34.6566013	46.5861035
48 C	36.0525172	34.2604454	46.1268460
49 C	36.8660071	35.3252633	45.4110073
50 N	36.2606462	35.8282117	44.1794788
51 C	36.7549888	36.9199877	43.5756885
52 N	37.9710152	37.3762547	43.9106177
53 N	36.0446905	37.5687495	42.6587536
54 O	31.9812810	33.4243265	46.2710085
55 H	34.2983190	33.7776473	48.5681928
56 H	33.9906732	34.8034223	45.7170825
57 H	34.6662093	35.6178958	47.1242584
58 H	36.6626345	33.9736847	46.9994903
59 H	36.0068065	33.3711777	45.4744463
60 H	37.0237240	36.1859344	46.0829289
61 H	37.8590813	34.8941785	45.2000171
62 H	35.5636015	35.2852879	43.6649779
63 H	38.6290068	36.8658878	44.5064471
64 H	38.1820282	38.3388980	43.6466872
65 H	35.0341578	37.4110137	42.5648876
66 H	36.4898885	38.2877283	42.0940817
67 H	34.1174604	31.5410162	47.8909754
68 H	34.0308519	31.9030881	46.2834369
69 H	35.4708810	32.1009257	47.1497720
70 O	34.8841708	34.0953378	41.5484503
71 H	34.2479569	34.7412563	41.1415846
72 H	34.3050379	33.5848004	42.1400122
73 H	29.0673618	31.2637718	41.3460386
74 H	31.3588011	37.1470383	39.2879857
75 H	30.4332085	29.4014565	35.8988528

A198L-EFIV-IM1
QM(B1)/MM Energy = -3330.500808219309 a.u.
QM(B2)/MM Energy = -3332.948769000000 a.u.
QM(B3)/MM Energy = -3332.328266133839 a.u.

1 C	29.9666908	31.5319825	41.9697050
2 H	29.8200081	32.5326588	42.4028460
3 H	29.9240003	30.8203327	42.8085630
4 C	31.2941332	31.5069630	41.2706072
5 N	31.9156185	30.3752264	40.7787459
6 H	31.5956032	29.4065348	40.8767434
7 C	33.0574041	30.7341846	40.1636943
8 H	33.7344817	30.0455161	39.6620225
9 N	33.2273365	32.0461411	40.2396716
10 C	32.1447863	32.5351191	40.9328675
11 H	32.0492955	33.5940494	41.1447927
12 C	32.0317884	36.9350224	38.4479593
13 H	31.6153980	36.3981474	37.5873005
14 H	32.4802680	37.8680603	38.0623283
15 C	33.1269526	36.1313926	39.1338140
16 O	33.5723396	36.5291344	40.2448380
17 O	33.5410085	35.1106088	38.5108738
18 C	31.1994971	30.0395588	35.3591341
19 H	31.9911153	29.3677992	34.9954510
20 H	30.6595876	30.4054911	34.4702963
21 C	31.7994393	31.1892518	36.1008022
22 N	31.1494897	32.3983136	36.2667886
23 H	30.1986803	32.6292928	35.9588244
24 C	31.9565930	33.2148515	36.9753225
25 H	31.6830812	34.2201347	37.2784782
26 N	33.1014259	32.6147784	37.2677289
27 C	33.0203058	31.3498295	36.7220899
28 H	33.8454037	30.6472579	36.8279827
29 Fe	34.3531329	33.2971225	38.9569369
30 O	37.9198030	31.3146778	38.7457560
31 C	36.5869255	31.5050181	38.6040004
32 O	36.2460134	32.6878037	39.0037821
33 O	35.8339668	30.6257845	38.1933679
34 C	38.4465146	30.0636800	38.2799970
35 C	38.5871366	30.0385304	36.7693426
36 C	39.1430191	28.7051013	36.2577720
37 O	39.7452601	27.9896377	37.0922854

