Supporting information for

Alternative pathway for the reaction catalyzed by DNA dealkylase AlkB from *ab initio* QM/MM calculations

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Scheme S1. Proposed Mechanism for Direct Dealkylation of 1-meA Catalyzed by AlkB.

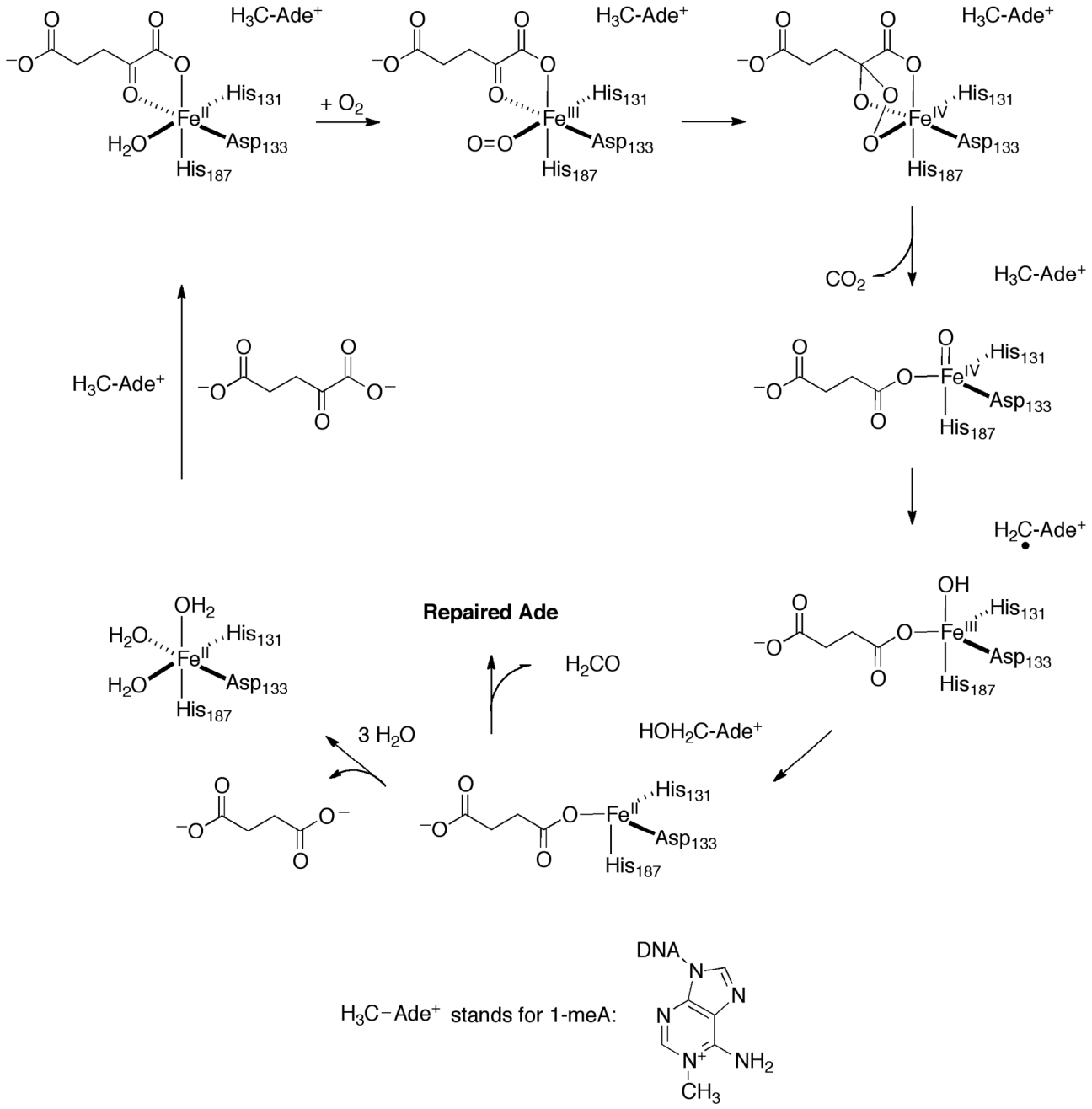


Figure S1. The active sites of crystal structures of AlkB with different substrates.

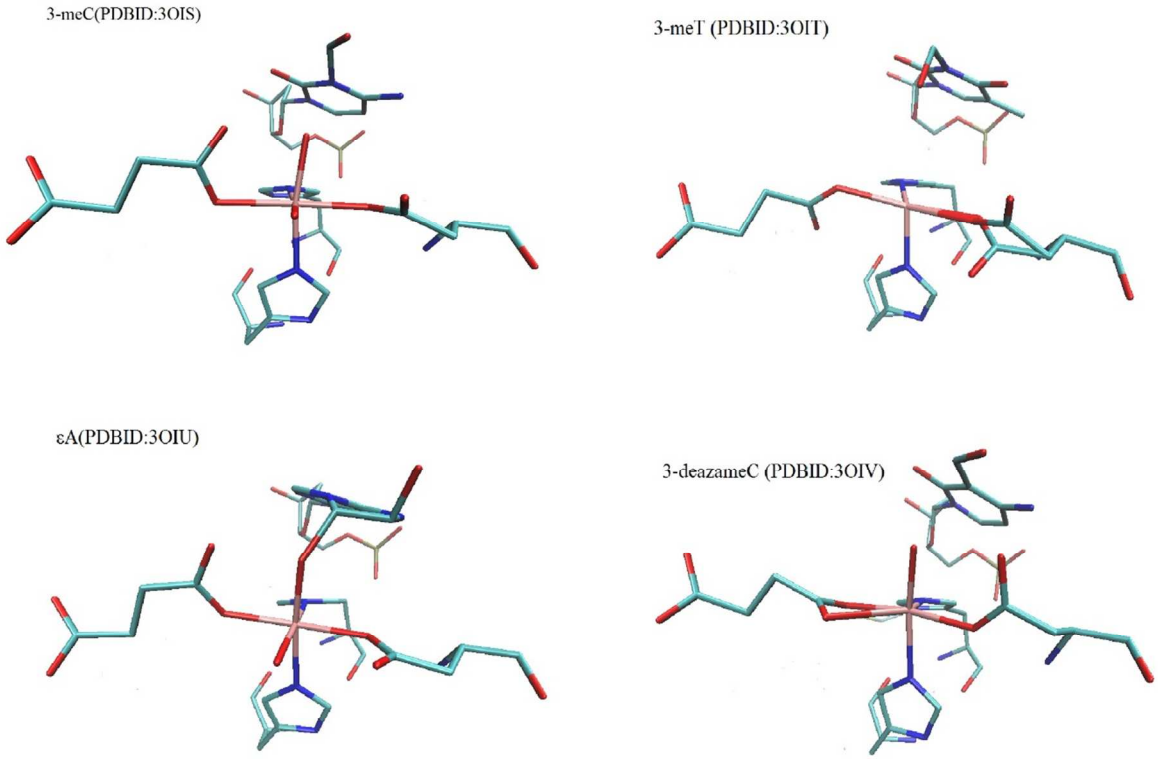


Figure S2. Electron configuration diagram of the iron(IV)-oxo moiety in the quintet and triplet states in an ideal octahedral ligand field. (HS, IS and LS represent high-spin, intermediate-spin and low-spin on Fe, respectively; AF and F stand for antiferromagnetic and ferromagnetic.)

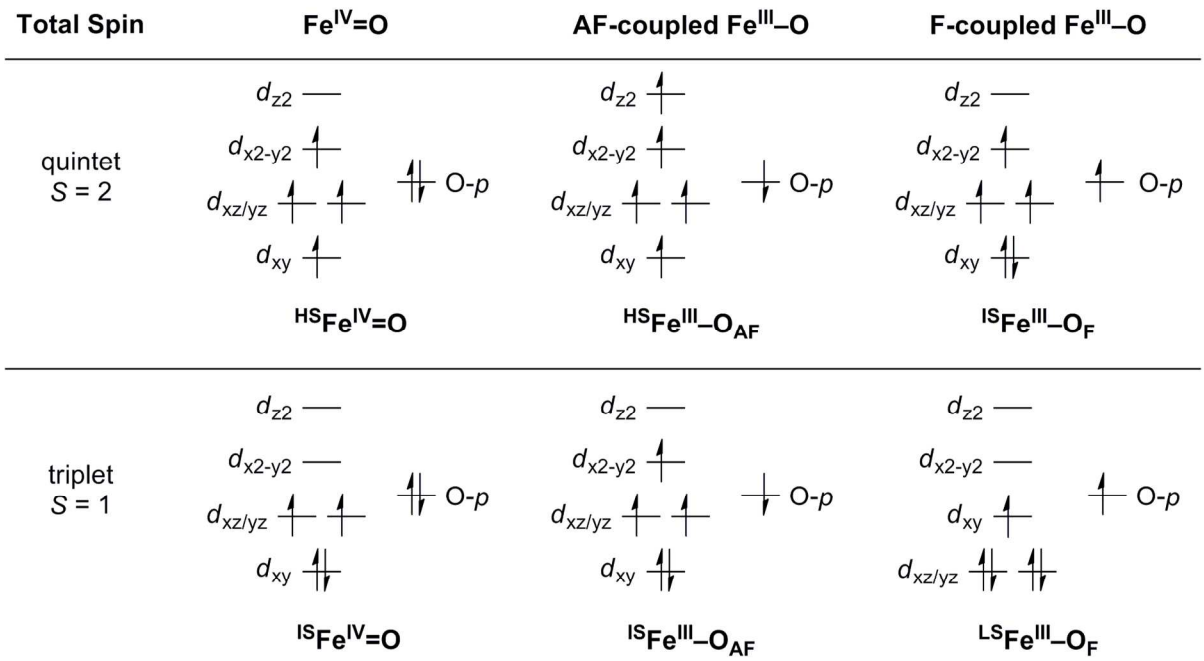


Figure S3. Relative energies (kcal/mol, the lowest state $^{IS}Fe^{III}$-O_F is taken as zero) of reactant, TS and I1 and Mulliken spin populations of key atoms (Fe, the first O is oxo, and the second O is the O of OH^- bound to the iron, and the carbon of methyl group of 1-meA) for the hydrogen abstraction step for H_2O pathway in quintet ($^{IS}Fe^{III}$-O_F and $^{HS}Fe^{III}$-O_{AF}) and triplet states ($^{LS}Fe^{III}$-O_F and $^{IS}Fe^{III}$-O_{AF}).

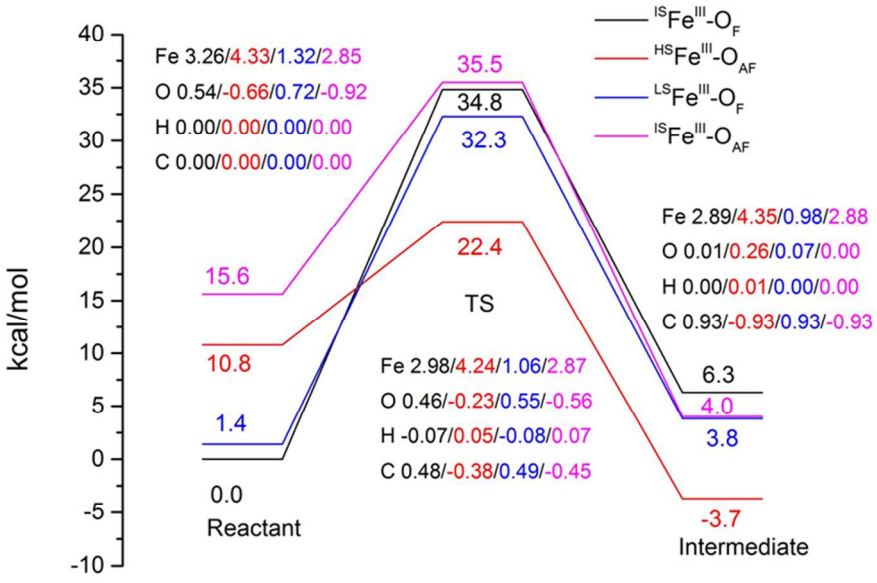


Table S1. Spin population for Fe and O (oxo) in $^{HS}Fe^{III}$-O_{AF} and $^{IS}Fe^{III}$-O_F states with different distances between Fe and O (d(Fe-O_{oxo})) for the H_2O pathway. The numbers in italics correspond to the optimized MECP. Except MECP, all other structures are obtained by only moving O with all other atoms fixed starting from the optimized $^{HS}Fe^{III}$-O_{AF} reactant.

d(Fe-O_{oxo})	Spin population (Fe, $^{HS}Fe^{III}$-O_{AF})	Spin population (O_{oxo}, $^{HS}Fe^{III}$-O_{AF})	Spin population (Fe, $^{IS}Fe^{III}$-O_F)	Spin population (O_{oxo}, $^{IS}Fe^{III}$-O_F)
1.800	4.33	-0.66	3.02	0.85
1.781	*4.32*	*-0.65*	*3.03*	*0.83*
1.780	4.32	-0.64	3.04	0.82
1.770	4.31	-0.64	3.06	0.80
1.765	4.31	-0.63	3.07	0.79
1.760	4.31	-0.63	3.08	0.78
1.740	4.29	-0.61	3.14	0.71
1.720	4.25	-0.56	3.22	0.62
1.700	4.23	-0.54	3.27	0.57
1.680	4.24	-0.54	3.27	0.56
1.660	4.23	-0.53	3.27	0.56
1.640	4.21	-0.51	3.26	0.56
1.620	4.19	-0.48	3.25	0.57
1.600	4.16	-0.45	3.24	0.57

Table S2. Atomic contributions of key atoms (O is the oxo; C is the carbon of the methyl group of 1-meA; when the contribution of the key atom is less than 1%, the atom is not shown) to the α-LUMO and β-LUMO for selected structures for the H_2O pathway.

Structure	Atomic Contribution (α-LUMO)	Atomic Contribution(β-LUMO)
$^{IS}Fe^{III}$-O_F reactant	Fe-45%,O-29%	Fe-88%, O-4%
$^{HS}Fe^{III}$-O_{AF} reactant	Fe-5%,O-86%	Fe-92%
$^{IS}Fe^{III}$-O_F MECP	Fe-85%, O-85%	Fe-92%
$^{HS}Fe^{III}$-O_{AF} MECP	Fe-54%,O-22%	Fe-21%,O-69%
$^{IS}Fe^{III}$-O_F TS	Fe-55%,O-15%	Fe-12%,O-31%,C-32%
$^{HS}Fe^{III}$-O_{AF} TS	Fe-5%,O-43%,C-28%	Fe-91%

Table S3. Atomic contributions of some key atoms (O is the oxo; C is the carbon of the methyl group of 1-meA; when the contribution of the key atom is less than 1%, the atom is not shown) to the α-LUMO and β-LUMO for selected structures for the OH^- pathway.

structure	Atomic Contribution (α-LUMO)	Atomic Contribution(β-LUMO)
$^{IS}Fe^{III}$-O_F reactant	Fe-22%,O-12%	Fe-2%
$^{HS}Fe^{III}$-O_{AF} reactant	Fe-5%,O-84%	----
$^{IS}Fe^{III}$-O_F T_{OH}	Fe-16%, O-57%	Fe-81%
$^{HS}Fe^{III}$-O_{AF} T_{OH}	Fe-5%,O-79%	----
$^{IS}Fe^{III}$-O_F TS	Fe-11%,O-2%	Fe-19%,O-23%,C-29%
$^{HS}Fe^{III}$-O_{AF} TS	Fe-2%,O-43%,C-43%	Fe-1%

Figure S4. Relative energies (kcal/mol) of the structures along the minimum energy path (MEP) shown in Scheme1b for the H_2O pathway in the quintet state. The energy of the $^{IS}Fe^{III}$-O_F reactant is taken as zero. For the TS structures, the values in parentheses are the energy differences between the TS and the immediate previous intermediate. The panel at the top right is the energy profile for the proton transfer to Glu136 starting from I2 with a different QM subsystem (Arg210, Glu136 and a bridging water are added to the QM system).

