

Supplementary Information

Mechanistic Insights into Dioxygen Activation, Oxygen Atom Exchange and Substrate Epoxidation by AsqJ Dioxygenase from Quantum Mechanics/Molecular Mechanics Calculations

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Parameter File for the Iron Center

BOND

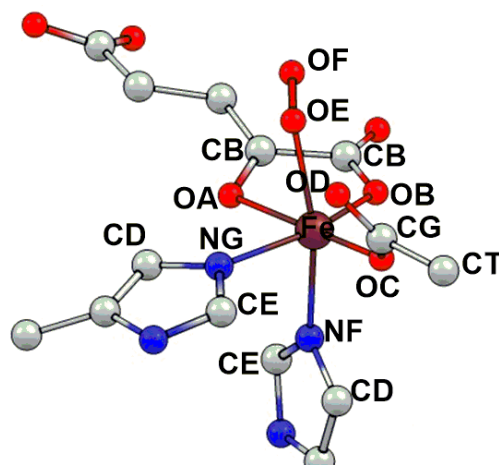
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Fe-OE 58.0 2.066
Fe-NF 77.86 2.072
Fe-NG 77.66 2.061

ANGLES

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OC-FE-NF 62.281 97.293
OC-FE-NG 43.758 92.373
OC-FE-OB 23.367 107.237
OC-FE-OA 32.296 175.430
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DIHE

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MD Simulation

The RMSD of backbone during MD simulations was shown in Figure S1. The backbone becomes stable after about 4ns.

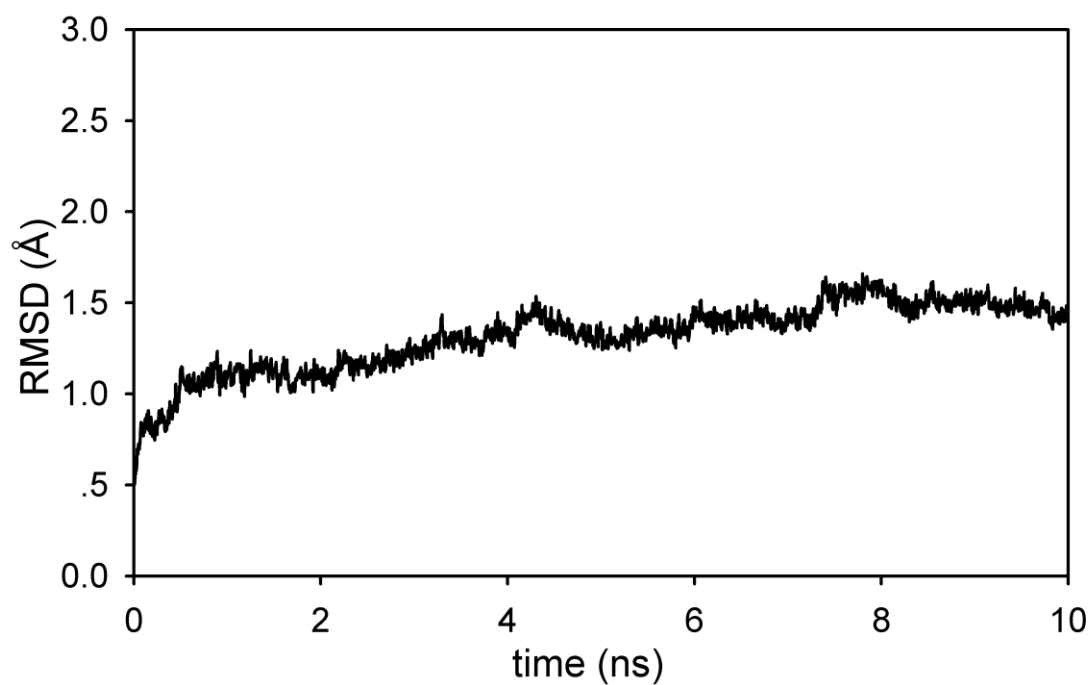


Figure S1. The RMSD plot of backbone during MD simulations.

Analysis of Electronic Structure of the Fe-O₂ Adducts.

