Electronic Supplementary Material (ESI) for Dalton Transactions.

Supplementary material for the paper

Functional Models of Nonheme Diiron Enzymes: Kinetic and Computational Evidence for the Formation of Oxoiron(IV) Species from Peroxo-diiron(III) Complexes, and Their Reactivity Towards Phenols and H_2O_2

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I. Catalase activity:

All reactions were carried out in a 50 mL reactor containing a stirring bar under air. Acetonitrile (30 mL) was added to the complex and the flask was closed with a rubber septum. Hydrogen peroxide was injected through the septum with a Hamilton syringe. The reactor was connected to a graduated burette filled with mercury and dioxygen evolution was measured volumetrically at time intervals of 30 or 60 sec. The reaction rates were calculated by the initial rate method.

Table S1. Kinetic data for the catalase-like activities **1** and **2**.

[1]	**[H_2O_2]**	**T**	**V_i**	***k_{cat}***
10^{-3} M	M	°C	10^{-5} M s^{-1}	10^{-3} M^{-1} s^{-1}
1	0.2	25	1.22	*2.73*
2.5	0.2	25	1.95	*2.76*
5	0.2	25	2.95	2.95
[**2**]	**[H_2O_2]**	**T**	**V_i**	***k***
10^{-3} M	M	°C	10^{-5} M s^{-1}	10^{-3} M^{-1} s^{-1}
1	0.2	25	2.28	5.09
2.5	0.2	25	3.62	5.12
5	0.2	25	5.10	5.10
1	0.15	25	1.64	4.89
1	0.2	25	2.28	5.09
1	0.25	25	2.83	5.06
1	0.3	25	3.40	5.07

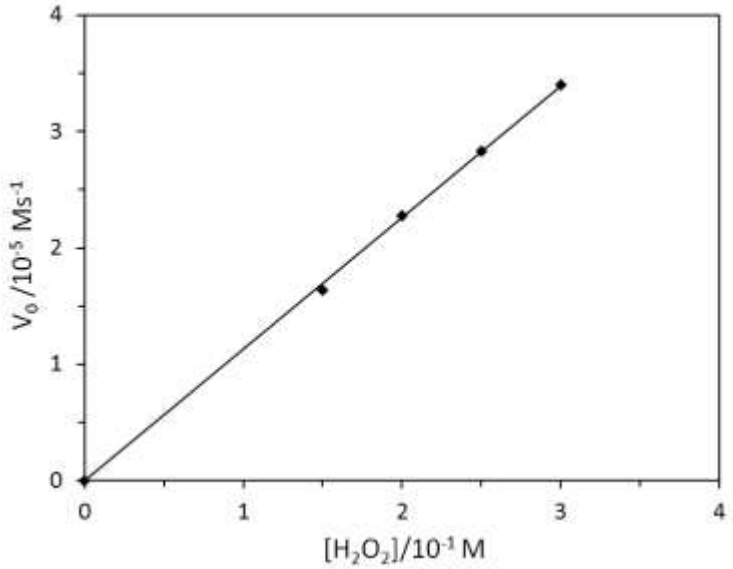

Fig. S1. Dependence of the initial reaction rate (V_0) on the H_2O_2 concentration for the disproportionation of H_2O_2 catalyzed by the in situ formed **4** at 298 K in MeCN. [**2**]$_0$ = 1 × 10^{-3} M.

II. Substrate oxidation studies

Table S2. Kinetic data for the oxidation of 2.6-DTBPh with **3**

[1] 10^{-3} M	[3] 10^{-3} M	[2.6-DTBPh] M	[H_2O_2] 10^{-3} M	T (°C)	V_0 10^{-7} M s^{-1}	V_i 10^{-7} M s^{-1}	V_{ox} 10^{-7} M s^{-1}	k_{ox} 10^{-4} $M^{-1/2}s^{-1}$
1	0.5	0.1	4	20	6.61	11.13	4.52	2.02
1	0.5	0.08	4	20	6.61	10.10	3.49	1.95
1	0.5	0.06	4	20	6.61	9.37	2.77	2.06
1	0.5	0.04	4	20	6.61	8.40	1.79	2.01
0.5	0.25	0.1	2	20	4.11	7.38	3.27	2.07
1	0.5	0.1	4	20	6.61	11.13	4.52	2.02
1.5	0.75	0.1	6	20	11.62	17.14	5.52	2.02
2	1	0.1	8	20	14.04	20.37	6.32	2.00
1	0.5	0.1	4	10	0.90	3.10	2.20	0.98
1	0.5	0.1	4	15	1.80	4.80	3.00	1.34
1	0.5	0.1	4	20	6.61	11.13	4.52	2.02
1	0.5	0.1	4	25	11.30	16.90	5.60	2.50

Table S3. Kinetic data for the oxidation of 2.6-DTBPh with **4**

[2] 10^{-3} M	[4] 10^{-3} M	[2.6-DTBPh] M	[H_2O_2] 10^{-3} M	T (°C)	V_0 10^{-7} M s^{-1}	V_i 10^{-7} M s^{-1}	V_{ox} 10^{-7} M s^{-1}	k_{ox} 10^{-5} $M^{-1/2}s^{-1}$
1	0.5	0.06	4	20	1.39	2.15	0.76	5.68
1	0.5	0.1	4	20	1.39	2.67	1.29	5.75
1	0.5	0.15	4	20	1.39	3.30	1.92	5.71
1	0.5	0.2	4	20	1.39	3.93	2.55	5.69
1	0.5	0.25	4	20	1.39	4.59	3.21	5.73
1	0.5	0.3	4	20	1.39	5.19	3.81	5.67
0.5	0.25	0.1	2	20	0.47	1.33	0.86	5.42
1	0.5	0.1	4	20	1.39	2.58	1.19	5.31
1.5	0.75	0.1	6	20	2.34	3.87	1.53	5.57
2	1	0.1	8	20	2.81	4.50	1.69	5.33
1	0.5	0.1	4	10	0.29	0.74	0.45	1.99
1	0.5	0.1	4	14	0.47	1.14	0.67	3.00
1	0.5	0.1	4	18	1.25	2.21	0.96	4.28
1	0.5	0.1	4	20	1.39	2.67	1.29	5.75
1	0.5	0.1	4	25	2.13	3.93	1.79	8.02

Table: S4. Kinetic data for the oxidation of 2-chloro-1,4-hydroquinone by **3**

[1] 10^{-3} M	[3] 10^{-3} M	[H_2Q-Cl] 10^{-2} M	T °C	V_i 10^{-4} M s^{-1}	k_{ox} $M^{-1/2}s^{-1}$
1	0.5	1	5	0.85	0.38
1	0.5	1.5	5	1.21	0.36
1	0.5	2	5	1.80	0.40
1	0.5	2.5	5	2.31	0.41
0.75	0.375	1	5	0.70	0.36
1	0.5	1	5	0.85	0.38
1.5	0.75	1	5	1.06	0.39
2	1	1	5	1.19	0.38
1	0.5	1	0	0.57	0.26
1	0.5	1	5	0.85	0.38
1	0.5	1	10	1.10	0.49
1	0.5	1	15	1.41	0.63

Table S5. Kinetic data for the oxidation of 2-chloro-1,4-hydroquinone by **4**

[2] 10^{-3} M	[4] 10^{-3} M	[H_2Q-Cl] 10^{-2} M	T (°C)	V_i 10^{-4} M s^{-1}	k_{ox} $M^{-1/2}s^{-1}$
0.75	0.375	1	5	0.11	0.06
1	0.5	1	5	0.13	0.06
1.5	0.75	1	5	0.17	0.06
2	1	1	5	0.19	0.06
1	0.5	1	5	0.13	0.06
1	0.5	1.5	5	0.19	0.06
1	0.5	2.0	5	0.24	0.05
1	0.5	2.5	5	0.31	0.06
1	0.5	1	0	0.09	0.04
1	0.5	1	5	0.13	0.06
2	0.5	1	10	0.22	0.10
3	0.5	1	15	0.31	0.14

Table S6. Reaction rates determined in the reactions of **3** or **4** (0.5 mM) with various *para*-substituted 2.6-di-tert-butylphenols (0.06 M) in MeCN at 5 ˚C.

2.6-DTBPh	[3] k_{ox} 10^{-4} $M^{-1/2}s^{-1}$	[4] k_{ox} 10^{-4} $M^{-1/2}s^{-1}$	BDE kcal mol^{-1}
^{t}Bu	2.65	0.90	81.2
H	2.06	0.57	82.3
Br	1.47	0.36	
CN	0.72	0.17	84.2

Table S7. Reaction rates determined in the reactions of **3** or **4** (0.5 mM) with various *meta*-substituted 1,4-hydroquinones (0.01 M) in MeCN at 5 ˚C.

H_2Q-X	[3] k_{ox} $M^{-1/2}s^{-1}$	[4] k_{ox} $M^{-1/2}s^{-1}$	BDE kcal mol^{-1}
^{t}Bu	1.16	0.33	79.6
Me	0.63	0.18	80.3
H	0.38	0.05	82.3
Cl	0.28	0.04	83.3
Br	0.30	0.04	83.2

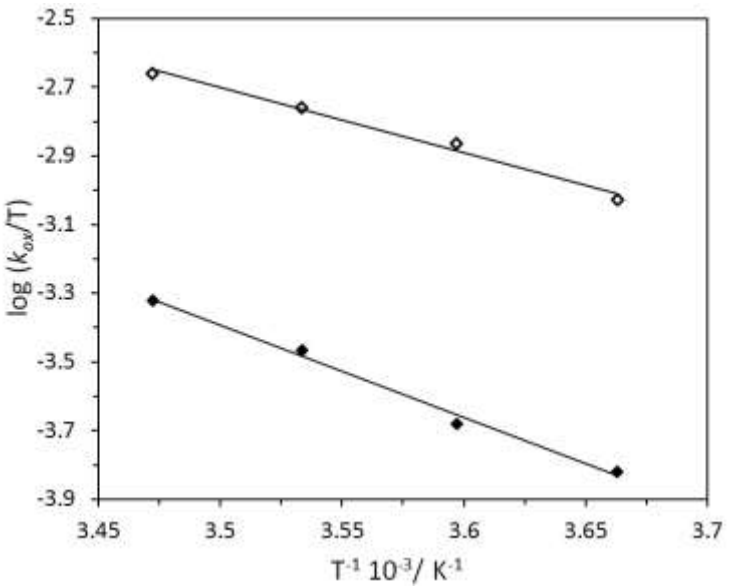

Fig. S2. Eyring plot for the oxidation of 2-chloro-1,4-hydroquinone by **3** (□) or **4** (■) in MeCN,

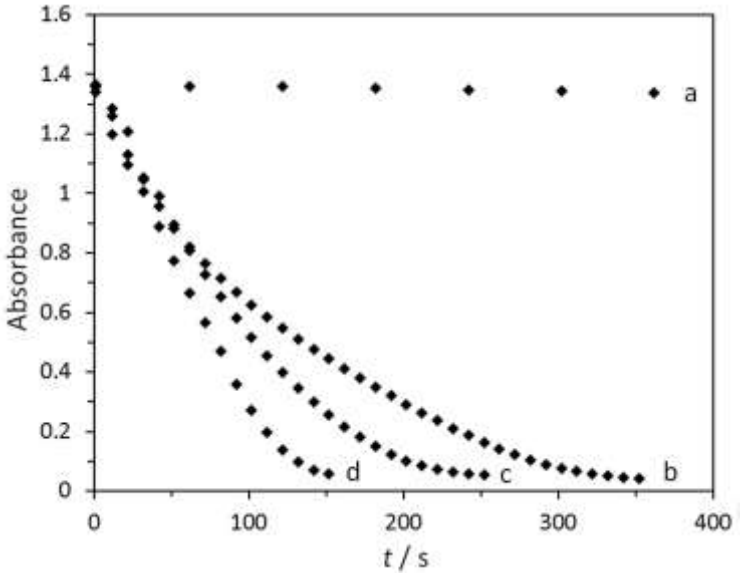

Fig.S3. Absorbance change versus time in the oxidation reactions of PPh_3, without substrate (a), $[PPh_3] = 5 \times 10^{-3}$ M (b), $[PPh_3] = 10 \times 10^{-3}$ M (c), $[PPh_3] = 15 \times 10^{-3}$ M (d). Reaction conditions: [**3**] =0.5×10^{-3} M, T = 20 °C, in MeCN

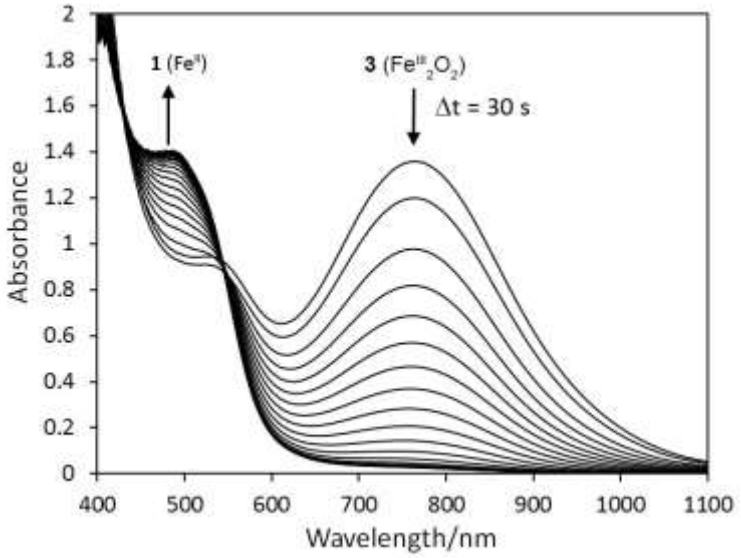

Fig.S4. UV-Vis spectral change after addition of PPh_3 to **3**. Reaction condition: [**3**] = 0.5 × 10-3 M, $[PPh_3] = 5 \times 10^{-3}$ M, T = 20 °C, Δ*t* = 30 s, in MeCN.

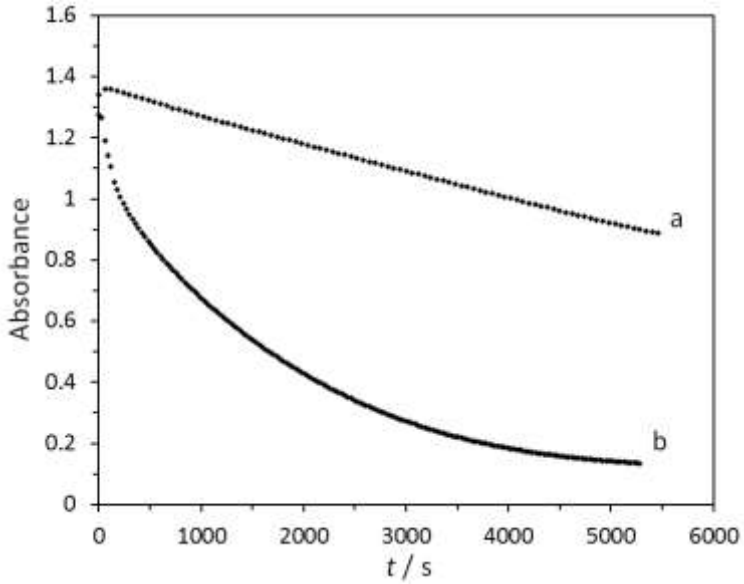

Fig.S5. Absorbance change versus time in the oxidation reactions of benzyl alcohol, without substrate (a), [$PhCH_2OH$] = 0.15 M (b). Reaction conditions: [**3**] =0.5 × 10^{-3} M, T = 20 °C, in MeCN.

III. Computational studies

Table S8. Partial charges for the 12 spin solutions of Fe_2O_2 models

	Partial charges			
Spin solution	**Fe1**	**Fe2**	**O1**	**O2**
S=0(1,-1)	1.44	1.44	-0.38	-0.38
S=1(1,1)	1.45	1.45	-0.39	-0.39
S=2(3,1)	1.44	1.46	-0.39	-0.40
S=3(5,1)	1.46	1.53	-0.37	-0.42
S=4(5,3)	1.53	1.48	-0.41	-0.37
S=5(5,5)	1.56	1.55	-0.40	-0.40
S=0(5,-5)	1.55	1.54	-0.39	-0.39
S=1(3,-1)	1.43	1.46	-0.38	-0.39
S=2(5,-1)	1.46	1.52	-0.36	-0.41
S=1(5,-3)	1.52	1.48	-0.40	-0.37
S=0(3,-3)	1.46	1.43	-0.40	-0.36
S=3(3,3)	1.47	1.47	-0.39	-0.36

Table S9. Energies (kcal/mol), selected bond lengths (Å), spin densities and partial charges for the transition states of the O-O homolytic bond breaking in Fe_2O_2 models

			Selected bond lengths				Spin densities				Partial charges			
Spin solution	**ΔG (vaccum)**	**ΔG (MeCN)**	**Fe1-O1**	**Fe2-O2**	**O-O**	**Fe-Fe**	**Fe1**	**Fe2**	**O1**	**O2**	**Fe1**	**Fe2**	**O1**	**O2**
S=0(1,-1)	15.3	17.5	1.69	1.69	1.86	4.57	0.95	-0.95	0.71	-0.71	1.44	1.43	-0.42	-0.42
S=2(3,1)	17.5	22.3	1.71	1.68	1.91	4.61	0.73	2.93	-0.36	0.58	1.42	1.48	-0.43	-0.43
S=3(5,1)	12.6	20.0	1.66	1.72	1.84	4.82	1.10	3.98	0.59	0.09	1.46	1.49	-0.39	-0.49
S=4(5,3)	10.9	20.8	1.71	1.67	1.82	4.82	3.95	3.03	0.09	0.45	1.50	1.50	-0.47	-0.39
S=5(5,5)	35.5	48.4	1.66	1.89	1.95	5.12	3.66	4.21	0.31	1.12	1.50	1.53	-0.43	-0.42
S=0(5,-5)	12.2	25.8	1.69	1.69	1.78	5.14	3.81	-3.81	0.16	-0.16	1.53	1.53	-0.42	-0.42
S=1(3,-1)	13.1	17.5	1.70	1.69	1.85	4.56	-0.96	2.90	-0.69	0.56	1.42	1.47	-0.42	-0.43
S=1(5,-1)	33.4	42.6	1.88	1.64	2.01	4.77	4.21	-3.02	1.14	-0.54	1.51	1.50	-0.45	-0.41
S=0(3,-3)	26.9	32.8	1.70	1.68	1.82	4.49	2.91	-2.93	0.53	-0.51	1.48	1.47	-0.42	-0.40
S=3(3,3)	32.0	38.8	1.73	1.66	1.89	4.57	2.79	2.99	-0.52	0.49	1.44	1.49	-0.44	-0.39

Note: No transition states could be located for S=1(1,1) and S=2(5,-1)

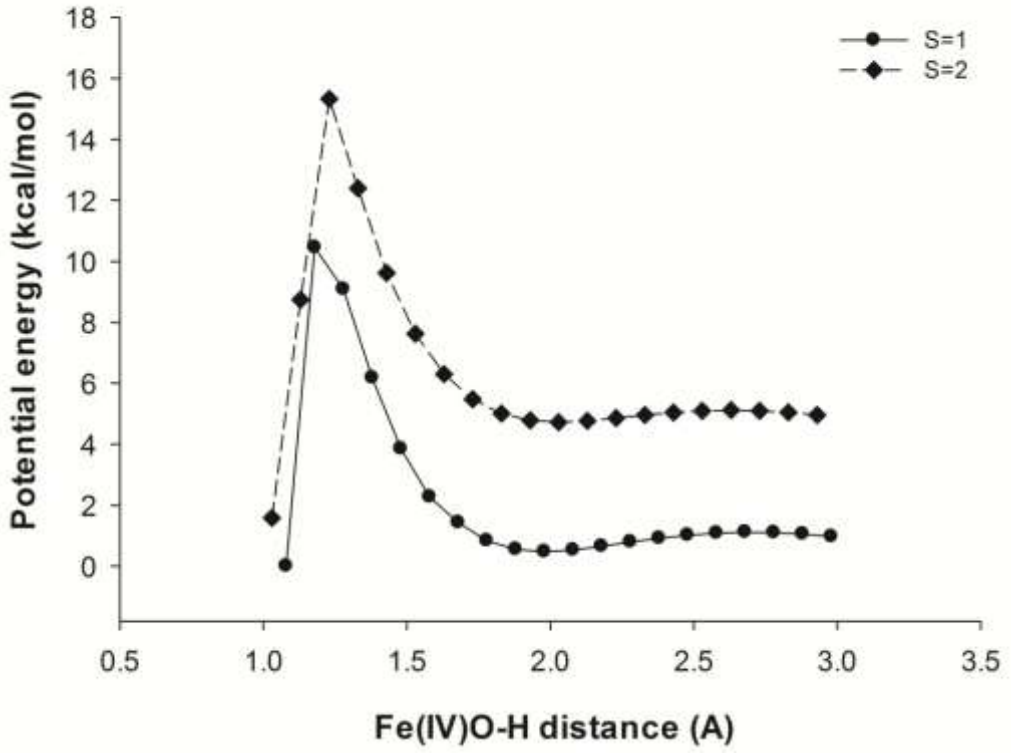

Fig. S6. Potential energy surfaces for the catalase reaction

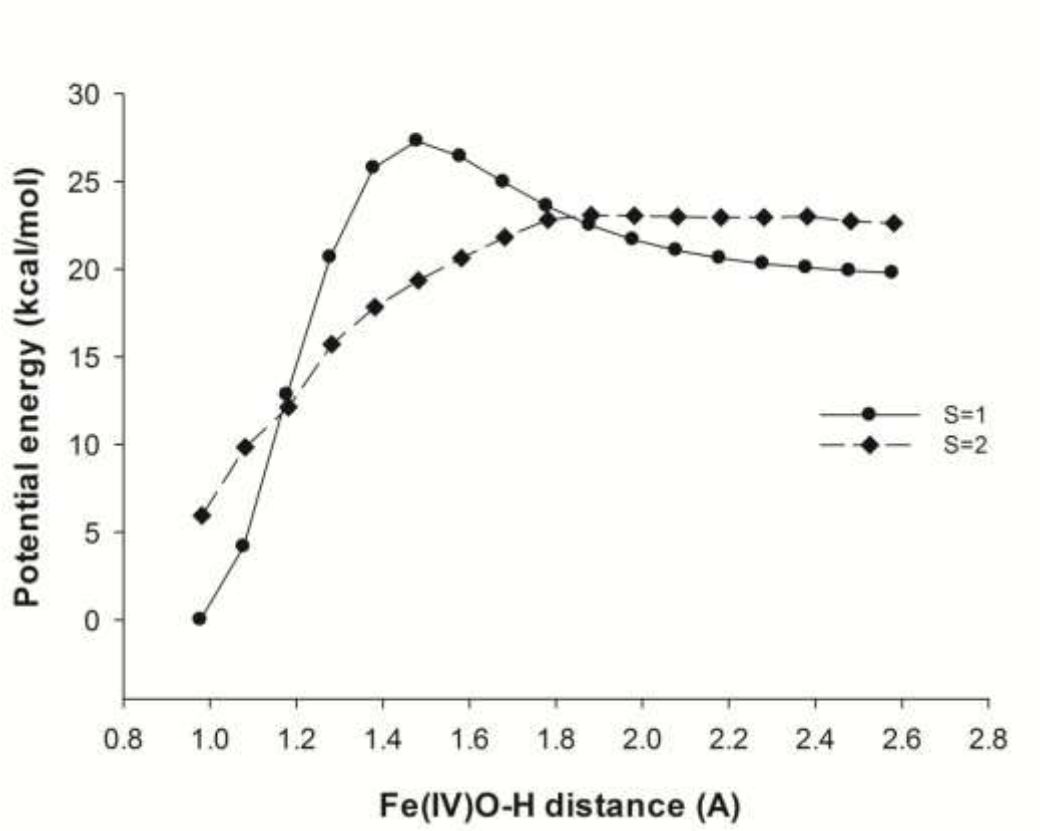

Fig. S7. Potential energy surfaces for the hydrogen atom abstraction from DTBPh

IV. Energies, imaginary frequencies and Cartesian coordinates for all optimised models

Fe_2O_2 S=0(1,-1)