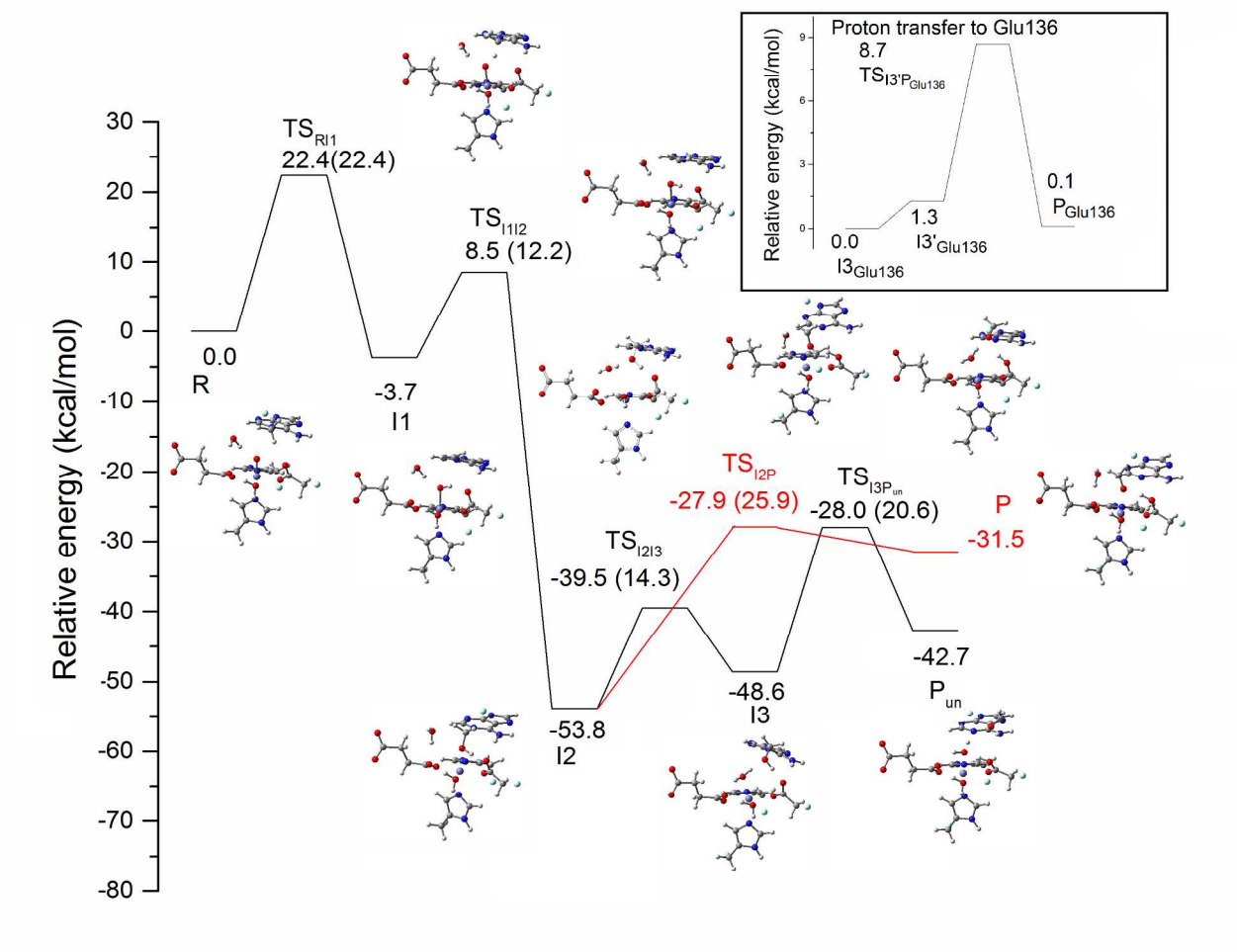
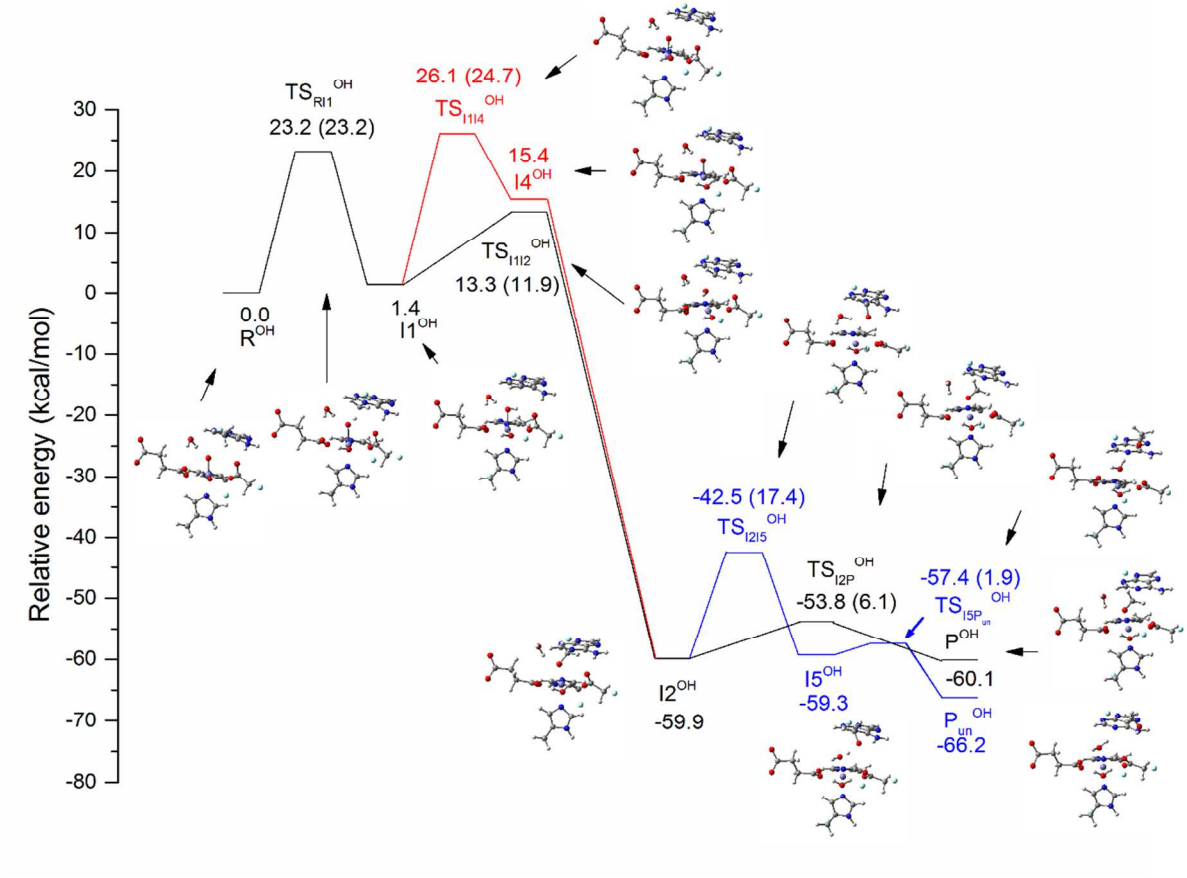


Figure S5. Relative energies (kcal/mol) of the structures shown in Scheme1c for OH^- pathway in the quintet state. The energy of the $^{IS}Fe^{III}$-O_F reactant is taken as zero. For the TS structures, the values in parentheses are the energy differences between the TS and the immediate previous intermediate.



Cartesian coordinates of QM part

The H_2O pathway

Refer to the supporting information of ref. 9 for R and TS_{R1} and I1 coordinates for the H_2O pathway. Cps represents the boundary carbon atoms.

$I2^{OH}$

H	-0.9631	3.6184	-4.4801
H	-0.1039	2.7171	-5.6961
C	0.0188	1.9446	-3.7634
N	0.7050	0.7789	-4.0326
H	1.2051	0.5777	-4.8996
C	0.6341	-0.0082	-2.9398
H	1.1071	-0.9742	-2.8475
N	-0.0677	0.5767	-1.9833
C	-0.4606	1.7905	-2.4939
H	-1.0292	2.4887	-1.8974
H	-0.6258	3.4011	2.8492
H	-2.3327	3.2414	3.2320
C	-1.6688	2.0545	1.6409
O	-0.9370	1.9163	0.6275
O	-2.4681	1.1600	2.0560
H	5.9720	0.7720	-0.6571
H	6.1576	2.4316	-0.1657
C	4.1749	1.7430	-0.2354
N	3.5752	2.8188	0.3855
H	4.0358	3.6954	0.6408
C	2.2963	2.4931	0.6541
H	1.6044	3.1518	1.1548
N	2.0263	1.2673	0.2310
C	3.1948	0.7940	-0.3203
H	3.2529	-0.1963	-0.7471
C	-4.4424	1.9545	-4.5416
H	-4.7551	2.6377	-5.3190
N	-4.6098	2.1312	-3.2501
C	-4.0633	1.0099	-2.6735
C	-3.8985	0.6172	-1.3195
N	-4.2535	1.3383	-0.2805
H	-4.7575	2.2255	-0.3821
H	-3.9275	1.1340	0.6602
N	-3.3151	-0.6261	-1.1743
C	-3.0856	-1.2563	0.1553
H	-3.0767	-2.3394	0.0215
H	-3.9406	-0.9997	0.7892
H	-2.0695	-0.0630	1.2806
C	-2.8270	-1.3384	-2.2435
H	-2.3369	-2.2675	-1.9736
N	-2.9117	-0.9963	-3.4860
C	-3.5531	0.1763	-3.6476
Fe	0.1630	0.2070	0.1381
O	1.0077	-7.4303	-0.0755
C	1.6989	-6.4349	0.2738
O	2.8788	-6.4925	0.6944
C	0.9710	-5.0922	0.2154
H	0.2481	-5.1313	-0.6043
H	0.3893	-5.0421	1.1414
C	1.8360	-3.8419	0.0955
H	2.6918	-3.9528	0.7695
H	2.2289	-3.7096	-0.9148
C	1.0658	-2.6081	0.5163
O	1.0236	-1.6065	-0.2649
O	0.4973	-2.6354	1.6469
O	-1.8806	-0.8580	0.6961
O	0.2288	-0.1719	2.2838
H	0.2609	-1.1695	2.2013
H	1.0542	0.0862	2.7055
O	-2.0604	-3.9349	1.2725
H	-1.2276	-3.4975	1.5087
H	-2.3275	-4.4381	2.0571
C	-0.0133	3.1128	-4.6820
C	-1.6296	3.3564	2.4038
C	5.5569	1.7696	-0.8009
N	-3.8011	0.7873	-4.8252
Cps	1.1654	4.0973	-4.5877
Cps	-1.9345	4.5740	1.5419
Cps	5.6516	2.1704	-2.2832
Cps	-3.3610	0.2605	-6.0735

TS_{I2I3}

H	-0.9277	3.5541	-4.4202
H	-0.0732	2.6504	-5.6401
C	0.1161	1.9203	-3.6921
N	0.7787	0.7413	-3.9737
H	1.2450	0.5270	-4.8554
C	0.7617	-0.0242	-2.8626
H	1.2290	-0.9934	-2.7728
N	0.1218	0.5907	-1.8826
C	-0.2868	1.7983	-2.3932
H	-0.8212	2.5051	-1.7768
H	-0.6299	3.3070	2.7602
H	-2.3304	3.1936	3.1903
C	-1.7704	2.0031	1.5570
O	-0.9540	1.7587	0.6329
O	-2.7276	1.2419	1.8888
H	6.0567	0.7943	-0.6423
H	6.2395	2.4601	-0.1763
C	4.2697	1.7411	-0.1544
N	3.6613	2.8147	0.4618
H	4.1022	3.7119	0.6775
C	2.4094	2.4565	0.7973
H	1.7171	3.1081	1.3054
N	2.1670	1.2074	0.4284
C	3.3277	0.7550	-0.1607
H	3.4022	-0.2457	-0.5567
C	-4.3106	2.1111	-4.6807
H	-4.4527	2.7972	-5.5035
N	-4.5781	2.3623	-3.4213
C	-4.2626	1.2004	-2.7649
C	-4.2931	0.8560	-1.3916
N	-4.5496	1.6764	-0.3959
H	-4.8942	2.6293	-0.5305
H	-4.2921	1.4571	0.5622
N	-4.0119	-0.4699	-1.1575
C	-4.2711	-1.0789	0.1811
H	-4.5519	-2.1118	-0.0154
H	-5.1374	-0.5586	0.6011
H	-2.9318	-0.1371	1.2970
C	-3.5348	-1.3113	-2.1423
H	-3.2248	-2.2875	-1.7867
N	-3.3925	-1.0020	-3.3910
C	-3.7990	0.2521	-3.6590
Fe	0.3448	0.1518	0.1795
O	1.0120	-7.4451	-0.0747
C	1.7252	-6.4729	0.2915
O	2.8958	-6.5685	0.7306
C	1.0687	-5.0943	0.2390
H	0.3043	-5.1015	-0.5452
H	0.5521	-4.9811	1.1989
C	2.0168	-3.9101	0.0561
H	2.8961	-4.0803	0.6858
H	2.3732	-3.8145	-0.9716
C	1.3521	-2.6210	0.4933
O	1.4972	-1.5633	-0.1832
O	0.6236	-2.6953	1.5301

O	-3.1677	-1.0694	0.9967
O	-0.1551	-0.4282	2.1916
H	0.1212	-1.4002	2.0447
H	0.4574	-0.0755	2.8455
O	-1.3558	-2.2426	-0.4969
H	-0.8772	-2.9144	-0.0004
H	-1.9388	-1.8461	0.1785
C	0.0301	3.0700	-4.6356
C	-1.6469	3.3034	2.3451
C	5.6211	1.7840	-0.7794
N	-3.8205	0.8528	-4.8704
Cps	1.1830	4.0898	-4.5829
Cps	-1.9388	4.5710	1.5391
Cps	5.6568	2.1687	-2.2679
Cps	-3.3463	0.2601	-6.0814

I3

H	-0.9476	3.6406	-4.4848
H	-0.1012	2.7708	-5.7330
C	0.0316	1.9438	-3.8217
N	0.7412	0.7944	-4.1094
H	1.2426	0.6122	-4.9801
C	0.6960	-0.0054	-3.0250
H	1.1917	-0.9606	-2.9401
N	-0.0112	0.5573	-2.0616
C	-0.4349	1.7665	-2.5521
H	-1.0144	2.4414	-1.9396
H	-0.6617	3.1797	2.6839
H	-2.3509	3.1499	3.1622
C	-1.8999	1.9738	1.4771
O	-1.1813	1.7717	0.4714
O	-2.8364	1.2067	1.8658
H	5.8999	0.8147	-0.6057
H	6.0820	2.4818	-0.1403
C	4.0995	1.7964	-0.2483
N	3.4833	2.8726	0.3585
H	3.9356	3.7539	0.6123
C	2.2069	2.5355	0.6226
H	1.5094	3.1916	1.1187
N	1.9540	1.3000	0.2138
C	3.1335	0.8345	-0.3260
H	3.2012	-0.1607	-0.7379
C	-4.1448	2.2145	-4.7452
H	-4.1680	2.8986	-5.5812
N	-4.4315	2.5107	-3.5008
C	-4.2882	1.3291	-2.8262
C	-4.4034	1.0169	-1.4529
N	-4.5612	1.8795	-0.4761
H	-4.7940	2.8636	-0.6232
H	-4.3723	1.6404	0.4929
N	-4.3335	-0.3313	-1.1960
C	-4.7672	-0.8666	0.1273
H	-5.2105	-1.8404	-0.0731
H	-5.5555	-0.2002	0.4888
H	-3.3766	-0.1177	1.3140
C	-3.9416	-1.2428	-2.1506
H	-3.8474	-2.2602	-1.7875
N	-3.6941	-0.9779	-3.3929
C	-3.9148	0.3164	-3.6911
Fe	0.1303	0.1490	0.0186
O	1.0650	-7.4290	-0.0722
C	1.7819	-6.4467	0.2632
O	2.9555	-6.5340	0.6962
C	1.1175	-5.0731	0.1706
H	0.3736	-5.1054	-0.6315
H	0.5729	-4.9453	1.1130
C	2.0552	-3.8793	-0.0093
H	2.9037	-4.0130	0.6693
H	2.4571	-3.8140	-1.0227
C	1.3499	-2.5862	0.3476
O	1.4075	-1.5893	-0.4198
O	0.6668	-2.5968	1.4277
O	-3.7187	-1.0116	1.0021
O	0.1325	-0.2018	2.2032
H	0.3752	-1.1640	2.0898
H	0.8810	0.2074	2.6485
O	-1.3237	-1.4538	-0.0371
H	-0.8638	-2.1210	0.5065
H	-2.2262	-1.3779	0.3295
C	-0.0025	3.1340	-4.7074
C	-1.6883	3.2433	2.2987
C	5.4958	1.8116	-0.7806
N	-3.8088	0.9031	-4.9037
Cps	1.1860	4.1035	-4.5900
Cps	-1.9349	4.5408	1.5238
Cps	5.6445	2.1802	-2.2674
Cps	-3.3514	0.2639	-6.0941

TS_{I3Pun}

H	-0.9448	-3.6072	4.4589
H	-0.0977	2.7244	-5.6959
C	0.0392	1.9212	-3.7763
N	0.7223	0.7572	-4.0692
H	1.2200	0.5704	-4.9408
C	0.6407	-0.0574	-3.0006
H	1.1068	-1.0285	-2.9292
N	-0.0611	0.5101	-2.0333
C	-0.4482	1.7378	-2.5150
H	-1.0366	2.4151	-1.9148
H	-0.6900	3.2609	2.7951
H	-2.4019	3.1889	3.1761
C	-1.7955	2.0044	1.5585
O	-1.1589	1.7796	0.5418
O	-2.6541	1.1512	2.0887
H	5.8822	0.7965	-0.6270
H	6.0302	2.4575	-0.1316
C	4.0627	1.7478	-0.2824
N	3.4499	2.7981	0.3710
H	3.9009	3.6764	0.6346
C	2.1809	2.4454	0.6476
H	1.4937	3.0770	1.1886
N	1.9266	1.2225	0.2023
C	3.0994	0.7822	-0.3739
H	3.1664	-0.2007	-0.8153
C	-4.3639	2.1927	-4.8387
H	-4.6024	2.7959	-5.7028
N	-4.5739	2.5424	-3.5939
C	-4.1239	1.4768	-2.8537
C	-4.0630	1.2193	-1.4712
N	-4.4044	2.0882	-0.5159
H	-4.8555	2.9831	-0.6775
H	-4.4132	1.7788	0.4416
N	-3.5982	0.0116	-1.1073
C	-4.7816	-1.0696	0.6303
H	-5.0102	-1.8879	-0.0656
H	-5.5111	-0.2473	0.6499
H	-2.8241	0.3383	1.5617
C	-3.1666	-0.8629	-2.0353
H	-2.7871	-1.8011	-1.6424
N	-3.1340	-0.7083	-3.3430
C	-3.6429	0.4789	-3.6848
Fe	0.1152	0.0423	0.0243
O	1.0597	-7.4971	-0.0730
C	1.7525	-6.4995	0.2655
O	2.9239	-6.5532	0.7078