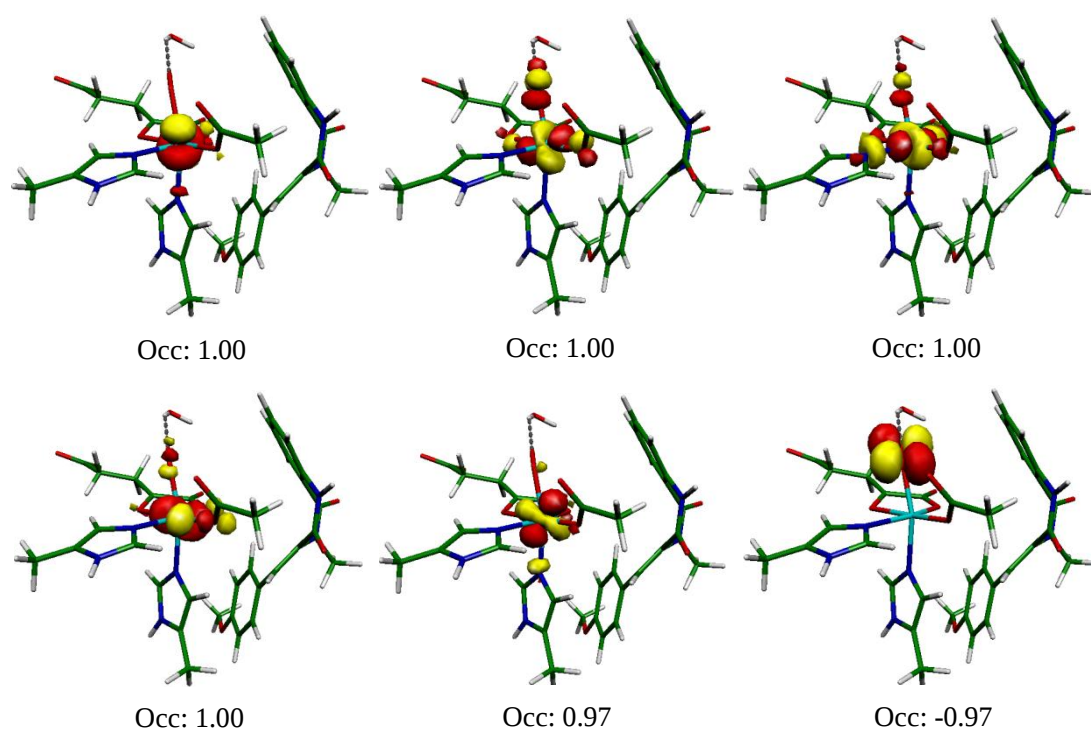


Figure S2. Singly occupied spin natural orbitals and their occupation numbers (Occ) for ⁵1 at the B3LYP(B1)/MM level.

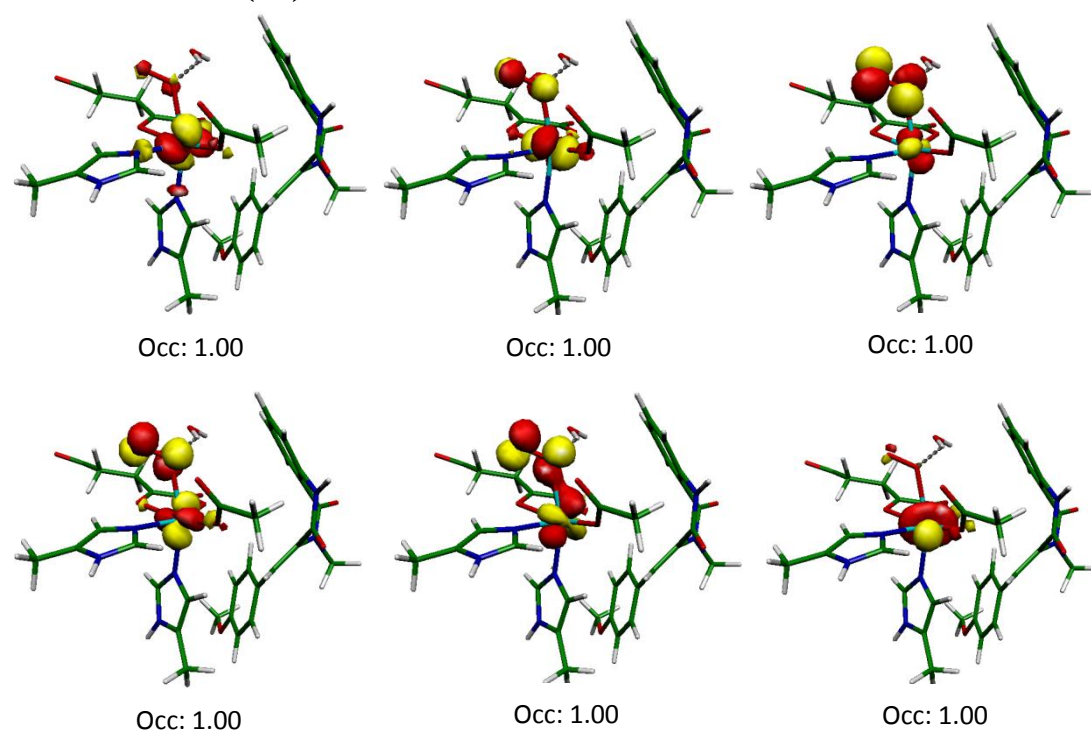


Figure S3. Singly occupied spin natural orbitals and their occupation numbers (Occ) for ⁷1 at the B3LYP(B1)/MM level.

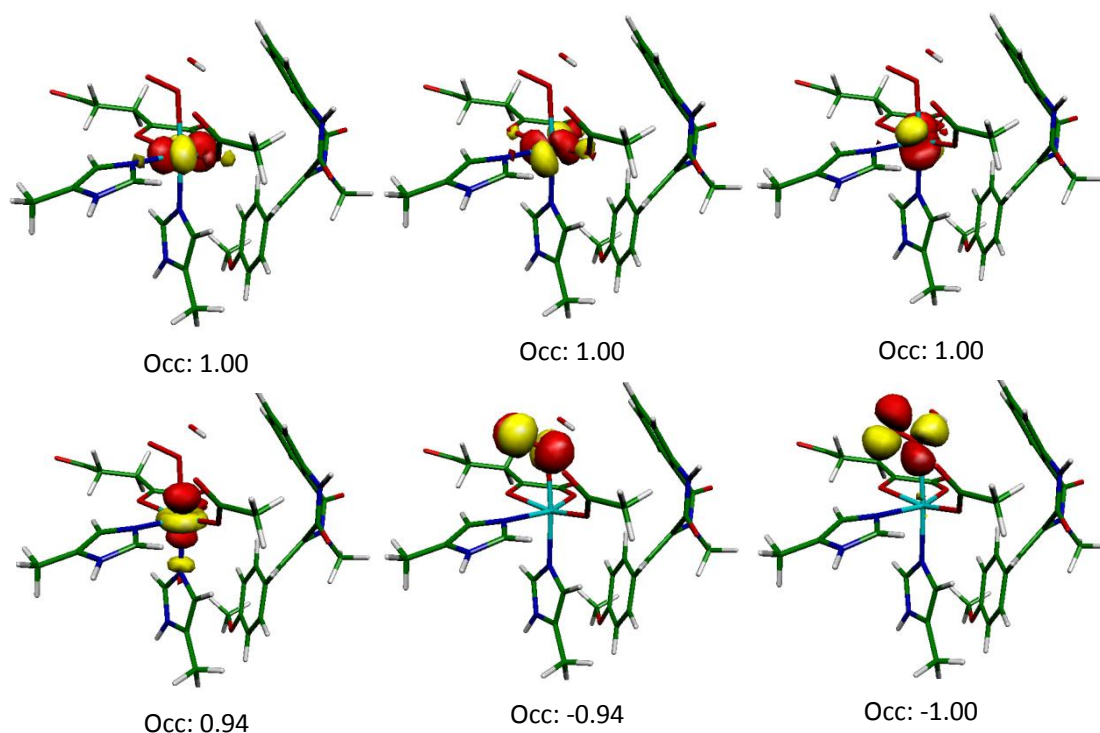


Figure S4. Singly occupied spin natural orbitals and their occupation numbers (Occ) for **1** at the B3LYP(B1)/MM level.