E(UB3LYP/6-31G(d,p))= -5450.13871521

no imaginary frequencies

	x	y	z
C	-0.04034	-3.23411	0.407391
H	-0.66066	-3.36505	-0.4696
C	1.014249	-4.10627	0.678858
H	1.211361	-4.93478	0.007797
C	1.787606	-3.9003	1.819141
H	2.604245	-4.57101	2.065735
C	1.495846	-2.81204	2.641658
H	2.090241	-2.6236	3.529161
C	0.428402	-1.98254	2.30456
C	0.008986	-0.8027	3.042611
C	-1.17715	0.983007	3.491269
C	-2.07813	2.057858	3.528071
H	-2.8127	2.19656	2.746572
C	-1.99081	2.932823	4.603475

H	-2.68548	3.76359	4.671307
C	-1.03107	2.76546	5.62647
H	-1.01291	3.464383	6.456004
C	-0.11715	1.719767	5.59907
H	0.616185	1.586355	6.387443
C	-0.20967	0.84162	4.516544
C	-3.12816	-2.08069	3.641846
H	-2.59286	-1.27419	4.126295
C	-3.89964	-2.96881	4.390066
H	-3.95604	-2.85567	5.466868
C	-4.58849	-3.98683	3.733115
H	-5.19388	-4.69685	4.287104
C	-4.49487	-4.07184	2.344471
H	-5.0308	-4.84674	1.807032
C	-3.70744	-3.14323	1.664943
C	-3.54636	-3.07379	0.223512
C	-2.83334	-2.28225	-1.68835
C	-2.23565	-1.56922	-2.73766
H	-1.61761	-0.70596	-2.53069
C	-2.49524	-2.00553	-4.03076
H	-2.0675	-1.46931	-4.87189
C	-3.31728	-3.12442	-4.2939
H	-3.48886	-3.42721	-5.32125
C	-3.91499	-3.84306	-3.26743
H	-4.54837	-4.70039	-3.46843
C	-3.65732	-3.3996	-1.96801
N	-0.34612	-2.20103	1.207027
N	-1.01617	-0.0726	2.594319
N	0.520809	-0.29337	4.187881
N	-3.01425	-2.16189	2.305555
N	-2.78747	-2.11165	-0.30614
N	-4.08505	-3.86708	-0.73347
Fe	-1.89569	-0.91301	1.027321
H	-4.69663	-4.65871	-0.58322
H	1.273063	-0.68902	4.735701
O	-0.9244	-0.01147	-0.18526
N	-3.45568	0.257319	1.005492
C	-4.47682	0.798942	0.973963
C	-5.75843	1.489001	0.937762
H	-5.81311	2.122633	0.047715
H	-6.5743	0.760507	0.90744
H	-5.87787	2.110008	1.830576
O	-1.15394	1.372212	-0.29672
Fe	0.057114	2.342767	-1.19958
N	-0.49979	3.931885	-0.07985
N	1.453452	2.19919	0.201566

N	-1.19102	2.884957	-2.66891
N	0.738239	0.90504	-2.32801
C	-1.56144	4.731401	-0.26217
C	0.355312	4.215622	0.940171
C	1.423612	3.235335	1.044507
C	2.56995	1.437129	0.544729
C	-0.69377	3.778691	-3.52681
C	-2.50041	2.630231	-3.07172
C	1.125356	0.169357	-3.13172
H	-2.2341	4.463446	-1.06645
C	-1.79852	5.855469	0.529481
C	0.185404	5.321613	1.770348
N	2.462302	3.202364	1.912201
C	3.094275	0.246623	0.019341
C	3.225642	2.077571	1.625043
C	0.679374	4.225894	-3.37559
N	-1.60512	4.128186	-4.46628
C	-3.48769	1.779082	-2.55468
C	-2.77193	3.420305	-4.21525
C	1.616846	-0.76198	-4.13734
H	-2.66439	6.477612	0.332397
C	-0.90602	6.163193	1.55401
H	0.887993	5.532442	2.569299
H	2.67532	3.894841	2.617671
H	2.599876	-0.26994	-0.79203
C	4.26853	-0.24037	0.579481
C	4.406093	1.590995	2.192215
C	1.330765	5.126482	-4.21742
N	1.296304	3.63611	-2.31463
H	-1.46428	4.781017	-5.22605
H	-3.28073	1.159394	-1.6927
C	-4.7111	1.752473	-3.21236
C	-4.00393	3.400124	-4.87358
H	0.947785	-1.62498	-4.20256
H	1.659506	-0.2695	-5.1135
H	2.622271	-1.10435	-3.87479
H	-1.05465	7.039697	2.176271
H	4.710179	-1.14904	0.183782
C	4.918933	0.422194	1.644191
H	4.907668	2.104033	3.006035
C	2.670577	5.426597	-3.9744
H	0.810321	5.585452	-5.0511
C	2.59254	3.919921	-2.104
H	-5.49494	1.091347	-2.85671
C	-4.96891	2.55068	-4.34955
H	-4.1993	4.01051	-5.74869

H	5.843675	0.013188	2.03729
C	3.312714	4.805349	-2.90483
H	3.201716	6.124365	-4.61356
H	3.071288	3.415621	-1.27455
H	-5.94104	2.495564	-4.82757
H	4.357817	4.996327	-2.68859

Fe_2O_2 S=1(1,1)

E(UB3LYP/6-31G(d,p))= -5450.13652874

no imaginary frequencies

	x	**y**	**z**
C	-3.02122	-0.09419	-2.72434
H	-2.91839	0.983132	-2.72048
C	-3.45742	-0.7713	-3.86364
H	-3.70652	-0.21117	-4.75798
C	-3.5769	-2.15868	-3.82359
H	-3.92953	-2.71155	-4.6882
C	-3.2308	-2.82987	-2.65051
H	-3.30178	-3.91092	-2.59777
C	-2.79985	-2.08614	-1.55421
C	-2.38062	-2.63063	-0.27324
C	-1.61155	-2.60195	1.777674
C	-1.09934	-2.29107	3.046069
H	-0.86784	-1.27033	3.318516
C	-0.90145	-3.34135	3.933582
H	-0.52351	-3.13298	4.929113
C	-1.19274	-4.67892	3.584747
H	-1.03829	-5.46379	4.317579
C	-1.6806	-5.0105	2.32708
H	-1.90855	-6.03683	2.05921
C	-1.87888	-3.95102	1.438384
C	-4.84069	-0.98503	1.440581
H	-4.231	-1.83074	1.731824
C	-6.19537	-0.94381	1.767511
H	-6.64232	-1.76953	2.309628
C	-6.94925	0.166323	1.391071
H	-8.0068	0.226961	1.626524
C	-6.31651	1.207584	0.713245
H	-6.87692	2.088814	0.420067
C	-4.95644	1.095922	0.426818
C	-4.15082	2.110084	-0.22913
C	-2.33818	3.031347	-1.03887

C	-1.04339	3.364659	-1.46249
H	-0.22329	2.677132	-1.30615
C	-0.87044	4.608863	-2.05571
H	0.119606	4.913585	-2.37974
C	-1.94443	5.508798	-2.2391
H	-1.7585	6.468718	-2.70873
C	-3.23224	5.194978	-1.82645
H	-4.05686	5.886315	-1.9629
C	-3.40344	3.945833	-1.22489
N	-2.71386	-0.72815	-1.58267
N	-1.95115	-1.8045	0.685421
N	-2.35514	-3.92144	0.133245
N	-4.22209	0.002658	0.771817
N	-2.84678	1.893712	-0.41499
N	-4.52679	3.323544	-0.6995
Fe	-2.19307	0.097105	0.187006
H	-5.45812	3.717217	-0.66939
H	-2.66403	-4.72346	-0.39972
O	-0.5303	0.315483	-0.47214
N	-1.84884	0.826979	1.962819
C	-1.79577	1.354329	2.990414
C	-1.72261	2.011516	4.28769
H	-0.81829	2.624516	4.342394
H	-2.59735	2.652858	4.431651
H	-1.70143	1.265312	5.087544
O	0.530331	0.315328	0.472393
Fe	2.193032	0.097134	-0.18695
N	2.714028	-0.72822	1.582629
N	1.951126	-1.80443	-0.68547
N	2.846819	1.893714	0.415022
N	1.848525	0.827167	-1.96265
C	3.021581	-0.09432	2.724288
C	2.799955	-2.08622	1.554104
C	2.380611	-2.63063	0.273142
C	1.611473	-2.60182	-1.77775
C	4.150857	2.110049	0.22907
C	2.338291	3.031354	1.038943
C	1.795159	1.354742	-2.99011
H	2.918825	0.983005	2.720484
C	3.457903	-0.7715	3.863496
C	3.230996	-2.83001	2.650322
N	2.355116	-3.92141	-0.13343
C	1.099192	-2.29087	-3.04611
C	1.878809	-3.95091	-1.43855
C	4.956444	1.095868	-0.4269
N	4.526901	3.323464	0.699506

C	1.043534	3.364718	1.462607
C	3.403592	3.945795	1.224938
C	1.721483	2.012117	-4.28726
H	3.707169	-0.21142	4.75782
C	3.577286	-2.15889	3.823382
H	3.301913	-3.91106	2.597521
H	2.664032	-4.72346	0.399475
H	0.867678	-1.27012	-3.31849
C	0.901267	-3.3411	-3.93367
C	1.680494	-5.01034	-2.3273
C	6.316545	1.207478	-0.71321
N	4.222084	0.00264	-0.77201
H	5.45825	3.717084	0.669399
H	0.223396	2.677238	1.306245
C	0.870647	4.608922	2.055848
C	3.232472	5.194931	1.826553
H	0.816762	2.624548	-4.34179
H	2.595791	2.654048	-4.43117
H	1.700714	1.266043	-5.08725
H	3.930008	-2.71181	4.687924
H	0.523269	-3.13268	-4.92917
C	1.192582	-4.67869	-3.58493
H	1.908458	-6.03668	-2.0595
C	6.949313	0.166202	-1.39099
H	6.876973	2.088671	-0.41995
C	4.84072	-0.98507	-1.44071
H	-0.11938	4.913695	2.379888
C	1.944682	5.508802	2.239238
H	4.057123	5.886228	1.962993
H	1.038087	-5.46352	-4.31779
C	6.195435	-0.9439	-1.76749
H	8.006892	0.226803	-1.62634
H	4.231037	-1.83076	-1.73201
H	1.758808	6.468723	2.708886
H	6.642409	-1.76965	-2.30957

Fe_2O_2 S=2(3,1)

E(UB3LYP/6-31G(d,p))= -5450.13075026

no imaginary frequencies

	x	**y**	**z**
C	-3.12529	0.444165	-2.68654
H	-2.80305	1.475678	-2.63117

C	-3.72065	-0.06338	-3.84122
H	-3.87367	0.586621	-4.69539
C	-4.11743	-1.39896	-3.86989
H	-4.59696	-1.81746	-4.74879
C	-3.88406	-2.19418	-2.74811
H	-4.17237	-3.2398	-2.7478
C	-3.28032	-1.61794	-1.63246
C	-2.94445	-2.30271	-0.39766
C	-2.13328	-2.52223	1.625542
C	-1.54489	-2.37739	2.89069
H	-1.13223	-1.42956	3.209112
C	-1.51513	-3.49361	3.717128
H	-1.08271	-3.41031	4.708766
C	-2.04724	-4.73742	3.310959
H	-2.01603	-5.57708	3.997166
C	-2.61909	-4.90658	2.056391
H	-3.03317	-5.85984	1.745232
C	-2.64727	-3.78142	1.229183
C	-4.95591	-0.26057	1.474688
H	-4.54859	-1.2459	1.658351
C	-6.24792	0.058303	1.890336
H	-6.85065	-0.69135	2.390538
C	-6.73818	1.341162	1.65459
H	-7.74088	1.619557	1.962127
C	-5.91122	2.267877	1.021405
H	-6.26385	3.276654	0.835447
C	-4.62909	1.875809	0.638185
C	-3.64913	2.730983	-0.00558
C	-1.73187	3.280943	-0.90915
C	-0.43312	3.343616	-1.43493
H	0.227418	2.489596	-1.37812
C	-0.03631	4.549259	-1.99898
H	0.965224	4.641902	-2.40652
C	-0.89148	5.672286	-2.05446
H	-0.53403	6.591068	-2.50686
C	-2.18069	5.626955	-1.54184
H	-2.84034	6.486973	-1.58421
C	-2.57883	4.414662	-0.97393
N	-2.92155	-0.30607	-1.59266
N	-2.34919	-1.61963	0.584434
N	-3.14292	-3.59673	-0.05565
N	-4.15383	0.617553	0.848952
N	-2.4381	2.247408	-0.29375
N	-3.77506	4.022984	-0.39119
Fe	-2.17822	0.312576	0.174482
H	-4.59792	4.602347	-0.2894

H	-3.59393	-4.3034	-0.62129
O	-0.54225	0.103749	-0.55375
N	-1.60401	0.893275	1.946235
C	-1.3857	1.346341	2.987076
C	-1.10789	1.918214	4.297121
H	-0.15775	2.459609	4.270414
H	-1.90614	2.611651	4.578442
H	-1.05169	1.127316	5.05085
O	0.569583	0.636646	0.151092
Fe	2.171865	-0.0652	-0.28244
N	2.648147	-1.16128	1.696483
N	1.557415	-1.98357	-0.61538
N	3.122863	1.558656	0.422304
N	2.12306	0.725584	-2.40713
C	3.167991	-0.67449	2.830559
C	2.450493	-2.49612	1.597341
C	1.861307	-2.88724	0.319332
C	1.010234	-2.68549	-1.68888
C	4.452115	1.514408	0.254226
C	2.84582	2.745089	1.102225
C	2.305943	1.183078	-3.45703
H	3.300585	0.401481	2.875477
C	3.529699	-1.48861	3.905511
C	2.785868	-3.38086	2.623554
N	1.553794	-4.14306	-0.09102
C	0.511853	-2.25506	-2.92718
C	1.017877	-4.06337	-1.36886
C	5.057779	0.384797	-0.43275
N	5.053342	2.60103	0.785785
C	1.639521	3.313917	1.534257
C	4.070294	3.414293	1.337725
C	2.534826	1.748295	-4.77976
H	3.95537	-1.04973	4.801074
C	3.341369	-2.8654	3.795259
H	2.628866	-4.4494	2.522028
H	1.715405	-4.99538	0.427866
H	0.48101	-1.20284	-3.17763
C	0.06412	-3.23087	-3.8092
C	0.568464	-5.04786	-2.25264
C	6.416634	0.240916	-0.70705
N	4.136613	-0.54228	-0.81644
H	6.045575	2.800211	0.782472
H	0.697887	2.822079	1.330796
C	1.714528	4.536688	2.19048
C	4.14933	4.64185	1.999009
H	1.724225	2.434505	-5.04101

H	3.482036	2.29569	-4.79354
H	2.580078	0.948153	-5.52469
H	3.622486	-3.53002	4.60579
H	-0.31116	-2.93577	-4.78364
C	0.09719	-4.60501	-3.48228
H	0.600871	-6.10335	-2.00375
C	6.845753	-0.88729	-1.40729
H	7.133258	0.990866	-0.38991
C	4.558708	-1.61569	-1.50474
H	0.802185	5.019307	2.525929
C	2.945839	5.189545	2.423063
H	5.094737	5.144846	2.171491
H	-0.24441	-5.33188	-4.21172
C	5.900771	-1.82624	-1.81787
H	7.898497	-1.02366	-1.63292
H	3.797852	-2.31993	-1.81766
H	2.951521	6.143576	2.939149
H	6.191419	-2.70992	-2.37477

Fe_2O_2 S=3(5,1)

E(UB3LYP/6-31G(d,p))= -5450.14082242

no imaginary frequencies

	x	**y**	**z**
C	3.272687	-0.24632	2.763526
H	3.274044	0.835265	2.73254
C	3.649359	-0.93306	3.918049
H	3.95942	-0.37654	4.795351
C	3.628606	-2.32582	3.915827
H	3.929333	-2.88784	4.794016
C	3.209672	-2.99044	2.762733
H	3.173175	-4.07422	2.738844
C	2.845895	-2.23739	1.648696
C	2.371513	-2.77275	0.383385
C	1.61372	-2.72574	-1.67234
C	1.140212	-2.40374	-2.95262
H	1.010546	-1.3743	-3.25703
C	0.844975	-3.45483	-3.81144
H	0.493003	-3.23898	-4.81483
C	1.002724	-4.80364	-3.42297
H	0.774443	-5.59045	-4.13405
C	1.451814	-5.14446	-2.15373
H	1.576937	-6.1796	-1.85423

C	1.749126	-4.08404	-1.29465
C	4.956234	-1.30213	-1.40346
H	4.297502	-2.12477	-1.65102
C	6.303372	-1.33965	-1.76029
H	6.696529	-2.20423	-2.28313
C	7.119581	-0.25688	-1.43771
H	8.17301	-0.25727	-1.69814
C	6.556459	0.835842	-0.77953
H	7.167433	1.695383	-0.5257
C	5.199994	0.802302	-0.45892
C	4.461765	1.870347	0.191244
C	2.715574	2.885882	1.038813
C	1.452992	3.27717	1.508235
H	0.603077	2.613975	1.415627
C	1.352988	4.539097	2.07912
H	0.391745	4.883689	2.446132
C	2.466592	5.401255	2.19426
H	2.337148	6.377245	2.649534
C	3.72396	5.028708	1.738559
H	4.579508	5.689482	1.827764
C	3.823089	3.760335	1.162028
N	2.894088	-0.87697	1.641525
N	2.024595	-1.93499	-0.59932
N	2.223166	-4.06462	0.011137
N	4.404469	-0.26268	-0.75513
N	3.157167	1.713844	0.427861
N	4.901659	3.079373	0.614728
Fe	2.403236	-0.04922	-0.13514
H	5.84707	3.432455	0.545693
H	2.445936	-4.87829	0.568879
O	0.763798	0.279594	0.55969
N	2.053695	0.682198	-1.9094
C	1.994387	1.214094	-2.93421
C	1.915905	1.874882	-4.22931
H	1.051188	2.544405	-4.25292
H	2.82396	2.459271	-4.40581
H	1.818395	1.1316	-5.02622
O	-0.32544	0.283724	-0.32124
Fe	-2.13166	0.235653	0.155928
N	-2.88667	-0.54489	-1.76521
N	-2.35519	-1.86481	0.518466
N	-2.72655	2.17821	-0.39087
N	-1.83305	0.821434	2.24134
C	-3.1107	0.168944	-2.88003
C	-3.2251	-1.85965	-1.75522
C	-2.91776	-2.5268	-0.49437