C	1.0549	-5.1435	0.1611
H	0.3265	-5.1927	-0.6542
H	0.4954	-5.0296	1.0967
C	1.9789	-3.9398	-0.0075
H	2.8272	-4.0786	0.6696
H	2.3755	-3.8622	-1.0218
C	1.2694	-2.6599	0.3652
O	1.2841	-1.6725	-0.4218
O	0.6383	-2.6531	1.4750
O	-3.8665	-1.1521	1.4445
O	0.2286	-0.1955	2.2548
H	0.4310	-1.1655	2.1665
H	1.0178	0.1977	2.6421
O	-1.4189	-1.4536	0.3595
H	-0.9171	-2.1352	0.8507
H	-2.3445	-1.4903	0.6603
C	0.0026	3.1050	-4.6769
C	-1.6939	3.2874	2.3502
C	5.4685	1.7905	-0.7964
N	-3.7965	0.9558	-4.9399
Cps	1.1848	4.0903	-4.5811
Cps	-1.9387	4.5431	1.5259
Cps	5.6499	2.1828	-2.2732
Cps	-3.3475	0.2650	-6.1047

P_{un}

H	-0.9555	3.5979	-4.4462
H	-0.1069	2.6967	-5.6695
C	0.0580	1.9399	-3.7306
N	0.7403	0.7733	-4.0123
H	1.2060	0.5636	-4.8960
C	0.7264	0.0036	-2.9080
H	1.2034	-0.9610	-2.8232
N	0.0704	0.6042	-1.9276
C	-0.3580	1.8058	-2.4379
H	-0.9191	2.5020	-1.8330
H	-0.6738	3.5393	2.9868
H	-2.3826	3.2407	3.2045
C	-1.4335	2.1096	1.7298
O	-0.7877	1.9998	0.6903
O	-1.9859	1.0908	2.3370
H	6.0921	0.7890	-0.6830
H	6.2788	2.4519	-0.2047
C	4.3042	1.7433	-0.1920
N	3.7048	2.8281	0.4128
H	4.1614	3.7120	0.6494
C	2.4285	2.5114	0.6848
H	1.7343	3.1722	1.1781
N	2.1655	1.2780	0.2813
C	3.3307	0.7903	-0.2609
H	3.3822	-0.2033	-0.6807
C	-4.4160	2.0226	-4.6302
H	-4.7604	2.6586	-5.4337
N	-4.5465	2.2702	-3.3471
C	-3.9565	1.1922	-2.7220
C	-3.7348	0.8492	-1.3668
N	-4.0584	1.6050	-0.3179
H	-4.6308	2.4437	-0.4112
H	-4.1070	1.1196	0.5774
N	-3.1037	-0.3303	-1.1476
C	-5.8935	0.1534	2.0625
H	-6.5230	-0.4874	2.7008
H	-6.3562	1.0706	1.6664
H	-1.7819	0.2620	1.7875
C	-2.7020	-1.0948	-2.1784
H	-2.1905	-2.0128	-1.8978
N	-2.8351	-0.8572	-3.4635
C	-3.4733	0.3025	-3.6643
Fe	0.3637	0.2124	0.1433
O	1.0169	-7.4530	-0.0654
C	1.7045	-6.4605	0.2975
O	2.8859	-6.5196	0.7136
C	0.9889	-5.1109	0.2562
H	0.2432	-5.1463	-0.5440
H	0.4457	-5.0261	1.2044
C	1.8825	-3.8879	0.0919
H	2.7253	-3.9838	0.7849
H	2.3030	-3.8141	-0.9132
C	1.1370	-2.6139	0.4243
O	1.2459	-1.6205	-0.3545
O	0.4252	-2.6044	1.4785
O	-4.7431	-0.1399	1.8125
O	0.6571	-0.1249	2.3497
H	0.6394	-1.1083	2.2988
H	1.5218	0.1170	2.6945
O	-1.4814	-0.8127	0.7668
H	-1.1641	-1.7103	0.9931
H	-2.2561	-0.7410	0.0808
C	-0.0049	3.0993	-4.6591
C	-1.6209	3.4139	2.4399
C	5.6572	1.7804	-0.8094
N	-3.7705	0.8482	-4.8664
Cps	1.1701	4.0941	-4.5836
Cps	-1.9347	4.5932	1.5419
Cps	5.6668	2.1790	-2.2925
Cps	-3.3517	0.2608	-6.0958

TS_{I2P}

H	-0.9375	3.5268	-4.4796
H	-0.0402	2.6267	-5.6697
C	0.1012	1.9067	-3.7203
N	0.8053	0.7482	-3.9719
H	1.2946	0.5355	-4.8416
C	0.7572	-0.0196	-2.8665
H	1.2343	-0.9818	-2.7611
N	0.0569	0.5753	-1.9160
C	-0.3661	1.7690	-2.4455
H	-0.9691	2.4558	-1.8715
H	-0.8106	3.3200	2.9400
H	-2.5482	3.1958	3.1187
C	-1.6898	2.0279	1.6092
O	-0.9532	1.8644	0.6396
O	-2.4356	1.0645	2.0931
H	5.9167	0.7748	-0.6521
H	6.0823	2.4328	-0.1543
C	4.1132	1.7307	-0.2552
N	3.5288	2.7731	0.4358
H	3.9852	3.6524	0.6859
C	2.2729	2.4152	0.7628
H	1.6017	3.0414	1.3298
N	2.0006	1.1996	0.3122
C	3.1448	0.7685	-0.3202
H	3.1954	-0.2077	-0.7787
C	-4.5807	2.0479	-4.7592
H	-4.9416	2.6133	-5.6060
N	-4.7699	2.3688	-3.5023
C	-4.1284	1.3833	-2.7872
C	-3.9688	1.1196	-1.4093
N	-4.4382	1.8842	-0.4189
H	-5.0123	2.7124	-0.5475
H	-4.4035	1.5054	0.5130
N	-3.2565	0.0257	-1.0794
C	-2.7565	-1.9952	0.7014
H	-2.6618	-2.6465	-0.1653
H	-3.7097	-2.0310	1.2392

H	-2.2614	0.1997	1.5991
C	-2.7143	-0.7288	-2.0453
H	-2.0961	-1.5561	-1.7090
N	-2.8056	-0.5963	-3.3544
C	-3.5402	0.4762	-3.6523
Fe	0.1564	0.1100	0.1583
O	1.0450	-7.4997	-0.1635
C	1.7274	-6.4734	0.1108
O	2.8570	-6.4761	0.6484
C	1.0356	-5.1529	-0.2464
H	0.6158	-5.2559	-1.2513
H	0.1842	-5.0893	0.4351
C	1.8826	-3.8893	-0.1266
H	2.6732	-4.1026	0.5997
H	2.3561	-3.6184	-1.0720
C	1.0795	-2.7218	0.3930
O	1.0174	-1.6652	-0.3068
O	0.5078	-2.8389	1.5179
O	-1.8819	-1.1878	1.0113
O	0.2583	-0.3682	2.2840
H	0.2613	-1.3602	2.1584
H	1.1014	-0.1584	2.6988
O	-1.9579	-4.0609	1.4595
H	-1.0503	-3.7784	1.6705
H	-2.2746	-4.6095	2.2042
C	0.0302	3.0521	-4.6659
C	-1.7557	3.3209	2.3771
C	5.5023	1.7707	-0.8085
N	-3.8437	0.9079	-4.8956
Cps	1.1745	4.0829	-4.5903
Cps	-1.9323	4.5753	1.5405
Cps	5.6517	2.1689	-2.2870
Cps	-3.3628	0.2592	-6.0728

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H	-0.9555	3.5979	-4.4462
H	-0.1069	2.6967	-5.6695
C	0.0580	1.9399	-3.7306
N	0.7403	0.7733	-4.0123
H	1.2060	0.5636	-4.8960
C	0.7264	0.0036	-2.9080
H	1.2034	-0.9610	-2.8232
N	0.0704	0.6042	-1.9276
C	-0.3580	1.8058	-2.4379
H	-0.9191	2.5020	-1.8330
H	-0.6738	3.5393	2.9868
H	-2.3826	3.2407	3.2045
C	-1.4335	2.1096	1.7298
O	-0.7877	1.9998	0.6903
O	-1.9859	1.0908	2.3370
H	6.0921	0.7890	-0.6830
H	6.2788	2.4519	-0.2047
C	4.3042	1.7433	-0.1920
N	3.7048	2.8281	0.4128
H	4.1614	3.7120	0.6494
C	2.4285	2.5114	0.6848
H	1.7343	3.1722	1.1781
N	2.1655	1.2780	0.2813
C	3.3307	0.7903	-0.2609
H	3.3822	-0.2033	-0.6807
C	-4.4160	2.0226	-4.6302
H	-4.7604	2.6586	-5.4337
N	-4.5465	2.2702	-3.3471
C	-3.9565	1.1922	-2.7220
C	-3.7348	0.8492	-1.3668
N	-4.0584	1.6050	-0.3179
H	-4.6308	2.4437	-0.4112
H	-4.1070	1.1196	0.5774
N	-3.1037	-0.3303	-1.1476
C	-5.8935	0.1534	2.0625
H	-6.5230	-0.4874	2.7008
H	-6.3562	1.0706	1.6664
H	-1.7819	0.2620	1.7875
C	-2.7020	-1.0948	-2.1784
H	-2.1905	-2.0128	-1.8978
N	-2.8351	-0.8572	-3.4635
C	-3.4733	0.3025	-3.6643
Fe	0.3637	0.2124	0.1433
O	1.0169	-7.4530	-0.0654
C	1.7045	-6.4605	0.2975
O	2.8859	-6.5196	0.7136
C	0.9889	-5.1109	0.2562
H	0.2432	-5.1463	-0.5440
H	0.4457	-5.0261	1.2044
C	1.8825	-3.8879	0.0919
H	2.7253	-3.9838	0.7849
H	2.3030	-3.8141	-0.9132
C	1.1370	-2.6139	0.4243
O	1.2459	-1.6205	-0.3545
O	0.4252	-2.6044	1.4785
O	-4.7431	-0.1399	1.8125
O	0.6571	-0.1249	2.3497
H	0.6394	-1.1083	2.2988
H	1.5218	0.1170	2.6945
O	-1.4814	-0.8127	0.7668
H	-1.1641	-1.7103	0.9931
H	-2.2561	-0.7410	0.0808
C	-0.0049	3.0993	-4.6591
C	-1.6209	3.4139	2.4399
C	5.6572	1.7804	-0.8094
N	-3.7705	0.8482	-4.8664
Cps	1.1701	4.0941	-4.5836
Cps	-1.9347	4.5932	1.5419
Cps	5.6668	2.1790	-2.2925
Cps	-3.3517	0.2608	-6.0958

Structures for 1-deazameA

Figure 7b

H	-0.8094	3.7669	-4.4538
H	0.0277	2.8304	-5.6587
C	0.1042	2.0725	-3.7138
N	0.7141	0.8623	-3.9889
H	1.1845	0.6246	-4.8576
C	0.5896	0.0804	-2.8929
H	0.9862	-0.9179	-2.7830
N	-0.0582	0.7145	-1.9361
C	-0.3749	1.9478	-2.4400
H	-0.9084	2.6624	-1.8309
H	-0.6834	3.6168	2.8290
H	-2.4126	3.4802	3.1364
C	-1.7139	2.2657	1.5711
O	-0.8921	2.1272	0.6225
O	-2.5861	1.4459	1.9326
H	5.9044	0.8252	-0.6141
H	6.0871	2.4885	-0.1358
C	4.1054	1.8125	-0.2632
N	3.4963	2.9083	0.3215
H	3.9488	3.7958	0.5372
C	2.2161	2.5744	0.6015
H	1.5034	3.2388	1.0662
N	1.9629	1.3345	0.2315
C	3.1318	0.8516	-0.2994
H	3.1762	-0.1525	-0.6950
C	-4.3240	2.0790	-4.7264
H	-4.5800	2.7487	-5.5359

N	-4.4928	2.3258	-3.4469
C	-4.0187	1.1933	-2.8009
C	-3.8964	0.8815	-1.4245
N	-4.2731	1.7497	-0.4594
H	-4.5633	2.6776	-0.7251
H	-3.8804	1.6460	0.4714
C	-3.3727	-0.4066	-1.1801
C	-3.1776	-0.9853	0.1978
H	-3.7935	-1.8881	0.2938
H	-3.4715	-0.2812	0.9728
H	-1.9086	-3.0533	0.4767
C	-2.9649	-1.2189	-2.2443
H	-2.5401	-2.1885	-1.9926
N	-3.0240	-0.9259	-3.5444
C	-3.5644	0.2719	-3.7349
Fe	0.0792	0.2331	0.2173
O	0.9877	-7.2262	-0.0703
C	1.7321	-6.3335	0.4206
O	2.9453	-6.5415	0.7155
C	1.1651	-4.9391	0.6850
H	0.0771	-4.9439	0.5954
H	1.4117	-4.6683	1.7157
C	1.7506	-3.8530	-0.2328
H	2.8414	-3.9732	-0.2617
H	1.3765	-3.9587	-1.2547
C	1.4444	-2.4337	0.2750
O	1.0498	-1.5705	-0.5711
O	1.6201	-2.2008	1.4882
O	-1.8171	-1.3599	0.3665
O	-0.3604	-0.3478	2.0606
H	0.3278	-1.0153	2.2094
H	-1.3899	-1.0214	1.2457
O	-2.2634	-3.9637	0.5567
H	-2.3397	-4.1477	1.4991
C	0.1244	3.2269	-4.6438
C	-1.6692	3.5806	2.3398
C	5.5028	1.8238	-0.7855
N	-3.7702	0.8602	-4.9491
Cps	1.3387	4.1842	-4.5528
Cps	-1.9228	4.8179	1.4757
Cps	5.6872	2.2031	-2.2706
Cps	-3.3353	0.2690	-6.1768

Figure 7c

H	-0.7663	3.7778	-4.4589
H	0.0826	2.8677	-5.6762
C	0.1867	2.0937	-3.7351
N	0.8310	0.9034	-4.0178
H	1.2867	0.6751	-4.8974
C	0.7788	0.1368	-2.9024
H	1.2226	-0.8429	-2.7995
N	0.1424	0.7592	-1.9348
C	-0.2396	1.9694	-2.4424
H	-0.7753	2.6755	-1.8247
H	-0.7783	3.8882	3.1167
H	-2.4408	3.4285	3.1428
C	-1.2131	2.2697	1.9270
O	-0.7012	2.1699	0.7752
O	-1.3636	1.3667	2.7766
H	6.0966	0.8750	-0.6939
H	6.2769	2.5435	-0.2321
C	4.2972	1.8468	-0.2805
N	3.6885	2.9424	0.3012
H	4.1454	3.8215	0.5404
C	2.3986	2.6190	0.5459
H	1.6844	3.2801	1.0128
N	2.1426	1.3918	0.1449
C	3.3149	0.8995	-0.3605
H	3.3595	-0.1046	-0.7563
C	-4.1764	2.2159	-4.7776
H	-4.2314	2.8919	-5.6198
N	-4.4408	2.5205	-3.5301
C	-4.2374	1.3448	-2.8281
C	-4.3192	1.0582	-1.4497
N	-4.5793	1.9675	-0.4877
H	-4.6845	2.9490	-0.6934
H	-4.2933	1.7001	0.4465
C	-4.1175	-0.3027	-1.1320
C	-4.3064	-0.7472	0.2952
H	-4.1412	-1.8343	0.3490
H	-5.3473	-0.5595	0.5912
H	-2.4947	-0.3053	0.8652
C	-3.7370	-1.2052	-2.1226
H	-3.5339	-2.2297	-1.8184
N	-3.5810	-0.9441	-3.4279
C	-3.8586	0.3239	-3.6980
Fe	0.2404	0.2771	0.1956
O	1.0285	-7.4599	-0.0499
C	1.7400	-6.4747	0.3087
O	2.9078	-6.5943	0.7577
C	1.0990	-5.0954	0.2269
H	0.2951	-5.1333	-0.5145
H	0.6261	-4.9175	1.2003
C	2.0206	-3.9128	-0.0601
H	2.9388	-4.0394	0.5263
H	2.3143	-3.8688	-1.1130
C	1.3714	-2.5809	0.3485
O	1.5204	-1.5811	-0.3987
O	0.7289	-2.6012	1.4381
O	-3.4653	-0.0544	1.1916
O	0.7884	-0.0593	2.3113
H	0.6991	-1.0274	2.2207
H	-0.0659	0.3025	2.6409
O	-1.3239	-0.8785	0.3258
H	-1.0315	-1.6716	0.7883
C	0.1752	3.2541	-4.6567
C	-1.6208	3.6428	2.4478
C	5.6712	1.8667	-0.8489
N	-3.8154	0.9161	-4.9318
Cps	1.3780	4.2246	-4.5526
Cps	-1.9327	4.7808	1.4849
Cps	5.7621	2.2412	-2.3424
Cps	-3.3508	0.2711	-6.1245

Figure 7d

H	-0.8014	3.7986	-4.4992
H	0.0449	2.8827	-5.7136
C	0.0872	2.0825	-3.7847
N	0.7178	0.8831	-4.0597
H	1.2086	0.6593	-4.9213
C	0.5704	0.0850	-2.9789
H	0.9773	-0.9098	-2.8730
N	-0.1120	0.6982	-2.0339
C	-0.4278	1.9342	-2.5283
H	-0.9851	2.6385	-1.9283
H	-0.6789	3.6525	2.8579
H	-2.4031	3.4868	3.1484
C	-1.6511	2.2387	1.6473
O	-0.9252	2.1005	0.6250
O	-2.3893	1.3671	2.1556
H	5.8696	0.8232	-0.6231