Scanned energy profile for the attack of the distal oxygen atom on the keto carbon of α -KG from **1**

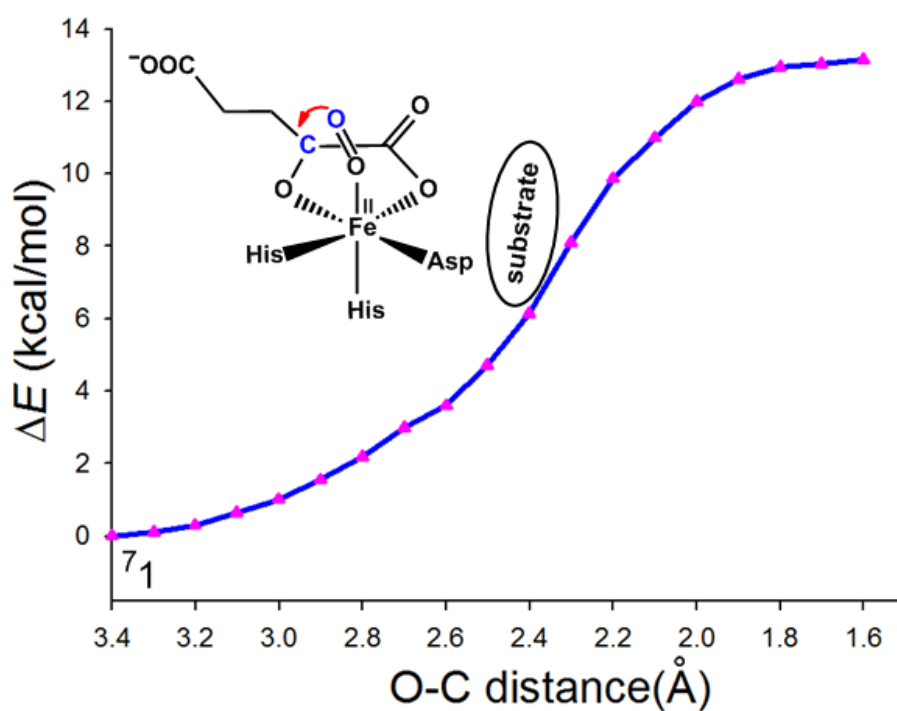


Figure S5. The UB3LYP(B1)/MM energy profile along the forming O-C bond starting from **1**.

Energies and Spin Densities for the Key Species.

Table S1. Absolute energies (in a.u.) for the key species in the dioxygen activation and the oxo group isomerization processes.

species	B3LYP/B1		B3LYP/B2		E_{disp}	E_{zpe}
	QM	QM/MM	QM	QM/MM		
⁵ 1	-3848.305556	-3977.223969	-3851.519793	-3980.438018	-0.125248	0.678957
⁵ TS1	-3848.295503	-3977.210186	-3851.510452	-3980.425151	-0.123305	0.691268
⁵ 3	-3848.371710	-3977.289845	-3851.592879	-3980.510975	-0.125055	0.686584
⁵ TS3	-3848.362395	-3977.280720	-3851.585179	-3980.503383	-0.125728	0.688623
⁵ 4	-3848.399687	-3977.311241	-3851.625397	-3980.536950	-0.127118	0.674440
⁵ TS4	-3848.378603	-3977.302487	-3851.605295	-3980.529086	-0.125862	0.686756
⁵ 5	-3848.392376	-3977.316879	-3851.620231	-3980.544568	-0.126434	0.678250
⁷ 1	-3848.298113	-3977.231799	-3185.509025	-3980.442647	-0.128892	0.686488
⁷ 2	-3848.296153	-3977.213018	-3851.513621	-3980.430401	-0.124510	0.692734
⁷ TS2	-3848.284493	-3977.208245	-3851.501960	-3980.425617	-0.124707	0.688469
⁷ 3	-3848.279516	-3977.21198	-3851.500797	-3980.433171	-0.127012	0.689768
⁷ TS3	-3848.251735	-3977.184324	-3851.474574	-3980.407116	-0.127667	0.689127
⁷ 4	-3848.360885	-3977.288490	-3851.579161	-3980.506636	-0.132207	0.687619
³ 1	-3848.298163	-3977.233446	-3851.510217	-3980.44545	-0.127933	0.692791
³ TS1	-3848.277413	-3977.195327	-3851.486178	-3980.403952	-0.125412	0.680786
³ 2	-3848.280196	-3977.197649	-3851.498558	-3980.415849	-0.125286	0.691632
³ TS2	-3848.260577	-3977.189299	-3851.474975	-3980.403640	-0.125944	0.689175
³ 3	-3848.309953	-3977.242219	-3851.532088	-3980.464189	-0.126586	0.693287
³ 3'	-3848.327673	-3977.255584	-3851.551272	-3980.479128	-0.126148	0.694165
³ TS3	-3848.325427	-3977.253499	-3851.550833	-3980.478691	-0.126677	0.686973
³ 4	-3848.362369	-3977.292209	-3851.581408	-3980.511076	-0.132723	0.686637

Table S2. Relative energies (in kcal/mol) for the key species in the dioxygen activation and the oxo group isomerization processes.