C	-2.19483	-2.78725	1.550307
C	-4.00397	2.515211	-0.17195
C	-2.12648	3.282825	-0.9978
C	-1.83919	1.253062	3.316706
H	-2.822	1.213445	-2.84636
C	-3.68737	-0.38223	-4.02296
C	-3.81139	-2.48108	-2.85857
N	-3.14163	-3.82756	-0.17847
C	-1.65613	-2.65474	2.838821
C	-2.70072	-4.03732	1.120831
C	-4.93724	1.597375	0.475828
N	-4.26428	3.770331	-0.60701
C	-0.81211	3.494929	-1.43334
C	-3.09655	4.299684	-1.14242
C	-1.85847	1.788474	4.669795
H	-3.85499	0.23594	-4.89774
C	-4.05009	-1.72843	-4.00821
H	-4.08653	-3.5298	-2.83068
H	-3.57346	-4.52341	-0.77125
H	-1.25531	-1.70845	3.181167
C	-1.6612	-3.77984	3.653238
C	-2.70696	-5.17238	1.935454
C	-6.27363	1.897799	0.745371
N	-4.37395	0.411558	0.813752
H	-5.15254	4.250848	-0.54885
H	-0.05899	2.727447	-1.30166
C	-0.52411	4.730136	-2.0034
C	-2.8137	5.53966	-1.71822
H	-0.89951	2.260746	4.901099
H	-2.65466	2.533256	4.763416
H	-2.04434	0.982924	5.386678
H	-4.51342	-2.18755	-4.87558
H	-1.26518	-3.71124	4.661136
C	-2.18067	-5.01769	3.211637
H	-3.10881	-6.12214	1.598919
C	-7.05762	0.944517	1.395858
H	-6.70629	2.851154	0.461525
C	-5.13515	-0.49171	1.447407
H	0.486004	4.943134	-2.33844
C	-1.50645	5.734141	-2.14772
H	-3.5667	6.313106	-1.82444
H	-2.1739	-5.86584	3.887985
C	-6.4775	-0.26924	1.758791
H	-8.09955	1.151361	1.617565
H	-4.64953	-1.42135	1.722383
H	-1.23422	6.681913	-2.59954

H	-7.04859	-1.03315	2.274529

Fe_2O_2 S=4(5,3)

E(UB3LYP/6-31G(d,p))= -5450.13510041

no imaginary frequencies

	x	**y**	**z**
C	3.134708	0.718371	2.847162
H	2.640955	1.678814	2.753755
C	3.822969	0.37214	4.009167
H	3.872212	1.069703	4.83765
C	4.446944	-0.8727	4.073779
H	5.00189	-1.17013	4.957712
C	4.349359	-1.73603	2.982104
H	4.826987	-2.7092	3.01568
C	3.63817	-1.32021	1.856599
C	3.447372	-2.11972	0.650787
C	2.757816	-2.64948	-1.3538
C	2.190624	-2.70807	-2.63525
H	1.618188	-1.878	-3.03086
C	2.396288	-3.86643	-3.37383
H	1.982917	-3.94218	-4.37422
C	3.142452	-4.953	-2.86475
H	3.285459	-5.83275	-3.48307
C	3.703271	-4.91843	-1.59433
H	4.278769	-5.75169	-1.20545
C	3.494292	-3.75085	-0.85656
C	5.14349	0.190885	-1.54003
H	4.84135	-0.83157	-1.73633
C	6.401476	0.651014	-1.93145
H	7.092727	-0.01911	-2.43018
C	6.742231	1.976671	-1.66963
H	7.712723	2.368453	-1.95637
C	5.810566	2.799159	-1.03577
H	6.055057	3.835932	-0.8311
C	4.572838	2.261213	-0.67933
C	3.502618	3.015544	-0.03418
C	1.549239	3.446706	0.856405
C	0.2445	3.421322	1.366998
H	-0.35413	2.520212	1.318885
C	-0.24756	4.60505	1.905341
H	-1.25758	4.631498	2.301309
C	0.522684	5.787273	1.947195

H	0.094539	6.685418	2.379156
C	1.817779	5.828511	1.445284
H	2.41039	6.736454	1.476273
C	2.307303	4.638791	0.903904
N	3.046264	-0.10067	1.787477
N	2.756612	-1.64449	-0.38764
N	3.906549	-3.37318	0.414031
N	4.244128	0.968391	-0.91968
N	2.32706	2.448442	0.265191
N	3.530523	4.318887	0.329074
Fe	2.130891	0.388269	-0.16205
H	4.306089	4.956871	0.208197
H	4.462633	-3.93739	1.042322
O	0.356117	0.068367	0.305487
N	1.668525	0.75879	-2.2718
C	1.554256	1.108456	-3.37054
C	1.426877	1.542392	-4.75395
H	2.175044	2.310276	-4.97278
H	1.58649	0.694614	-5.42704
H	0.429689	1.956115	-4.92817
O	-0.80612	0.562864	-0.28432
Fe	-2.37677	-0.20002	0.219775
N	-2.84459	-1.27249	-1.75667
N	-1.66355	-2.09594	0.508776
N	-4.30053	-0.75897	0.814828
N	-3.40522	1.40317	-0.41413
N	-2.26011	0.57547	2.343561
C	-3.40982	-0.78205	-2.86738
C	-2.56505	-2.59565	-1.70269
C	-1.92975	-2.98894	-0.44781
C	-1.05649	-2.79492	1.551565
C	-4.66064	-1.86606	1.48483
C	-5.26531	0.146648	0.491022
C	-4.72411	1.312997	-0.18842
C	-3.19431	2.613345	-1.0767
C	-2.42869	1.024791	3.399323
H	-3.60526	0.285086	-2.87698
C	-3.73821	-1.58282	-3.96268
C	-2.86315	-3.46611	-2.7521
N	-1.54161	-4.23512	-0.08028
C	-0.56294	-2.37287	2.794604
C	-0.98795	-4.16067	1.189955
H	-3.86533	-2.55212	1.748504
C	-5.98253	-2.13155	1.83893
C	-6.6075	-0.05181	0.809791
N	-5.38007	2.39406	-0.66261

C	-2.02827	3.223276	-1.55964
C	-4.44798	3.250506	-1.23761
C	-2.64032	1.578344	4.729757
H	-4.20202	-1.14223	-4.83818
C	-3.46615	-2.94838	-3.89917
H	-2.6402	-4.52576	-2.68736
H	-1.65313	-5.07921	-0.62519
H	-0.59097	-1.32921	3.079275
C	-0.0443	-3.34608	3.639619
C	-0.46616	-5.14242	2.035783
H	-6.22311	-3.0408	2.378232
C	-6.97247	-1.21373	1.490996
H	-7.36009	0.681311	0.540075
H	-6.37707	2.560451	-0.61377
H	-1.06414	2.749592	-1.43177
C	-2.17142	4.454936	-2.18601
C	-4.595	4.488395	-1.86643
H	-1.85636	2.303876	4.964595
H	-3.61231	2.078484	4.775888
H	-2.62129	0.776954	5.474471
H	-3.71814	-3.60299	-4.7272
H	0.329283	-3.05824	4.616882
C	-0.00105	-4.70917	3.270778
H	-0.4383	-6.18955	1.753688
H	-8.01114	-1.39278	1.749613
H	-1.29224	4.963295	-2.56792
C	-3.42994	5.078295	-2.33886
H	-5.56193	4.966089	-1.98203
H	0.396481	-5.43559	3.971674
H	-3.48835	6.040788	-2.83559

Fe_2O_2 S=5(5,5)

E(UB3LYP/6-31G(d,p))= -5450.14196146

no imaginary frequencies

	x	**y**	**z**
C	3.354398	-0.19338	2.918249
H	3.252624	0.885216	2.875445
C	3.839595	-0.82563	4.061955
H	4.123466	-0.23701	4.927066
C	3.958831	-2.21471	4.061266
H	4.343317	-2.73889	4.930226
C	3.576607	-2.92615	2.924103

H	3.659678	-4.00744	2.907817
C	3.095842	-2.22258	1.81912
C	2.655079	-2.83775	0.571731
C	1.856696	-2.988	-1.45825
C	1.322059	-2.77814	-2.73775
H	1.075094	-1.78167	-3.08258
C	1.121555	-3.89556	-3.53798
H	0.7217	-3.77021	-4.53886
C	1.433715	-5.19911	-3.09104
H	1.270631	-6.0401	-3.75655
C	1.949512	-5.42889	-1.82193
H	2.189586	-6.42974	-1.47937
C	2.151044	-4.30146	-1.02239
C	5.185695	-1.21617	-1.39528
H	4.560709	-2.06826	-1.63912
C	6.54212	-1.20942	-1.72384
H	6.984085	-2.06535	-2.22151
C	7.304287	-0.0883	-1.40117
H	8.362623	-0.04868	-1.63761
C	6.683308	0.990324	-0.77078
H	7.259895	1.87318	-0.51632
C	5.320464	0.904774	-0.48051
C	4.547438	1.967228	0.156933
C	2.821405	3.021323	1.003182
C	1.565663	3.430307	1.470934
H	0.705439	2.77674	1.386065
C	1.480685	4.701287	2.02739
H	0.525209	5.059964	2.395781
C	2.603262	5.552158	2.124233
H	2.486891	6.535355	2.567319
C	3.855032	5.161103	1.664372
H	4.716924	5.815429	1.738347
C	3.935495	3.884468	1.105776
N	2.994644	-0.86879	1.815216
N	2.193797	-2.0971	-0.44034
N	2.647075	-4.1585	0.266363
N	4.57944	-0.19001	-0.78173
N	3.238436	1.829205	0.406507
N	4.999544	3.177607	0.558545
Fe	2.352546	-0.00146	-0.10824
H	5.947909	3.519384	0.47451
H	2.95949	-4.91361	0.861787
O	0.579873	0.413271	0.396726
N	2.1189	0.597851	-2.19432
C	2.188508	1.007555	-3.27604
C	2.285721	1.512642	-4.63738

H	3.199369	2.104222	-4.74981
H	2.318457	0.677001	-5.34307
H	1.422323	2.143344	-4.86738
O	-0.53082	0.182572	-0.39899
Fe	-2.34418	0.208575	0.115156
N	-3.09878	-0.51117	-1.82227
N	-2.64455	-1.88211	0.444796
N	-4.54486	0.490806	0.801153
N	-2.8352	2.18781	-0.40043
N	-1.96357	0.748249	2.196315
C	-3.2864	0.231333	-2.92514
C	-3.4621	-1.8194	-1.84696
C	-3.19364	-2.51656	-0.59384
C	-2.52399	-2.82644	1.462995
C	-5.34076	-0.3915	1.422281
C	-5.05465	1.710054	0.496911
C	-4.08551	2.593097	-0.14526
C	-2.18379	3.26923	-0.99595
C	-1.92797	1.169939	3.274884
H	-2.97698	1.268448	-2.8635
C	-3.85029	-0.28461	-4.09061
C	-4.03619	-2.4059	-2.97517
N	-3.44502	-3.81809	-0.308
C	-2.01751	-2.72773	2.767163
C	-3.03829	-4.0597	0.996837
H	-4.89704	-1.34963	1.668061
C	-6.66733	-0.11273	1.75479
C	-6.3719	2.066299	0.789752
N	-4.28042	3.872067	-0.54242
C	-0.87254	3.410205	-1.46814
C	-3.09498	4.3451	-1.09227
C	-1.89658	1.691428	4.633135
H	-3.98851	0.355172	-4.95486
C	-4.23714	-1.62391	-4.11259
H	-4.33042	-3.44978	-2.97604
H	-3.86765	-4.49752	-0.92603
H	-1.60989	-1.7958	3.138991
C	-2.0596	-3.86836	3.558247
C	-3.08148	-5.21054	1.787466
H	-7.26871	-0.86131	2.258358
C	-7.19273	1.13561	1.427608
H	-6.76229	3.044892	0.5316
H	-5.13813	4.401229	-0.45512
H	-0.1656	2.593257	-1.38827
C	-0.52683	4.638408	-2.02013
C	-2.75301	5.57917	-1.64773

H	-0.9231	2.144789	4.839888
H	-2.6765	2.448634	4.758442
H	-2.07465	0.881643	5.347218
H	-4.68996	-2.05585	-4.99924
H	-1.68652	-3.82587	4.57621
C	-2.58521	-5.0893	3.078979
H	-3.487	-6.14744	1.42085
H	-8.22132	1.385871	1.66624
H	0.481745	4.793218	-2.38929
C	-1.44862	5.703899	-2.11086
H	-3.46072	6.398198	-1.71717
H	-2.606	-5.95111	3.737426
H	-1.13231	6.643246	-2.55144

Fe_2O_2 S=0(5,-5)

E(UB3LYP/6-31G(d,p))= -5450.14538243

no imaginary frequencies

	x	**y**	**z**
C	3.334485	0.002058	2.929909
H	3.157473	1.069654	2.864078
C	3.850009	-0.57208	4.090584
H	4.082336	0.051639	4.946397
C	4.066848	-1.94911	4.118617
H	4.477868	-2.42802	5.001471
C	3.748689	-2.70758	2.992248
H	3.909156	-3.7802	2.998019
C	3.231504	-2.06171	1.868622
C	2.85039	-2.73063	0.629321
C	2.095002	-2.97497	-1.40708
C	1.568752	-2.82702	-2.69889
H	1.264943	-1.85613	-3.07049
C	1.454398	-3.97115	-3.47771
H	1.062913	-3.8929	-4.48665
C	1.844475	-5.24203	-2.99854
H	1.746503	-6.10531	-3.64806
C	2.355919	-5.4112	-1.71843
H	2.656887	-6.38665	-1.35162
C	2.470127	-4.25695	-0.9399
C	5.256252	-0.97614	-1.39222
H	4.685093	-1.86816	-1.62441
C	6.608943	-0.88855	-1.72487
H	7.102261	-1.72115	-2.21378

C	7.30048	0.281487	-1.41749
H	8.353851	0.384139	-1.65711
C	6.614551	1.326758	-0.79826
H	7.135452	2.246672	-0.55525
C	5.260358	1.15979	-0.50357
C	4.42337	2.180459	0.121141
C	2.635963	3.134761	0.957108
C	1.358511	3.470051	1.424678
H	0.540692	2.762187	1.357836
C	1.193096	4.742873	1.958578
H	0.217867	5.044749	2.326062
C	2.258055	5.666644	2.0341
H	2.079836	6.647986	2.460389
C	3.530688	5.349176	1.574755
H	4.348753	6.059032	1.632777
C	3.691694	4.070589	1.038609
N	3.035178	-0.71845	1.83712
N	2.355097	-2.04359	-0.40323
N	2.936251	-4.05534	0.351819
N	4.588189	0.017293	-0.78905
N	3.127499	1.961961	0.379663
N	4.797498	3.424733	0.498817
Fe	2.359362	0.070688	-0.10307
H	5.721129	3.825986	0.403265
H	3.289769	-4.77566	0.966933
O	0.578631	0.351108	0.366601
N	2.081029	0.623313	-2.20479
C	2.125549	1.02183	-3.29203
C	2.195481	1.512361	-4.6605
H	2.974596	2.276377	-4.7417
H	2.437955	0.688576	-5.33873
H	1.236932	1.948932	-4.95464
O	-0.56545	0.270953	-0.37945
Fe	-2.35872	0.139911	0.101886
N	-3.07805	-0.60057	-1.84026
N	-2.51386	-1.97123	0.403163
N	-4.5727	0.252188	0.809828
N	-2.99354	2.082473	-0.38127
N	-2.01346	0.679229	2.198518
C	-3.31988	0.141656	-2.93286
C	-3.36217	-1.92805	-1.87794
C	-3.03875	-2.62331	-0.63677
C	-2.32592	-2.91906	1.407574
C	-5.30193	-0.69067	1.423524
C	-5.16784	1.436674	0.524263
C	-4.26725	2.394507	-0.11082

C	-2.42435	3.215803	-0.96514
C	-2.01017	1.089516	3.282219
H	-3.07309	1.194882	-2.86168
C	-3.86199	-0.39385	-4.09979
C	-3.91079	-2.53487	-3.00823
N	-3.21114	-3.94083	-0.36452
C	-1.80959	-2.8066	2.706852
C	-2.77449	-4.17419	0.932024
H	-4.79103	-1.61842	1.655357
C	-6.64267	-0.50913	1.766219
C	-6.50503	1.697051	0.82822
N	-4.55443	3.662477	-0.48635
C	-1.13087	3.456125	-1.4465
C	-3.40991	4.226064	-1.03764
C	-2.02056	1.595867	4.646669
H	-4.04563	0.246367	-4.95523
C	-4.16845	-1.75355	-4.13453
H	-4.14196	-3.59445	-3.01911
H	-3.6021	-4.63597	-0.98588
H	-1.45302	-1.85678	3.08595
C	-1.77599	-3.95711	3.483811
C	-2.74165	-5.3349	1.708755
H	-7.18754	-1.30391	2.263264
C	-7.25561	0.703691	1.457913
H	-6.96352	2.649283	0.584072
H	-5.44612	4.1288	-0.38343
H	-0.36671	2.690098	-1.38759
C	-0.87793	4.713268	-1.9834
C	-3.16105	5.489135	-1.57698
H	-1.05912	2.059626	4.884261
H	-2.81338	2.341472	4.759982
H	-2.20639	0.775596	5.346667
H	-4.6025	-2.20173	-5.0225
H	-1.3938	-3.90522	4.497974
C	-2.23678	-5.20057	2.995533
H	-3.09777	-6.28907	1.335404
H	-8.2977	0.878721	1.704857
H	0.112904	4.942809	-2.36128
C	-1.87319	5.712385	-2.04929
H	-3.92559	6.256831	-1.62817
H	-2.20012	-6.0698	3.64347
H	-1.62811	6.677794	-2.47875

Fe_2O_2 S=1(3,-1)

E(UB3LYP/6-31G(d,p))= -5450.13212909

no imaginary frequencies

	x	y	z
C	3.334485	0.002058	2.929909
H	3.157473	1.069654	2.864078
C	3.850009	-0.57208	4.090584
H	4.082336	0.051639	4.946397
C	4.066848	-1.94911	4.118617
H	4.477868	-2.42802	5.001471
C	3.748689	-2.70758	2.992248
H	3.909156	-3.7802	2.998019
C	3.231504	-2.06171	1.868622
C	2.85039	-2.73063	0.629321
C	2.095002	-2.97497	-1.40708
C	1.568752	-2.82702	-2.69889
H	1.264943	-1.85613	-3.07049
C	1.454398	-3.97115	-3.47771
H	1.062913	-3.8929	-4.48665
C	1.844475	-5.24203	-2.99854
H	1.746503	-6.10531	-3.64806
C	2.355919	-5.4112	-1.71843
H	2.656887	-6.38665	-1.35162
C	2.470127	-4.25695	-0.9399
C	5.256252	-0.97614	-1.39222
H	4.685093	-1.86816	-1.62441
C	6.608943	-0.88855	-1.72487
H	7.102261	-1.72115	-2.21378
C	7.30048	0.281487	-1.41749
H	8.353851	0.384139	-1.65711
C	6.614551	1.326758	-0.79826
H	7.135452	2.246672	-0.55525
C	5.260358	1.15979	-0.50357
C	4.42337	2.180459	0.121141
C	2.635963	3.134761	0.957108
C	1.358511	3.470051	1.424678
H	0.540692	2.762187	1.357836
C	1.193096	4.742873	1.958578
H	0.217867	5.044749	2.326062
C	2.258055	5.666644	2.0341
H	2.079836	6.647986	2.460389
C	3.530688	5.349176	1.574755
H	4.348753	6.059032	1.632777
C	3.691694	4.070589	1.038609
N	3.035178	-0.71845	1.83712
N	2.355097	-2.04359	-0.40323

N	2.936251	-4.05534	0.351819
N	4.588189	0.017293	-0.78905
N	3.127499	1.961961	0.379663
N	4.797498	3.424733	0.498817
Fe	2.359362	0.070688	-0.10307
H	5.721129	3.825986	0.403265
H	3.289769	-4.77566	0.966933
O	0.578631	0.351108	0.366601
N	2.081029	0.623313	-2.20479
C	2.125549	1.02183	-3.29203
C	2.195481	1.512361	-4.6605
H	2.974596	2.276377	-4.7417
H	2.437955	0.688576	-5.33873
H	1.236932	1.948932	-4.95464
O	-0.56545	0.270953	-0.37945
Fe	-2.35872	0.139911	0.101886
N	-3.07805	-0.60057	-1.84026
N	-2.51386	-1.97123	0.403163
N	-4.5727	0.252188	0.809828
N	-2.99354	2.082473	-0.38127
N	-2.01346	0.679229	2.198518
C	-3.31988	0.141656	-2.93286
C	-3.36217	-1.92805	-1.87794
C	-3.03875	-2.62331	-0.63677
C	-2.32592	-2.91906	1.407574
C	-5.30193	-0.69067	1.423524
C	-5.16784	1.436674	0.524263
C	-4.26725	2.394507	-0.11082
C	-2.42435	3.215803	-0.96514
C	-2.01017	1.089516	3.282219
H	-3.07309	1.194882	-2.86168
C	-3.86199	-0.39385	-4.09979
C	-3.91079	-2.53487	-3.00823
N	-3.21114	-3.94083	-0.36452
C	-1.80959	-2.8066	2.706852
C	-2.77449	-4.17419	0.932024
H	-4.79103	-1.61842	1.655357
C	-6.64267	-0.50913	1.766219
C	-6.50503	1.697051	0.82822
N	-4.55443	3.662477	-0.48635
C	-1.13087	3.456125	-1.4465
C	-3.40991	4.226064	-1.03764
C	-2.02056	1.595867	4.646669
H	-4.04563	0.246367	-4.95523
C	-4.16845	-1.75355	-4.13453
H	-4.14196	-3.59445	-3.01911

H	-3.6021	-4.63597	-0.98588
H	-1.45302	-1.85678	3.08595
C	-1.77599	-3.95711	3.483811
C	-2.74165	-5.3349	1.708755
H	-7.18754	-1.30391	2.263264
C	-7.25561	0.703691	1.457913
H	-6.96352	2.649283	0.584072
H	-5.44612	4.1288	-0.38343
H	-0.36671	2.690098	-1.38759
C	-0.87793	4.713268	-1.9834
C	-3.16105	5.489135	-1.57698
H	-1.05912	2.059626	4.884261
H	-2.81338	2.341472	4.759982
H	-2.20639	0.775596	5.346667
H	-4.6025	-2.20173	-5.0225
H	-1.3938	-3.90522	4.497974
C	-2.23678	-5.20057	2.995533
H	-3.09777	-6.28907	1.335404
H	-8.2977	0.878721	1.704857
H	0.112904	4.942809	-2.36128
C	-1.87319	5.712385	-2.04929
H	-3.92559	6.256831	-1.62817
H	-2.20012	-6.0698	3.64347
H	-1.62811	6.677794	-2.47875