H	6.0185	2.4863	-0.1315
C	4.0490	1.7868	-0.3189
N	3.4246	2.8559	0.2979
H	3.8665	3.7404	0.5425
C	2.1407	2.5015	0.5437
H	1.4179	3.1413	1.0266
N	1.8975	1.2778	0.1185
C	3.0781	0.8250	-0.4126
H	3.1381	-0.1647	-0.8408
C	-4.3325	2.0632	-4.6899
H	-4.6241	2.7196	-5.4984
N	-4.4689	2.3208	-3.4089
C	-3.9504	1.2063	-2.7648
C	-3.7835	0.9087	-1.3899
N	-4.1508	1.7738	-0.4189
H	-4.5157	2.6851	-0.6469
H	-3.8139	1.6311	0.5233
C	-3.2190	-0.3630	-1.1438
C	-2.9766	-0.9140	0.2454
H	-3.4884	-1.8874	0.3025
H	-3.4657	-0.2638	0.9795
H	-1.5974	-2.8204	0.4872
C	-2.8226	-1.1748	-2.2116
H	-2.3693	-2.1320	-1.9592
N	-2.9286	-0.8988	-3.5144
C	-3.5021	0.2837	-3.7031
Fe	-0.1307	0.1573	0.0598
O	1.0340	-7.2438	-0.0769
C	1.7804	-6.3426	0.3982
O	2.9908	-6.5474	0.7022
C	1.2172	-4.9458	0.6400
H	0.1349	-4.9308	0.5155
H	1.4298	-4.6828	1.6801
C	1.8377	-3.8610	-0.2551
H	2.9303	-3.9601	-0.2188
H	1.5243	-3.9847	-1.2949
C	1.4738	-2.4454	0.2147
O	1.0672	-1.6074	-0.6408
O	1.6348	-2.1986	1.4347
O	-1.6199	-1.0966	0.5415
O	0.2007	-0.1749	2.2687
H	0.8441	-0.9018	2.0838
H	-0.6607	-0.6052	2.1288
O	-1.8682	-3.7728	0.5106
H	-2.0379	-3.9656	1.4382
C	0.1303	3.2543	-4.6886
C	-1.6575	3.5902	2.3544
C	5.4619	1.8183	-0.8015
N	-3.7606	0.8542	-4.9180
Cps	1.3527	4.1951	-4.5596
Cps	-1.9241	4.8118	1.4765
Cps	5.6890	2.2033	-2.2799
Cps	-3.3447	0.2687	-6.1565

Structures for proton being transferred to Glu136

$I3_{Glu136}$

H	-0.9242	3.6422	-4.4912
H	-0.0723	2.7554	-5.7247
C	0.0378	1.9475	-3.8015
N	0.7383	0.7882	-4.0733
H	1.2445	0.5943	-4.9378
C	0.6763	-0.0003	-2.9799
H	1.1606	-0.9605	-2.8813
N	-0.0314	0.5782	-2.0270
C	-0.4388	1.7868	-2.5325
H	-1.0135	2.4728	-1.9276
H	-0.8066	3.3106	2.8111
H	-2.5467	3.2752	3.1023
C	-1.8625	2.0165	1.5504
O	-1.1506	1.8531	0.5218
O	-2.6471	1.1515	2.0231
H	5.8524	0.8136	-0.5488
H	6.0161	2.4814	-0.0822
C	4.0421	1.7818	-0.2091
N	3.4181	2.8555	0.3951
H	3.8602	3.7458	0.6336
C	2.1476	2.5068	0.6715
H	1.4443	3.1591	1.1648
N	1.9062	1.2656	0.2752
C	3.0860	0.8082	-0.2705
H	3.1581	-0.1900	-0.6745
C	-4.0480	2.2358	-4.7732
H	-4.0469	2.8970	-5.6276
N	-4.3426	2.5713	-3.5411
C	-4.2295	1.4049	-2.8339
C	-4.4524	1.1390	-1.4587
N	-4.6851	2.0637	-0.5576
H	-4.7210	3.0320	-0.8527
H	-4.9264	1.9012	0.4386
N	-4.4168	-0.1977	-1.1531
C	-4.8376	-0.6942	0.1980
H	-5.3410	-1.6424	0.0130
H	-5.5632	0.0162	0.5948
H	-3.4113	-0.0340	1.4165
C	-4.0190	-1.1432	-2.0739
H	-3.9676	-2.1513	-1.6778
N	-3.7187	-0.9305	-3.3169
C	-3.8755	0.3614	-3.6656
Fe	0.0598	0.1650	0.0687
O	1.1145	-7.4896	-0.0418
C	1.8082	-6.4909	0.2988
O	2.9717	-6.5553	0.7588
C	1.1151	-5.1337	0.1783
H	0.3848	-5.1927	-0.6344
H	0.5512	-5.0129	1.1102
C	2.0166	-3.9122	0.0055
H	2.8599	-4.0205	0.6961
H	2.4296	-3.8356	-1.0028
C	1.2702	-2.6365	0.3551
O	1.3335	-1.6248	-0.3901
O	0.5611	-2.6820	1.4179
O	-3.7753	-0.8938	1.0406
O	0.0045	-0.3379	2.2543
H	0.2750	-1.2886	2.0872
H	0.6841	0.0504	2.8128
O	-1.4134	-1.4081	-0.0283
H	-0.9716	-2.1114	0.4811
H	-2.2971	-1.2906	0.3792
H	-5.1892	2.7815	7.1494
H	-6.7219	3.2584	6.5331
C	-5.0714	3.4330	5.2028
O	-5.6262	2.5082	4.5075
O	-4.0780	4.0896	4.8565
H	-4.0448	-2.3573	5.6567
C	-3.4680	-0.6965	4.6894
N	-3.6008	0.6161	4.5464
H	-4.4328	1.0638	4.9261
H	-3.2331	1.0356	3.6902
N	-2.5837	-1.3665	3.9386
H	-2.5132	-2.3726	4.0317
H	-1.9658	-0.8717	3.3059
O	-5.7470	1.9213	1.9773
H	-5.5362	2.1490	2.9332
H	-6.6816	1.6868	1.9633

C	0.0198	3.1283	-4.7016
C	-1.7902	3.3334	2.3149
C	5.4426	1.8074	-0.7300
N	-3.7443	0.9135	-4.8973
C	-5.6837	3.5961	6.5927
N	-4.1900	-1.3503	5.5850
Cps	1.2133	4.0941	-4.5834
Cps	-1.9727	4.5858	1.4583
Cps	5.6144	2.1767	-2.2145
Cps	-3.3111	0.2475	-6.0862
Cps	-5.5222	4.9369	7.2924
Cps	-5.1167	-0.7070	6.5039

I3'$_{Glu136}$

H	-0.9306	3.6371	-4.4705
H	-0.0828	2.7330	-5.6938
C	0.0359	1.9532	-3.7594
N	0.7215	0.7842	-4.0284
H	1.2218	0.5807	-4.8936
C	0.6601	0.0057	-2.9266
H	1.1337	-0.9596	-2.8258
N	-0.0311	0.5990	-1.9708
C	-0.4285	1.8081	-2.4830
H	-0.9848	2.5066	-1.8749
H	-0.7905	3.4809	2.9898
H	-2.5233	3.2741	3.1514
C	-1.5545	2.0191	1.7545
O	-0.9572	1.9493	0.6364
O	-1.9803	1.0345	2.3978
H	5.9734	0.8188	-0.6069
H	6.1429	2.4870	-0.1420
C	4.1667	1.7822	-0.2137
N	3.5507	2.8652	0.3788
H	3.9999	3.7506	0.6224
C	2.2683	2.5400	0.6257
H	1.5620	3.1966	1.1091
N	2.0168	1.3073	0.2166
C	3.1950	0.8261	-0.3007
H	3.2562	-0.1706	-0.7122
C	-4.1644	2.2011	-4.8112
H	-4.2373	2.8453	-5.6756
N	-4.4556	2.5365	-3.5790
C	-4.2259	1.3998	-2.8529
C	-4.4350	1.1346	-1.4791
N	-4.7910	2.0543	-0.6122
H	-4.9037	3.0085	-0.9312
H	-4.9701	1.8999	0.3861
N	-4.2772	-0.1832	-1.1412
C	-4.8125	-0.7055	0.1647
H	-4.7701	-1.7901	0.0625
H	-5.8592	-0.3928	0.1963
H	-4.5671	0.4205	1.7294
C	-3.7622	-1.0957	-2.0368
H	-3.5820	-2.0771	-1.6151
N	-3.4976	-0.8819	-3.2891
C	-3.7951	0.3750	-3.6692
Fe	0.1633	0.2342	0.1575
O	1.0634	-7.4871	-0.0309
C	1.7377	-6.4827	0.3326
O	2.9097	-6.5360	0.7730
C	1.0104	-5.1393	0.2636
H	0.2616	-5.2002	-0.5318
H	0.4671	-5.0441	1.2110
C	1.8743	-3.8962	0.0795
H	2.7246	-3.9676	0.7670
H	2.2855	-3.8218	-0.9300
C	1.1016	-2.6283	0.4093
O	1.2017	-1.6241	-0.3477
O	0.3815	-2.6552	1.4612
O	-4.0963	-0.2983	1.2523
O	0.6674	-0.1727	2.3040
H	0.6178	-1.1529	2.2555
H	1.5776	0.0396	2.5288
O	-1.5587	-1.0272	0.4159
H	-1.1364	-1.7629	0.9053
H	-2.1541	-0.5501	1.0256
H	-5.2002	2.7510	7.1045
H	-6.7436	3.2318	6.5178
C	-5.1140	3.4155	5.1636
O	-5.6845	2.4891	4.4728
O	-4.1305	4.0694	4.7992
H	-4.1202	-2.3658	5.6528
C	-3.4983	-0.7107	4.7066
N	-3.6121	0.6005	4.5501
H	-4.4370	1.0758	4.9030
H	-3.0492	1.0379	3.8127
N	-2.6087	-1.3829	3.9679
H	-2.5124	-2.3849	4.0745
H	-2.0667	-0.8648	3.2890
O	-5.6500	1.7566	2.0713
H	-5.5224	2.1111	3.0345
H	-6.5673	1.4577	2.0369
C	0.0137	3.1215	-4.6764
C	-1.7249	3.3804	2.4107
C	5.5494	1.8102	-0.7689
N	-3.7517	0.9066	-4.9160
C	-5.7043	3.5684	6.5604
N	-4.2434	-1.3555	5.5896
Cps	1.2051	4.0926	-4.5780
Cps	-1.9618	4.5734	1.4908
Cps	5.6477	2.1871	-2.2567
Cps	-3.3088	0.2447	-6.1021
Cps	-5.5266	4.9060	7.2564
Cps	-5.1455	-0.6948	6.5205

$TS_{I3'PGlu136}$

H	-0.9257	3.6104	-4.4541
H	-0.0731	2.6957	-5.6660
C	0.0504	1.9416	-3.7211
N	0.7206	0.7628	-3.9860
H	1.2180	0.5513	-4.8499
C	0.6434	-0.0130	-2.8806
H	1.1027	-0.9855	-2.7803
N	-0.0401	0.5905	-1.9268
C	-0.4183	1.8028	-2.4440
H	-0.9731	2.5070	-1.8413
H	-0.8097	3.5646	3.0541
H	-2.5359	3.3079	3.1687
C	-1.4904	2.0295	1.8758
O	-0.9600	1.9239	0.7284
O	-1.7775	1.0813	2.6354
H	5.9596	0.8123	-0.6112
H	6.1166	2.4787	-0.1354
C	4.1435	1.7678	-0.2366
N	3.5183	2.8516	0.3447
H	3.9652	3.7356	0.5949
C	2.2316	2.5234	0.5717
H	1.5187	3.1747	1.0525
N	1.9857	1.2927	0.1565
C	3.1724	0.8112	-0.3390
H	3.2401	-0.1857	-0.7493
C	-4.1609	2.2121	-4.8300
H	-4.2130	2.8611	-5.6921

N	-4.4646	2.5421	-3.5991
C	-4.2569	1.3966	-2.8796
C	-4.4565	1.1281	-1.5095
N	-4.8127	2.0583	-0.6518
H	-4.9291	3.0034	-0.9895
H	-4.9687	1.8882	0.3459
N	-4.2871	-0.1833	-1.1705
C	-4.6776	-0.6716	0.2388
H	-4.5438	-1.7594	0.1590
H	-5.7588	-0.4650	0.2820
H	-4.6792	0.8403	1.8235
C	-3.8058	-1.0977	-2.0690
H	-3.6360	-2.0829	-1.6523
N	-3.5517	-0.8905	-3.3286
C	-3.8303	0.3724	-3.6942
Fe	0.1259	0.1980	0.2563
O	1.0892	-7.4923	-0.0080
C	1.7599	-6.4963	0.3846
O	2.9398	-6.5546	0.8038
C	1.0201	-5.1605	0.3772
H	0.2552	-5.2103	-0.4027
H	0.4970	-5.0947	1.3384
C	1.8613	-3.9032	0.1952
H	2.7055	-3.9445	0.8930
H	2.2873	-3.8337	-0.8084
C	1.0569	-2.6446	0.4957
O	1.1825	-1.6426	-0.2608
O	0.3029	-2.6735	1.5213
O	-3.9560	-0.0913	1.2004
O	0.8042	-0.1921	2.3334
H	0.5921	-1.1514	2.3264
H	1.7630	-0.1486	2.3966
O	-1.6233	-1.0175	0.3438
H	-1.2955	-1.7673	0.8724
H	-2.3932	-0.5847	0.8023
H	-5.2431	2.7512	7.0779
H	-6.7783	3.2725	6.4964
C	-5.1296	3.4674	5.1696
O	-5.8123	2.6201	4.4191
O	-4.1011	4.0127	4.8161
H	-4.1921	-2.3953	5.6186
C	-3.5432	-0.7526	4.6593
N	-3.5788	0.5726	4.5709
H	-4.0968	1.0395	5.2932
H	-2.8908	1.0378	3.9535
N	-2.7543	-1.4351	3.8329
H	-2.7311	-2.4467	3.8714
H	-2.3020	-0.9139	3.0893
O	-5.3938	1.6493	2.0821
H	-5.4037	2.3490	3.5345
H	-6.2672	1.2387	2.0528
C	0.0224	3.0993	-4.6540
C	-1.7210	3.4183	2.4483
C	5.5334	1.8028	-0.7729
N	-3.7642	0.9143	-4.9324
C	-5.7340	3.5879	6.5500
N	-4.2804	-1.3806	5.5645
Cps	1.2053	4.0858	-4.5741
Cps	-1.9655	4.5773	1.4902
Cps	5.6476	2.1874	-2.2572
Cps	-3.3088	0.2440	-6.1022
Cps	-5.5268	4.9066	7.2558
Cps	-5.1453	-0.6943	6.5204

P_{Glu136}

H	-0.9426	3.5182	-4.3575
H	-0.0973	2.5844	-5.5594
C	0.0902	1.8957	-3.5953
N	0.7607	0.7175	-3.8527
H	1.2256	0.4875	-4.7287
C	0.7244	-0.0339	-2.7301
H	1.1896	-1.0022	-2.6249
N	0.0707	0.5878	-1.7658
C	-0.3329	1.7860	-2.2999
H	-0.8908	2.4940	-1.7052
H	-0.6867	3.5654	2.9073
H	-2.4239	3.4476	3.2426
C	-1.7213	2.1331	1.7576
O	-0.8509	1.9121	0.8698
O	-2.6468	1.3462	2.0759
H	6.0159	0.8303	-0.5949
H	6.1777	2.4980	-0.1327
C	4.2094	1.7765	-0.1603
N	3.5980	2.8593	0.4371
H	4.0393	3.7566	0.6459
C	2.3350	2.5103	0.7521
H	1.6325	3.1650	1.2437
N	2.0909	1.2637	0.3864
C	3.2537	0.7996	-0.1800
H	3.3170	-0.2016	-0.5795
C	-4.3905	1.9430	-4.7070
H	-4.7299	2.5768	-5.5139
N	-4.5428	2.1924	-3.4272
C	-3.9498	1.1190	-2.7946
C	-3.7249	0.7981	-1.4344
N	-4.1019	1.5723	-0.4156
H	-4.5498	2.4570	-0.5897
H	-3.7418	1.3711	0.5155
N	-3.0774	-0.3560	-1.1799
C	-6.5358	-1.1610	3.5818
H	-7.2746	-1.9700	3.4836
H	-6.3104	-0.8262	4.5992
H	-5.6191	1.0734	2.1804
C	-2.6420	-1.1133	-2.1988
H	-2.1086	-2.0144	-1.9046
N	-2.7662	-0.9004	-3.4967
C	-3.4342	0.2355	-3.7260
Fe	0.2059	0.2094	0.4043
O	1.0519	-7.4936	-0.0137
C	1.7233	-6.4936	0.3657
O	2.8917	-6.5507	0.8155
C	0.9958	-5.1497	0.3102
H	0.2500	-5.1990	-0.4890
H	0.4520	-5.0690	1.2586
C	1.8627	-3.9046	0.1513
H	2.7345	-4.0165	0.8056
H	2.2372	-3.7860	-0.8684
C	1.1144	-2.6506	0.5743
O	1.1947	-1.6085	-0.1409
O	0.4338	-2.7210	1.6418
O	-6.0050	-0.6840	2.6031
O	0.5943	-0.2126	2.5445
H	0.5119	-1.1897	2.4648
H	1.4974	-0.0422	2.8271
O	-1.5477	-0.9922	0.9820
H	-1.2187	-1.9038	1.0161
H	-2.2744	-0.8730	0.3213
H	-5.1221	2.9003	7.2444
H	-6.7388	3.3219	6.8178
C	-5.2680	3.5972	5.3194
O	-5.9232	2.6204	4.6895
O	-4.3973	4.2648	4.8035
H	-3.9996	-2.3601	5.5686
C	-3.5209	-0.6884	4.5333
N	-3.6941	0.6220	4.4178