species	B3LYP/B1		B3LYP/B2	
	QM	QM/MM	QM	QM/MM
⁵1	0.0	0.0	0.0	0.0
⁵TS1	6.3	8.6	5.9	8.1
⁵3	-41.5	-41.3	-45.9	-45.8
⁵TS3	-35.7	-35.6	-41.0	-41.0
⁵4	-59.1	-54.8	-66.3	-62.1
⁵TS4	-45.8	-49.3	-53.7	-57.1
⁵5	-54.5	-58.3	-63.0	-66.9
⁷1	4.7	-4.9	6.8	-2.9
⁷2	5.9	6.9	3.9	4.8
⁷TS2	13.2	9.9	11.2	7.8
⁷3	16.3	7.5	11.9	3.0
⁷TS3	33.8	24.9	28.4	19.4
⁷4	-34.7	-40.5	-37.3	-43.1
³1	4.6	-5.9	6.0	-4.7
³TS1	17.7	18.0	21.1	21.4
³2	15.9	16.5	13.3	13.9
³TS2	28.2	21.8	28.1	21.6
³3	-2.8	-11.5	-7.7	-16.4
³3'	-13.9	-19.8	-19.8	-25.8
³TS3	-12.5	-18.5	-19.5	-25.5
³4	-35.7	-42.8	-38.7	-45.8

Table S3. Spin density distribution for the key species in the dioxygen activation and the oxo group isomerization processes at the B3LYP(B1)/MM level.

species	Fe	O1	O2	AKG ^a	C ^b	sub	L ^c	other
⁵ 1	4.20	-0.25	-0.49	0.08	0.17	0.00	0.25	0.05
⁵ TS1	4.23	-0.16	-0.26	-0.02	-0.11	0.00	0.26	0.06
⁵ 3	3.80	0.07	0.01	0.02	0.00	0.00	0.08	0.02
⁵ TS3	3.91	0.04	-0.14	0.03	0.00	0.00	0.12	0.03
⁵ 4	3.08	0.75	0.02	0.02	0.01	0.00	0.09	0.03
⁵ TS4	3.16	0.69	0.02	0.04	0.00	0.00	0.11	0.02
⁵ 5	3.14	0.69	0.00	0.00	0.00	0.00	0.10	0.02
⁷ 1	3.93	0.86	0.95	0.02	0.08	0.00	0.13	0.04
⁷ 2	4.21	0.67	0.45	0.16	0.21	0.00	0.24	0.05
⁷ TS2	4.22	0.45	0.27	0.36	0.39	0.00	0.25	0.05
⁷ 3	4.24	0.23	0.03	0.09	1.06	0.02	0.28	0.04
⁷ TS3	4.25	0.21	0.03	0.10	1.06	0.02	0.29	0.04
⁷ 4	4.18	1.22	0.20	0.11	0.01	0.00	0.23	0.04
³ 1	3.75	-0.90	-1.01	0.02	0.05	0.00	0.07	0.02
³ TS1	2.94	-0.46	-0.54	0.06	-0.03	0.00	0.01	0.03
³ 2	2.91	-0.53	-0.39	-0.01	-0.03	0.00	0.02	0.03
³ TS2	2.82	-0.03	-0.09	-0.27	-0.51	0.00	0.06	0.02
³ 3	1.94	0.02	0.01	0.02	0.00	0.00	0.01	0.00
³ 3'	1.99	0.02	-0.01	-0.02	0.00	0.00	-0.01	0.03
³ TS3	2.10	0.00	-0.09	-0.03	0.00	0.00	0.00	0.03
³ 4	2.84	-0.79	-0.07	-0.03	0.01	0.00	0.03	0.03

^a The spin density for C₁, O₄ and O₅ are not included.

^b The spin density for C₁, O₄ and O₅.

^c The ligated N atoms of His134 and His211, and ligated O atom of Asp 136.

Table S4. Mulliken charge for the key species in the dioxygen activation and the oxo group isomerization processes at the B3LYP(B1)/MM level.

species	Fe	O1	O2	AKG ^a	C ^b	sub	L ^c	other
⁵ 1	0.93	-0.18	-0.19	-1.10	-0.44	-0.01	-0.97	0.95
⁵ TS1	0.93	-0.24	-0.16	-1.19	-0.31	0.00	-0.97	0.95
⁵ 3	0.82	-0.40	-0.17	-0.92	0.00	-0.01	-0.97	0.65
⁵ TS3	0.86	-0.39	-0.22	-0.99	0.00	-0.01	-0.99	0.73
⁵ 4	0.85	-0.33	-0.34	-1.10	0.02	0.00	-0.91	0.82
⁵ TS4	0.86	-0.36	-0.29	-1.14	0.02	-0.02	-0.92	0.85
⁵ 5	0.90	-0.39	-0.31	-1.14	0.01	-0.03	-0.91	0.86
⁷ 1	0.86	-0.07	0.00	-1.03	-0.54	-0.03	-0.99	0.81
⁷ 2	0.91	-0.13	-0.10	-1.20	-0.40	-0.03	-0.98	0.93
⁷ TS2	0.94	-0.24	-0.15	-1.16	-0.28	-0.04	-0.97	0.92
⁷ 3	0.95	-0.34	-0.09	-0.86	-0.55	-0.08	-0.94	0.91
⁷ TS3	0.95	-0.31	-0.14	-0.87	-0.54	-0.08	-0.93	0.91
⁷ 4	0.93	-0.37	-0.26	-1.16	-0.01	0.00	-0.97	0.86
³ 1	0.81	-0.03	0.05	-1.04	-0.55	-0.03	-0.98	0.76
³ TS1	0.77	-0.15	-0.10	-1.15	-0.35	-0.04	-0.90	0.92
³ 2	0.78	-0.13	-0.10	-1.17	-0.35	-0.04	-0.90	0.92
³ TS2	0.78	-0.27	-0.18	-1.08	-0.23	-0.04	-0.90	0.92
³ 3	0.75	-0.41	-0.12	-0.96	0.06	-0.05	-0.91	0.64
³ 3'	0.72	-0.39	-0.12	-0.90	0.01	-0.05	-0.91	0.63
³ TS3	0.73	-0.38	-0.15	-0.93	0.01	-0.05	-0.90	0.66
³ 4	0.81	-0.32	-0.28	-1.15	-0.01	-0.02	-0.91	0.89

^a C₁, O₄ and O₅ are not included.