38 O	38.9410549	28.4354541	35.0452767
39 H	37.6085006	30.2028519	36.2965024
40 H	39.2551903	30.8540475	36.4356658
41 H	39.4234947	29.9508299	38.7654711
42 H	37.7939130	29.2449719	38.6173937
43 N	34.4076386	32.2237845	47.0177965
44 C	33.8822672	33.4973927	47.6133853
45 C	32.3313055	33.4316548	47.5926599
46 O	31.7163816	33.6895261	48.6434042
47 C	34.3681900	34.7040418	46.8069771
48 C	35.8874265	34.8106877	46.6417886
49 C	36.3431735	36.1277086	46.0168961
50 N	35.9522901	36.2680422	44.6093200
51 C	36.6249269	36.9960712	43.7053445
52 N	37.9423982	37.2385684	43.8134734
53 N	35.9664909	37.4942642	42.6562359
54 O	31.8135452	33.1501036	46.4822138
55 H	34.2383500	33.5309791	48.6519874
56 H	33.8663842	34.6781937	45.8254616
57 H	33.9916662	35.5985269	47.3246589
58 H	36.3743420	34.7303138	47.6284913
59 H	36.2844030	33.9851350	46.0280596
60 H	35.9375578	36.9773774	46.5971434
61 H	37.4362952	36.1865220	46.0843620
62 H	34.9736525	36.0958060	44.3579957
63 H	38.5248680	36.8435307	44.5576700
64 H	38.2544857	38.1151005	43.3906821
65 H	34.9661371	37.3031332	42.5781488
66 H	36.4683654	37.8113615	41.8294299
67 H	34.1453367	31.4075493	47.6038060
68 H	33.9975884	32.0529573	46.0867760
69 H	35.4491750	32.1804312	46.9771633
70 O	35.0423993	34.4432439	40.8675964
71 H	34.6005937	35.3220925	40.7150716
72 H	34.6053360	34.0861425	41.6562663
73 H	29.1047728	31.2860927	41.3494608
74 H	31.2317745	37.1500282	39.1563499
75 H	30.4611310	29.4512672	35.9039237

A198L-EFIV-TS2
QM(B1)/MM Energy = -3330.454777 a.u.
QM(B2)/MM Energy = -3332.904805000000 a.u.
QM(B3)/MM Energy = -3332.292022935338 a.u.

1 C	29.9843506	31.5594182	42.0668842
2 H	29.8412845	32.5537977	42.5153019
3 H	29.9728796	30.8372284	42.8955573
4 C	31.2783226	31.5311825	41.3067699
5 N	31.9086780	30.3576502	40.9492268
6 H	31.6354302	29.4074934	41.2171606
7 C	32.9548694	30.6464859	40.1648769
8 H	33.5978169	29.8950509	39.7188452
9 N	33.0628772	31.9577640	39.9924092
10 C	32.0246671	32.5240099	40.7080197
11 H	31.8789118	33.5998491	40.7431232
12 C	32.7315164	36.9155708	38.8137877
13 H	32.4096644	36.9507530	37.7651964
14 H	33.4763596	37.7137198	38.9688907
15 C	33.4232264	35.5919734	39.1481816
16 O	34.0799757	35.4826082	40.2027523
17 O	33.3238394	34.6863160	38.2623631
18 C	30.7900202	29.7981125	35.1656437
19 H	31.5245598	29.1082483	34.7311930
20 H	30.1265179	30.1288723	34.3509858
21 C	31.5065959	30.9510271	35.7662186
22 N	30.9641974	32.2110255	35.9159792
23 H	30.0179159	32.5040307	35.6489059
24 C	31.8634969	32.9856174	36.5489732
25 H	31.7045667	34.0206731	36.8387431
26 N	32.9664626	32.2954092	36.8075278
27 C	32.7620308	31.0282968	36.3162600
28 H	33.5136586	30.2503340	36.4233597
29 Fe	34.1957048	32.8173778	38.4216638
30 O	37.4459554	31.4371972	38.7381614
31 C	36.1770045	30.1154782	38.5487848
32 O	35.1730074	30.6959229	38.2134589
33 O	36.6814212	29.0828130	38.8298033
34 C	38.7281693	30.9762244	38.3019223
35 C	38.7559312	30.5572641	36.8274574
36 C	39.2497302	29.1256251	36.5006222
37 O	39.8522450	28.4690128	37.3755125
38 O	38.9931349	28.7485097	35.3247930
39 H	37.7344942	30.6194138	36.4221898
40 H	39.3622324	31.2468247	36.2146730
41 H	39.4553814	31.7854386	38.5060440
42 H	39.0108797	30.1055243	38.9152490
43 N	34.3489442	32.1387589	46.9296998
44 C	33.8528601	33.3976546	47.5769143
45 C	32.3014185	33.3705885	47.5874730
46 O	31.7175310	33.7923938	48.6025439
47 C	34.3754113	34.6203076	46.8089749
48 C	35.9008373	34.6389475	46.6514195
49 C	36.4860198	35.8927289	46.0058945
50 N	36.1979958	35.9688508	44.5696644
51 C	36.7834063	36.8382268	43.7345541
52 N	38.0076651	37.3282020	43.9765559
53 N	36.1381513	37.2234695	42.6280949
54 O	31.7416635	32.9578776	46.5389228
55 H	34.2217006	33.3903043	48.6120670
56 H	33.8728635	34.6535413	45.8272231
57 H	34.0453201	35.5124655	47.3598203
58 H	36.3678642	34.5328492	47.6445971
59 H	36.2405271	33.7781732	46.0549115
60 H	36.1082138	36.7996753	46.5140256
61 H	37.5749513	35.8679255	46.1480692
62 H	35.3085266	35.5915206	44.2187804
63 H	38.6082519	36.9795768	44.7295368
64 H	38.2230760	38.2387624	43.5653768
65 H	35.2352798	36.7902312	42.4157679
66 H	36.6438156	37.6738140	41.8686668
67 H	34.0557861	31.3005409	47.4674481
68 H	33.9567433	32.0251948	45.9757136