Fe_2O_2 S=2(5,-1)

E(UB3LYP/6-31G(d,p))= -5450.14276598

no imaginary frequencies

	x	**y**	**z**
C	3.270686	-0.27419	2.761873
H	3.28954	0.807276	2.731973
C	3.636371	-0.96802	3.915636
H	3.955726	-0.41744	4.793352
C	3.592532	-2.36026	3.912149
H	3.884031	-2.92795	4.789812
C	3.162546	-3.0169	2.758571
H	3.108239	-4.09991	2.73383
C	2.811005	-2.25718	1.645083
C	2.328256	-2.78431	0.379385
C	1.57199	-2.7251	-1.67658
C	1.104578	-2.39561	-2.95724
H	0.991533	-1.36427	-3.26181

C	0.793112	-3.44177	-3.81617
H	0.445232	-3.22032	-4.81976
C	0.929123	-4.79305	-3.42763
H	0.688873	-5.57604	-4.13898
C	1.372118	-5.14102	-2.15832
H	1.480945	-6.17801	-1.85887
C	1.68577	-4.08545	-1.29894
C	4.935665	-1.35089	-1.40168
H	4.26498	-2.16335	-1.65061
C	6.282509	-1.40825	-1.7569
H	6.663348	-2.27816	-2.28001
C	7.114364	-0.33799	-1.43253
H	8.167994	-0.35391	-1.6917
C	6.566835	0.762644	-0.77433
H	7.190323	1.612786	-0.51929
C	5.209673	0.749221	-0.45537
C	4.486667	1.827883	0.194377
C	2.754782	2.8691	1.040662
C	1.49811	3.278917	1.510144
H	0.637466	2.629421	1.418302
C	1.416551	4.54179	2.081874
H	0.460441	4.900039	2.449103
C	2.542834	5.387165	2.197942
H	2.427712	6.364673	2.653802
C	3.794742	4.996091	1.74278
H	4.66008	5.643843	1.833068
C	3.875226	3.726729	1.165532
N	2.881487	-0.89765	1.639434
N	1.994976	-1.9412	-0.60327
N	2.159513	-4.07373	0.006898
N	4.398726	-0.30374	-0.75318
N	3.179477	1.690886	0.429311
N	4.944026	3.029883	0.619
Fe	2.401334	-0.06018	-0.13702
H	5.894702	3.368855	0.551246
H	2.368988	-4.89093	0.564637
O	0.77304	0.29126	0.543942
N	2.062494	0.676728	-1.91112
C	2.007458	1.211945	-2.93448
C	1.934457	1.876927	-4.22763
H	1.078891	2.558314	-4.24669
H	2.849961	2.449359	-4.40498
H	1.824433	1.137108	-5.02614
O	-0.31952	0.255013	-0.30803
Fe	-2.13045	0.252267	0.162035
N	-2.8757	-0.52625	-1.765

N	-2.36709	-1.85471	0.521369
N	-2.70149	2.203834	-0.38881
N	-1.82398	0.836921	2.251004
C	-3.09098	0.190084	-2.88001
C	-3.22172	-1.8391	-1.75812
C	-2.92686	-2.51038	-0.49627
C	-2.22227	-2.78	1.552454
C	-3.97719	2.548224	-0.1737
C	-2.09378	3.305128	-0.99327
C	-1.83938	1.265227	3.327687
H	-2.79736	1.23315	-2.84331
C	-3.66517	-0.35618	-4.02645
C	-3.80566	-2.45583	-2.8655
N	-3.16313	-3.81077	-0.18478
C	-1.69356	-2.65296	2.845822
C	-2.73396	-4.02585	1.117281
C	-4.91874	1.635787	0.470353
N	-4.22945	3.805257	-0.60921
C	-0.77673	3.510106	-1.42427
C	-3.05716	4.327955	-1.14071
C	-1.87068	1.796375	4.682297
H	-3.82584	0.264146	-4.90101
C	-4.03481	-1.70056	-4.01526
H	-4.08671	-3.50304	-2.84038
H	-3.59727	-4.50176	-0.78141
H	-1.28978	-1.70959	3.193018
C	-1.71325	-3.77879	3.658781
C	-2.75491	-5.16179	1.930653
C	-6.25366	1.945776	0.736219
N	-4.36561	0.445068	0.808536
H	-5.11522	4.290646	-0.55423
H	-0.02719	2.739359	-1.29051
C	-0.47909	4.743744	-1.99267
C	-2.76488	5.566481	-1.71511
H	-0.90506	2.244252	4.933516
H	-2.64998	2.560176	4.763955
H	-2.08949	0.993148	5.392451
H	-4.4965	-2.1561	-4.88539
H	-1.32539	-3.71424	4.670117
C	-2.23782	-5.01245	3.211151
H	-3.16122	-6.10816	1.589949
C	-7.04703	0.99766	1.382858
H	-6.67825	2.902789	0.452516
C	-5.13594	-0.45327	1.438367
H	0.533525	4.951039	-2.32372
C	-1.45512	5.753509	-2.14005

H	-3.51286	6.34448	-1.82355
H	-2.24269	-5.86143	3.886477
C	-6.47746	-0.22103	1.745857
H	-8.08805	1.212232	1.601498
H	-4.65833	-1.38709	1.713084
H	-1.17573	6.699873	-2.59043
H	-7.05605	-0.98134	2.258526

Fe_2O_2 S=1(5,-3)

E(UB3LYP/6-31G(d,p))= -5450.13605350

no imaginary frequencies

	x	**y**	**z**
C	3.139907	0.716769	2.849085
H	2.644641	1.676437	2.755318
C	3.832334	0.374356	4.009983
H	3.883035	1.073917	4.836694
C	4.458151	-0.86933	4.075646
H	5.01617	-1.16411	4.958512
C	4.358278	-1.73505	2.986043
H	4.837428	-2.70747	3.020247
C	3.642881	-1.32242	1.861999
C	3.45041	-2.12559	0.65837
C	2.759211	-2.66276	-1.34324
C	2.190793	-2.72537	-2.62395
H	1.617153	-1.89675	-3.02114
C	2.398009	-3.88502	-3.36017
H	1.984095	-3.96382	-4.36011
C	3.146924	-4.96882	-2.84934
H	3.291161	-5.8497	-3.46576
C	3.70939	-4.92999	-1.57971
H	4.287415	-5.76101	-1.18981
C	3.498884	-3.76113	-0.84441
C	5.138772	0.189251	-1.53712
H	4.8372	-0.8333	-1.73397
C	6.396684	0.6502	-1.9274
H	7.088795	-0.01923	-2.42587
C	6.736275	1.976009	-1.66467
H	7.706661	2.368663	-1.95056
C	5.803626	2.797452	-1.03108
H	6.04728	3.834356	-0.82613
C	4.565977	2.258623	-0.67534
C	3.495694	3.012852	-0.02955

C	1.545223	3.446389	0.863446
C	0.241551	3.422609	1.37731
H	-0.3593	2.522852	1.329578
C	-0.24702	4.605415	1.920509
H	-1.25587	4.632473	2.319466
C	0.525644	5.786054	1.964072
H	0.100295	6.683717	2.399775
C	1.819747	5.825942	1.459813
H	2.414487	6.732424	1.492745
C	2.30587	4.6368	0.91386
N	3.048859	-0.10423	1.791437
N	2.756631	-1.65517	-0.37991
N	3.912244	-3.3789	0.424486
N	4.238511	0.965752	-0.91673
N	2.31931	2.447847	0.268396
N	3.527508	4.315698	0.337134
Fe	2.130754	0.381125	-0.16596
H	4.304945	4.951703	0.218545
H	4.47168	-3.93944	1.053032
O	0.347946	0.034913	0.278794
N	1.672178	0.753969	-2.28239
C	1.574182	1.099973	-3.38396
C	1.46817	1.529365	-4.77075
H	2.217001	2.299398	-4.97942
H	1.642217	0.680211	-5.43848
H	0.47266	1.938889	-4.96335
O	-0.81524	0.561188	-0.25645
Fe	-2.38517	-0.20145	0.213123
N	-2.82915	-1.27593	-1.76145
N	-1.67848	-2.0869	0.521866
N	-4.31111	-0.75451	0.789017
N	-3.3967	1.401657	-0.43013
N	-2.29902	0.585912	2.346598
C	-3.38267	-0.78996	-2.88002
C	-2.54818	-2.59854	-1.69923
C	-1.92772	-2.98492	-0.43521
C	-1.08247	-2.77846	1.576168
C	-4.68049	-1.86123	1.45477
C	-5.27006	0.155495	0.459339
C	-4.71814	1.319643	-0.2144
C	-3.17261	2.610905	-1.09071
C	-2.47666	1.042027	3.398054
H	-3.57977	0.276782	-2.8955
C	-3.69731	-1.59536	-3.97593
C	-2.83293	-3.47317	-2.74882
N	-1.53922	-4.2273	-0.05685

C	-0.60719	-2.34959	2.823883
C	-1.00309	-4.1452	1.220455
H	-3.89014	-2.55065	1.72411
C	-6.00613	-2.12179	1.798368
C	-6.61527	-0.03814	0.767654
N	-5.36315	2.404945	-0.6927
C	-1.99962	3.214034	-1.56527
C	-4.42126	3.255888	-1.26008
C	-2.69946	1.603831	4.723275
H	-4.15204	-1.15873	-4.85815
C	-3.42364	-2.96026	-3.90444
H	-2.60936	-4.53227	-2.67763
H	-1.6381	-5.07394	-0.60031
H	-0.64359	-1.30521	3.104707
C	-0.09508	-3.31733	3.678982
C	-0.48785	-5.12145	2.076594
H	-6.25422	-3.03087	2.33454
C	-6.98989	-1.19971	1.444328
H	-7.36282	0.698378	0.493243
H	-6.3595	2.577594	-0.65155
H	-1.039	2.734873	-1.43208
C	-2.13107	4.447188	-2.19138
C	-4.55644	4.495125	-1.88878
H	-1.90952	2.320246	4.965933
H	-3.66549	2.116517	4.75418
H	-2.70071	0.805414	5.471421
H	-3.66525	-3.61815	-4.73297
H	0.265084	-3.02411	4.659643
C	-0.04081	-4.68157	3.315814
H	-0.45128	-6.16938	1.798494
H	-8.03117	-1.37517	1.694767
H	-1.24608	4.950297	-2.56671
C	-3.38455	5.07846	-2.35237
H	-5.5197	4.978592	-2.01078
H	0.351318	-5.40344	4.024391
H	-3.43362	6.04177	-2.84852

Fe_2O_2 S=0(3,-3)

E(UB3LYP/6-31G(d,p))= -5450.12243367

no imaginary frequencies

	x	**y**	**z**
C	3.136862	-0.61388	2.922163

H	3.291575	0.45976	2.899577
C	3.455563	-1.36305	4.05557
H	3.871033	-0.87538	4.930389
C	3.238631	-2.74013	4.030816
H	3.486155	-3.35564	4.889651
C	2.700016	-3.32046	2.882132
H	2.524949	-4.39035	2.845267
C	2.406894	-2.4991	1.792008
C	1.842473	-2.96087	0.527735
C	1.052796	-2.86939	-1.51381
C	0.594288	-2.51022	-2.78962
H	0.608613	-1.47913	-3.11729
C	0.123167	-3.52768	-3.60936
H	-0.22546	-3.28776	-4.6085
C	0.09389	-4.87519	-3.18527
H	-0.266	-5.63778	-3.86782
C	0.522681	-5.24665	-1.91777
H	0.503242	-6.28113	-1.59175
C	0.994391	-4.21972	-1.09616
C	4.641806	-1.85274	-1.24318
H	3.893015	-2.59833	-1.47856
C	5.987687	-2.073	-1.53314
H	6.293657	-3.0081	-1.98865
C	6.915994	-1.07799	-1.23132
H	7.97089	-1.21991	-1.44302
C	6.467468	0.11211	-0.6569
H	7.171107	0.903943	-0.4234
C	5.106765	0.260628	-0.39523
C	4.484697	1.437346	0.189675
C	2.86653	2.689089	0.987915
C	1.661451	3.246282	1.436544
H	0.729147	2.711358	1.315971
C	1.725999	4.504183	2.023025
H	0.814422	4.973669	2.378152
C	2.944511	5.203498	2.169718
H	2.941556	6.184046	2.6335
C	4.148109	4.663735	1.735552
H	5.085402	5.197303	1.850766
C	4.080378	3.398563	1.148933
N	2.630987	-1.16404	1.810465
N	1.605101	-2.11618	-0.47883
N	1.494505	-4.22944	0.197798
N	4.201292	-0.71767	-0.67626
N	3.156391	1.468207	0.376003
N	5.070191	2.570793	0.631141
Fe	2.233327	-0.19905	-0.22

H	6.059	2.784761	0.604824
H	1.588928	-5.04586	0.786109
O	0.61707	0.555563	0.063224
N	2.293038	0.413939	-2.44739
C	2.528484	0.727071	-3.53933
C	2.823618	1.108176	-4.9141
H	1.998314	1.694286	-5.32833
H	3.737863	1.70807	-4.94871
H	2.966596	0.212433	-5.52605
O	-0.51351	-0.25646	-0.15653
Fe	-2.14525	0.396887	0.221884
N	-3.15657	-0.05497	-1.79837
N	-2.69863	-1.56849	0.370536
N	-4.01097	0.986037	0.913835
N	-2.08533	2.344953	-0.30558
N	-1.58194	0.878618	2.381679
C	-3.35014	0.75379	-2.84874
C	-3.6743	-1.30567	-1.84678
C	-3.37968	-2.08949	-0.65173
C	-2.58092	-2.57167	1.330639
C	-4.91942	0.231837	1.555633
C	-4.27776	2.308464	0.733888
C	-3.20664	2.999169	0.036948
C	-1.30871	3.253172	-1.03191
C	-1.45524	1.252139	3.472059
H	-2.91116	1.74337	-2.78214
C	-4.0707	0.366463	-3.97954
C	-4.41147	-1.77048	-2.93712
N	-3.72701	-3.37722	-0.40436
C	-1.97065	-2.58706	2.593263
C	-3.24358	-3.72503	0.849044
H	-4.6659	-0.80973	1.70374
C	-6.12661	0.749103	2.022983
C	-5.46269	2.895637	1.17445
N	-3.19049	4.277048	-0.39947
C	-0.07103	3.119901	-1.67526
C	-2.00301	4.485209	-1.08811
C	-1.30565	1.718578	4.844298
H	-4.20334	1.059843	-4.8025
C	-4.61557	-0.91569	-4.02042
H	-4.82915	-2.77154	-2.9496
H	-4.25502	-3.98116	-1.01951
H	-1.45562	-1.71405	2.974196
C	-2.06285	-3.75969	3.332622
C	-3.33714	-4.90637	1.588801
H	-6.82879	0.097911	2.531345

C	-6.40581	2.100429	1.825909
H	-5.65405	3.952066	1.019982
H	-3.92737	4.960132	-0.27987
H	0.473554	2.186969	-1.63531
C	0.421673	4.235278	-2.34098
C	-1.50772	5.61024	-1.75025
H	-2.11606	2.409274	5.095153
H	-1.34259	0.870395	5.534247
H	-0.34926	2.235331	4.963323
H	-5.19122	-1.24738	-4.87842
H	-1.61707	-3.80329	4.321001
C	-2.73699	-4.90003	2.841704
H	-3.86046	-5.77994	1.214852
H	-7.33808	2.531913	2.1758
H	1.378345	4.171169	-2.84919
C	-0.2783	5.461038	-2.37774
H	-2.05328	6.547214	-1.78194
H	-2.79535	-5.78872	3.461126
H	0.149822	6.303045	-2.91094

Fe_2O_2 S=3(3,3)

E(UB3LYP/6-31G(d,p))= -5450.12036608

no imaginary frequencies

	x	**y**	**z**
C	3.175971	-0.6923	2.816957
H	3.355826	0.377384	2.841345
C	3.507749	-1.50255	3.904217
H	3.957935	-1.06712	4.789409
C	3.258941	-2.87162	3.819462
H	3.516199	-3.53342	4.640187
C	2.67459	-3.38336	2.660186
H	2.47175	-4.44572	2.577809
C	2.372108	-2.50329	1.619944
C	1.761926	-2.88917	0.350788
C	0.927128	-2.68106	-1.66519
C	0.453393	-2.24938	-2.91254
H	0.475379	-1.20216	-3.18369
C	-0.0424	-3.2177	-3.77659
H	-0.40154	-2.92236	-4.75695
C	-0.08114	-4.5851	-3.42281
H	-0.45855	-5.3072	-4.13923
C	0.3643	-5.0278	-2.18369

H	0.34163	-6.07836	-1.91389
C	0.862766	-4.05086	-1.31808
C	4.521725	-1.75792	-1.49253
H	3.736045	-2.44477	-1.78146
C	5.853377	-2.01786	-1.81262
H	6.110636	-2.92403	-2.34945
C	6.831139	-1.09861	-1.43536
H	7.876743	-1.27355	-1.66754
C	6.444743	0.060022	-0.7602
H	7.187462	0.795015	-0.46906
C	5.09414	0.253337	-0.47634
C	4.529212	1.416525	0.188032
C	2.964661	2.709096	1.02671
C	1.780422	3.315697	1.468147
H	0.823204	2.839199	1.304798
C	1.896929	4.552714	2.090351
H	1.002717	5.062181	2.434409
C	3.146778	5.183308	2.280784
H	3.184238	6.149949	2.771468
C	4.329258	4.596617	1.849521
H	5.289382	5.080789	1.991947
C	4.20897	3.354626	1.222849
N	2.628609	-1.17669	1.694588
N	1.507701	-1.98873	-0.60259
N	1.391912	-4.13396	-0.03773
N	4.141052	-0.6547	-0.82745
N	3.203615	1.497976	0.375482
N	5.163575	2.502562	0.678904
Fe	2.202954	-0.10115	-0.29529
H	6.160134	2.677617	0.655071
H	1.492862	-4.9814	0.503956
O	0.621396	0.690166	0.088434
N	2.17861	0.663415	-2.43681
C	2.352434	1.113008	-3.49163
C	2.570122	1.666182	-4.8213
H	1.744599	2.330808	-5.09205
H	3.505282	2.233947	-4.84145
H	2.633344	0.857295	-5.55565
O	-0.51178	0.167201	-0.57414
Fe	-2.08979	0.387379	0.251489
N	-3.05989	-0.24028	-1.67554
N	-2.39639	-1.67495	0.503962
N	-4.01653	0.753958	1.017953
N	-2.34791	2.386071	-0.23343
N	-1.42304	0.846219	2.258105
C	-3.3436	0.527967	-2.73518

C	-3.44689	-1.53672	-1.69546
C	-3.0532	-2.26962	-0.49483
C	-2.17657	-2.65404	1.473145
C	-4.78422	-0.11163	1.701723
C	-4.50054	2.00807	0.799371
C	-3.55613	2.858076	0.094342
C	-1.68881	3.416992	-0.90321
C	-1.25539	1.290223	3.315351
H	-3.00196	1.556285	-2.68814
C	-4.03734	0.050943	-3.84849
C	-4.14796	-2.09141	-2.76761
N	-3.28132	-3.57943	-0.22686
C	-1.54368	-2.60091	2.723792
C	-2.74453	-3.86799	1.020241
H	-4.36365	-1.09173	1.88449
C	-6.05539	0.216278	2.170899
C	-5.76482	2.405028	1.233562
N	-3.71996	4.136396	-0.31619
C	-0.41051	3.487644	-1.47394
C	-2.55448	4.535585	-0.95829
C	-1.04557	1.847091	4.644454
H	-4.24947	0.713217	-4.68041
C	-4.45268	-1.27936	-3.86018
H	-4.46162	-3.12976	-2.75991
H	-3.77528	-4.23218	-0.82009
H	-1.10191	-1.68149	3.087309
C	-1.51714	-3.7676	3.478898
C	-2.71899	-5.04364	1.774269
H	-6.63198	-0.52188	2.716944
C	-6.55903	1.492292	1.926627
H	-6.12886	3.408586	1.041678
H	-4.54621	4.70684	-0.19145
H	0.264682	2.643379	-1.4233
C	-0.05328	4.686807	-2.07783
C	-2.19809	5.741539	-1.56518
H	-1.87723	2.506904	4.908986
H	-0.98947	1.042215	5.383434
H	-0.11428	2.420194	4.666249
H	-5.00494	-1.6811	-4.7035
H	-1.05282	-3.75739	4.4596
C	-2.0969	-4.9689	3.014812
H	-3.17317	-5.9639	1.422378
H	-7.54704	1.77697	2.273515
H	0.930962	4.786583	-2.52381
C	-0.92862	5.794501	-2.12579
H	-2.87097	6.591569	-1.59993