^b C₁, O₄ and O₅.

^c The ligated N atoms of His134 and His211, and ligated O atom of Asp 136.

Table S5. Absolute energies (in a.u.) for the key species in the oxygen atom exchange and epoxidation processes.

species	B3LYP/B1		B3LYP/B2		E_{disp}	E_{zpe}
	QM	QM/MM	QM	QM/MM		
⁵ 6	-3812.695088	-3941.611767	-3815.915431	-3944.831986	-0.132683	0.726004
⁵ TS5	-3812.673923	-3941.593293	-3815.890060	-3944.809412	-0.132600	0.720756
⁵ 7	-3812.685404	-3941.602876	-3815.907249	-3944.824548	-0.131348	0.725608
⁵ TS6	-3812.672757	-3941.590831	-3815.897521	-3944.815533	-0.131332	0.722471
⁵ 8	-3812.683798	-3941.604834	-3815.906209	-3944.827188	-0.132316	0.724184
⁵ TS7	-3812.680664	-3941.597415	-3815.899920	-3944.816462	-0.129961	0.720605
⁵ 9	-3812.708320	-3941.622542	-3815.928567	-3944.842724	-0.130840	0.726832
⁵ TS8	-3812.670623	-3941.587512	-3815.886414	-3944.799888	-0.138337	0.726947
⁵ 10	-3812.711168	-3941.627219	-3815.918966	-3944.834901	-0.137500	0.732561
⁵ TS9	-3812.698874	-3941.612672	-3815.904932	-3944.818708	-0.137200	0.726602
⁵ 11	-3812.744114	-3941.660720	-3815.956225	-3944.870255	-0.128581	0.742469

Table S6. Relative energies (in kcal/mol) for the key species in the oxygen atom exchange and epoxidation processes.

species	B3LYP/B1		B3LYP/B2	
	QM	QM/MM	QM	QM/MM
⁵ 6	0.0	0.0	0.0	0.0
⁵ TS5	13.3	11.6	15.9	14.2
⁵ 7	6.1	5.6	5.1	4.7
⁵ TS6	14.0	13.1	11.2	10.3
⁵ 8	7.1	4.4	5.8	3.0
⁵ TS7	9.1	9.0	9.7	9.7
⁵ 9	-8.3	-6.8	-8.2	-6.7
⁵ TS8	15.4	15.2	18.2	16.4
⁵ 10	-10.1	-9.7	-2.2	20.1
⁵ TS9	-2.4	-0.6	6.6	-1.8
⁵ 11	-30.8	-30.7	-25.6	-24.0

Table S7. Spin density distribution for the key species in the oxygen atom exchange and epoxidation processes at the B3LYP/B1 level.

species	Fe	O4^a	O1^b	C4^c	Sub^d	L^e	other
⁵ 6	3.18	0.04	0.60	0.00	0.00	0.15	0.04
⁵ TS5	3.33	0.05	0.37	0.00	0.00	0.17	0.07
⁵ 7	3.40	0.16	0.18	0.00	0.00	0.19	0.07
⁵ TS6	3.48	0.11	0.13	0.00	0.00	0.20	0.08
⁵ 8	3.39	0.24	0.12	0.00	0.00	0.17	0.07
⁵ TS7	3.34	0.35	0.10	0.00	0.00	0.14	0.07
⁵ 9	3.16	0.63	0.05	0.00	0.00	0.12	0.03
⁵ TS8	3.96	0.04	0.06	-0.40	-0.31	0.21	0.03
⁵ 10	4.23	0.26	0.07	-0.91	-0.90	0.30	0.04
⁵ TS9	4.04	0.13	0.04	-0.39	-0.42	0.18	0.03
⁵ 11	3.84	0.00	0.03	0.00	0.00	0.09	0.04

^a The ligated O atom of the added water molecule.

^b The O atom of iron-oxo.

^c The C atom of the substrate C3=C4 unit.

^d The spin density for C4 are also included.

^e The ligated N atoms of His134 and His211, and ligated O atom of Asp 136.

Table S8. Mulliken charge for the key species in the oxygen atom exchange and epoxidation processes at the B3LYP/B1 level.

species	Fe	O4 ^a	O1 ^b	C4 ^c	Sub ^d	L ^e	other
⁵ 6	0.84	-0.60	-0.38	0.03	-0.02	-1.24	0.41
⁵ TS5	0.83	-0.63	-0.46	0.03	-0.01	-1.22	0.49
⁵ 7	0.81	-0.55	-0.46	0.03	-0.01	-1.22	0.44
⁵ TS6	0.80	-0.53	-0.48	0.03	-0.03	-1.22	0.45
⁵ 8	0.83	-0.50	-0.56	0.03	-0.02	-1.25	0.48
⁵ TS7	0.85	-0.49	-0.62	0.03	-0.01	-1.24	0.52
⁵ 9	0.85	-0.39	-0.59	0.02	-0.02	-1.25	0.40
⁵ TS8	0.92	-0.45	-0.63	-0.01	0.13	-1.24	0.26
⁵ 10	0.97	-0.51	-0.64	-0.10	0.14	-1.27	0.32
⁵ TS9	0.95	-0.46	-0.66	-0.05	0.31	-1.29	0.15
⁵ 11	0.85	-0.28	-0.65	0.05	0.30	-1.34	0.12

^a The ligated O atom of the added water molecule.

^b The O atom of iron-oxo.

^c The C atom of the substrate C3=C4 unit.

^d C4 are also included.

^e The ligated N atoms of His134 and His211, and ligated O atom of Asp 136.