H	-4.4115	1.0311	4.9944
H	-3.3232	1.1053	3.5803
N	-2.7134	-1.3438	3.7062
H	-2.6450	-2.3516	3.7920
H	-2.3416	-0.8966	2.8633
O	-5.9867	1.9756	2.1701
H	-5.7758	2.5357	3.7027
H	-6.8952	1.8411	1.8613
C	0.0120	3.0228	-4.5632
C	-1.6797	3.4927	2.4418
C	5.5784	1.8163	-0.7492
N	-3.7269	0.7773	-4.9363
C	-5.7128	3.6962	6.7588
N	-4.1647	-1.3555	5.4931
Cps	1.1735	4.0396	-4.5401
Cps	-1.9545	4.6635	1.4921
Cps	5.6527	2.1932	-2.2376
Cps	-3.2941	0.2208	-6.1788
Cps	-5.5120	5.0425	7.4128
Cps	-5.0736	-0.7199	6.4501

The OH^- pathway

R^{OH} ($^{HS}Fe^{III}$-O_{AF})

H	-0.7389	3.7674	-4.4960
H	0.1286	2.8740	-5.7140
C	0.2195	2.0791	-3.7834
N	0.8470	0.8856	-4.0796
H	1.3190	0.6714	-4.9568
C	0.7834	0.1033	-2.9776
H	1.2123	-0.8845	-2.8993
N	0.1503	0.7203	-2.0032
C	-0.2132	1.9440	-2.4946
H	-0.7331	2.6532	-1.8681
H	-0.7020	3.4499	2.6848
H	-2.4142	3.3312	3.0389
C	-1.7915	2.2070	1.3822
O	-0.9265	2.0597	0.4660
O	-2.7211	1.4113	1.6456
H	5.8522	0.8308	-0.6018
H	6.0270	2.4949	-0.1228
C	4.0498	1.8207	-0.2979
N	3.4334	2.8980	0.3097
H	3.8849	3.7795	0.5557
C	2.1584	2.5526	0.5860
H	1.4526	3.2047	1.0756
N	1.9097	1.3189	0.1840
C	3.0841	0.8545	-0.3586
H	3.1476	-0.1465	-0.7562
C	-4.3015	2.1291	-4.6839
H	-4.3901	2.8260	-5.5053
N	-4.5888	2.3823	-3.4294
C	-4.3236	1.2033	-2.7759
C	-4.3564	0.8628	-1.4012
N	-4.6101	1.6866	-0.4075
H	-4.9127	2.6466	-0.5635
H	-4.2274	1.4955	0.5210
N	-4.0874	-0.4563	-1.1551
C	-4.1708	-0.9608	0.2216
H	-3.8482	-2.0008	0.2377
H	-5.2028	-0.8601	0.5652
H	-3.4838	-0.3817	0.8371
C	-3.6437	-1.3074	-2.1296
H	-3.3941	-2.3001	-1.7754
N	-3.5168	-1.0213	-3.3915
C	-3.8775	0.2438	-3.6633
Fe	-0.0086	0.1753	0.2518
O	0.9694	-7.3359	-0.1008
C	1.6884	-6.3708	0.2812
O	2.8793	-6.4927	0.6715
C	1.0147	-5.0051	0.3246
H	0.1656	-5.0004	-0.3615
H	0.5960	-4.9163	1.3335
C	1.8837	-3.7771	0.0645
H	2.8167	-3.8863	0.6284
H	2.1535	-3.6762	-0.9900
C	1.1741	-2.5111	0.5415
O	1.2401	-1.4635	-0.1853
O	0.5574	-2.5791	1.6300
O	-1.4372	-0.7881	-0.5130
O	-0.2104	-0.0384	2.0528
H	-1.3716	-3.4066	0.9333
H	0.0952	-0.9438	2.2415
O	-1.8918	-3.3991	0.1190
H	-1.6002	-2.5513	-0.2776
C	0.2085	3.2534	-4.6913
C	-1.6981	3.4725	2.2245
C	5.4613	1.8315	-0.7885
N	-3.8570	0.8546	-4.8725
Cps	1.3957	4.2303	-4.5647
Cps	-1.9473	4.7757	1.4569
Cps	5.6920	2.2051	-2.2681
Cps	-3.3634	0.2678	-6.0793

R^{OH}($^{IS}Fe^{III}$-O_F)

H	-0.7382	3.7633	-4.5032
H	0.1364	2.8553	-5.7053
C	0.2169	2.0846	-3.7635
N	0.8284	0.8789	-4.0466
H	1.2965	0.6500	-4.9221
C	0.7643	0.1098	-2.9372
H	1.1837	-0.8801	-2.8368
N	0.1446	0.7532	-1.9689
C	-0.2091	1.9763	-2.4707
H	-0.7136	2.6963	-1.8448
H	-0.7045	3.4453	2.6807
H	-2.4162	3.3215	3.0291
C	-1.7863	2.2150	1.3582
O	-0.9807	2.1243	0.3890
O	-2.6690	1.3791	1.6724
H	5.8347	0.8357	-0.5952
H	6.0005	2.5015	-0.1167
C	4.0247	1.8229	-0.3169
N	3.4018	2.8877	0.3063
H	3.8511	3.7630	0.5761
C	2.1177	2.5443	0.5456
H	1.4054	3.1847	1.0410
N	1.8713	1.3248	0.1024
C	3.0543	0.8654	-0.4249
H	3.1215	-0.1282	-0.8402
C	-4.3472	2.1057	-4.6785
H	-4.4957	2.7874	-5.5040
N	-4.6084	2.3623	-3.4188
C	-4.2660	1.2066	-2.7582
C	-4.2675	0.8714	-1.3813
N	-4.5557	1.6775	-0.3831
H	-4.8943	2.6266	-0.5340
H	-4.1500	1.4918	0.5399
N	-3.9387	-0.4370	-1.1342
C	-4.0976	-0.9672	0.2297

H	-3.7908	-2.0119	0.2406
H	-5.1472	-0.8602	0.5123
H	-3.4324	-0.4096	0.8844
C	-3.4492	-1.2653	-2.1057
H	-3.1352	-2.2397	-1.7488
N	-3.3467	-0.9762	-3.3703
C	-3.7918	0.2609	-3.6467
Fe	0.0025	0.1946	0.0869
O	0.9650	-7.3366	-0.1002
C	1.6902	-6.3774	0.2848
O	2.8801	-6.5068	0.6756
C	1.0365	-5.0033	0.3295
H	0.1637	-4.9956	-0.3259
H	0.6610	-4.8868	1.3526
C	1.9217	-3.8015	0.0103
H	2.8591	-3.9055	0.5668
H	2.1782	-3.7514	-1.0513
C	1.2366	-2.5037	0.4384
O	1.2929	-1.5037	-0.3487
O	0.6495	-2.5178	1.5486
O	-1.2930	-0.7341	-0.2142
O	0.0507	0.0468	1.8628
H	-1.3305	-3.5121	1.0031
H	0.1447	-0.9176	2.0096
O	-1.8509	-3.3741	0.2018
H	-1.5517	-2.4735	-0.0401
C	0.2106	3.2484	-4.6872
C	-1.6996	3.4709	2.2166
C	5.4446	1.8355	-0.7878
N	-3.8439	0.8529	-4.8649
Cps	1.3952	4.2291	-4.5643
Cps	-1.9471	4.7769	1.4563
Cps	5.6907	2.2052	-2.2671
Cps	-3.3624	0.2681	-6.0781

$R^{OH}(^{IS}Fe^{III}\text{-}O_{AF})$

H	-0.7361	3.7474	-4.4967
H	0.1409	2.8458	-5.7026
C	0.2334	2.0751	-3.7599
N	0.8599	0.8742	-4.0391
H	1.3249	0.6465	-4.9168
C	0.8135	0.1089	-2.9280
H	1.2464	-0.8742	-2.8150
N	0.1889	0.7523	-1.9610
C	-0.1871	1.9683	-2.4665
H	-0.7030	2.6807	-1.8410
H	-0.7092	3.4368	2.6779
H	-2.4202	3.3268	3.0363
C	-1.8107	2.2258	1.3491
O	-1.0254	2.1482	0.3671
O	-2.7002	1.3914	1.6591
H	5.8414	0.8363	-0.5946
H	6.0139	2.5022	-0.1187
C	4.0360	1.8273	-0.3062
N	3.4141	2.8991	0.3068
H	3.8649	3.7766	0.5683
C	2.1317	2.5595	0.5545
H	1.4187	3.2057	1.0414
N	1.8861	1.3335	0.1270
C	3.0679	0.8668	-0.3989
H	3.1305	-0.1325	-0.8016
C	-4.3177	2.1207	-4.6801
H	-4.4256	2.8147	-5.5017
N	-4.5958	2.3726	-3.4231
C	-4.3078	1.1989	-2.7689
C	-4.3196	0.8608	-1.3920
N	-4.5718	1.6779	-0.3936
H	-4.8885	2.6340	-0.5471
H	-4.1561	1.4940	0.5269
N	-4.0286	-0.4566	-1.1491
C	-4.1025	-0.9645	0.2279
H	-3.7772	-2.0037	0.2413
H	-5.1328	-0.8663	0.5768
H	-3.4144	-0.3811	0.8387
C	-3.5819	-1.3010	-2.1267
H	-3.3107	-2.2892	-1.7744
N	-3.4681	-1.0132	-3.3898
C	-3.8547	0.2450	-3.6591
Fe	0.0364	0.2739	0.0169
O	0.9634	-7.3473	-0.0999
C	1.6900	-6.3883	0.2830
O	2.8783	-6.5188	0.6795
C	1.0479	-5.0109	0.3139
H	0.1682	-5.0043	-0.3320
H	0.6846	-4.8726	1.3386
C	1.9468	-3.8288	-0.0342
H	2.8890	-3.9415	0.5127
H	2.1912	-3.8001	-1.0997
C	1.2907	-2.5124	0.3809
O	1.3395	-1.5289	-0.4163
O	0.7248	-2.5033	1.5070
O	-1.3565	-0.7145	-0.5038
O	-0.0843	0.0098	1.7622
H	-1.2357	-3.3754	0.9339
H	0.2194	-0.9129	1.8914
O	-1.8041	-3.3427	0.1526
H	-1.5062	-2.5014	-0.2454
C	0.2155	3.2392	-4.6846
C	-1.7067	3.4706	2.2197
C	5.4526	1.8367	-0.7858
N	-3.8555	0.8528	-4.8702
Cps	1.3949	4.2277	-4.5643
Cps	-1.9478	4.7775	1.4572
Cps	5.6912	2.2053	-2.2667
Cps	-3.3636	0.2679	-6.0790

$R^{OH}(^{LS}Fe^{III}\text{-}O_{F})$

H	-0.7305	3.7392	-4.4745
H	0.1433	2.8207	-5.6695
C	0.2488	2.0806	-3.7154
N	0.8465	0.8677	-3.9965
H	1.3009	0.6291	-4.8758
C	0.7980	0.1126	-2.8736
H	1.2023	-0.8835	-2.7785
N	0.2041	0.7683	-1.8998
C	-0.1508	1.9859	-2.4119
H	-0.6422	2.7175	-1.7894
H	-0.6709	3.4456	2.6625
H	-2.3805	3.3012	3.0251
C	-1.7525	2.1712	1.3819
O	-0.8693	2.0109	0.4786
O	-2.6885	1.3918	1.6522
H	5.8599	0.8215	-0.6197
H	6.0301	2.4831	-0.1296
C	4.0531	1.8066	-0.3063
N	3.4450	2.8769	0.3212
H	3.8993	3.7549	0.5724
C	2.1675	2.5313	0.5985
H	1.4692	3.1790	1.1045
N	1.9082	1.3081	0.1785
C	3.0775	0.8478	-0.3758
H	3.1349	-0.1459	-0.7937
C	-4.3246	2.1263	-4.6910

H	-4.4399	2.8121	-5.5184
N	-4.5994	2.3888	-3.4356
C	-4.3005	1.2235	-2.7716
C	-4.3239	0.8920	-1.3951
N	-4.5922	1.7136	-0.4028
H	-4.9028	2.6709	-0.5584
H	-4.2084	1.5192	0.5243
N	-4.0391	-0.4231	-1.1410
C	-4.1992	-0.9354	0.2286
H	-3.9094	-1.9842	0.2414
H	-5.2444	-0.8078	0.5186
H	-3.5153	-0.3882	0.8740
C	-3.5654	-1.2691	-2.1055
H	-3.2801	-2.2499	-1.7403
N	-3.4409	-0.9861	-3.3699
C	-3.8415	0.2640	-3.6533
Fe	-0.0717	0.2266	0.1328
O	0.9702	-7.2690	-0.1092
C	1.6792	-6.2923	0.2664
O	2.8695	-6.4042	0.6582
C	0.9767	-4.9314	0.3026
H	0.1352	-4.9512	-0.3928
H	0.5471	-4.8568	1.3086
C	1.8017	-3.6653	0.0506
H	2.7398	-3.7436	0.6115
H	2.0606	-3.5472	-1.0048
C	1.0492	-2.4271	0.5516
O	1.0335	-1.3869	-0.2019
O	0.4970	-2.5121	1.6665
O	-1.4261	-0.5453	-0.2789
O	-0.0731	0.0890	1.9152
H	-1.4728	-3.3583	0.8621
H	0.1866	-0.8265	2.1051
O	-1.8968	-3.2083	0.0085
H	-1.6322	-2.2771	-0.1635
C	0.2223	3.2311	-4.6581
C	-1.6698	3.4543	2.2084
C	5.4662	1.8223	-0.7994
N	-3.8543	0.8599	-4.8710
Cps	1.3969	4.2289	-4.5602
Cps	-1.9446	4.7625	1.4547
Cps	5.6984	2.2060	-2.2781
Cps	-3.3665	0.2684	-6.0784

$TS_{RI1}{}^{OH}$ ($^{HS}Fe^{III}$-O_{AF})

H	-0.7466	3.7452	-4.5291
H	0.1412	2.8507	-5.7317
C	0.2196	2.0689	-3.7942
N	0.8669	0.8822	-4.0717
H	1.3448	0.6642	-4.9449
C	0.8131	0.1151	-2.9576
H	1.2585	-0.8639	-2.8655
N	0.1671	0.7349	-1.9932
C	-0.2142	1.9452	-2.5046
H	-0.7456	2.6578	-1.8923
H	-0.6627	3.4515	2.6444
H	-2.3674	3.3357	3.0458
C	-1.8000	2.2285	1.3588
O	-0.9638	2.0843	0.4162
O	-2.7426	1.4456	1.6199
H	5.8384	0.8388	-0.6067
H	6.0346	2.5054	-0.1443
C	4.0484	1.8528	-0.3107
N	3.4345	2.9456	0.2710
H	3.8909	3.8267	0.5111
C	2.1553	2.6125	0.5452
H	1.4515	3.2794	1.0174
N	1.9024	1.3732	0.1658
C	3.0767	0.8927	-0.3605
H	3.1373	-0.1139	-0.7442
C	-4.3576	2.1163	-4.6953
H	-4.4484	2.8187	-5.5120
N	-4.6522	2.3562	-3.4390
C	-4.3804	1.1745	-2.7927
C	-4.3378	0.8469	-1.4144
N	-4.5328	1.6852	-0.4224
H	-4.8837	2.6274	-0.5862
H	-4.0523	1.5367	0.4781
N	-4.0154	-0.4689	-1.1769
C	-3.7648	-0.9460	0.1640
H	-3.8636	-2.0267	0.2187
H	-4.3439	-0.4156	0.9113
H	-2.5387	-0.7333	0.2667
C	-3.6046	-1.3204	-2.1778
H	-3.3093	-2.3033	-1.8301
N	-3.5389	-1.0338	-3.4380
C	-3.9246	0.2293	-3.6874
Fe	-0.0171	0.2102	0.2487
O	0.9710	-7.2887	-0.0946
C	1.6955	-6.3361	0.3078
O	2.8886	-6.4774	0.6847
C	1.0313	-4.9639	0.3937
H	0.1600	-4.9476	-0.2618
H	0.6478	-4.8796	1.4174
C	1.8873	-3.7273	0.1133
H	2.8192	-3.8101	0.6828
H	2.1589	-3.6411	-0.9419
C	1.1568	-2.4620	0.5684
O	1.1847	-1.4327	-0.1942
O	0.5647	-2.5067	1.6679
O	-1.4805	-0.7895	-0.3879
O	-0.1668	0.0757	2.0722
H	-1.3853	-3.4864	0.8827
H	0.1448	-0.8219	2.2804
O	-1.8195	-3.4584	0.0212
H	-1.5441	-2.5679	-0.2864
C	0.2063	3.2363	-4.7101
C	-1.6715	3.4782	2.2145
C	5.4591	1.8420	-0.8021
N	-3.8999	0.8473	-4.8865
Cps	1.3855	4.2212	-4.5761
Cps	-1.9420	4.7795	1.4508
Cps	5.6876	2.2016	-2.2853
Cps	-3.3739	0.2619	-6.0751

$TS_{RI1}{}^{OH}$ ($^{IS}Fe^{III}$-O_F)

H	-0.7531	3.7542	-4.5636
H	0.1548	2.8519	-5.7448
C	0.1831	2.0751	-3.8042
N	0.8377	0.8840	-4.0507
H	1.3333	0.6542	-4.9112
C	0.7497	0.1233	-2.9379
H	1.1969	-0.8506	-2.8042
N	0.0720	0.7582	-2.0014
C	-0.2951	1.9667	-2.5314
H	-0.8423	2.6829	-1.9381
H	-0.6611	3.4280	2.6157
H	-2.3560	3.3221	3.0503
C	-1.8299	2.2453	1.3224
O	-1.1089	2.1856	0.2889
O	-2.7013	1.4035	1.6579
H	5.7412	0.8782	-0.5623
H	5.9311	2.5518	-0.1191
C	3.9471	1.9094	-0.3601
N	3.3241	2.9923	0.2343
H	3.7801	3.8648	0.5050
C	2.0322	2.6707	0.4555