H	-2.06669	-5.85066	3.646147
H	-0.60224	6.708621	-2.60998

Fe_2O_2 S=0(1,-1) TS

E(UB3LYP/6-31G(d,p))= -5450.11350277

i506.23

	x	**y**	**z**
C	3.324676	0.035571	2.686217
H	3.175279	1.107129	2.661506
C	3.864769	-0.59124	3.809169
H	4.147959	0.003066	4.670665
C	4.038895	-1.97363	3.79605
H	4.470229	-2.48744	4.648998
C	3.644163	-2.69123	2.666728
H	3.758961	-3.76939	2.635926
C	3.107581	-1.9977	1.583863
C	2.623799	-2.59269	0.349698
C	1.713522	-2.64408	-1.6417
C	1.099271	-2.38458	-2.87589
H	0.813729	-1.37947	-3.155
C	0.869921	-3.46525	-3.71781
H	0.41258	-3.29697	-4.6873
C	1.228322	-4.78331	-3.35633
H	1.045029	-5.59313	-4.05453
C	1.817285	-5.06437	-2.13044
H	2.095054	-6.07555	-1.85237
C	2.046928	-3.97457	-1.28704
C	4.945328	-0.91146	-1.51249
H	4.360544	-1.79439	-1.73846
C	6.278936	-0.82408	-1.91078
H	6.73693	-1.65046	-2.44258
C	6.997502	0.333405	-1.61706
H	8.038085	0.431417	-1.90882
C	6.351955	1.372759	-0.94783
H	6.885464	2.288813	-0.71792
C	5.01456	1.211491	-0.58758
C	4.196803	2.213525	0.074047
C	2.386095	3.084307	0.945786
C	1.099967	3.372415	1.424114
H	0.307153	2.642471	1.327733
C	0.900568	4.625663	1.989131
H	-0.08386	4.895703	2.357736

C	1.940407	5.577466	2.088934
H	1.735069	6.542298	2.540044
C	3.218834	5.30873	1.618675
H	4.016446	6.040165	1.691987
C	3.416929	4.049625	1.046967
N	2.9682	-0.64403	1.5858
N	2.104748	-1.80798	-0.59823
N	2.612344	-3.89464	-0.02073
N	4.315973	0.074199	-0.85242
N	2.914502	1.949716	0.334958
N	4.539685	3.458346	0.484341
Fe	2.280807	0.118052	-0.15555
H	5.450442	3.889474	0.395637
H	2.971091	-4.67371	0.515004
O	0.750546	0.292932	0.546396
N	1.835839	0.781093	-1.93607
C	1.715212	1.27267	-2.97508
C	1.558628	1.884344	-4.28691
H	0.641634	2.480225	-4.31124
H	2.412232	2.53488	-4.49989
H	1.507297	1.110945	-5.05904
O	-0.75423	0.249072	-0.54861
Fe	-2.28089	0.049195	0.154908
N	-2.94999	-0.73057	-1.5852
N	-2.06851	-1.87153	0.60291
N	-2.95324	1.866512	-0.33848
N	-1.85058	0.726451	1.933314
C	-3.31563	-0.06073	-2.68853
C	-3.06566	-2.08644	-1.5793
C	-2.57262	-2.66873	-0.34276
C	-1.66132	-2.69698	1.648752
C	-4.24169	2.103005	-0.08186
C	-2.44754	3.011337	-0.94926
C	-1.74203	1.22256	2.971491
H	-3.18447	1.01329	-2.66684
C	-3.84257	-0.70037	-3.81051
C	-3.58805	-2.79265	-2.66091
N	-2.53653	-3.96907	0.031615
C	-1.05143	-2.42207	2.88175
C	-1.96938	-4.03459	1.298049
C	-5.03924	1.085333	0.580546
N	-4.6102	3.339317	-0.49571
C	-1.16598	3.326753	-1.42238
C	-3.49871	3.953804	-1.05577
C	-1.60089	1.840104	4.282359
H	-4.1341	-0.11386	-4.67457

C	-3.99302	-2.0855	-3.79321
H	-3.68402	-3.87256	-2.62699
H	-2.87974	-4.75649	-0.5021
H	-0.78539	-1.41077	3.157896
C	-0.8004	-3.49576	3.726424
C	-1.71804	-5.11737	2.144338
C	-6.38038	1.219159	0.938091
N	-4.31704	-0.03609	0.849522
H	-5.53023	3.751002	-0.4103
H	-0.35797	2.614439	-1.32093
C	-0.99161	4.58331	-1.98839
C	-3.32584	5.215976	-1.6289
H	-0.69794	2.457032	4.306746
H	-2.4695	2.471145	4.49328
H	-1.5326	1.069511	5.055977
H	-4.41375	-2.60938	-4.64533
H	-0.34555	-3.31601	4.695021
C	-1.13357	-4.82149	3.368893
H	-1.97621	-6.13454	1.869281
C	-7.00492	0.168139	1.609033
H	-6.93275	2.123163	0.705046
C	-4.92659	-1.03318	1.511007
H	-0.01157	4.874641	-2.35248
C	-2.05164	5.511883	-2.09433
H	-4.13887	5.929774	-1.70661
H	-0.93386	-5.62567	4.069102
C	-6.26245	-0.97305	1.906917
H	-8.04783	0.244849	1.89889
H	-4.32381	-1.90311	1.740163
H	-1.86557	6.480327	-2.54606
H	-6.70367	-1.80759	2.440151

Fe_2O_2 S=1(1,1) TS

No TS located

Fe_2O_2 S=2(3,1) TS

E(UB3LYP/6-31G(d,p))= -5450.10105648

i432.38

	x	**y**	**z**
C	3.347823	0.559124	2.671719

H	2.947292	1.56316	2.62319
C	4.024451	0.106144	3.804019
H	4.16232	0.772428	4.648134
C	4.517594	-1.1971	3.824326
H	5.059128	-1.57285	4.686342
C	4.298724	-2.01712	2.717428
H	4.66198	-3.03915	2.712214
C	3.610918	-1.49682	1.623025
C	3.275696	-2.21594	0.407383
C	2.403863	-2.51387	-1.58072
C	1.757868	-2.42459	-2.82253
H	1.266026	-1.51221	-3.13157
C	1.776157	-3.54883	-3.63789
H	1.299566	-3.50788	-4.61179
C	2.411274	-4.74736	-3.24339
H	2.411453	-5.59503	-3.92033
C	3.04248	-4.86203	-2.01164
H	3.533546	-5.78061	-1.70845
C	3.022944	-3.72853	-1.19561
C	5.095832	-0.06932	-1.55737
H	4.745571	-1.07872	-1.73123
C	6.354337	0.329513	-2.00718
H	6.989383	-0.37996	-2.52568
C	6.769166	1.640405	-1.78109
H	7.743894	1.981296	-2.11455
C	5.903391	2.513615	-1.1234
H	6.197668	3.542181	-0.94422
C	4.659403	2.04045	-0.7077
C	3.641097	2.833291	-0.04176
C	1.704607	3.261931	0.889135
C	0.409447	3.237114	1.424711
H	-0.17999	2.330871	1.387567
C	-0.06794	4.420966	1.972538
H	-1.07	4.449786	2.388389
C	0.705926	5.602735	2.001137
H	0.288044	6.501078	2.442724
C	1.990569	5.642475	1.475638
H	2.585856	6.548951	1.497095
C	2.469685	4.452968	0.922333
N	3.158153	-0.21429	1.592051
N	2.594359	-1.58853	-0.55563
N	3.554384	-3.49518	0.06672
N	4.257973	0.756045	-0.90914
N	2.473286	2.272434	0.28005
N	3.681421	4.137008	0.323886
Fe	2.289105	0.328032	-0.14551

H	4.457649	4.77226	0.193526
H	4.073587	-4.16363	0.620318
O	0.779937	0.073048	0.612476
N	1.625407	0.843858	-1.90301
C	1.335043	1.27094	-2.93656
C	0.96782	1.806869	-4.23957
H	-0.00784	2.297371	-4.17637
H	1.714142	2.537068	-4.56658
H	0.919977	1.002097	-4.97901
O	-0.83414	0.557705	-0.29608
Fe	-2.28112	-0.09425	0.243629
N	-2.8268	-1.22878	-1.67736
N	-1.63064	-2.00434	0.600993
N	-3.32644	1.496949	-0.40545
N	-2.1948	0.672665	2.347446
C	-3.38761	-0.76187	-2.79974
C	-2.60264	-2.5583	-1.56876
C	-1.9611	-2.92443	-0.3088
C	-1.02875	-2.68312	1.659688
C	-4.65027	1.417048	-0.20949
C	-3.09024	2.696448	-1.07646
C	-2.33785	1.124468	3.405527
H	-3.53748	0.311474	-2.85245
C	-3.7684	-1.5941	-3.854
C	-2.95646	-3.45979	-2.57419
N	-1.62364	-4.16997	0.107181
C	-0.47748	-2.2292	2.866468
C	-1.03702	-4.06572	1.360948
C	-5.20771	0.269601	0.487912
N	-5.28707	2.4936	-0.71851
C	-1.90529	3.298004	-1.52076
C	-4.33486	3.336808	-1.28176
C	-2.5174	1.681437	4.739078
H	-4.22619	-1.17194	-4.74169
C	-3.55548	-2.96649	-3.73388
H	-2.77881	-4.52446	-2.46609
H	-1.79085	-5.03135	-0.39479
H	-0.43781	-1.17255	3.09528
C	0.016153	-3.18765	3.742854
C	-0.54111	-5.03284	2.238793
C	-6.55512	0.087659	0.794695
N	-4.25051	-0.62903	0.848037
H	-6.28352	2.668957	-0.69205
H	-0.94856	2.825973	-1.33824
C	-2.02126	4.524986	-2.16309
C	-4.45507	4.568409	-1.92881

H	-1.70352	2.374744	4.969551
H	-3.46896	2.21858	4.794641
H	-2.52351	0.877203	5.48097
H	-3.84963	-3.64467	-4.52836
H	0.433773	-2.8742	4.694083
C	-0.02111	-4.56714	3.439752
H	-0.57228	-6.09195	2.005889
C	-6.93442	-1.05124	1.506295
H	-7.30011	0.816621	0.494273
C	-4.62486	-1.71177	1.547842
H	-1.12722	5.032438	-2.5106
C	-3.27227	5.149006	-2.36801
H	-5.41501	5.050337	-2.07975
H	0.35897	-5.27968	4.164208
C	-5.95246	-1.9608	1.894776
H	-7.97687	-1.21766	1.75793
H	-3.83685	-2.39291	1.844702
H	-3.31014	6.107324	-2.87469
H	-6.20294	-2.8509	2.46091

Fe_2O_2 S=3(5,1) TS

E(UB3LYP/6-31G(d,p))= -5450.11243687

i478.18

	x	**y**	**z**
C	-3.76831	0.675811	-2.43722
H	-3.54383	1.733324	-2.39866
C	-4.43094	0.119384	-3.53102
H	-4.73731	0.758098	-4.35177
C	-4.68906	-1.24965	-3.54411
H	-5.21198	-1.70827	-4.37703
C	-4.25721	-2.02736	-2.46922
H	-4.43381	-3.09749	-2.4615
C	-3.59857	-1.40464	-1.41161
C	-3.06582	-2.06483	-0.23342
C	-2.03267	-2.22785	1.69254
C	-1.33244	-2.04407	2.893692
H	-0.95443	-1.07136	3.176054
C	-1.14311	-3.1566	3.703149
H	-0.62141	-3.04384	4.647795
C	-1.62365	-4.43481	3.341244
H	-1.46692	-5.27077	4.014615
C	-2.3016	-4.6424	2.147463

H	-2.67569	-5.62184	1.868843
C	-2.49212	-3.52015	1.337995
C	-5.06273	-0.16699	1.876215
H	-4.56732	-1.11987	2.014591
C	-6.32676	0.061819	2.41801
H	-6.82399	-0.72442	2.974795
C	-6.92624	1.306689	2.232624
H	-7.91107	1.515207	2.637912
C	-6.23484	2.287599	1.522256
H	-6.67553	3.267353	1.372569
C	-4.97221	1.98442	1.014068
C	-4.11697	2.901366	0.281437
C	-2.32391	3.564058	-0.7963
C	-1.08545	3.698549	-1.44111
H	-0.38847	2.871145	-1.47707
C	-0.80498	4.929611	-2.01893
H	0.143107	5.075704	-2.52557
C	-1.71765	6.007532	-1.96978
H	-1.45181	6.948715	-2.43893
C	-2.94851	5.890513	-1.33817
H	-3.65065	6.716508	-1.30306
C	-3.2303	4.652041	-0.75713
N	-3.37529	-0.06242	-1.38786
N	-2.42251	-1.34271	0.688673
N	-3.13011	-3.3703	0.1136
N	-4.39276	0.763649	1.176916
N	-2.91729	2.489296	-0.13644
N	-4.34376	4.189561	-0.06793
Fe	-2.44731	0.594008	0.277667
H	-5.17758	4.726887	0.130708
H	-3.58491	-4.10749	-0.40846
O	-1.00928	0.679005	-0.54585
N	-1.75379	1.187225	2.00908
C	-1.42285	1.682983	2.999119
C	-1.00192	2.303171	4.246324
H	-0.03938	2.802269	4.099555
H	-1.74363	3.042604	4.563355
H	-0.90383	1.546298	5.030154
O	0.613231	0.042374	0.055343
Fe	2.222966	-0.38378	-0.37042
N	2.855969	-1.30532	1.536352
N	1.99909	-2.47708	-0.7232
N	3.212977	1.386162	0.150205
N	2.137948	0.192903	-2.49238
C	3.256504	-0.6542	2.638373
C	2.915881	-2.65995	1.522039

C	2.434346	-3.24569	0.275289
C	1.606258	-3.33934	-1.74406
C	4.536398	1.445339	-0.03871
C	2.838576	2.604385	0.716079
C	2.236449	0.587523	-3.57726
H	3.18637	0.427339	2.60778
C	3.747533	-1.31349	3.764436
C	3.39912	-3.39109	2.608447
N	2.359526	-4.56369	-0.04001
C	1.066717	-3.09053	-3.01476
C	1.840701	-4.67034	-1.32326
C	5.267807	0.340375	-0.65154
N	5.041394	2.628777	0.383781
C	1.583746	3.096084	1.097681
C	3.995059	3.40047	0.873932
C	2.373924	1.069428	-4.9441
H	4.068041	-0.74413	4.629667
C	3.826503	-2.70537	3.744997
H	3.453154	-4.47387	2.575608
H	2.645911	-5.33798	0.543388
H	0.871507	-2.07926	-3.34954
C	0.797191	-4.18861	-3.8209
C	1.570959	-5.77841	-2.13035
C	6.641345	0.347632	-0.90033
N	4.470776	-0.70371	-0.98491
H	6.01058	2.914822	0.339001
H	0.69331	2.49893	0.943263
C	1.543234	4.378581	1.634369
C	3.959658	4.68549	1.418721
H	3.103063	1.884395	-4.97942
H	2.720869	0.257799	-5.59078
H	1.412338	1.435611	-5.31437
H	4.215826	-3.25092	4.598538
H	0.389748	-4.03401	-4.81459
C	1.048318	-5.51071	-3.38909
H	1.765934	-6.79348	-1.80113
C	7.214552	-0.75922	-1.52712
H	7.261395	1.192364	-0.61979
C	5.03136	-1.75516	-1.59749
H	0.588596	4.809076	1.920301
C	2.709321	5.158197	1.798676
H	4.853589	5.288425	1.53645
H	0.832042	-6.33604	-4.05904
C	6.39508	-1.82656	-1.88825
H	8.279648	-0.78105	-1.73347
H	4.36326	-2.56372	-1.87299

H	2.627758	6.153461	2.222231
H	6.798121	-2.70034	-2.388

Fe_2O_2 S=4(5,3) TS

E(UB3LYP/6-31G(d,p))= -5450.10700009

i566.79

	x	**y**	**z**
C	3.198561	0.291202	2.751959
H	2.844426	1.313296	2.679835
C	3.785292	-0.18964	3.92212
H	3.89724	0.463702	4.780061
C	4.228328	-1.51095	3.956666
H	4.700896	-1.91439	4.846398
C	4.0578	-2.31183	2.8275
H	4.394949	-3.34268	2.836849
C	3.459258	-1.75854	1.694979
C	3.216331	-2.47517	0.447222
C	2.553326	-2.82166	-1.60705
C	2.038559	-2.74863	-2.90958
H	1.597828	-1.83362	-3.28526
C	2.121259	-3.8912	-3.69473
H	1.743945	-3.86791	-4.71179
C	2.694962	-5.08868	-3.21132
H	2.747423	-5.95218	-3.86584
C	3.200054	-5.18424	-1.9209
H	3.644383	-6.10256	-1.55209
C	3.115188	-4.03206	-1.13536
C	5.357062	-0.35116	-1.41592
H	4.953293	-1.32679	-1.66154
C	6.688628	-0.04034	-1.69635
H	7.332723	-0.78111	-2.1568
C	7.162636	1.229939	-1.37564
H	8.192889	1.506019	-1.57532
C	6.286951	2.14922	-0.7977
H	6.635488	3.145723	-0.5482
C	4.968799	1.759601	-0.5549
C	3.944023	2.628448	0.013977
C	1.97955	3.269747	0.738529
C	0.638578	3.385124	1.126815
H	-0.04085	2.548252	1.019816
C	0.229469	4.617296	1.624295
H	-0.80471	4.754266	1.923568

C	1.115915	5.709629	1.744434
H	0.749199	6.650959	2.139478
C	2.448856	5.609375	1.36452
H	3.129643	6.448977	1.454397
C	2.855337	4.372381	0.861399
N	3.044895	-0.46839	1.65785
N	2.643445	-1.86935	-0.59364
N	3.515799	-3.76833	0.167747
N	4.508945	0.518886	-0.8499
N	2.692983	2.194883	0.207643
N	4.082654	3.920977	0.392254
Fe	2.270425	0.199473	-0.29673
H	4.929084	4.472152	0.338915
H	3.971194	-4.42539	0.786486
O	0.594882	0.125927	0.060642
N	2.074905	0.70687	-2.42642
C	2.073864	1.11881	-3.50928
C	2.089714	1.62673	-4.87348
H	2.505443	2.638643	-4.88849
H	2.709867	0.98141	-5.50301
H	1.074337	1.652896	-5.27863
O	-1.08344	0.730837	-0.28091
Fe	-2.51011	0.067041	0.274083
N	-3.05625	-1.02561	-1.63507
N	-1.87308	-1.84374	0.630212
N	-4.47268	-0.44442	0.922423
N	-3.54666	1.680785	-0.33027
N	-2.3568	0.857096	2.361298
C	-3.60747	-0.53017	-2.74998
C	-2.8006	-2.35253	-1.56818
C	-2.1711	-2.74429	-0.31059
C	-1.28473	-2.54142	1.685109
C	-4.84717	-1.53853	1.604947
C	-5.42095	0.484194	0.617906
C	-4.86296	1.633193	-0.07435
C	-3.30578	2.887328	-0.98966
C	-2.43299	1.397743	3.383997
H	-3.77769	0.54085	-2.76953
C	-3.95066	-1.33454	-3.83813
C	-3.11489	-3.22521	-2.61063
N	-1.82192	-3.99408	0.078964
C	-0.77731	-2.11522	2.92068
C	-1.26302	-3.91489	1.347251
H	-4.06561	-2.24436	1.856573
C	-6.16747	-1.7677	1.990349
C	-6.76082	0.322647	0.966272

N	-5.489	2.739245	-0.52744
C	-2.12961	3.457278	-1.49403
C	-4.54014	3.567723	-1.11822
C	-2.5319	2.06521	4.674257
H	-4.40245	-0.89156	-4.71864
C	-3.70672	-2.70468	-3.76231
H	-2.91041	-4.28803	-2.53783
H	-1.96869	-4.84442	-0.44781
H	-0.77122	-1.06712	3.189516
C	-0.29063	-3.09059	3.78207
C	-0.77479	-4.89894	2.210026
H	-6.41861	-2.66772	2.540226
C	-7.14108	-0.82642	1.660564
H	-7.49919	1.074488	0.709029
H	-6.47827	2.940468	-0.45421
H	-1.17959	2.947995	-1.39664
C	-2.24313	4.698309	-2.10868
C	-4.65735	4.814152	-1.73562
H	-1.6766	2.731349	4.818705
H	-3.45304	2.653918	4.719818
H	-2.54894	1.322768	5.477855
H	-3.97028	-3.36074	-4.58555
H	0.092567	-2.79811	4.754141
C	-0.2942	-4.4604	3.437351
H	-0.78504	-5.95132	1.946761
H	-8.17793	-0.9772	1.94325
H	-1.35516	5.176025	-2.50886
C	-3.48207	5.366166	-2.22919
H	-5.60918	5.326054	-1.82749
H	0.077315	-5.18768	4.151525
H	-3.51735	6.333495	-2.71864

Fe_2O_2 S=5(5,5) TS

E(UB3LYP/6-31G(d,p))= -5450.09169327

i479.74

	x	**y**	**z**
C	3.392596	0.66744	-2.59822
H	3.416523	-0.41455	-2.53197
C	3.76795	1.329055	-3.76757
H	4.096508	0.760134	-4.63006
C	3.719916	2.721923	-3.79551
H	4.016713	3.269195	-4.68437

C	3.284711	3.407646	-2.66128
H	3.238324	4.491315	-2.66576
C	2.923746	2.673449	-1.53074
C	2.447763	3.250481	-0.27755
C	1.708588	3.327024	1.781555
C	1.254619	3.068771	3.082943
H	1.16098	2.054909	3.450967
C	0.934833	4.162666	3.876455
H	0.591633	4.001226	4.893003
C	1.052659	5.48855	3.402326
H	0.802602	6.311158	4.063805
C	1.488066	5.763887	2.112394
H	1.582519	6.78208	1.750287
C	1.809367	4.660502	1.318187
C	5.17443	1.962477	1.521416
H	4.470295	2.746685	1.77306
C	6.535928	2.114901	1.785055
H	6.899334	3.030525	2.237894
C	7.404463	1.074741	1.460169
H	8.469717	1.160676	1.648344
C	6.881244	-0.08827	0.894813
H	7.538465	-0.91382	0.643617
C	5.507085	-0.16522	0.666765
C	4.81937	-1.32601	0.117996
C	3.141472	-2.5647	-0.56063
C	1.897507	-3.10338	-0.91355
H	0.9887	-2.52526	-0.78948
C	1.893182	-4.40546	-1.40006
H	0.94986	-4.86673	-1.67363
C	3.079521	-5.15892	-1.54175
H	3.022687	-6.17136	-1.92701
C	4.319725	-4.63705	-1.19489
H	5.230307	-5.2169	-1.29991
C	4.321658	-3.33087	-0.7027
N	2.989693	1.320655	-1.49981
N	2.126588	2.47556	0.760088
N	2.27396	4.563521	0.013084
N	4.661511	0.85507	0.96498
N	3.490883	-1.31562	-0.04847
N	5.353083	-2.50897	-0.26251
Fe	2.512993	0.430377	0.476573
H	6.331482	-2.76375	-0.22639
H	2.469823	5.343161	-0.59991
O	0.957499	-0.06255	0.156859
N	2.491219	-0.13142	2.592323
C	2.590814	-0.57691	3.657135