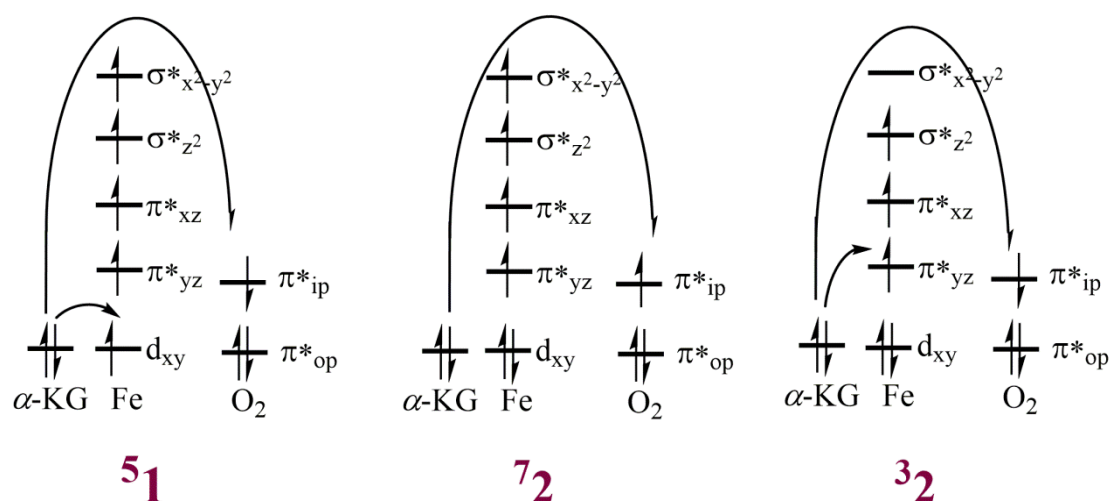


Figure S6. Schematics of electron transfer in the formation of the iron-peracid species at three spin states

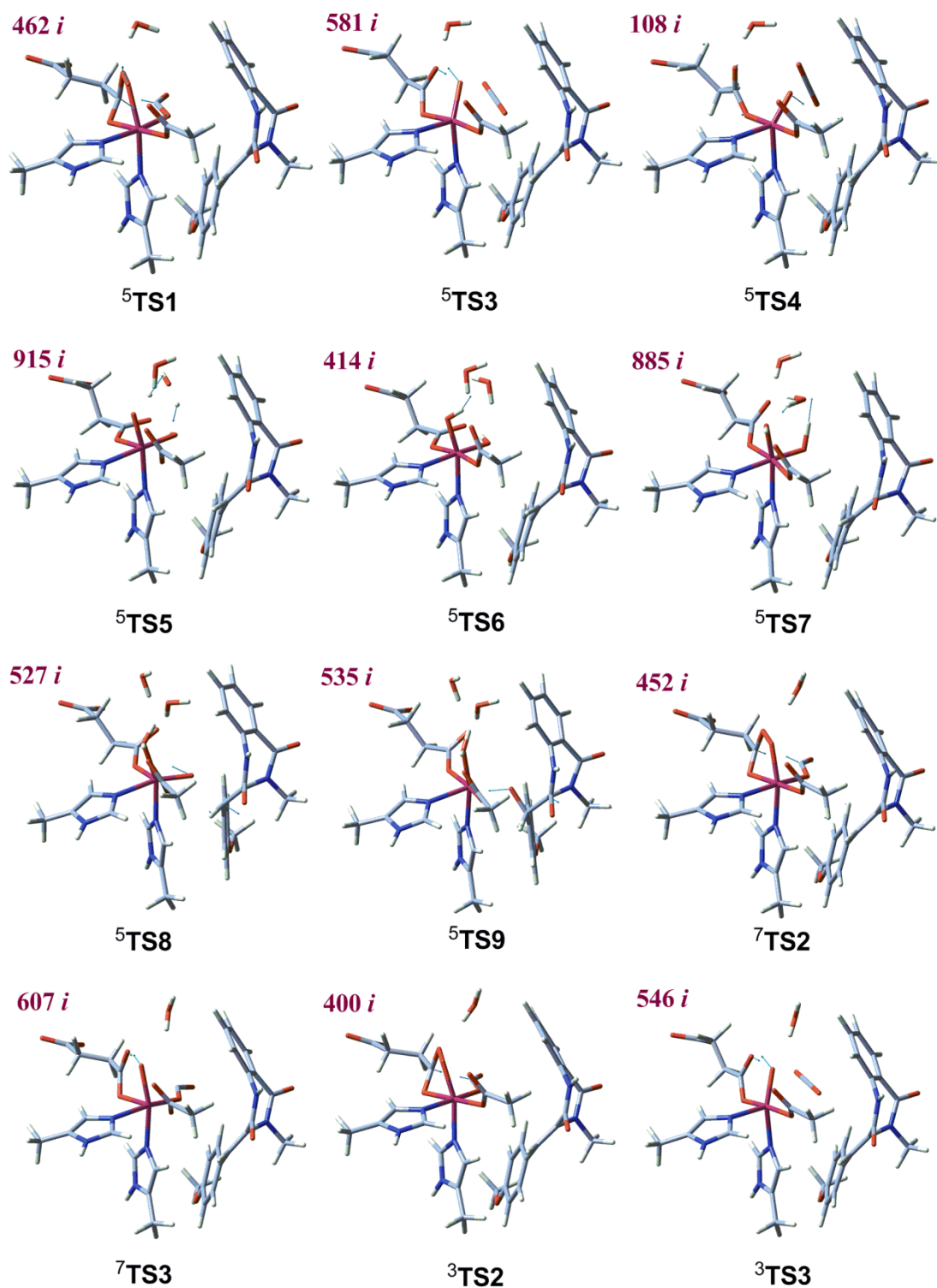
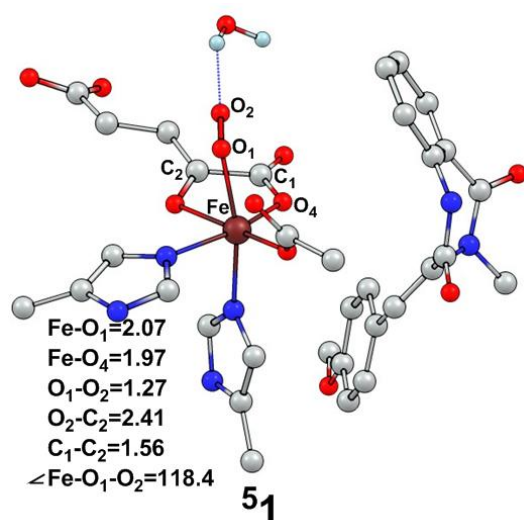


Figure S7. The normal modes of vibrations along the imaginary frequency for transition states.