H	1.3197	3.3271	0.9288
N	1.7809	1.4456	0.0287
C	2.9677	0.9624	-0.4694
H	3.0299	-0.0420	-0.8579
C	-4.3650	2.1209	-4.7039
H	-4.4893	2.8106	-5.5271
N	-4.6407	2.3722	-3.4452
C	-4.3269	1.2080	-2.7855
C	-4.2694	0.8947	-1.4049
N	-4.4864	1.7232	-0.4089
H	-4.8580	2.6602	-0.5591
H	-4.0170	1.5591	0.4950
N	-3.9094	-0.4121	-1.1541
C	-3.7078	-0.8772	0.1881
H	-3.7330	-1.9624	0.2432
H	-4.3324	-0.3694	0.9123
H	-2.3357	-0.6523	0.2984
C	-3.4930	-1.2642	-2.1510
H	-3.1796	-2.2392	-1.7963
N	-3.4408	-0.9861	-3.4159
C	-3.8630	0.2616	-3.6763
Fe	0.0147	0.3181	0.0658
O	0.9763	-7.2690	-0.0964
C	1.7067	-6.3241	0.3138
O	2.8999	-6.4761	0.6881
C	1.0649	-4.9426	0.4087
H	0.1642	-4.9216	-0.2059
H	0.7341	-4.8266	1.4477
C	1.9418	-3.7398	0.0601
H	2.8754	-3.8183	0.6264
H	2.2065	-3.7168	-1.0004
C	1.2502	-2.4282	0.4418
O	1.2827	-1.4652	-0.3880
O	0.6849	-2.3950	1.5649
O	-1.3142	-0.7936	-0.1766
O	0.0908	0.1839	1.8234
H	-1.3984	-3.5444	0.9968
H	0.2207	-0.7807	1.9658
O	-1.8237	-3.4454	0.1369
H	-1.4663	-2.5740	-0.1309
C	0.2003	3.2398	-4.7231
C	-1.6786	3.4707	2.2048
C	5.3829	1.8815	-0.7922
N	-3.8801	0.8612	-4.8869
Cps	1.3829	4.2176	-4.5675
Cps	-1.9499	4.7766	1.4553
Cps	5.6875	2.2107	-2.2730
Cps	-3.3666	0.2666	-6.0780

$TS_{RI1}{}^{OH}$ ($^{IS}Fe^{III}$-O_{AF})

H	-0.7466	3.7180	-4.5347
H	0.1616	2.8270	-5.7247
C	0.2346	2.0583	-3.7797
N	0.9082	0.8792	-4.0325
H	1.3852	0.6519	-4.9041
C	0.8853	0.1371	-2.9039
H	1.3536	-0.8273	-2.7785
N	0.2312	0.7730	-1.9532
C	-0.1887	1.9612	-2.4875
H	-0.7352	2.6709	-1.8864
H	-0.6731	3.4073	2.6238
H	-2.3756	3.3090	3.0392
C	-1.8407	2.2376	1.3124
O	-1.0860	2.1594	0.3056
O	-2.7596	1.4310	1.6102
H	5.8154	0.9078	-0.5470
H	6.0189	2.5874	-0.1407
C	4.0282	1.9414	-0.3118
N	3.4063	3.0387	0.2533
H	3.8598	3.9211	0.4956
C	2.1191	2.7130	0.5004
H	1.4085	3.3839	0.9566
N	1.8713	1.4729	0.1198
C	3.0551	0.9858	-0.3779
H	3.1218	-0.0246	-0.7487
C	-4.3491	2.1423	-4.7222
H	-4.4395	2.8419	-5.5417
N	-4.6422	2.3853	-3.4655
C	-4.3700	1.2061	-2.8140
C	-4.3093	0.8822	-1.4350
N	-4.4986	1.7186	-0.4435
H	-4.8531	2.6606	-0.6042
H	-4.0134	1.5652	0.4579
N	-3.9708	-0.4326	-1.1982
C	-3.6726	-0.9006	0.1333
H	-3.7427	-1.9833	0.1912
H	-4.2316	-0.3769	0.8986
H	-2.4265	-0.6599	0.1787
C	-3.5755	-1.2865	-2.2024
H	-3.2728	-2.2680	-1.8576
N	-3.5281	-1.0033	-3.4631
C	-3.9174	0.2596	-3.7062
Fe	0.0146	0.3346	0.0358
O	1.2100	-7.1545	-0.0469
C	1.9592	-6.2211	0.3559
O	3.1764	-6.3776	0.6378
C	1.3050	-4.8557	0.5597
H	0.3860	-4.8254	-0.0252
H	0.9989	-4.8076	1.6119
C	2.1320	-3.6006	0.2578
H	3.0161	-3.5978	0.9054
H	2.4868	-3.5692	-0.7753
C	1.3137	-2.3441	0.5728
O	1.3002	-1.3892	-0.2681
O	0.6890	-2.3442	1.6625
O	-1.4051	-0.6769	-0.5057
O	-0.1196	0.1813	1.7904
H	-1.2036	-3.3465	0.7864
H	0.2193	-0.7140	1.9888
O	-1.6257	-3.3696	-0.0819
H	-1.3795	-2.4820	-0.4163
C	0.2128	3.2181	-4.7041
C	-1.6856	3.4550	2.2036
C	5.4471	1.9052	-0.7824
N	-3.8936	0.8716	-4.9055
Cps	1.3823	4.2126	-4.5599
Cps	-1.9456	4.7626	1.4533
Cps	5.6994	2.2061	-2.2754
Cps	-3.3635	0.2676	-6.0801

$TS_{RI1}{}^{OH}$ ($^{LS}Fe^{III}$-O_{F})

H	-0.7450	3.7005	-4.5213
H	0.1620	2.8116	-5.7132
C	0.2402	2.0408	-3.7702
N	0.8833	0.8496	-4.0415
H	1.3574	0.6258	-4.9155
C	0.8412	0.0924	-2.9207
H	1.2879	-0.8848	-2.8199
N	0.2062	0.7260	-1.9564
C	-0.1816	1.9313	-2.4770
H	-0.7051	2.6504	-1.8665
H	-0.6519	3.4366	2.6396
H	-2.3589	3.2749	3.0131
C	-1.7349	2.1880	1.3410
O	-0.8966	2.0636	0.3945

O	-2.6488	1.3823	1.6235
H	5.8051	0.8966	-0.5693
H	5.9804	2.5733	-0.1384
C	4.0015	1.9054	-0.3384
N	3.3783	2.9864	0.2560
H	3.8292	3.8662	0.5104
C	2.0929	2.6518	0.5000
H	1.3813	3.3056	0.9774
N	1.8460	1.4224	0.0875
C	3.0287	0.9494	-0.4256
H	3.0970	-0.0511	-0.8225
C	-4.3686	2.1475	-4.7210
H	-4.4809	2.8392	-5.5446
N	-4.6479	2.3973	-3.4621
C	-4.3486	1.2278	-2.8045
C	-4.2808	0.9075	-1.4284
N	-4.4763	1.7421	-0.4312
H	-4.8477	2.6794	-0.5791
H	-4.0120	1.5735	0.4692
N	-3.9295	-0.4007	-1.1841
C	-3.7053	-0.8620	0.1566
H	-3.7226	-1.9471	0.2002
H	-4.3423	-0.3692	0.8810
H	-2.3451	-0.6016	0.2586
C	-3.5282	-1.2567	-2.1835
H	-3.2151	-2.2345	-1.8334
N	-3.4815	-0.9726	-3.4466
C	-3.8928	0.2800	-3.6951
Fe	0.0511	0.3173	0.1065
O	1.1210	-7.1606	-0.0498
C	1.8494	-6.2144	0.3628
O	3.0577	-6.3588	0.6860
C	1.1690	-4.8517	0.5299
H	0.2569	-4.8523	-0.0666
H	0.8524	-4.7912	1.5781
C	1.9646	-3.5776	0.2125
H	2.8820	-3.5786	0.8117
H	2.2644	-3.5228	-0.8371
C	1.1542	-2.3323	0.6049
O	1.1620	-1.3247	-0.1916
O	0.5411	-2.3826	1.6898
O	-1.3341	-0.6898	-0.2560
O	0.0529	0.2359	1.8857
H	-1.4775	-3.4549	0.6693
H	0.2369	-0.6950	2.0914
O	-1.7368	-3.3566	-0.2544
H	-1.4186	-2.4413	-0.4215
C	0.2158	3.2041	-4.6930
C	-1.6550	3.4480	2.1952
C	5.4261	1.8924	-0.7961
N	-3.8965	0.8833	-4.9000
Cps	1.3799	4.2079	-4.5575
Cps	-1.9461	4.7620	1.4618
Cps	5.6945	2.2149	-2.2824
Cps	-3.3734	0.2747	-6.0744

$I1^{OH}$ ($^{HS}Fe^{III}$-O_{AF})

H	-0.7213	3.7683	-4.4760
H	0.1426	2.8780	-5.6989
C	0.2551	2.0867	-3.7660
N	0.8644	0.8868	-4.0738
H	1.3153	0.6668	-4.9602
C	0.8374	0.1164	-2.9601
H	1.2596	-0.8747	-2.8899
N	0.2455	0.7459	-1.9691
C	-0.1292	1.9656	-2.4603
H	-0.6210	2.6838	-1.8217
H	-0.7609	3.4072	2.7094
H	-2.4845	3.2888	3.0024
C	-1.7871	2.1917	1.3465
O	-0.9089	2.0937	0.4455
O	-2.6982	1.3491	1.5765
H	5.9359	0.8366	-0.6598
H	6.1259	2.4985	-0.1792
C	4.1419	1.8316	-0.3088
N	3.5432	2.9113	0.3113
H	4.0044	3.7885	0.5553
C	2.2653	2.5794	0.5932
H	1.5714	3.2351	1.0955
N	1.9998	1.3544	0.1804
C	3.1629	0.8791	-0.3726
H	3.2099	-0.1177	-0.7842
C	-4.3662	2.1116	-4.6874
H	-4.4728	2.7952	-5.5177
N	-4.6646	2.3748	-3.4374
C	-4.3723	1.2128	-2.7657
C	-4.4174	0.8915	-1.3886
N	-4.6587	1.7124	-0.3868
H	-4.9644	2.6733	-0.5367
H	-4.1972	1.5277	0.5131
N	-4.1576	-0.4396	-1.1209
C	-4.3757	-0.9675	0.1475
H	-3.8937	-1.9091	0.3837
H	-5.0885	-0.4638	0.7817
H	-2.1506	-0.2074	0.4029
C	-3.5965	-1.2743	-2.0806
H	-3.2897	-2.2416	-1.6992
N	-3.4525	-0.9800	-3.3335
C	-3.8826	0.2579	-3.6370
Fe	0.0848	0.2019	0.2691
O	0.9707	-7.2976	-0.0982
C	1.6818	-6.3336	0.3020
O	2.8777	-6.4481	0.6779
C	1.0004	-4.9721	0.3858
H	0.1350	-4.9569	-0.2803
H	0.6104	-4.8924	1.4072
C	1.8672	-3.7466	0.1107
H	2.8060	-3.8494	0.6663
H	2.1248	-3.6557	-0.9476
C	1.1627	-2.4781	0.5816
O	1.2056	-1.4525	-0.1857
O	0.5824	-2.5106	1.6867
O	-1.5516	-0.6391	-0.2238
O	-0.0129	0.1379	2.1076
H	-1.4288	-3.3596	1.0319
H	0.2541	-0.7640	2.3451
O	-1.9750	-3.2263	0.2477
H	-1.7201	-2.3002	0.0018
C	0.2276	3.2589	-4.6769
C	-1.7401	3.4408	2.2158
C	5.5408	1.8379	-0.8312
N	-3.8821	0.8495	-4.8582
Cps	1.4099	4.2437	-4.5570
Cps	-1.9573	4.7560	1.4578
Cps	5.7250	2.2168	-2.3152
Cps	-3.3757	0.2655	-6.0629

$I1^{OH}$ ($^{IS}Fe^{III}$-O_F)

H	-0.7274	3.7470	-4.4920
H	0.1475	2.8633	-5.7123
C	0.2540	2.0700	-3.7796
N	0.8792	0.8744	-4.0768
H	1.3267	0.6506	-4.9642
C	0.8726	0.1131	-2.9606
H	1.3114	-0.8687	-2.8631

N	0.2740	0.7518	-1.9766
C	-0.1275	1.9613	-2.4743
H	-0.6302	2.6727	-1.8375
H	-0.7812	3.3915	2.7029
H	-2.5035	3.2763	2.9839
C	-1.7989	2.2199	1.2944
O	-1.0203	2.2094	0.3174
O	-2.6400	1.3086	1.5834
H	5.9514	0.8534	-0.6399
H	6.1123	2.5218	-0.1683
C	4.1375	1.8231	-0.3167
N	3.5099	2.8939	0.2917
H	3.9581	3.7712	0.5588
C	2.2238	2.5582	0.5188
H	1.5057	3.1986	1.0061
N	1.9856	1.3364	0.0768
C	3.1703	0.8654	-0.4310
H	3.2339	-0.1307	-0.8419
C	-4.3936	2.0802	-4.6644
H	-4.5455	2.7578	-5.4926
N	-4.6704	2.3364	-3.4079
C	-4.3190	1.1880	-2.7407
C	-4.3320	0.8640	-1.3637
N	-4.6020	1.6663	-0.3559
H	-4.9495	2.6147	-0.4977
H	-4.1184	1.4909	0.5374
N	-4.0098	-0.4565	-1.1009
C	-4.2196	-1.0011	0.1619
H	-3.7070	-1.9287	0.3938
H	-4.9497	-0.5207	0.7945
H	-1.9361	-0.0581	0.3978
C	-3.4271	-1.2670	-2.0692
H	-3.0658	-2.2182	-1.6913
N	-3.3184	-0.9653	-3.3248
C	-3.8110	0.2510	-3.6208
Fe	0.2493	0.2796	0.0654
O	0.9460	-7.3566	-0.1198
C	1.6642	-6.3927	0.2681
O	2.8478	-6.5182	0.6775
C	1.0164	-5.0141	0.2869
H	0.1430	-5.0137	-0.3692
H	0.6468	-4.8685	1.3087
C	1.9144	-3.8329	-0.0664
H	2.8572	-3.9374	0.4823
H	2.1617	-3.8136	-1.1314
C	1.2628	-2.5091	0.3338
O	1.3562	-1.5268	-0.4649
O	0.6754	-2.4799	1.4452
O	-1.3512	-0.5700	-0.1820
O	0.2720	0.1640	1.8346
H	-1.2828	-3.3803	0.8839
H	0.3608	-0.8007	1.9720
O	-1.8757	-3.1410	0.1608
H	-1.5754	-2.2098	-0.0056
C	0.2245	3.2425	-4.6894
C	-1.7568	3.4411	2.2015
C	5.5429	1.8478	-0.8201
N	-3.8665	0.8368	-4.8438
Cps	1.4021	4.2320	-4.5596
Cps	-1.9590	4.7684	1.4636
Cps	5.7256	2.2190	-2.3065
Cps	-3.3708	0.2643	-6.0581

$I1^{OH}$ ($^{IS}Fe^{III}$-O_{AF})

H	-0.7245	-3.7502	4.4893
H	0.1496	2.8649	-5.7092
C	0.2566	2.0739	-3.7753
N	0.8795	0.8767	-4.0710
H	1.3276	0.6515	-4.9578
C	0.8692	0.1158	-2.9544
H	1.3063	-0.8667	-2.8568
N	0.2705	0.7558	-1.9713
C	-0.1270	1.9663	-2.4704
H	-0.6297	2.6788	-1.8350
H	-0.7799	3.3811	2.6934
H	-2.5012	3.2742	2.9838
C	-1.8112	2.2180	1.2883
O	-1.0420	2.2085	0.3040
O	-2.6525	1.3082	1.5807
H	5.9412	0.8522	-0.6404
H	6.1080	2.5199	-0.1686
C	4.1311	1.8281	-0.3179
N	3.5069	2.8996	0.2926
H	3.9570	3.7763	0.5586
C	2.2207	2.5659	0.5228
H	1.5057	3.2072	1.0133
N	1.9793	1.3446	0.0811
C	3.1621	0.8721	-0.4298
H	3.2238	-0.1242	-0.8402
C	-4.4013	2.0821	-4.6692
H	-4.5591	2.7556	-5.4996
N	-4.6768	2.3418	-3.4131
C	-4.3181	1.1978	-2.7420
C	-4.3316	0.8774	-1.3640
N	-4.6091	1.6799	-0.3586
H	-4.9563	2.6279	-0.5034
H	-4.1292	1.5050	0.5371
N	-4.0040	-0.4412	-1.0969
C	-4.2178	-0.9850	0.1655
H	-3.7030	-1.9096	0.4053
H	-4.9518	-0.5054	0.7941
H	-1.9427	-0.0568	0.3949
C	-3.4135	-1.2496	-2.0620
H	-3.0479	-2.1975	-1.6816
N	-3.3059	-0.9518	-3.3187
C	-3.8062	0.2604	-3.6194
Fe	0.2417	0.2879	0.0756
O	0.9532	-7.3160	-0.0968
C	1.6751	-6.3633	0.3103
O	2.8658	-6.4985	0.6981
C	1.0341	-4.9835	0.3819
H	0.1270	-4.9665	-0.2257
H	0.7221	-4.8422	1.4230
C	1.9251	-3.8089	-0.0111
H	2.8832	-3.9094	0.5111
H	2.1402	-3.8033	-1.0832
C	1.2868	-2.4801	0.3903
O	1.3507	-1.5127	-0.4300
O	0.7383	-2.4312	1.5204
O	-1.3515	-0.5758	-0.1723
O	0.2513	0.2037	1.8471
H	-1.2867	-3.3473	1.0172
H	0.3866	-0.7533	2.0029
O	-1.8704	-3.1350	0.2789
H	-1.5674	-2.2135	0.0717
C	0.2273	3.2456	-4.6868
C	-1.7580	3.4362	2.1974
C	5.5367	1.8480	-0.8209
N	-3.8677	0.8408	-4.8449
Cps	1.4046	4.2360	-4.5596
Cps	-1.9586	4.7636	1.4599
Cps	5.7233	2.2180	-2.3070
Cps	-3.3725	0.2652	-6.0583