C	2.726351	-1.12402	4.999144
H	3.387321	-1.99572	4.979392
H	3.154858	-0.37057	5.666948
H	1.74823	-1.42827	5.38205
O	-0.66035	-1.15574	0.157694
Fe	-2.4023	-0.68614	-0.41285
N	-3.23057	0.056344	1.499771
N	-2.45977	1.398242	-0.69158
N	-4.61142	-0.79107	-1.13556
N	-3.0595	-2.64442	0.070536
N	-2.06143	-1.196	-2.49982
C	-3.53775	-0.67727	2.578826
C	-3.47883	1.388791	1.524403
C	-3.06688	2.065595	0.298842
C	-2.21954	2.329415	-1.70385
C	-5.32213	0.159	-1.76012
C	-5.20691	-1.98472	-0.8963
C	-4.32541	-2.9498	-0.2468
C	-2.51641	-3.78409	0.670145
C	-1.99206	-1.66767	-3.55604
H	-3.30811	-1.7351	2.522412
C	-4.1258	-0.12431	3.71712
C	-4.06638	2.015167	2.623149
N	-3.23789	3.370304	-0.01489
C	-1.61504	2.19961	-2.96182
C	-2.71965	3.584602	-1.28698
H	-4.808	1.093257	-1.95804
C	-6.64724	-0.02254	-2.15641
C	-6.53024	-2.24653	-1.25735
N	-4.62974	-4.21889	0.109517
C	-1.24476	-4.03362	1.204203
C	-3.50871	-4.79058	0.698144
C	-1.91794	-2.25171	-4.88665
H	-4.36487	-0.75785	4.563869
C	-4.40126	1.241549	3.735485
H	-4.26445	3.08162	2.623728
H	-3.69428	4.067107	0.558625
H	-1.21496	1.250042	-3.2945
C	-1.55625	3.333728	-3.76326
C	-2.66157	4.727972	-2.08573
H	-7.17831	0.778031	-2.65897
C	-7.26281	-1.24554	-1.89503
H	-6.99045	-3.20699	-1.05214
H	-5.51932	-4.68071	-0.02633
H	-0.47703	-3.26886	1.187494
C	-1.0204	-5.29485	1.743457

C	-3.28776	-6.05874	1.237785
H	-0.87462	-2.42857	-5.16291
H	-2.45568	-3.20465	-4.90277
H	-2.37463	-1.57604	-5.61621
H	-4.86772	1.70164	4.600548
H	-1.11019	3.265755	-4.75003
C	-2.07366	4.576066	-3.3363
H	-3.06334	5.681279	-1.7593
H	-8.29326	-1.42236	-2.18565
H	-0.04807	-5.52736	2.16476
C	-2.02137	-6.29082	1.760438
H	-4.05745	-6.8228	1.252059
H	-2.01811	5.43036	-4.00261
H	-1.7976	-7.26011	2.19285

Fe_2O_2 S=0(5,-5) TS

E(UB3LYP/6-31G(d,p))= -5450.11220926

i653.90

	x	**y**	**z**
C	3.066608	-0.3224	2.993038
H	2.86347	0.741736	3.035102
C	3.40867	-1.03773	4.140195
H	3.479728	-0.5287	5.094758
C	3.661906	-2.40387	4.02808
H	3.94191	-2.98933	4.897803
C	3.549956	-3.01297	2.778365
H	3.739274	-4.07573	2.67316
C	3.198591	-2.23007	1.677905
C	3.030381	-2.73251	0.318342
C	2.591833	-2.71008	-1.82503
C	2.253519	-2.39849	-3.14983
H	1.986013	-1.38927	-3.43614
C	2.26826	-3.43424	-4.07449
H	2.018642	-3.22794	-5.11001
C	2.60573	-4.75658	-3.70842
H	2.613316	-5.53041	-4.46853
C	2.930366	-5.08815	-2.39952
H	3.189508	-6.10331	-2.11851
C	2.913025	-4.04271	-1.47317
C	5.642333	-0.69797	-0.91977
H	5.167463	-1.57799	-1.33789
C	7.025745	-0.52865	-0.99416

H	7.638853	-1.28806	-1.46639
C	7.591669	0.625173	-0.45578
H	8.663958	0.787638	-0.49234
C	6.755074	1.577258	0.127872
H	7.175144	2.485852	0.545831
C	5.381535	1.334563	0.1584
C	4.389757	2.250061	0.709849
C	2.415027	3.015506	1.283331
C	1.054173	3.228142	1.537009
H	0.316914	2.484459	1.259508
C	0.707323	4.428818	2.14542
H	-0.33728	4.639785	2.349532
C	1.672662	5.394781	2.503964
H	1.351453	6.316597	2.976858
C	3.026929	5.193528	2.265992
H	3.768885	5.934377	2.543612
C	3.37181	3.988817	1.651465
N	2.972761	-0.89788	1.786046
N	2.689123	-1.91758	-0.68215
N	3.177543	-4.01044	-0.1106
N	4.830038	0.203274	-0.34962
N	3.085759	1.942869	0.695296
N	4.601045	3.461825	1.271368
Fe	2.565388	0.125183	-0.13518
H	5.496667	3.916498	1.392575
H	3.44369	-4.80545	0.454333
O	0.88988	0.261798	0.000841
N	2.694758	0.910254	-2.17126
C	2.880006	1.409997	-3.19996
C	3.123864	2.025504	-4.49628
H	3.785088	2.88945	-4.3799
H	3.601845	1.30356	-5.16549
H	2.180393	2.355015	-4.94051
O	-0.88988	0.261793	-0.00077
Fe	-2.56539	0.125239	0.135202
N	-2.97272	-0.89784	-1.78603
N	-2.68923	-1.91751	0.682192
N	-4.83005	0.203423	0.349539
N	-3.08566	1.942943	-0.69532
N	-2.69481	0.91034	2.171261
C	-3.06649	-0.32237	-2.99303
C	-3.19861	-2.23001	-1.67788
C	-3.03048	-2.73244	-0.3183
C	-2.59202	-2.71	1.825087
C	-5.64241	-0.69778	0.919664
C	-5.38149	1.334719	-0.15853

C	-4.38965	2.250181	-0.70993
C	-2.41486	3.015563	-1.28331
C	-2.88007	1.410099	3.199954
H	-2.8633	0.741761	-3.0351
C	-3.40852	-1.0377	-4.14019
C	-3.54996	-3.01291	-2.77834
N	-3.17771	-4.01036	0.110655
C	-2.25374	-2.39841	3.149895
C	-2.91324	-4.04263	1.473236
H	-5.16759	-1.57781	1.337834
C	-7.02582	-0.52842	0.993978
C	-6.75502	1.577455	-0.12809
N	-4.60087	3.461956	-1.27145
C	-1.05399	3.228157	-1.53691
C	-3.37159	3.98891	-1.65148
C	-3.12394	2.025625	4.496257
H	-3.47951	-0.52868	-5.09477
C	-3.66182	-2.40383	-4.02807
H	-3.73933	-4.07567	-2.67313
H	-3.44386	-4.80537	-0.45428
H	-1.98621	-1.38919	3.436211
C	-2.26855	-3.43415	4.07457
C	-2.93065	-5.08806	2.399593
H	-7.63898	-1.28779	1.466187
C	-7.59168	0.625409	0.455539
H	-7.17504	2.486051	-0.5461
H	-5.49647	3.916664	-1.39269
H	-0.31677	2.484446	-1.25938
C	-0.70707	4.428829	-2.14529
C	-3.02664	5.193619	-2.26597
H	-2.1805	2.355354	4.940391
H	-3.78535	2.889429	4.379894
H	-3.60171	1.303619	5.165553
H	-3.94181	-2.98929	-4.8978
H	-2.01896	-3.22784	5.110093
C	-2.60605	-4.75648	3.708503
H	-3.18981	-6.10321	2.118587
H	-8.66396	0.787905	0.492028
H	0.337554	4.639765	-2.34934
C	-1.67236	5.39483	-2.50387
H	-3.76856	5.934496	-2.54362
H	-2.61369	-5.5303	4.468614
H	-1.35109	6.316643	-2.97673

Fe_2O_2 S=1(3,-1) TS

E(UB3LYP/6-31G(d,p))= -5450.10803726

i532.11

	x	y	z
C	-3.32253	0.521657	-2.66347
H	-2.93232	1.530203	-2.62456
C	-3.99727	0.051936	-3.78996
H	-4.14386	0.709308	-4.63958
C	-4.4774	-1.25634	-3.79743
H	-5.01745	-1.64506	-4.65461
C	-4.24747	-2.06427	-2.68395
H	-4.60041	-3.0898	-2.6688
C	-3.56195	-1.52783	-1.59587
C	-3.21577	-2.23389	-0.37551
C	-2.33083	-2.50894	1.609656
C	-1.67696	-2.40468	2.846336
H	-1.19003	-1.48596	3.144443
C	-1.68009	-3.52274	3.670214
H	-1.197	-3.47048	4.640361
C	-2.30789	-4.7296	3.289163
H	-2.29663	-5.5719	3.972688
C	-2.94573	-4.85935	2.062378
H	-3.4307	-5.78452	1.769533
C	-2.94111	-3.73213	1.237297
C	-5.0681	-0.1022	1.546997
H	-4.70378	-1.10444	1.732873
C	-6.33537	0.281878	1.984789
H	-6.96317	-0.43199	2.506075
C	-6.76814	1.584227	1.743351
H	-7.7501	1.913609	2.067039
C	-5.91086	2.464351	1.083745
H	-6.21924	3.486813	0.893659
C	-4.65694	2.0063	0.681032
C	-3.64497	2.809421	0.017658
C	-1.70629	3.263678	-0.89608
C	-0.40517	3.257574	-1.41755
H	0.201168	2.363323	-1.36656
C	0.058216	4.445509	-1.96847
H	1.064546	4.488626	-2.37259
C	-0.73517	5.61372	-2.01402
H	-0.32754	6.516058	-2.45704
C	-2.02589	5.635152	-1.5027
H	-2.63614	6.531238	-1.53668
C	-2.49069	4.441498	-0.94609

N	-3.12202	-0.24045	-1.57763
N	-2.53584	-1.5932	0.579221
N	-3.48118	-3.51346	-0.02379
N	-4.23855	0.729597	0.896283
N	-2.46459	2.265529	-0.28801
N	-3.70313	4.109536	-0.35804
Fe	-2.2572	0.32714	0.152958
H	-4.49076	4.733001	-0.23962
H	-3.99756	-4.19066	-0.56931
O	-0.75163	0.080561	-0.5867
N	-1.62208	0.864344	1.916653
C	-1.35062	1.297967	2.952667
C	-1.00582	1.841771	4.258452
H	-0.02764	2.328953	4.209647
H	-1.75582	2.576413	4.566606
H	-0.97406	1.04186	5.004042
O	0.797861	0.565076	0.293776
Fe	2.261226	-0.08557	-0.25151
N	2.796639	-1.24179	1.662656
N	1.606772	-1.99058	-0.62915
N	3.292409	1.502538	0.420786
N	2.1832	0.705652	-2.35384
C	3.35497	-0.7889	2.791994
C	2.567798	-2.5692	1.539627
C	1.931044	-2.92043	0.272869
C	1.010994	-2.65833	-1.69837
C	4.617311	1.427666	0.229297
C	3.051225	2.695411	1.102017
C	2.336151	1.1661	-3.4069
H	3.509221	0.283209	2.85633
C	3.728405	-1.63334	3.83915
C	2.913609	-3.48242	2.537283
N	1.594364	-4.16149	-0.15757
C	0.468817	-2.19165	-2.90446
C	1.015421	-4.04391	-1.41364
C	5.181	0.28813	-0.47619
N	5.249827	2.500846	0.750675
C	1.8635	3.290796	1.547456
C	4.293628	3.336663	1.317826
C	2.527694	1.734102	-4.73417
H	4.184881	-1.22224	4.732699
C	3.510222	-3.00353	3.704219
H	2.732108	-4.54521	2.41768
H	1.759867	-5.02818	0.335718
H	0.434135	-1.1328	-3.12388
C	-0.02078	-3.14039	-3.79361

C	0.523859	-5.00139	-2.30449
C	6.530275	0.11209	-0.77808
N	4.227814	-0.60954	-0.84939
H	6.245959	2.678653	0.729672
H	0.908662	2.818049	1.357513
C	1.974509	4.512487	2.200646
C	4.408934	4.56281	1.976088
H	1.716533	2.430239	-4.96571
H	3.480209	2.270694	-4.77714
H	2.539246	0.936231	-5.48283
H	3.798724	-3.69102	4.49275
H	-0.43128	-2.81677	-4.74454
C	0.012175	-4.52288	-3.50401
H	0.552513	-6.0629	-2.08237
C	6.915694	-1.01953	-1.49799
H	7.272184	0.839919	-0.46747
C	4.608075	-1.68528	-1.55684
H	1.078103	5.015415	2.548725
C	3.223416	5.137336	2.415733
H	5.367365	5.045238	2.134831
H	-0.36415	-5.22753	-4.23809
C	5.937917	-1.92806	-1.89935
H	7.95976	-1.18125	-1.74595
H	3.823032	-2.36568	-1.86315
H	3.257411	6.091382	2.930687
H	6.193462	-2.81256	-2.47195

Fe_2O_2 S=2(5,-1) TS

no TS located

Fe_2O_2 S=1(5,-3) TS

no TS located

Fe_2O_2 S=0(3,-3) TS

E(UB3LYP/6-31G(d,p))= -5450.09931213

i601.22

	x	**y**	**z**
C	3.406797	-0.8022	2.76371

H	3.631941	0.259037	2.778289
C	3.752699	-1.62592	3.836532
H	4.260569	-1.20971	4.699454
C	3.440296	-2.9826	3.766755
H	3.70472	-3.65459	4.576807
C	2.780495	-3.46823	2.637175
H	2.525591	-4.52034	2.567967
C	2.469153	-2.57624	1.609517
C	1.77742	-2.93592	0.374653
C	0.833116	-2.69506	-1.58803
C	0.299342	-2.24436	-2.80372
H	0.335844	-1.19692	-3.07174
C	-0.2776	-3.19327	-3.63854
H	-0.68454	-2.88304	-4.5954
C	-0.33777	-4.56013	-3.28593
H	-0.77889	-5.2677	-3.98009
C	0.165612	-5.02083	-2.07591
H	0.12498	-6.0709	-1.80638
C	0.744985	-4.06312	-1.23985
C	4.47875	-1.90881	-1.5904
H	3.65115	-2.56177	-1.83854
C	5.781104	-2.22626	-1.97455
H	5.972682	-3.14282	-2.52107
C	6.814735	-1.35009	-1.64765
H	7.83937	-1.56999	-1.92958
C	6.511187	-0.17561	-0.95798
H	7.297546	0.527335	-0.70471
C	5.184968	0.075004	-0.61049
C	4.702913	1.262268	0.075779
C	3.233414	2.621168	0.981728
C	2.096424	3.272739	1.477652
H	1.115407	2.829561	1.365757
C	2.291507	4.503319	2.092635
H	1.436625	5.045253	2.483577
C	3.573153	5.083772	2.221078
H	3.672365	6.047218	2.709418
C	4.709911	4.451213	1.734443
H	5.694116	4.896786	1.83094
C	4.510608	3.215065	1.116828
N	2.788818	-1.26339	1.669265
N	1.499486	-2.02566	-0.56236
N	1.344313	-4.16689	0.00758
N	4.177546	-0.79043	-0.91134
N	3.392194	1.400579	0.324827
N	5.402902	2.322775	0.531671
Fe	2.267503	-0.14921	-0.26999

H	6.403754	2.45586	0.461415
H	1.452182	-5.01933	0.539964
O	0.847811	0.601332	0.284583
N	2.160961	0.590776	-2.39127
C	2.293992	1.022508	-3.45909
C	2.460303	1.553563	-4.80491
H	1.658734	2.262419	-5.03111
H	3.423095	2.066603	-4.88787
H	2.432479	0.737574	-5.53334
O	-0.69589	0.113276	-0.53764
Fe	-2.15666	0.435756	0.234185
N	-3.24902	-0.08899	-1.66919
N	-2.61658	-1.58662	0.475092
N	-4.07614	0.911996	1.030858
N	-2.29571	2.424512	-0.20158
N	-1.48172	0.832074	2.271378
C	-3.51382	0.709937	-2.71063
C	-3.72912	-1.35395	-1.68371
C	-3.34204	-2.12657	-0.50662
C	-2.41035	-2.59128	1.4199
C	-4.90028	0.095752	1.70801
C	-4.46823	2.200988	0.833814
C	-3.46309	2.986246	0.137773
C	-1.55081	3.41016	-0.8479
C	-1.2809	1.22275	3.343551
H	-3.09647	1.710186	-2.66869
C	-4.28099	0.296291	-3.80073
C	-4.50952	-1.84348	-2.73266
N	-3.63423	-3.42499	-0.24685
C	-1.72031	-2.59633	2.640901
C	-3.06556	-3.76305	0.973248
H	-4.55141	-0.91523	1.873947
C	-6.14157	0.509534	2.190854
C	-5.69608	2.685324	1.282333
N	-3.51912	4.280181	-0.24825
C	-0.26746	3.384949	-1.40811
C	-2.32235	4.595674	-0.88151
C	-1.0355	1.707691	4.69463
H	-4.47325	0.980508	-4.61961
C	-4.79334	-0.99992	-3.8068
H	-4.89961	-2.85557	-2.7201
H	-4.18111	-4.04203	-0.83188
H	-1.20764	-1.71119	2.995544
C	-1.72859	-3.77578	3.375723
C	-3.07655	-4.95087	1.70841
H	-6.76797	-0.19154	2.730892

C	-6.55097	1.82258	1.96831
H	-5.98621	3.71594	1.108386
H	-4.29503	4.914673	-0.1093
H	0.331711	2.484791	-1.36696
C	0.190997	4.563228	-1.98478
C	-1.86453	5.780061	-1.46178
H	-1.77515	2.469493	4.958251
H	-1.11497	0.881812	5.4079
H	-0.03501	2.144052	4.761246
H	-5.40371	-1.35159	-4.63223
H	-1.21999	-3.8103	4.333672
C	-2.39845	-4.93322	2.920955
H	-3.59693	-5.83761	1.362284
H	-7.51304	2.174098	2.326703
H	1.183798	4.591991	-2.42199
C	-0.59095	5.739277	-2.01489
H	-2.46469	6.683326	-1.48221
H	-2.39156	-5.82625	3.53691
H	-0.18775	6.633252	-2.47839

Fe_2O_2 S=3(3,3) TS

E(UB3LYP/6-31G(d,p))= -5450.09047570

i462.25

	x	**y**	**z**
C	3.37444	-0.84693	2.843728
H	3.662448	0.199154	2.845873
C	3.639831	-1.66872	3.940914
H	4.148102	-1.26721	4.810557
C	3.248921	-3.00566	3.886173
H	3.448988	-3.67572	4.716032
C	2.596808	-3.47465	2.745071
H	2.281893	-4.51112	2.686968
C	2.372312	-2.58589	1.692241
C	1.716084	-2.93178	0.434738
C	0.905766	-2.6855	-1.58956
C	0.465277	-2.23221	-2.84097
H	0.551176	-1.18936	-3.11643
C	-0.07551	-3.17543	-3.70602
H	-0.40874	-2.86471	-4.69078
C	-0.19279	-4.53683	-3.34739
H	-0.60441	-5.23987	-4.06387
C	0.217278	-4.99851	-2.10285

H	0.132796	-6.04476	-1.82872
C	0.76231	-4.04734	-1.23703
C	4.471279	-1.98843	-1.574
H	3.632808	-2.63364	-1.80444
C	5.76122	-2.31851	-1.98718
H	5.931617	-3.23739	-2.53673
C	6.81055	-1.45294	-1.6827
H	7.82651	-1.68299	-1.98698
C	6.534111	-0.27708	-0.98465
H	7.332622	0.417468	-0.7468
C	5.218716	-0.01342	-0.60701
C	4.766237	1.174054	0.097623
C	3.33331	2.52554	1.062255
C	2.210394	3.180842	1.586338
H	1.221632	2.753622	1.475122
C	2.428075	4.395009	2.224869
H	1.585547	4.939193	2.638945
C	3.718887	4.956926	2.347859
H	3.836454	5.908056	2.85587
C	4.840737	4.323037	1.830107
H	5.83091	4.756457	1.920568
C	4.619437	3.102606	1.188292
N	2.764043	-1.29207	1.738594
N	1.514398	-2.0222	-0.52403
N	1.279563	-4.15463	0.04687
N	4.195552	-0.86779	-0.88746
N	3.465294	1.322008	0.372949
N	5.490496	2.214864	0.567883
Fe	2.297711	-0.19634	-0.22777
H	6.492623	2.331857	0.492002
H	1.354548	-5.00902	0.581752
O	0.858998	0.651696	0.219305
N	2.294985	0.624919	-2.42316
C	2.498596	1.073496	-3.47339
C	2.756155	1.624366	-4.79804
H	1.912501	2.241092	-5.12032
H	3.659229	2.241368	-4.77867
H	2.899181	0.81347	-5.51835
O	-0.76987	0.065305	-0.53535
Fe	-2.20527	0.447425	0.199963
N	-3.32849	-0.02178	-1.70063
N	-2.74019	-1.54804	0.433688
N	-4.11613	0.985987	0.987582
N	-2.26225	2.429075	-0.2243
N	-1.54529	0.814406	2.25107
C	-3.5599	0.789109	-2.74084