Cartesian Coordinates of the QM Region of Key Species

⁵1

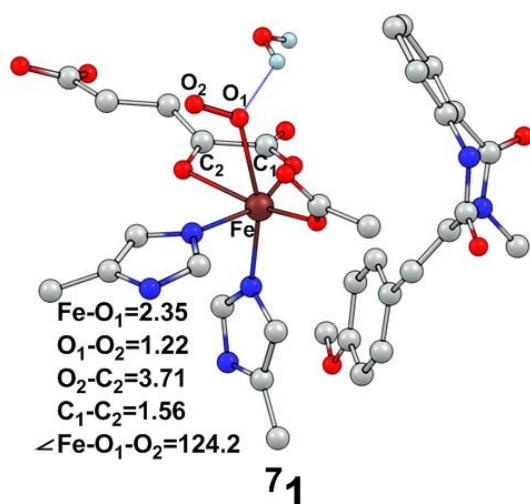


O	2.252641	-1.501046	7.488441
H	1.399409	-1.284877	7.908394
H	2.024570	-2.211420	6.859555
Fe	-0.746434	-6.043998	7.401640
C	0.017054	-3.991420	9.223660
O	0.000294	-3.047266	10.001413
O	-0.997041	-4.517788	8.624267
C	1.350305	-4.728030	8.905810
O	1.250266	-5.870899	8.443557
C	2.625592	-4.067173	9.320679
C	3.946044	-4.700695	8.895725
C	5.198486	-4.142488	9.619717
O	6.315923	-4.482038	9.167311
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H	4.106629	-4.589721	7.808717
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C	-4.051317	-6.440404	4.587404
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O	0.965254	-3.802094	6.709438

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H	-1.542524	-8.604664	5.427255
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O	-2.637366	-6.332570	14.816606	H	-5.585911	-3.113058	5.931198
O	-6.239967	-5.041632	7.219681	H	-3.400932	-2.391267	5.056879
O	-5.287961	-0.728012	10.076597	H	-1.165610	0.328022	7.548792
C	-6.228816	-3.096257	10.913795	H	-2.714356	-0.147734	9.444529
H	-4.618081	-6.189393	8.941460	H	-7.253772	-2.893094	10.549631
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H	-1.518096	-0.790177	5.344998	h	-4.676368	-7.209146	5.041731
H	-1.869923	-5.745104	16.601929	h	-2.960917	-11.177130	9.953524
H	-0.986918	-5.092724	15.182233	h	2.318844	-11.272774	7.196105
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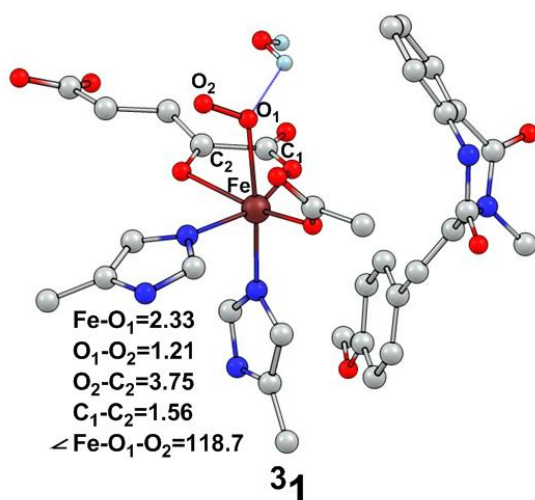
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Fe	-0.889497	-6.021434	7.464739	C	-4.141843	-6.491578	4.554861
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O	-0.031843	-2.980074	10.079697	H	-4.655170	-5.518029	4.663060
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C	2.663993	-3.820070	9.343639	O	0.192259	-4.730089	5.833837
C	3.976541	-4.485990	8.940576	O	1.193403	-5.078303	5.239271
C	5.238699	-4.020185	9.702095	C	-3.256985	-10.231943	10.386065
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O	5.111655	-3.340487	10.759889	H	-4.263509	-9.988788	10.004528
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				H	-0.889676	-9.258995	11.675203
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				H	2.643734	-11.073463	5.491256
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C	-0.585707	-8.627514	5.826028	O	-2.680588	-6.340012	14.727809
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H	2.050484	-7.612095	7.312121	H	-4.555450	-6.134229	8.804827
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C	-5.465016	-4.066729	7.564985	H	-1.024008	-5.112554	15.106297
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C	-3.994027	-5.527374	10.839352	H	-3.244914	-2.228685	5.087358
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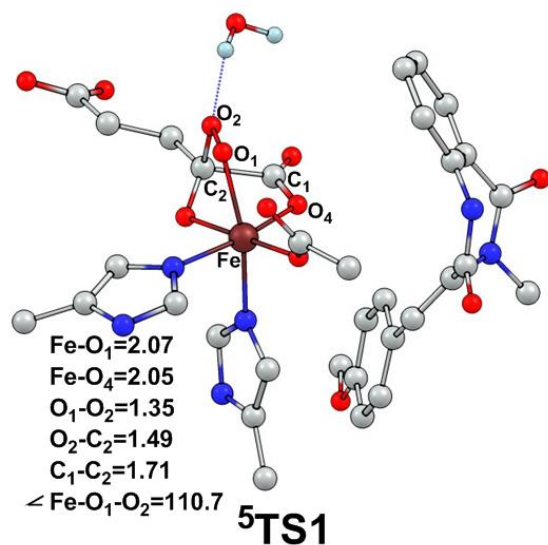
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H	0.017045	-2.503875	6.861417	O	-0.870244	-4.346314	8.547329
Fe	-0.802833	-6.032802	7.441013	C	1.487282	-4.498899	8.837004
				O	1.470236	-5.545817	8.205773
				C	2.741851	-3.820277	9.312661
				C	4.057030	-4.485169	8.919766
				C	5.308357	-4.026874	9.701562
				O	6.414949	-4.426336	9.270947
				O	5.169320	-3.336964	10.750876
				H	2.683432	-2.785745	8.930242
				H	2.663999	-3.722306	10.409863
				H	4.261128	-4.361858	7.842128
				H	3.981000	-5.577501	9.075130
				C	-4.129907	-6.494548	4.562177