$I1^{OH}$ ($^{LS}Fe^{III}$-O_{F})

H	-0.7150	3.7198	-4.4562
H	0.1614	2.8131	-5.6580
C	0.2890	2.0692	-3.7078
N	0.8711	0.8524	-4.0065
H	1.3096	0.6165	-4.8948
C	0.8590	0.1000	-2.8813
H	1.2648	-0.8961	-2.7924
N	0.3015	0.7608	-1.8894
C	-0.0673	1.9782	-2.3926
H	-0.5334	2.7128	-1.7544
H	-0.7121	3.4603	2.7239
H	-2.4334	3.2696	2.9977
C	-1.6715	2.1771	1.3708
O	-0.7611	2.0828	0.5029
O	-2.5815	1.3295	1.5957
H	5.9176	0.8327	-0.6540
H	6.0978	2.4946	-0.1683
C	4.1169	1.8203	-0.3134
N	3.5155	2.8912	0.3210
H	3.9748	3.7664	0.5748
C	2.2367	2.5580	0.5955
H	1.5385	3.2025	1.1049
N	1.9734	1.3388	0.1635
C	3.1385	0.8682	-0.3907
H	3.1851	-0.1248	-0.8105
C	-4.3749	2.0994	-4.6756
H	-4.5119	2.7762	-5.5069
N	-4.6510	2.3656	-3.4211
C	-4.3228	1.2140	-2.7479
C	-4.3373	0.8988	-1.3692
N	-4.5771	1.7191	-0.3655
H	-4.9138	2.6707	-0.5101
H	-4.1067	1.5400	0.5298
N	-4.0497	-0.4260	-1.0992
C	-4.2613	-0.9561	0.1686
H	-3.7580	-1.8882	0.4025
H	-4.9734	-0.4541	0.8050
H	-1.9934	-0.0631	0.4296
C	-3.4845	-1.2552	-2.0628
H	-3.1456	-2.2120	-1.6782
N	-3.3670	-0.9621	-3.3199
C	-3.8317	0.2629	-3.6232
Fe	0.1879	0.3208	0.1386
O	0.9818	-7.2723	-0.1187
C	1.6832	-6.2829	0.2414
O	2.8737	-6.3769	0.6356
C	0.9797	-4.9248	0.2526
H	0.1328	-4.9569	-0.4368
H	0.5607	-4.8237	1.2609
C	1.8162	-3.6767	-0.0320
H	2.7686	-3.7714	0.5017
H	2.0495	-3.5729	-1.0951
C	1.1104	-2.4148	0.4770
O	1.1467	-1.3732	-0.2632
O	0.5526	-2.4921	1.5932
O	-1.4120	-0.5113	-0.2004
O	0.1468	0.1521	1.9177
H	-1.4022	-3.3028	0.8766
H	0.3092	-0.7873	2.0917
O	-1.9256	-3.0737	0.0993
H	-1.6211	-2.1358	-0.0533
C	0.2420	3.2218	-4.6462
C	-1.6860	3.4456	2.2190
C	5.5214	1.8333	-0.8269
N	-3.8702	0.8458	-4.8488
Cps	1.4049	4.2342	-4.5527
Cps	-1.9514	4.7507	1.4557
Cps	5.7223	2.2154	-2.3102
Cps	-3.3752	0.2645	-6.0600

$TS_{I114}{}^{OH}$

H	-0.7337	3.8167	-4.5641
H	0.1578	2.9374	-5.7742
C	0.1917	2.1102	-3.8549
N	0.8624	0.9341	-4.1253
H	1.3530	0.7216	-4.9935
C	0.7901	0.1532	-3.0282
H	1.2508	-0.8174	-2.9234
N	0.1054	0.7591	-2.0785
C	-0.2791	1.9719	-2.5828
H	-0.8332	2.6699	-1.9739
H	-0.6798	3.4149	2.6322
H	-2.3871	3.2801	3.0172
C	-1.8115	2.2136	1.3055
O	-0.9519	2.0860	0.3747
O	-2.7755	1.4523	1.5340
H	5.8926	0.8743	-0.6176
H	6.0884	2.5472	-0.1768
C	4.0993	1.8875	-0.3216
N	3.4766	2.9858	0.2423
H	3.9295	3.8705	0.4772
C	2.1966	2.6510	0.5132
H	1.4885	3.3254	0.9695
N	1.9484	1.4024	0.1547
C	3.1318	0.9227	-0.3587
H	3.2015	-0.0891	-0.7257
C	-4.4151	2.1201	-4.7345
H	-4.5884	2.7705	-5.5804
N	-4.6851	2.4075	-3.4825
C	-4.3081	1.2857	-2.7836
C	-4.3110	1.0011	-1.4001
N	-4.6156	1.8289	-0.4229
H	-4.9724	2.7659	-0.6000
H	-4.1418	1.6888	0.4816
N	-3.9544	-0.3030	-1.0975
C	-4.1267	-0.8184	0.1749
H	-3.6920	-1.7842	0.3842
H	-4.7437	-0.2671	0.8630
H	-1.2225	-0.6173	1.2076
C	-3.3785	-1.1321	-2.0513
H	-3.0139	-2.0716	-1.6566
N	-3.2822	-0.8657	-3.3176
C	-3.7923	0.3339	-3.6397
Fe	-0.0174	0.2277	0.0010
O	0.9685	-7.1600	-0.0726
C	1.7162	-6.2486	0.3757
O	2.9196	-6.4335	0.7048
C	1.1144	-4.8557	0.5763
H	0.1321	-4.8041	0.1068
H	0.9520	-4.7290	1.6532
C	1.9694	-3.6749	0.0960
H	2.9522	-3.7509	0.5727
H	2.1297	-3.6939	-0.9848
C	1.3326	-2.3473	0.5091
O	1.2955	-1.3846	-0.3360
O	0.8774	-2.2788	1.6676
O	-1.4361	-0.8620	0.0082
O	-0.5210	-0.0913	2.0319
H	-1.5984	-3.5542	1.1743
H	0.1003	-0.8161	2.2322
O	-1.9454	-3.4225	0.2863
H	-1.6232	-2.5048	0.0793
C	0.2127	3.2957	-4.7429
C	-1.6855	3.4431	2.1946
C	5.5100	1.8737	-0.8218
N	-3.8687	0.8808	-4.8774
Cps	1.4104	4.2478	-4.5647
Cps	-1.9585	4.7563	1.4542
Cps	5.7265	2.2164	-2.3130

Cps	-3.3716	0.2629	-6.0657

$I4^{OH}$

H	-0.7378	3.8157	-4.5358
H	0.1349	2.9297	-5.7547
C	0.1830	2.1042	-3.8371
N	0.8116	0.9113	-4.1312
H	1.2989	0.7009	-5.0011
C	0.7181	0.1152	-3.0446
H	1.1442	-0.8732	-2.9598
N	0.0632	0.7275	-2.0805
C	-0.2808	1.9605	-2.5617
H	-0.8039	2.6691	-1.9375
H	-0.7125	3.5090	2.7367
H	-2.4266	3.3407	3.0368
C	-1.7022	2.2047	1.4350
O	-0.9127	2.1011	0.4592
O	-2.4852	1.3042	1.8388
H	5.9002	0.8296	-0.6370
H	6.0692	2.4929	-0.1503
C	4.0905	1.8119	-0.3245
N	3.4717	2.8841	0.2878
H	3.9235	3.7591	0.5530
C	2.1825	2.5449	0.5178
H	1.4739	3.1965	1.0049
N	1.9267	1.3258	0.0822
C	3.1115	0.8616	-0.4338
H	3.1777	-0.1315	-0.8521
C	-4.3451	2.0971	-4.6483
H	-4.5089	2.7765	-5.4729
N	-4.5899	2.3565	-3.3849
C	-4.2358	1.2022	-2.7240
C	-4.2185	0.8726	-1.3489
N	-4.4538	1.6850	-0.3309
H	-4.8115	2.6299	-0.4611
H	-4.0008	1.4843	0.5630
N	-3.9158	-0.4495	-1.0952
C	-4.0259	-0.9772	0.1798
H	-3.6714	-1.9855	0.3370
H	-4.6551	-0.4493	0.8787
H	-1.6550	-2.4793	0.0540
C	-3.3774	-1.2675	-2.0794
H	-3.0408	-2.2307	-1.7171
N	-3.2932	-0.9662	-3.3397
C	-3.7648	0.2587	-3.6194
Fe	-0.1044	0.1274	-0.0140
O	0.9382	-7.2844	-0.1017
C	1.6567	-6.3412	0.3301
O	2.8525	-6.4833	0.7017
C	1.0070	-4.9661	0.4583
H	0.0796	-4.9365	-0.1138
H	0.7298	-4.8524	1.5126
C	1.8766	-3.7742	0.0594
H	2.8438	-3.8671	0.5651
H	2.0717	-3.7570	-1.0159
C	1.2346	-2.4549	0.4751
O	1.2396	-1.4866	-0.3447
O	0.7356	-2.3997	1.6316
O	-1.4905	-0.8753	-0.0968
O	0.1616	0.0458	2.1265
H	0.3871	-0.9315	2.1113
H	-0.7523	0.1118	2.4256
O	-1.9376	-3.4250	0.2329
H	-1.5266	-3.5927	1.0872
C	0.2046	3.2907	-4.7252
C	-1.6936	3.4974	2.2404
C	5.5015	1.8288	-0.8140
N	-3.8399	0.8476	-4.8414
Cps	1.4052	4.2429	-4.5645
Cps	-1.9503	4.7806	1.4566
Cps	5.7104	2.2108	-2.2950
Cps	-3.3686	0.2676	-6.0631

$TS_{I1I2}{}^{OH}$

H	-0.7516	3.7532	-4.5091
H	0.1367	2.8296	-5.6879
C	0.1778	2.0774	-3.7389
N	0.8304	0.8841	-3.9811
H	1.3391	0.6567	-4.8338
C	0.6851	0.1039	-2.8867
H	1.1212	-0.8771	-2.7723
N	-0.0266	0.7171	-1.9598
C	-0.3539	1.9420	-2.4870
H	-0.9277	2.6530	-1.9122
H	-0.6718	3.5103	2.7369
H	-2.3822	3.3778	3.1012
C	-1.7474	2.2143	1.4895
O	-0.9713	2.0937	0.4875
O	-2.5905	1.3701	1.8506
H	5.9040	0.8363	-0.6552
H	6.0996	2.4982	-0.1754
C	4.1104	1.8489	-0.3390
N	3.5143	2.9337	0.2740
H	3.9841	3.8019	0.5358
C	2.2237	2.6264	0.5150
H	1.5322	3.2880	1.0130
N	1.9459	1.4099	0.0799
C	3.1154	0.9163	-0.4430
H	3.1587	-0.0796	-0.8567
C	-4.2977	2.1476	-4.6701
H	-4.4572	2.8352	-5.4895
N	-4.5073	2.4122	-3.3978
C	-4.1580	1.2479	-2.7361
C	-4.0752	0.9411	-1.3768
N	-4.3771	1.7476	-0.3580
H	-4.7968	2.6595	-0.5221
H	-3.9248	1.6290	0.5444
N	-3.6835	-0.3893	-1.1160
C	-3.4315	-0.8611	0.1374
H	-3.5421	-1.9306	0.2631
H	-3.7178	-0.2261	0.9564
H	-1.4093	-1.2958	1.0818
C	-3.3334	-1.2542	-2.1633
H	-3.0408	-2.2435	-1.8372
N	-3.3523	-0.9589	-3.4241
C	-3.7591	0.2892	-3.6572
Fe	0.0418	0.3223	0.3071
O	0.9782	-7.2717	-0.0924
C	1.6894	-6.3181	0.3295
O	2.8826	-6.4449	0.7086
C	1.0011	-4.9574	0.4367
H	0.1361	-4.9545	-0.2281
H	0.6051	-4.9023	1.4576
C	1.8404	-3.7043	0.1822
H	2.7594	-3.7673	0.7759
H	2.1411	-3.6166	-0.8649
C	1.0823	-2.4434	0.6042
O	1.1327	-1.4212	-0.1612
O	0.4407	-2.4885	1.6830
O	-1.5750	-0.8853	0.2201
O	0.1479	0.2289	2.1362
H	-1.4512	-3.7019	1.1061
H	0.4266	-0.6529	2.4165
O	-1.9624	-3.6519	0.2883
H	-1.5908	-2.8573	-0.1236
C	0.1982	3.2346	-4.6737

C	-1.6709	3.5013	2.2802
C	5.5204	1.8406	-0.8353
N	-3.8405	0.8880	-4.8705
Cps	1.3856	4.2172	-4.5568
Cps	-1.9441	4.7565	1.4558
Cps	5.7249	2.2157	-2.3171
Cps	-3.3762	0.2634	-6.0631

$I2^{OH}$

H	-0.7777	3.7757	-4.5102
H	0.0878	2.8652	-5.7160
C	0.1258	2.0681	-3.7870
N	0.7762	0.8776	-4.0495
H	1.3000	0.6686	-4.8980
C	0.6174	0.0736	-2.9756
H	1.0497	-0.9104	-2.8652
N	-0.1036	0.6695	-2.0452
C	-0.4177	1.9080	-2.5436
H	-0.9778	2.6141	-1.9477
H	-0.7093	3.6051	2.8363
H	-2.4271	3.4524	3.1169
C	-1.6669	2.2367	1.5988
O	-1.0481	2.1238	0.5113
O	-2.2801	1.3019	2.1831
H	5.8863	0.8288	-0.6387
H	6.0593	2.4906	-0.1507
C	4.0788	1.8194	-0.3286
N	3.4741	2.8936	0.2943
H	3.9360	3.7638	0.5601
C	2.1822	2.5738	0.5218
H	1.4843	3.2273	1.0216
N	1.9118	1.3625	0.0720
C	3.0882	0.8827	-0.4486
H	3.1361	-0.1088	-0.8740
C	-4.4164	2.0403	-4.6876
H	-4.7326	2.6801	-5.4990
N	-4.5651	2.3009	-3.4094
C	-4.0100	1.2173	-2.7690
C	-3.8117	0.9224	-1.3939
N	-4.1526	1.7123	-0.3937
H	-4.6604	2.5858	-0.5239
H	-3.8321	1.5180	0.5482
N	-3.2113	-0.2854	-1.1810
C	-2.8835	-0.8740	0.2166
H	-3.4584	-1.8127	0.2295
H	-3.3332	-0.1706	0.9239
H	-1.5966	-2.9509	0.5500
C	-2.7595	-1.0795	-2.1935
H	-2.2483	-1.9716	-1.8462
N	-2.8844	-0.8466	-3.4673
C	-3.5208	0.3143	-3.6936
Fe	0.0056	0.2151	0.0945
O	1.0271	-7.2774	-0.0765
C	1.7404	-6.3621	0.4195
O	2.9525	-6.5193	0.7335
C	1.1046	-4.9999	0.6891
H	0.0485	-5.0098	0.4243
H	1.1550	-4.8236	1.7675
C	1.7908	-3.8311	-0.0244
H	2.8640	-3.8619	0.1991
H	1.6888	-3.9119	-1.1103
C	1.2440	-2.4723	0.4192
O	1.1365	-1.5565	-0.4524
O	0.9399	-2.3435	1.6324
O	-1.5771	-1.0644	0.3540
O	0.3284	0.0972	2.2457
H	0.5413	-0.8733	2.1751
H	-0.5873	0.1775	2.5378
O	-2.0783	-3.7971	0.4821
H	-2.1501	-4.1380	1.3857
C	0.1625	3.2442	-4.6928
C	-1.6839	3.5704	2.3241
C	5.4909	1.8288	-0.8158
N	-3.7881	0.8509	-4.9067
Cps	1.3664	4.2010	-4.5607
Cps	-1.9309	4.8105	1.4764
Cps	5.7020	2.2091	-2.2954
Cps	-3.3557	0.2692	-6.1388