69 H	35.3882725	32.0764115	46.9089827
70 O	36.1184069	33.3711267	38.3308481
71 H	36.2901378	34.1106210	38.9292288
72 H	36.8817186	32.4852243	38.4383761
73 H	29.1209348	31.3083241	41.4508224
74 H	31.8509072	37.0956176	39.4303732
75 H	30.1415281	29.2610671	35.8578195

A198L-EFIV-3HP
QM(B1)/MM Energy = -3330.473203962700 a.u.
QM(B2)/MM Energy = -3332.937023000000 a.u.
QM(B3)/MM Energy = -3332.315164181494 a.u.

1 C	29.9119570	31.5283334	42.0968719
2 H	29.7622418	32.5132322	42.5637793
3 H	29.8965211	30.7891177	42.9106062
4 C	31.2093970	31.5290385	41.3417575
5 N	31.8219671	30.3811075	40.8845713
6 H	31.5498375	29.4154078	41.0926928
7 C	32.8639994	30.7256883	40.1125373
8 H	33.4800212	30.0016607	39.5897513
9 N	32.9860736	32.0436844	40.0501465
10 C	31.9653677	32.5598826	40.8235062
11 H	31.8435507	33.6315280	40.9516545
12 C	32.5598273	36.9289296	38.8116344
13 H	32.2397107	36.9747653	37.7630655
14 H	33.3213588	37.7154837	38.9540496
15 C	33.2386017	35.6043204	39.1377234
16 O	33.6513217	35.3492942	40.2819804
17 O	33.4023804	34.8176237	38.1439181
18 C	30.8401275	29.8216300	35.1920073
19 H	31.5876879	29.1353574	34.7729024
20 H	30.1899600	30.1445303	34.3637403
21 C	31.5285023	30.9882113	35.8031725
22 N	30.9741789	32.2464840	35.9002427
23 H	30.0324691	32.5243699	35.6024481
24 C	31.8501085	33.0456360	36.5411603
25 H	31.6717996	34.0898622	36.7815442
26 N	32.9464735	32.3724453	36.8605183
27 C	32.7640003	31.0917387	36.3972142
28 H	33.5079556	30.3135695	36.5445090
29 Fe	34.1274163	32.9843183	38.5410400
30 O	38.4246392	32.0922405	38.7777390
31 C	35.5836992	28.6147874	38.3379588
32 O	34.5216757	28.6357872	37.8566480
33 O	36.6292330	28.5414479	38.8326675
34 C	38.9136372	30.8029099	38.4300041
35 C	38.6886974	30.4560984	36.9640248
36 C	39.1606028	29.0553076	36.5228735
37 O	39.8343072	28.3801339	37.3327585
38 O	38.8127508	28.7006666	35.3622401
39 H	37.6127093	30.5153600	36.7205491
40 H	39.1879888	31.2032730	36.3209548
41 H	39.9897913	30.7920340	38.6353845
42 H	38.4721307	30.0182545	39.0684060
43 N	34.3398473	32.1564245	46.8964182
44 C	33.8416216	33.3954773	47.5794401
45 C	32.2904998	33.3640950	47.6002175
46 O	31.7122710	33.7544485	48.6308287
47 C	34.3427071	34.6408863	46.8360739
48 C	35.8662541	34.7078857	46.6779097
49 C	36.3937928	36.0027937	46.0625316
50 N	36.0754140	36.1237967	44.6363955
51 C	36.7198952	36.9333353	43.7829183
52 N	37.9944056	37.3020546	43.9713416
53 N	36.0724048	37.3832040	42.7032313
54 O	31.7239121	32.9864666	46.5416440
55 H	34.2191280	33.3652378	48.6110473
56 H	33.8388889	34.6807146	45.8551712
57 H	33.9905484	35.5147648	47.4016559
58 H	36.3373650	34.5989515	47.6689439
59 H	36.2359125	33.8736518	46.0613640
60 H	35.9926447	36.8756784	46.6111162
61 H	37.4850839	36.0203968	46.1813748
62 H	35.1385117	35.8526616	44.3174892
63 H	38.5906392	36.9233697	44.7130605
64 H	38.2705630	38.1837117	43.5356242
65 H	35.1205940	37.0414481	42.5439352
66 H	36.5882755	37.7846247	41.9234982
67 H	34.0524198	31.3029539	47.4133489
68 H	33.9435611	32.0692936	45.9420316
69 H	35.3795761	32.0973886	46.8677312
70 O	35.7562254	31.9833152	38.2791157
71 H	35.9744609	31.9195852	37.3387286
72 H	37.4667648	32.1133494	38.5455428
73 H	29.0537038	31.2869914	41.4697972
74 H	31.6926125	37.1232371	39.4427050
75 H	30.1807114	29.2790733	35.8694064

References

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