C	-3.84506	-1.27239	-1.72377
C	-3.48791	-2.05959	-0.54755
C	-2.57017	-2.55915	1.379366
C	-4.9777	0.199277	1.652997
C	-4.45199	2.291342	0.796108
C	-3.41046	3.03625	0.110801
C	-1.47412	3.387002	-0.86415
C	-1.31335	1.200999	3.318351
H	-3.11282	1.776059	-2.69271
C	-4.32982	0.401745	-3.83861
C	-4.63018	-1.73478	-2.78122
N	-3.82977	-3.34462	-0.28547
C	-1.87898	-2.59171	2.599159
C	-3.27191	-3.7041	0.93364
H	-4.67168	-0.8261	1.815004
C	-6.20414	0.661545	2.12959
C	-5.66165	2.823719	1.239684
N	-3.41182	4.33091	-0.27188
C	-0.19002	3.314765	-1.41801
C	-2.20015	4.601099	-0.89802
C	-1.02963	1.681172	4.66333
H	-4.49391	1.093968	-4.65687
C	-4.87957	-0.87897	-3.8543
H	-5.04746	-2.73604	-2.7774
H	-4.40096	-3.94078	-0.86921
H	-1.33151	-1.72786	2.953928
C	-1.9327	-3.77028	3.333368
C	-3.32836	-4.8909	1.668274
H	-6.86338	-0.01611	2.660393
C	-6.55648	1.992297	1.913397
H	-5.9072	3.866778	1.071455
H	-4.16283	4.995417	-0.13512
H	0.377809	2.394738	-1.37363
C	0.313909	4.477358	-1.98865
C	-1.696	5.769489	-1.4717
H	-1.74791	2.458087	4.94171
H	-1.11077	0.857391	5.378856
H	-0.01912	2.096947	4.707247
H	-5.49153	-1.20996	-4.68707
H	-1.42416	-3.82509	4.290395
C	-2.64817	-4.90051	2.879552
H	-3.8829	-5.75658	1.321882
H	-7.5057	2.381112	2.267608
H	1.308993	4.46877	-2.42122
C	-0.42233	5.682339	-2.01907
H	-2.26209	6.694497	-1.49134

H	-2.67463	-5.79365	3.494763
H	0.016552	6.561885	-2.47777

^{3}Fe(IV)O

E(UB3LYP/6-31G(d,p))= -2725.17601797

no imaginary frequencies

	x	**y**	**z**
C	0.987612	2.73096	-0.12741
H	1.964104	2.266777	-0.09722
C	0.847824	4.117098	-0.10487
H	1.731086	4.742117	-0.04317
C	-0.42881	4.670555	-0.17346
H	-0.56845	5.746279	-0.16194
C	-1.52907	3.820022	-0.26719
H	-2.53316	4.224512	-0.33065
C	-1.31472	2.443538	-0.28582
C	-2.34138	1.425708	-0.40557
C	-3.15794	-0.60129	-0.54385
C	-3.40061	-1.9814	-0.58848
H	-2.59319	-2.69513	-0.50368
C	-4.71481	-2.39706	-0.7464
H	-4.93461	-3.45846	-0.7882
C	-5.78043	-1.47652	-0.85574
H	-6.7911	-1.84973	-0.98012
C	-5.56378	-0.10666	-0.80594
H	-6.38064	0.602163	-0.88675
C	-4.23967	0.307059	-0.64815
C	-0.98878	-0.35369	2.595033
H	-1.97639	-0.27391	2.156008
C	-0.82247	-0.51046	3.970628
H	-1.69108	-0.54717	4.617954
C	0.46866	-0.61897	4.48403
H	0.632778	-0.73987	5.549653
C	1.552443	-0.57369	3.607873
H	2.566253	-0.6589	3.983846
C	1.304667	-0.41708	2.24459
C	2.315453	-0.36783	1.200003
C	3.082489	-0.21291	-0.85115
C	3.26273	-0.08134	-2.23585
H	2.414785	0.054117	-2.89617
C	4.566866	-0.13694	-2.70655
H	4.7504	-0.04054	-3.77127

C	5.668216	-0.31644	-1.83826
H	6.668397	-0.35283	-2.25651
C	5.505148	-0.44752	-0.46521
H	6.352287	-0.58491	0.197901
C	4.192733	-0.39259	0.009215
N	-0.06717	1.90606	-0.2038
N	-1.98801	0.139014	-0.38899
N	-3.67826	1.57286	-0.55305
N	0.045169	-0.30208	1.743478
N	1.935181	-0.19699	-0.0659
N	3.664008	-0.48553	1.291872
Fe	-0.01039	-0.09119	-0.40271
H	4.196142	-0.62324	2.139649
H	-4.18172	2.446674	-0.61741
O	0.122323	0.048301	-2.01032
N	-0.01059	-2.05668	-0.52743
C	0.130001	-3.17801	-0.76727
C	0.291355	-4.58903	-1.08289
H	1.347744	-4.80896	-1.26209
H	-0.06768	-5.20447	-0.25313
H	-0.279	-4.82985	-1.98498

^{3}Fe(IV)O+HOOH

E(UB3LYP/6-31G(d,p))= -2876.73647918

no imaginary frequencies

	x	**y**	**z**
C	0.979123	2.341128	1.299773
H	1.97932	2.003254	1.065047
C	0.762244	3.531699	1.987849
H	1.610296	4.126091	2.307314
C	-0.54653	3.937844	2.243914
H	-0.74508	4.862387	2.775532
C	-1.60022	3.143598	1.799233
H	-2.62801	3.438723	1.975619
C	-1.31069	1.964548	1.116722
C	-2.28136	1.032751	0.577573
C	-2.98094	-0.79159	-0.41061
C	-3.14848	-2.038	-1.02892
H	-2.30253	-2.67413	-1.24991
C	-4.44261	-2.43124	-1.34058
H	-4.60491	-3.38923	-1.82294
C	-5.55957	-1.62037	-1.04385

H	-6.55172	-1.96909	-1.30884
C	-5.41653	-0.39222	-0.41362
H	-6.27328	0.228339	-0.17502
C	-4.11358	0.000537	-0.10384
C	-0.50603	-1.79752	2.333722
H	-1.53807	-1.61446	2.059115
C	-0.18004	-2.55799	3.456388
H	-0.96899	-2.97182	4.073754
C	1.163627	-2.77093	3.758698
H	1.450353	-3.35697	4.625557
C	2.140589	-2.22193	2.928594
H	3.192786	-2.37583	3.142152
C	1.736182	-1.47407	1.823786
C	2.619193	-0.84519	0.854658
C	3.139458	0.326062	-0.92754
C	3.155568	1.105786	-2.09297
H	2.232328	1.448316	-2.54361
C	4.399102	1.406817	-2.62988
H	4.456117	2.007008	-3.53163
C	5.59938	0.953718	-2.0358
H	6.546405	1.217002	-2.49451
C	5.599351	0.181555	-0.88142
H	6.521889	-0.16413	-0.42793
C	4.347844	-0.12262	-0.34141
N	-0.03227	1.563776	0.882694
N	-1.85039	-0.11072	0.037268
N	-3.62489	1.129005	0.536652
N	0.424682	-1.26035	1.532333
N	2.089298	-0.14162	-0.14557
N	3.97349	-0.85639	0.778773
Fe	0.10999	-0.08737	-0.23961
H	4.604477	-1.32025	1.417237
H	-4.1585	1.960086	0.750572
O	0.043133	0.801089	-1.59878
N	0.198111	-1.76064	-1.27904
C	0.356993	-2.6211	-2.03326
C	0.537923	-3.69946	-2.99279
H	1.524471	-3.61728	-3.45809
H	0.456719	-4.66791	-2.49113
H	-0.22849	-3.62998	-3.77047
O	-2.37373	3.331924	-1.4612
H	-2.60388	3.969757	-2.15753
O	-2.45311	2.083427	-2.20247
H	-1.50798	1.837896	-2.2592

^{3}Fe(IV)O+HOOH_TS

E(UB3LYP/6-31G(d,p))= -2876.72033650

i1826.54

	x	y	z
C	0.936521	2.327926	1.225324
H	1.927952	1.963504	0.99237
C	0.750447	3.529577	1.903269
H	1.613393	4.106843	2.214106
C	-0.54666	3.970073	2.158702
H	-0.72197	4.903426	2.682978
C	-1.62036	3.198102	1.72103
H	-2.64008	3.522247	1.896149
C	-1.35939	2.009185	1.045089
C	-2.34897	1.108195	0.489807
C	-3.07828	-0.65883	-0.57859
C	-3.26136	-1.86496	-1.26841
H	-2.42113	-2.48907	-1.53858
C	-4.5609	-2.2275	-1.59464
H	-4.7345	-3.15315	-2.13287
C	-5.6683	-1.42433	-1.24645
H	-6.66524	-1.74798	-1.52495
C	-5.50978	-0.23114	-0.55482
H	-6.35896	0.386619	-0.28375
C	-4.20113	0.130397	-0.2312
C	-0.80229	-1.6861	2.306767
H	-1.80677	-1.46859	1.964795
C	-0.58004	-2.41876	3.47155
H	-1.42325	-2.77377	4.052709
C	0.731619	-2.681	3.862939
H	0.938001	-3.24662	4.765466
C	1.780355	-2.20881	3.075181
H	2.809623	-2.40252	3.356972
C	1.479733	-1.4854	1.92177
C	2.448345	-0.94001	0.985839
C	3.126927	0.118608	-0.80938
C	3.249816	0.837327	-2.0077
H	2.369991	1.195404	-2.52695
C	4.535249	1.050872	-2.48394
H	4.674146	1.600636	-3.40871
C	5.675539	0.570565	-1.79968
H	6.659241	0.765	-2.21341
C	5.570613	-0.1446	-0.61393
H	6.44709	-0.51335	-0.09234
C	4.276572	-0.36138	-0.13519

N	-0.09269	1.570702	0.814277
N	-1.9362	-0.01418	-0.10355
N	-3.69317	1.229934	0.448172
N	0.198512	-1.22121	1.544077
N	2.011207	-0.25769	-0.07111
N	3.803107	-1.02306	0.991653
Fe	0.033922	-0.1164	-0.24646
H	4.372255	-1.4877	1.685058
H	-4.23146	2.018029	0.779867
O	0.11044	0.734045	-1.71202
N	0.127278	-1.82073	-1.23799
C	0.309104	-2.71476	-1.94672
C	0.523266	-3.83392	-2.85165
H	1.587274	-3.91812	-3.0906
H	0.185384	-4.76452	-2.38694
H	-0.03629	-3.66868	-3.77712
O	-0.72971	3.696231	-1.74716
H	-0.48375	3.980749	-2.64771
O	-1.4268	2.508769	-1.96658
H	-0.64064	1.643065	-1.92126

^{2}Fe(III)OH+OOH

E(UB3LYP/6-31G(d,p))=-2876.74427016

no imaginary frequencies

	x	**y**	**z**
C	0.901331	1.872984	1.897801
H	1.897841	1.629518	1.553422
C	0.69563	2.804517	2.913124
H	1.54802	3.288086	3.37601
C	-0.60782	3.100299	3.308155
H	-0.79853	3.820562	4.096631
C	-1.668	2.462659	2.667264
H	-2.69274	2.681313	2.946823
C	-1.38602	1.544575	1.657376
C	-2.35979	0.81993	0.864579
C	-3.05353	-0.55684	-0.6863
C	-3.20554	-1.49124	-1.7205
H	-2.34524	-1.94003	-2.19716
C	-4.49799	-1.81248	-2.10938
H	-4.64973	-2.52947	-2.90909
C	-5.62782	-1.23	-1.49376
H	-6.61873	-1.51171	-1.833

C	-5.49988	-0.30645	-0.46521
H	-6.36681	0.140299	0.009243
C	-4.19754	0.014606	-0.07776
C	-0.73911	-2.34797	1.729011
H	-1.75006	-2.06247	1.464496
C	-0.49828	-3.39539	2.616247
H	-1.33199	-3.93003	3.056477
C	0.819945	-3.73378	2.916806
H	1.041715	-4.54211	3.605592
C	1.854695	-3.02046	2.31465
H	2.889	-3.26735	2.528175
C	1.535446	-1.98787	1.433261
C	2.490855	-1.16762	0.708306
C	3.139961	0.385312	-0.69243
C	3.239679	1.427958	-1.62621
H	2.344766	1.89818	-2.01398
C	4.517986	1.797474	-2.01865
H	4.640749	2.597723	-2.74073
C	5.671736	1.159463	-1.50739
H	6.648917	1.486469	-1.84648
C	5.588984	0.12395	-0.58549
H	6.476034	-0.36472	-0.1974
C	4.302523	-0.25055	-0.19096
N	-0.11231	1.241691	1.284633
N	-1.92298	-0.03031	-0.06614
N	-3.71274	0.876412	0.897004
N	0.247392	-1.64867	1.147952
N	2.035497	-0.21183	-0.09793
N	3.848134	-1.22473	0.689907
Fe	0.054431	-0.06931	-0.21897
H	4.429048	-1.86454	1.212673
H	-4.2737	1.462876	1.498529
O	0.121174	1.238517	-1.41006
N	0.194924	-1.35143	-1.70536
C	0.405976	-1.94636	-2.67292
C	0.660395	-2.68294	-3.90207
H	1.730213	-2.66589	-4.12865
H	0.333703	-3.72113	-3.79566
H	0.116093	-2.21614	-4.72817
O	-1.18177	4.294532	-2.11168
H	-1.7361	5.104877	-2.15702
O	-1.61813	3.623637	-1.05419
H	-0.46646	1.993712	-1.21576

^{2}Fe(III)OH

E(UB3LYP/6-31G(d,p))= -2725.82424075

no imaginary frequencies

	x	y	z
C	-1.39266	-2.73946	0.41283
H	-2.30125	-2.16387	0.296154
C	-1.43362	-4.07035	0.826596
H	-2.38856	-4.53244	1.0485
C	-0.24195	-4.78247	0.936468
H	-0.2423	-5.82073	1.250615
C	0.956754	-4.1406	0.629186
H	1.899136	-4.67256	0.699753
C	0.917735	-2.80832	0.224985
C	2.067144	-1.99767	-0.13369
C	3.141402	-0.19423	-0.76174
C	3.56065	1.089895	-1.13576
H	2.852343	1.898469	-1.25885
C	4.920832	1.289797	-1.33104
H	5.277168	2.272208	-1.62197
C	5.858681	0.249494	-1.15698
H	6.911101	0.452586	-1.32235
C	5.465311	-1.02542	-0.77191
H	6.18548	-1.82365	-0.62889
C	4.097277	-1.2213	-0.5771
C	0.922779	0.927115	1.980696
H	1.887688	0.544386	1.673067
C	0.776579	1.627858	3.177049
H	1.638815	1.785246	3.814676
C	-0.48195	2.112425	3.52715
H	-0.62865	2.660208	4.451989
C	-1.55503	1.883782	2.667498
H	-2.54543	2.250426	2.914558
C	-1.33173	1.174638	1.488381
C	-2.33534	0.851842	0.489742
C	-3.10503	-0.036	-1.36084
C	-3.30185	-0.71662	-2.57149
H	-2.48194	-1.23504	-3.05255
C	-4.58618	-0.70904	-3.09658
H	-4.78017	-1.22578	-4.03044
C	-5.6554	-0.0516	-2.44632
H	-6.64147	-0.07507	-2.89766
C	-5.47904	0.617303	-1.24198
H	-6.30285	1.114581	-0.74165
C	-4.18635	0.610057	-0.71341

N	-0.24504	-2.11101	0.125204
N	1.882036	-0.7201	-0.47492
N	3.374267	-2.33931	-0.17973
N	-0.10289	0.695493	1.146937
N	-1.97026	0.142233	-0.57654
N	-3.65708	1.155886	0.450251
Fe	-0.03598	-0.28917	-0.69733
H	-4.17286	1.678671	1.144018
H	3.760911	-3.2519	0.017422
O	-0.15461	-1.15399	-2.24883
N	0.211612	1.407587	-1.62271
C	0.256401	2.372345	-2.25921
C	0.32479	3.583904	-3.06298
H	-0.61376	3.720661	-3.60802
H	0.493197	4.451548	-2.41856
H	1.145548	3.506309	-3.78217
H	-0.08127	-0.5625	-3.01334

^{5}Fe(IV)O

E(UB3LYP/6-31G(d,p))= -2725.17080986

no imaginary frequencies

	x	**y**	**z**
C	0.894881	2.916164	-0.00451
H	1.890412	2.490939	0.057864
C	0.698714	4.296859	0.010547
H	1.549218	4.963394	0.095458
C	-0.60054	4.789241	-0.09415
H	-0.79008	5.857407	-0.08905
C	-1.65946	3.889971	-0.21252
H	-2.67711	4.254843	-0.29823
C	-1.37974	2.522951	-0.22186
C	-2.37997	1.46918	-0.35674
C	-3.21287	-0.55135	-0.50186
C	-3.45633	-1.931	-0.54301
H	-2.64918	-2.64498	-0.44626
C	-4.77073	-2.34313	-0.71399
H	-4.99419	-3.4039	-0.75323
C	-5.8313	-1.41926	-0.83899
H	-6.84192	-1.78944	-0.97259
C	-5.61114	-0.04922	-0.79242
H	-6.42538	0.661266	-0.88426
C	-4.2875	0.360297	-0.62142

C	-0.93078	-0.5567	2.563981
H	-1.91816	-0.49252	2.122657
C	-0.76084	-0.76144	3.93314
H	-1.62916	-0.85353	4.575282
C	0.53169	-0.84474	4.446177
H	0.697836	-1.00167	5.506777
C	1.61599	-0.72724	3.576233
H	2.630884	-0.79259	3.953144
C	1.367199	-0.52625	2.219945
C	2.381496	-0.39974	1.183372
C	3.16121	-0.13302	-0.85434
C	3.34709	0.06108	-2.22909
H	2.501067	0.18718	-2.89397
C	4.65783	0.080212	-2.68732
H	4.847308	0.227427	-3.74515
C	5.756937	-0.08755	-1.81497
H	6.761663	-0.06477	-2.22308
C	5.586772	-0.28118	-0.44938
H	6.432756	-0.40973	0.216904
C	4.268685	-0.30015	0.009748
N	-0.11763	2.047593	-0.10981
N	-2.03737	0.17946	-0.33144
N	-3.71598	1.620792	-0.52248
N	0.104151	-0.43591	1.720688
N	2.00419	-0.19857	-0.08365
N	3.728849	-0.46514	1.283379
Fe	0.016496	-0.1574	-0.40412
H	4.259078	-0.61577	2.130802
H	-4.21293	2.497927	-0.5886
O	0.119573	0.008125	-2.00136
N	-0.04214	-2.35039	-0.55505
C	0.109978	-3.42919	-0.94907
C	0.287869	-4.78497	-1.44611
H	1.344943	-4.96332	-1.66342
H	-0.05117	-5.5071	-0.69797
H	-0.29075	-4.91751	-2.36505

^{5}Fe(IV)O+HOOH

E(UB3LYP/6-31G(d,p))= -2876.72970981

no imaginary frequencies

	x	**y**	**z**
C	0.869487	2.633098	1.123956

H	1.892246	2.305948	0.973311
C	0.584214	3.893871	1.644462
H	1.392603	4.563257	1.915077
C	-0.75003	4.267671	1.799355
H	-1.00798	5.241672	2.201519
C	-1.75314	3.376001	1.426256
H	-2.79678	3.646171	1.538852
C	-1.38595	2.133831	0.908632
C	-2.32054	1.103978	0.470414
C	-3.02356	-0.83463	-0.26802
C	-3.1836	-2.15446	-0.70938
H	-2.33433	-2.81502	-0.8251
C	-4.47448	-2.5831	-0.9892
H	-4.63367	-3.59868	-1.33572
C	-5.5913	-1.73451	-0.83192
H	-6.58052	-2.11357	-1.06429
C	-5.45301	-0.42911	-0.37933
H	-6.31072	0.221355	-0.24792
C	-4.15391	-0.00207	-0.10167
C	-0.43896	-1.57542	2.49148
H	-1.47108	-1.45819	2.1841
C	-0.10424	-2.18368	3.701403
H	-0.88875	-2.54642	4.355458
C	1.240282	-2.31243	4.042096
H	1.532784	-2.7796	4.976597
C	2.212329	-1.83391	3.162921
H	3.265249	-1.92549	3.406493
C	1.802169	-1.2393	1.971618
C	2.682157	-0.69958	0.945817
C	3.203838	0.271116	-0.9559
C	3.218983	0.905718	-2.2043
H	2.295953	1.156583	-2.71253
C	4.464563	1.189407	-2.74868
H	4.521974	1.679799	-3.7145
C	5.664778	0.857742	-2.08069
H	6.61267	1.101502	-2.54823
C	5.664507	0.227925	-0.84188
H	6.58759	-0.02551	-0.33214
C	4.411566	-0.05729	-0.29673
N	-0.09089	1.769132	0.771781
N	-1.89226	-0.11017	0.109482
N	-3.66332	1.200217	0.383352
N	0.487745	-1.10839	1.643025
N	2.149498	-0.14238	-0.14711
N	4.033224	-0.66743	0.897186
Fe	0.138136	-0.18457	-0.25177

H	4.665489	-1.02794	1.598807
H	-4.19217	2.056606	0.470694
O	0.035197	0.493278	-1.71595
N	0.216122	-2.21937	-1.10111
C	0.381285	-3.10649	-1.82764
C	0.574711	-4.22286	-2.74052
H	1.558743	-4.14829	-3.21227
H	0.507905	-5.16919	-2.19642
H	-0.19438	-4.19839	-3.51814
O	-2.38659	3.113821	-1.88664
H	-2.63721	3.647775	-2.6593
O	-2.47158	1.774659	-2.44586
H	-1.52717	1.529797	-2.49265