TS_{I2I5}^{OH}

H	-0.7808	3.7577	-4.4751
H	0.0732	2.8261	-5.6715
C	0.1373	2.0659	-3.7259
N	0.7499	0.8555	-3.9948
H	1.2521	0.6308	-4.8528
C	0.6029	0.0611	-2.9133
H	1.0142	-0.9326	-2.8141
N	-0.0779	0.6827	-1.9656
C	-0.3762	1.9280	-2.4667
H	-0.9125	2.6461	-1.8640
H	-0.7047	3.8777	3.0241
H	-2.3948	3.5366	3.1961
C	-1.3489	2.2904	1.9106
O	-0.8608	2.1311	0.7506
O	-1.5513	1.3994	2.7655
H	5.9783	0.8624	-0.6216
H	6.1635	2.5355	-0.1791
C	4.1794	1.8601	-0.2792
N	3.5673	2.9689	0.2696
H	4.0314	3.8441	0.5167
C	2.2703	2.6724	0.4779
H	1.5584	3.3493	0.9235
N	2.0091	1.4406	0.0813
C	3.1917	0.9233	-0.3796
H	3.2449	-0.0867	-0.7581
C	-4.2691	2.1385	-4.7268
H	-4.4307	2.8198	-5.5502
N	-4.4838	2.4044	-3.4600
C	-4.1524	1.2418	-2.8037
C	-4.1025	0.8916	-1.4302
N	-4.2400	1.6634	-0.3732
H	-4.6111	2.6121	-0.4033
H	-3.8660	1.2646	0.5000
N	-3.8469	-0.4377	-1.2220
C	-3.9708	-0.9422	0.2416
H	-3.9446	-2.0380	0.1267
H	-5.0083	-0.6490	0.4922
H	-1.9814	-1.7455	0.4877
C	-3.4016	-1.2711	-2.1932
H	-3.0796	-2.2449	-1.8353
N	-3.3063	-0.9715	-3.4622
C	-3.7326	0.2785	-3.7074
Fe	0.1951	0.3796	0.1656
O	1.0404	-7.3527	-0.0224
C	1.7523	-6.3859	0.3709
O	2.9340	-6.5016	0.7818
C	1.0894	-5.0134	0.3983
H	0.2214	-5.0303	-0.2647
H	0.7092	-4.8833	1.4177
C	1.9700	-3.8086	0.0603
H	2.9006	-3.8950	0.6326
H	2.2364	-3.7751	-0.9990
C	1.2729	-2.5140	0.4707
O	1.2757	-1.5077	-0.2908
O	0.7008	-2.5608	1.6025
O	-3.0104	-0.4004	0.9743

O	0.3388	-0.1259	2.0974
H	0.3780	-1.1185	2.1160
H	-0.4646	0.2650	2.5299
O	-1.6798	-2.5962	0.0962
H	-1.0060	-2.8927	0.7208
C	0.1600	3.2286	-4.6581
C	-1.6194	3.6831	2.4390
C	5.5706	1.8563	-0.8044
N	-3.8038	0.8732	-4.9229
Cps	1.3586	4.2003	-4.5616
Cps	-1.9306	4.8107	1.4757
Cps	5.7018	2.2085	-2.2967
Cps	-3.3564	0.2685	-6.1387

$I5^{OH}$

H	-0.7533	3.7682	-4.4713
H	0.1080	2.8560	-5.6789
C	0.1945	2.0828	-3.7404
N	0.8362	0.8916	-4.0207
H	1.3218	0.6760	-4.8897
C	0.7561	0.1115	-2.9196
H	1.1998	-0.8686	-2.8217
N	0.0943	0.7240	-1.9581
C	-0.2647	1.9470	-2.4605
H	-0.7988	2.6562	-1.8451
H	-0.7610	3.7752	3.0239
H	-2.4511	3.4252	3.1271
C	-1.3610	2.2228	1.8247
O	-0.8048	2.1181	0.6925
O	-1.6224	1.2848	2.6133
H	6.0834	0.8677	-0.6960
H	6.2648	2.5346	-0.2303
C	4.2856	1.8432	-0.2867
N	3.6888	2.9290	0.3212
H	4.1528	3.8031	0.5712
C	2.4021	2.6165	0.5710
H	1.7037	3.2767	1.0612
N	2.1328	1.3965	0.1467
C	3.2989	0.9032	-0.3778
H	3.3416	-0.0941	-0.7899
C	-4.3080	2.1342	-4.7065
H	-4.4276	2.8247	-5.5293
N	-4.5786	2.3880	-3.4481
C	-4.2775	1.2201	-2.7893
C	-4.3268	0.8598	-1.4154
N	-4.5893	1.6144	-0.3772
H	-4.9124	2.5793	-0.4414
H	-4.3342	1.1840	0.5355
N	-4.0502	-0.4687	-1.1960
C	-4.2893	-1.0068	0.2390
H	-3.9960	-2.0679	0.1531
H	-5.3876	-0.9527	0.3330
H	-2.1856	-0.6195	0.7170
C	-3.5733	-1.2905	-2.1615
H	-3.3030	-2.2815	-1.8154
N	-3.4245	-0.9931	-3.4225
C	-3.8220	0.2655	-3.6815
Fe	0.2892	0.3154	0.1762
O	1.0545	-7.4378	-0.0504
C	1.7526	-6.4511	0.3234
O	2.9198	-6.5500	0.7735
C	1.0775	-5.0826	0.2569
H	0.3085	-5.1210	-0.5210
H	0.5582	-4.9544	1.2139
C	1.9828	-3.8710	0.0461
H	2.8512	-3.9749	0.7065
H	2.3635	-3.8128	-0.9771
C	1.2666	-2.5677	0.4012
O	1.3967	-1.5672	-0.3546
O	0.5653	-2.5881	1.4600
O	-3.6137	-0.2851	1.1252
O	0.6137	-0.0326	2.2735
H	0.6027	-1.0086	2.2719
H	-0.2538	0.2892	2.6070
O	-1.3522	-0.9871	0.2609
H	-0.9759	-1.7065	0.7984
C	0.1916	3.2476	-4.6608
C	-1.6530	3.6007	2.3995
C	5.6621	1.8609	-0.8520
N	-3.8389	0.8683	-4.8945
Cps	1.3842	4.2213	-4.5506
Cps	-1.9362	4.7760	1.4742
Cps	5.7567	2.2368	-2.3428
Cps	-3.3592	0.2729	-6.1039

$TS_{I5Pun}{}^{OH}$

H	-0.7466	-3.7601	4.4628
H	0.1233	2.8167	-5.6390
C	0.2056	2.0990	-3.6784
N	0.8400	0.8987	-3.9362
H	1.3243	0.6648	-4.8005
C	0.7303	0.1256	-2.8339
H	1.1592	-0.8598	-2.7261
N	0.0596	0.7497	-1.8837
C	-0.2789	1.9738	-2.4045
H	-0.8269	2.6882	-1.8080
H	-0.8239	3.8466	3.0959
H	-2.5155	3.4865	3.1311
C	-1.3522	2.2668	1.9142
O	-0.8119	2.1225	0.7822
O	-1.5770	1.3575	2.7511
H	6.0521	0.8606	-0.7118
H	6.2376	2.5263	-0.2433
C	4.2576	1.8432	-0.3121
N	3.6681	2.9265	0.3089
H	4.1343	3.8006	0.5558
C	2.3900	2.6060	0.5921
H	1.7001	3.2632	1.0985
N	2.1167	1.3829	0.1784
C	3.2730	0.8968	-0.3758
H	3.3118	-0.0999	-0.7898
C	-4.5678	1.9978	-4.6951
H	-4.9428	2.5863	-5.5201
N	-4.7254	2.2825	-3.4235
C	-4.0751	1.2636	-2.7563
C	-3.8396	0.9761	-1.3892
N	-4.2551	1.7130	-0.3578
H	-4.8088	2.5613	-0.4363
H	-4.0168	1.3871	0.5679
N	-3.1323	-0.1425	-1.1303
C	-5.4404	-0.8752	0.7316
H	-5.5684	-1.6860	-0.0098
H	-6.2190	-0.0993	0.7402
H	-2.2719	-0.7517	0.3283
C	-2.6544	-0.8976	-2.1249
H	-2.0635	-1.7546	-1.8085
N	-2.7983	-0.7231	-3.4263
C	-3.5204	0.3757	-3.6643
Fe	0.2525	0.3236	0.2780
O	1.0506	-7.4386	-0.0534
C	1.7343	-6.4448	0.3271
O	2.9085	-6.5248	0.7613
C	1.0261	-5.0915	0.2894
H	0.2554	-5.1385	-0.4860
H	0.5084	-4.9946	1.2511
C	1.8959	-3.8520	0.0914

H	2.7583	-3.9294	0.7633
H	2.2883	-3.7813	-0.9262
C	1.1328	-2.5753	0.4439
O	1.2178	-1.5723	-0.3205
O	0.4415	-2.6115	1.5052
O	-4.4981	-0.8358	1.4868
O	0.7025	-0.0175	2.3860
H	0.6165	-0.9880	2.3791
H	-0.1423	0.3432	2.7277
O	-1.4318	-0.8404	0.8253
H	-1.1506	-1.7540	0.9928
C	0.2025	3.2423	-4.6342
C	-1.6867	3.6514	2.4365
C	5.6393	1.8566	-0.8734
N	-3.8440	0.8599	-4.8874
Cps	1.3876	4.2358	-4.5579
Cps	-1.9475	4.7983	1.4775
Cps	5.7589	2.2341	-2.3636
Cps	-3.3700	0.2667	-6.0976

P_{un}^{OH}

H	-0.7435	3.7800	-4.4867
H	0.1179	2.8757	-5.6994
C	0.1980	2.0865	-3.7665
N	0.8363	0.8954	-4.0547
H	1.3112	0.6791	-4.9298
C	0.7575	0.1089	-2.9602
H	1.1946	-0.8748	-2.8749
N	0.1028	0.7188	-1.9911
C	-0.2587	1.9451	-2.4868
H	-0.7984	2.6485	-1.8701
H	-0.8806	3.5983	3.0003
H	-2.5948	3.3232	3.0022
C	-1.4815	2.1622	1.6695
O	-0.8159	2.1057	0.6026
O	-1.8756	1.1680	2.3379
H	6.1137	0.8613	-0.6953
H	6.2971	2.5268	-0.2261
C	4.3166	1.8358	-0.2660
N	3.7261	2.9212	0.3487
H	4.1941	3.7919	0.6046
C	2.4364	2.6183	0.5912
H	1.7439	3.2813	1.0857
N	2.1584	1.4035	0.1559
C	3.3227	0.9048	-0.3688
H	3.3592	-0.0876	-0.7926
C	-4.3439	2.1942	-4.7900
H	-4.5642	2.8080	-5.6519
N	-4.5370	2.5384	-3.5396
C	-4.1100	1.4506	-2.8085
C	-4.0116	1.1994	-1.4168
N	-4.2933	2.0943	-0.4726
H	-4.7321	2.9878	-0.6668
H	-4.3470	1.7774	0.4904
N	-3.5738	-0.0251	-1.0522
C	-5.8636	0.0901	1.7382
H	-5.5884	-0.4377	0.8091
H	-6.5901	-0.3978	2.4087
H	-2.2465	-0.6286	0.2946
C	-3.2081	-0.9054	-2.0000
H	-2.8441	-1.8557	-1.6218
N	-3.2029	-0.7589	-3.3154
C	-3.6714	0.4463	-3.6527
Fe	0.3191	0.3355	0.1272
O	1.0098	-7.4033	-0.0648
C	1.6951	-6.4126	0.3192
O	2.8704	-6.4972	0.7505
C	0.9999	-5.0520	0.2875
H	0.2209	-5.0846	-0.4804
H	0.4951	-4.9415	1.2544
C	1.9004	-3.8394	0.0740
H	2.7751	-3.9468	0.7249
H	2.2738	-3.7811	-0.9517
C	1.2043	-2.5297	0.4309
O	1.3773	-1.5299	-0.3171
O	0.4900	-2.5317	1.4838
O	-5.3883	1.1692	2.0128
O	0.5726	0.0273	2.2649
H	0.5781	-0.9524	2.2509
H	-0.3123	0.3126	2.5581
O	-1.3417	-0.9804	0.2311
H	-1.1275	-1.6797	0.8683
C	0.1998	3.2588	-4.6786
C	-1.7517	3.5009	2.3291
C	5.6889	1.8540	-0.8435
N	-3.8162	0.9427	-4.9094
Cps	1.3972	4.2281	-4.5572
Cps	-1.9524	4.7301	1.4645
Cps	5.7608	2.2350	-2.3334
Cps	-3.3686	0.2706	-6.0922

TS_{I2P}^{OH}

H	-0.8240	-3.7761	4.5894
H	0.0912	2.8610	-5.7526
C	0.0713	2.0832	-3.8167
N	0.7875	0.9199	-4.0196
H	1.3340	0.7010	-4.8512
C	0.6277	0.1436	-2.9262
H	1.1056	-0.8125	-2.7732
N	-0.1513	0.7328	-2.0386
C	-0.5097	1.9359	-2.5903
H	-1.1361	2.6336	-2.0543
H	-0.7845	3.7291	2.9960
H	-2.5041	3.5347	3.1544
C	-1.5690	2.2624	1.8034
O	-1.1257	2.1288	0.6367
O	-1.8519	1.3238	2.6035
H	5.7890	0.9039	-0.5715
H	6.0414	2.5770	-0.1605
C	4.0329	1.9981	-0.3556
N	3.4559	3.1090	0.2256
H	3.9430	3.9661	0.4913
C	2.1437	2.8560	0.4047
H	1.4633	3.5469	0.8762
N	1.8371	1.6531	-0.0420
C	3.0074	1.1098	-0.5045
H	3.0284	0.1087	-0.9076
C	-4.2319	2.3224	-4.9558
H	-4.3759	2.9290	-5.8392
N	-4.4543	2.7014	-3.7184
C	-4.1446	1.5980	-2.9539
C	-4.1295	1.3426	-1.5634
N	-4.3899	2.2587	-0.6295
H	-4.7342	3.1885	-0.8333
H	-4.4740	1.9600	0.3268
N	-3.8006	0.0911	-1.1989
C	-2.7610	-0.6960	0.5839
H	-3.4659	-1.5349	0.5757
H	-3.0371	0.2072	1.1325
H	-1.3407	-3.1783	0.8027
C	-3.4599	-0.8313	-2.1127
H	-3.1925	-1.8044	-1.7109
N	-3.3902	-0.6864	-3.4187
C	-3.7487	0.5517	-3.7630
Fe	0.0874	0.4091	0.1224
O	1.0915	-7.1968	-0.1087

C	1.7830	-6.2032	0.2582
O	2.9682	-6.2893	0.6666
C	1.0808	-4.8440	0.2498
H	0.2548	-4.8748	-0.4649
H	0.6250	-4.7326	1.2402
C	1.9526	-3.6154	-0.0099
H	2.8754	-3.7224	0.5709
H	2.2336	-3.5237	-1.0625
C	1.2602	-2.3329	0.4412
O	1.2287	-1.3500	-0.3562
O	0.7635	-2.3382	1.6037
O	-1.6006	-0.8819	0.2122
O	0.5145	0.1769	2.1855
H	0.5640	-0.8132	2.1647
H	-0.3256	0.4515	2.5953
O	-2.0963	-3.7590	0.6480
H	-2.2418	-4.2118	1.4955
C	0.1240	3.2478	-4.7297
C	-1.7120	3.6377	2.4060
C	5.4523	1.9130	-0.8056
N	-3.7962	1.0334	-5.0222
Cps	1.3255	4.2008	-4.5610
Cps	-1.9307	4.8106	1.4763
Cps	5.7018	2.2089	-2.2961
Cps	-3.3562	0.2690	-6.1386

P^{OH}

H	-0.8280	3.7530	-4.4521
H	0.0151	2.8097	-5.6474
C	0.1043	2.0724	-3.6943
N	0.7542	0.8786	-3.9439
H	1.2460	0.6459	-4.8040
C	0.6438	0.1082	-2.8397
H	1.0844	-0.8706	-2.7210
N	-0.0416	0.7301	-1.8986
C	-0.3887	1.9486	-2.4253
H	-0.9486	2.6624	-1.8390
H	-0.7704	3.8324	3.0649
H	-2.4798	3.5542	3.1909
C	-1.4398	2.2720	1.9204
O	-0.9491	2.1082	0.7754
O	-1.6999	1.3572	2.7533
H	5.9603	0.8722	-0.6169
H	6.1735	2.5413	-0.1764
C	4.1798	1.8943	-0.2615
N	3.5962	2.9970	0.3284
H	4.0687	3.8710	0.5633
C	2.3033	2.7062	0.5755
H	1.6175	3.3843	1.0588
N	2.0175	1.4846	0.1674
C	3.1798	0.9682	-0.3446
H	3.2093	-0.0360	-0.7408
C	-4.3529	2.2094	-4.8765
H	-4.5929	2.8133	-5.7401
N	-4.5531	2.5564	-3.6267
C	-4.1009	1.4823	-2.8902
C	-4.0249	1.2164	-1.5016
N	-4.3731	2.0756	-0.5410
H	-4.8018	2.9775	-0.7076
H	-4.3611	1.7559	0.4126
N	-3.5404	0.0100	-1.1592
C	-2.6467	-0.7792	0.7285
H	-3.3436	-1.6236	0.6850
H	-2.9599	0.1255	1.2606
H	-1.2563	-3.3203	1.0510
C	-3.1050	-0.8511	-2.0908
H	-2.6881	-1.7767	-1.7012
N	-3.1053	-0.6950	-3.4017
C	-3.6266	0.4899	-3.7310
Fe	0.2052	0.3432	0.2408
O	1.0288	-7.2993	-0.1087
C	1.7230	-6.3308	0.3105
O	2.9136	-6.4360	0.7023
C	1.0390	-4.9731	0.3994
H	0.1347	-4.9800	-0.2103
H	0.7078	-4.8654	1.4378
C	1.8926	-3.7607	0.0377
H	2.8564	-3.8417	0.5546
H	2.1048	-3.7147	-1.0339
C	1.2271	-2.4599	0.4769
O	1.2890	-1.4561	-0.2896
O	0.6572	-2.4710	1.6066
O	-1.4682	-0.9553	0.4242
O	0.5976	0.0313	2.3181
H	0.5586	-0.9555	2.2579
H	-0.2266	0.3654	2.7148
O	-2.0587	-3.8199	0.8429
H	-2.2405	-4.3478	1.6419
C	0.1105	3.2208	-4.6383
C	-1.6764	3.6689	2.4563
C	5.5673	1.8720	-0.8000
N	-3.7920	0.9720	-4.9881
Cps	1.3152	4.1860	-4.5581
Cps	-1.9309	4.8054	1.4842
Cps	5.7070	2.2163	-2.2932
Cps	-3.3506	0.2734	-6.1559

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