^{5}Fe(IV)O+HOOH_TS

E(UB3LYP/6-31G(d,p))= -2876.71239662

i1876.80

	x	**y**	**z**
C	0.858235	2.671741	1.168279
H	1.877967	2.315064	1.070865
C	0.586156	3.957477	1.634401
H	1.400111	4.615889	1.91521
C	-0.74244	4.369729	1.721586
H	-0.99107	5.363914	2.077576
C	-1.75327	3.489131	1.340081
H	-2.79249	3.793262	1.397872
C	-1.39664	2.219773	0.883587
C	-2.33868	1.198637	0.439479
C	-3.06002	-0.72537	-0.3229
C	-3.229	-2.03624	-0.78847
H	-2.38244	-2.69576	-0.92534
C	-4.52365	-2.45391	-1.06582
H	-4.68971	-3.46198	-1.43049
C	-5.63588	-1.6036	-0.88513
H	-6.62844	-1.9744	-1.11659
C	-5.48863	-0.30575	-0.41414
H	-6.34226	0.347271	-0.26908
C	-4.18515	0.110323	-0.13933
C	-0.57745	-1.51994	2.50474
H	-1.60048	-1.3843	2.175369
C	-0.28029	-2.12624	3.724663
H	-1.08505	-2.4675	4.365468

C	1.054481	-2.28137	4.092867
H	1.317793	-2.74763	5.03647
C	2.054443	-1.83203	3.229958
H	3.099972	-1.94613	3.494767
C	1.682334	-1.23814	2.025982
C	2.592049	-0.73019	1.010516
C	3.165661	0.20133	-0.89408
C	3.216659	0.813729	-2.15301
H	2.305505	1.067682	-2.67976
C	4.477071	1.064941	-2.67799
H	4.562262	1.536902	-3.65097
C	5.658581	0.722404	-1.98213
H	6.619432	0.940561	-2.43574
C	5.623432	0.112502	-0.73424
H	6.531866	-0.15081	-0.20359
C	4.355241	-0.14025	-0.20812
N	-0.10713	1.818327	0.807894
N	-1.92241	-0.01262	0.056568
N	-3.68275	1.306355	0.350399
N	0.376655	-1.07965	1.671723
N	2.08928	-0.17906	-0.09917
N	3.944744	-0.72489	0.987387
Fe	0.091344	-0.18502	-0.19666
H	4.557286	-1.08632	1.705657
H	-4.22525	2.13633	0.543214
O	0.0718	0.495424	-1.74528
N	0.159289	-2.28128	-1.02791
C	0.364941	-3.16912	-1.74377
C	0.609883	-4.28588	-2.6446
H	1.615068	-4.20619	-3.06822
H	0.522678	-5.23184	-2.10284
H	-0.12024	-4.26864	-3.45896
O	-1.67733	2.896449	-2.45318
H	-1.37395	3.118526	-3.3541
O	-1.91476	1.527241	-2.52065
H	-0.92338	1.011283	-2.1836

^{4}Fe(III)OH+OOH

E(UB3LYP/6-31G(d,p))= -2876.73688683

no imaginary frequencies

	x	**y**	**z**
C	0.979422	2.580359	1.443164

H	1.994717	2.242201	1.265494
C	0.727185	3.810665	2.05185
H	1.552147	4.44111	2.363285
C	-0.59589	4.204337	2.241106
H	-0.82941	5.155586	2.707561
C	-1.62208	3.36149	1.815331
H	-2.65805	3.656832	1.941546
C	-1.28194	2.147026	1.218008
C	-2.2423	1.171826	0.710916
C	-2.99325	-0.65443	-0.24458
C	-3.17359	-1.88196	-0.8962
H	-2.32716	-2.45896	-1.24532
C	-4.4784	-2.3223	-1.07481
H	-4.65559	-3.26805	-1.57579
C	-5.58647	-1.5731	-0.62288
H	-6.58725	-1.95745	-0.7874
C	-5.42534	-0.35696	0.028033
H	-6.27575	0.218975	0.376318
C	-4.11237	0.082341	0.205662
C	-0.50175	-1.91971	2.201495
H	-1.53056	-1.73651	1.916132
C	-0.18732	-2.73875	3.284403
H	-0.98252	-3.19755	3.860414
C	1.153028	-2.94953	3.602682
H	1.430392	-3.57999	4.440959
C	2.139171	-2.3423	2.82577
H	3.188682	-2.49765	3.050737
C	1.750042	-1.53812	1.756409
C	2.644779	-0.85071	0.839615
C	3.182882	0.424767	-0.86124
C	3.209167	1.25624	-1.98962
H	2.285622	1.570063	-2.45899
C	4.458896	1.634107	-2.46
H	4.5261	2.276967	-3.33121
C	5.653826	1.204114	-1.83858
H	6.605648	1.527751	-2.24598
C	5.643306	0.37723	-0.72245
H	6.561936	0.047163	-0.24983
C	4.385818	-0.00266	-0.24904
N	0.002288	1.760253	1.041944
N	-1.84044	0.05853	0.088533
N	-3.59076	1.21649	0.809963
N	0.438664	-1.32344	1.453718
N	2.122682	-0.12621	-0.15165
N	3.99909	-0.80329	0.821315
Fe	0.132149	-0.13931	-0.2305

H	4.624052	-1.26117	1.469949
H	-4.13044	1.96225	1.225638
O	0.082755	0.700553	-1.77409
N	0.205069	-2.19185	-1.33663
C	0.466973	-2.99162	-2.13392
C	0.786285	-3.99745	-3.13803
H	1.776579	-3.80084	-3.55825
H	0.779707	-4.99391	-2.68778
H	0.047489	-3.96428	-3.94371
O	-3.13553	2.6754	-3.17724
H	-2.57099	2.616838	-3.97963
O	-2.53558	1.954974	-2.24331
H	-0.79113	1.032298	-2.05281

^{4}Fe(III)OH

E(UB3LYP/6-31G(d,p))= -2725.81261266

no imaginary frequencies

	x	**y**	**z**
C	-1.34176	-2.89194	0.451995
H	-2.26843	-2.33496	0.368354
C	-1.34097	-4.23828	0.817982
H	-2.27644	-4.74069	1.035513
C	-0.12372	-4.91156	0.887927
H	-0.08503	-5.95938	1.166249
C	1.050667	-4.22091	0.590501
H	2.007711	-4.72881	0.63854
C	0.963436	-2.8758	0.23141
C	2.105195	-2.032	-0.11125
C	3.223318	-0.24152	-0.68446
C	3.662926	1.044363	-1.02797
H	2.964819	1.864776	-1.13894
C	5.027169	1.226683	-1.2136
H	5.401568	2.209308	-1.48026
C	5.946465	0.166471	-1.0609
H	7.002823	0.356063	-1.2172
C	5.531123	-1.11171	-0.70982
H	6.238235	-1.92464	-0.58571
C	4.159125	-1.28902	-0.52404
C	0.869101	1.030528	1.907722
H	1.836259	0.67465	1.577045
C	0.727495	1.721901	3.109188
H	1.598862	1.903323	3.727664

C	-0.53746	2.165065	3.48936
H	-0.68089	2.704338	4.419712
C	-1.62138	1.906548	2.652536
H	-2.61632	2.242421	2.923582
C	-1.40652	1.209754	1.464418
C	-2.43098	0.870684	0.491401
C	-3.243	-0.0051	-1.34405
C	-3.45994	-0.66571	-2.56119
H	-2.64212	-1.14911	-3.0814
C	-4.76037	-0.67994	-3.04582
H	-4.97212	-1.18181	-3.98391
C	-5.8235	-0.0615	-2.34896
H	-6.82249	-0.10068	-2.76976
C	-5.62568	0.590449	-1.13809
H	-6.44511	1.059189	-0.60422
C	-4.31693	0.603939	-0.65178
N	-0.21913	-2.22195	0.170433
N	1.949692	-0.74258	-0.41655
N	3.408895	-2.39903	-0.16088
N	-0.16889	0.770644	1.095564
N	-2.08478	0.18692	-0.59949
N	-3.75858	1.14459	0.502564
Fe	-0.06941	-0.21877	-0.72627
H	-4.26233	1.648487	1.219127
H	3.775255	-3.32336	0.017834
O	-0.19529	-1.06626	-2.27287
N	0.313779	1.63288	-1.75296
C	0.365595	2.577409	-2.42214
C	0.439036	3.76308	-3.26249
H	-0.4883	3.869449	-3.83306
H	0.581497	4.652429	-2.64195
H	1.277419	3.672119	-3.95937
H	0.013513	-0.49464	-3.02902

^{3}Fe(IV)O+HODTBPh_TS

E(UB3LYP/6-31G(d,p))= -3347.17365058

i899.78

	x	**y**	**z**
C	-2.0489	-2.29906	-0.15407
H	-2.86676	-1.59446	-0.08592
C	-2.27041	-3.67067	-0.03242
H	-3.27473	-4.03621	0.147621

C	-1.19334	-4.5441	-0.15583
H	-1.33515	-5.61644	-0.07406
C	0.075491	-4.01808	-0.39388
H	0.930899	-4.67539	-0.5056
C	0.219341	-2.63644	-0.49633
C	1.469099	-1.93152	-0.72264
C	2.788763	-0.20165	-0.93642
C	3.378356	1.066963	-1.02291
H	2.773381	1.963023	-1.05478
C	4.764666	1.128517	-1.06833
H	5.251555	2.095829	-1.13287
C	5.56349	-0.03526	-1.03199
H	6.643001	0.062056	-1.07241
C	4.998831	-1.30082	-0.93768
H	5.611076	-2.19538	-0.90123
C	3.604946	-1.35692	-0.88322
C	1.081614	0.581665	1.97087
H	1.919768	0.104922	1.48045
C	1.201592	1.057204	3.275744
H	2.139296	0.937808	3.806121
C	0.107398	1.681679	3.870206
H	0.168064	2.066152	4.882806
C	-1.07193	1.80438	3.139398
H	-1.94023	2.285852	3.575863
C	-1.1134	1.295992	1.84085
C	-2.27513	1.322827	0.972235
C	-3.47358	0.903667	-0.80408
C	-3.98335	0.465925	-2.03169
H	-3.34048	-0.03145	-2.74296
C	-5.32977	0.696846	-2.27794
H	-5.76185	0.368518	-3.21745
C	-6.16008	1.346292	-1.33759
H	-7.2059	1.506504	-1.57682
C	-5.67295	1.776384	-0.11
H	-6.31277	2.265059	0.616712
C	-4.32025	1.53523	0.137865
N	-0.83182	-1.78362	-0.37148
N	1.459354	-0.60484	-0.84371
N	2.730309	-2.42673	-0.75303
N	-0.04759	0.690518	1.254189
N	-2.20136	0.797107	-0.2496
N	-3.52185	1.786825	1.24407
Fe	-0.38534	0.142674	-0.80851
H	-3.82596	2.21269	2.107682
H	2.992992	-3.39909	-0.67753
O	-0.76064	-0.21957	-2.42406

N	0.088661	1.963142	-1.32573
C	0.210935	2.989563	-1.842
C	0.365462	4.258891	-2.53416
H	-0.46736	4.924261	-2.29087
H	1.304451	4.738993	-2.24563
H	0.373858	4.065563	-3.61087
C	1.657888	0.401953	-7.6396
C	0.517446	0.342017	-8.44104
C	-0.75229	0.438194	-7.87025
C	-0.93757	0.611157	-6.50157
C	0.250685	0.694068	-5.681
C	1.57019	0.562522	-6.26156
H	2.623893	0.315243	-8.11707
H	0.616958	0.214826	-9.5144
H	-1.60798	0.386789	-8.52832
C	2.851768	0.576319	-5.4062
C	3.010352	1.929559	-4.6698
C	2.801975	-0.60049	-4.40239
C	4.122819	0.385095	-6.26217
H	3.041864	2.755368	-5.38823
H	2.191271	2.103986	-3.97296
H	3.952678	1.937555	-4.11256
H	2.736157	-1.55358	-4.93756
H	3.719433	-0.6147	-3.80528
H	1.947714	-0.5241	-3.72861
H	4.996702	0.383737	-5.60415
H	4.121671	-0.56622	-6.80264
H	4.263392	1.194631	-6.98471
C	-2.37102	0.668868	-5.93769
C	-2.6469	-0.66647	-5.1994
C	-2.57825	1.892677	-5.01111
C	-3.42905	0.791969	-7.05838
H	-2.50589	-1.51156	-5.88016
H	-1.99139	-0.81547	-4.33822
H	-3.68731	-0.69821	-4.85678
H	-2.32846	2.817419	-5.54183
H	-3.62998	1.957635	-4.71673
H	-1.97554	1.845824	-4.10558
H	-4.42007	0.870938	-6.60227
H	-3.27711	1.685369	-7.67158
H	-3.45134	-0.08153	-7.71587
O	0.193035	1.025915	-4.38232
H	-0.31432	0.460046	-3.65118

^{2}Fe(III)OH+ODTBPh

E(UB3LYP/6-31G(d,p))= -3347.21717548

no imaginary frequencies

	x	y	z
C	-1.93898	-2.38251	0.407253
H	-2.76381	-1.68532	0.468703
C	-2.13392	-3.74583	0.629173
H	-3.12264	-4.11075	0.882005
C	-1.05115	-4.61239	0.510003
H	-1.17239	-5.67855	0.668887
C	0.196854	-4.08776	0.176952
H	1.0567	-4.74011	0.070775
C	0.31351	-2.71459	-0.02279
C	1.540035	-2.01019	-0.35428
C	2.820794	-0.2785	-0.74582
C	3.38945	0.991122	-0.9129
H	2.778456	1.884248	-0.90285
C	4.765999	1.059063	-1.08545
H	5.237919	2.027377	-1.21395
C	5.572652	-0.0991	-1.09553
H	6.643394	0.002899	-1.23521
C	5.028836	-1.36523	-0.91891
H	5.649437	-2.2547	-0.91298
C	3.646323	-1.42773	-0.73705
C	1.032279	0.810203	2.154346
H	1.901235	0.336703	1.716215
C	1.102214	1.405763	3.412908
H	2.035833	1.387198	3.963151
C	-0.03577	2.015387	3.93654
H	-0.01404	2.488196	4.912674
C	-1.20789	2.009122	3.183359
H	-2.10924	2.476421	3.564853
C	-1.19993	1.39089	1.93353
C	-2.33519	1.289548	1.035477
C	-3.41972	0.671808	-0.7623
C	-3.83911	0.127052	-1.98372
H	-3.13953	-0.40161	-2.61792
C	-5.17427	0.298002	-2.32213
H	-5.5411	-0.11427	-3.25612
C	-6.0768	0.990627	-1.48365
H	-7.11047	1.098099	-1.79464
C	-5.67697	1.531809	-0.26868
H	-6.37205	2.0576	0.376808
C	-4.33534	1.354129	0.075296

N	-0.74303	-1.86754	0.095945
N	1.509586	-0.6863	-0.51115
N	2.795372	-2.49762	-0.48932
N	-0.09018	0.793521	1.419329
N	-2.18309	0.657483	-0.12613
N	-3.60909	1.729453	1.19826
Fe	-0.34199	0.01373	-0.52328
H	-3.97298	2.227674	1.99783
H	3.070648	-3.46704	-0.41926
O	-0.71781	-0.62064	-2.13542
N	0.077314	1.743595	-1.29588
C	0.185895	2.704227	-1.92973
C	0.323515	3.904681	-2.73856
H	-0.4843	3.932967	-3.47539
H	0.274014	4.795719	-2.10698
H	1.280688	3.881685	-3.26668
C	1.676493	0.835762	-7.88183
C	0.554189	1.08645	-8.68754
C	-0.73511	1.164327	-8.13727
C	-0.95492	1.013573	-6.78092
C	0.220083	0.801231	-5.90815
C	1.564532	0.680755	-6.51315
H	2.642475	0.764148	-8.36464
H	0.684136	1.208893	-9.75846
H	-1.56436	1.338246	-8.81066
C	2.793922	0.400154	-5.63526
C	3.003769	1.569949	-4.6418
C	2.601756	-0.92799	-4.85945
C	4.082796	0.266451	-6.47225
H	3.139812	2.515228	-5.17871
H	2.148802	1.659462	-3.97045
H	3.90291	1.392021	-4.04344
H	2.486611	-1.76725	-5.55291
H	3.487776	-1.12369	-4.24489
H	1.723792	-0.8918	-4.2137
H	4.92383	0.055154	-5.80518
H	4.023523	-0.55534	-7.19235
H	4.322863	1.185519	-7.01581
C	-2.37517	1.029808	-6.19473
C	-2.67218	-0.35719	-5.57002
C	-2.51936	2.144175	-5.12745
C	-3.44302	1.291494	-7.27699
H	-2.60757	-1.14441	-6.32765
H	-1.97306	-0.5979	-4.76762
H	-3.69196	-0.37089	-5.16964
H	-2.29976	3.125632	-5.56296

H	-3.54883	2.171126	-4.75542
H	-1.84877	1.968497	-4.28606
H	-4.43344	1.289835	-6.8124
H	-3.31153	2.264338	-7.76088
H	-3.44632	0.517148	-8.04967
O	0.082378	0.733897	-4.65116
H	-0.45012	-0.04735	-2.88097

^{4}Fe(III)OH+ODTBPh

E(UB3LYP/6-31G(d,p))= -3347.20769890

no imaginary frequencies

	x	**y**	**z**
C	-1.83881	-2.51783	0.372605
H	-2.68985	-1.84857	0.425203
C	-1.98929	-3.89126	0.566143
H	-2.96771	-4.30224	0.786602
C	-0.86665	-4.70847	0.461886
H	-0.94649	-5.78131	0.601555
C	0.367286	-4.12863	0.170352
H	1.252985	-4.74817	0.081896
C	0.433708	-2.74666	-0.00714
C	1.657052	-2.00738	-0.30655
C	2.965794	-0.30225	-0.68062
C	3.545012	0.962155	-0.85473
H	2.939395	1.86036	-0.85623
C	4.922468	1.017788	-1.02543
H	5.40391	1.980728	-1.15925
C	5.71814	-0.14833	-1.02741
H	6.790131	-0.05651	-1.16496
C	5.163007	-1.40955	-0.8487
H	5.776501	-2.30395	-0.8408
C	3.779259	-1.45889	-0.67009
C	0.962492	0.963679	2.084881
H	1.847315	0.542174	1.62693
C	1.017787	1.545899	3.349394
H	1.959444	1.572565	3.88533
C	-0.14488	2.083143	3.897157
H	-0.136	2.543507	4.879445
C	-1.32489	2.021175	3.1599
H	-2.24412	2.433403	3.561323
C	-1.30566	1.422002	1.900435
C	-2.45875	1.285028	1.027322

C	-3.57464	0.677296	-0.74793
C	-4.0066	0.153444	-1.97369
H	-3.3087	-0.33301	-2.64327
C	-5.35495	0.287888	-2.2747
H	-5.73246	-0.10858	-3.21135
C	-6.25781	0.923806	-1.39262
H	-7.30229	1.004121	-1.67433
C	-5.84567	1.443796	-0.17197
H	-6.54221	1.926262	0.504999
C	-4.49002	1.303689	0.131384
N	-0.65732	-1.95403	0.09929
N	1.646553	-0.68475	-0.45269
N	2.910374	-2.51444	-0.43258
N	-0.16964	0.893629	1.365155
N	-2.31849	0.689597	-0.15452
N	-3.74157	1.675356	1.242125
Fe	-0.3436	0.105838	-0.57358
H	-4.09811	2.144643	2.062398
H	3.170512	-3.48783	-0.36508
O	-0.68783	-0.53511	-2.17452
N	0.168408	1.94669	-1.39833
C	0.276381	2.869039	-2.08965
C	0.41364	4.023997	-2.96035
H	-0.42457	4.042261	-3.6627
H	0.419541	4.944654	-2.37078
H	1.346098	3.941871	-3.52559
C	1.662581	0.791063	-7.85922
C	0.55195	1.083589	-8.6671
C	-0.73563	1.206137	-8.12037
C	-0.96425	1.062725	-6.76482
C	0.201847	0.813328	-5.89
C	1.542312	0.639233	-6.49087
H	2.626079	0.683146	-8.34003
H	0.688836	1.202052	-9.73761
H	-1.55659	1.408186	-8.79597
C	2.757417	0.304834	-5.61139
C	3.0155	1.45702	-4.60884
C	2.509205	-1.01972	-4.84525
C	4.041494	0.123852	-6.44729
H	3.190658	2.400143	-5.13869
H	2.167403	1.576293	-3.9338
H	3.907182	1.238048	-4.01303
H	2.36258	-1.8491	-5.54457
H	3.384804	-1.25455	-4.22977
H	1.632615	-0.95451	-4.19997
H	4.871875	-0.12413	-5.7796

H	3.951459	-0.69132	-7.1717
H	4.319016	1.035603	-6.98539
C	-2.38563	1.122241	-6.18318
C	-2.72648	-0.25435	-5.55771
C	-2.50392	2.240083	-5.11644
C	-3.44124	1.41403	-7.26984
H	-2.67988	-1.04532	-6.31266
H	-2.04024	-0.51351	-4.74967
H	-3.74867	-0.23635	-5.16385
H	-2.25774	3.215621	-5.55147
H	-3.53395	2.294055	-4.7488
H	-1.84259	2.047167	-4.27161
H	-4.43269	1.443485	-6.80854
H	-3.27873	2.381505	-7.7551
H	-3.46561	0.638634	-8.04106
O	0.060457	0.762644	-4.63239
H	-0.42786	0.033591	-2.93075