H	-4.096142 -6.706329 3.482461	C	-3.857255 -6.970787 12.815128
H	-4.623354 -5.512250 4.684005	C	-3.143290 -4.612322 11.497641
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O	-2.532168 -6.291943 6.363260	N	-5.100430 -3.014738 6.822929
O	-1.786053 -6.244986 4.247449	C	-4.047948 -2.118488 7.098724
O	-0.087306 -4.582244 5.771425	C	-3.160551 -1.781087 6.061878
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C	1.390534 -8.205074 6.738923	H	-1.147008 0.407118 7.732769
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C	-4.894998 -1.704321 9.466283	H	-7.290914 -2.902422 10.499981
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C	-2.667675 -4.856383 12.787917	h	-4.750725 -7.255681 5.034752
C	-5.486878 -4.082472 7.577933	h	-2.951269 -11.167870 9.959780
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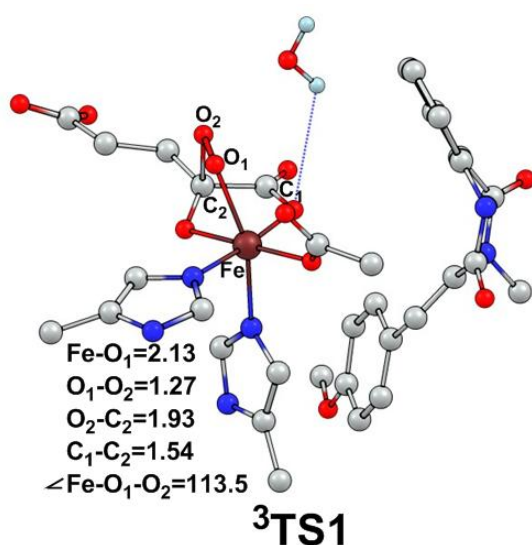


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C	-3.283352	-10.187863	10.350537
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H	-1.528397	-0.795789	5.336881	H	-7.255438	-2.890660	10.553068
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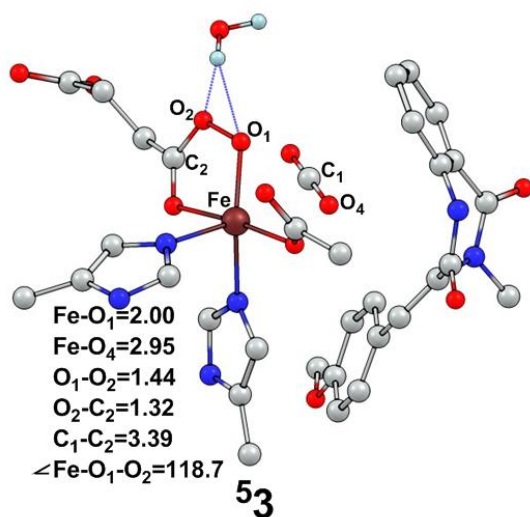
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Fe	-0.528680	-6.144049	7.442231	H	-4.424269	-5.404695	4.920070
C	0.020026	-3.985580	8.977886	C	-2.487065	-6.293767	5.179851
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O	1.219799	-5.963334	8.586595	O	1.537103	-4.217725	6.868371
C	2.613536	-4.038862	9.252299	C	-3.280031	-10.208497	10.375500
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O	5.024681	-3.461264	10.682296	H	-0.905635	-9.254039	11.652369
H	2.555107	-2.983358	8.935219	C	-2.333522	-9.096064	10.052773
H	2.530528	-4.024156	10.353157	C	-0.571897	-7.755711	10.179760
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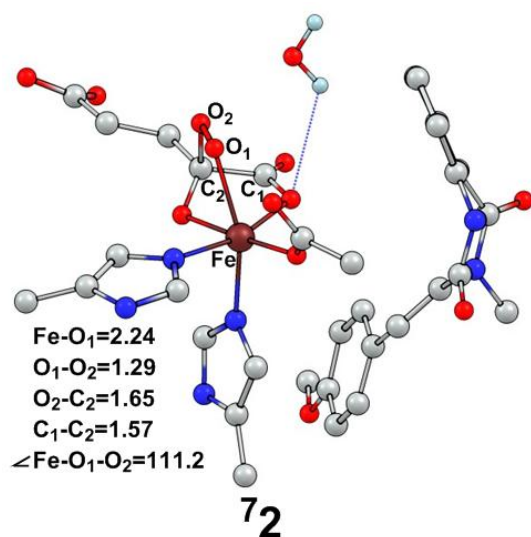
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Fe	-0.598215	-6.053097	7.191553	C	4.451770	-4.210803	8.574033
C	-0.937373	-3.421183	9.292828	C	5.584748	-4.045426	9.609737
O	-0.036359	-2.893548	9.813047	O	6.696572	-4.551150	9.324792
O	-1.861866	-3.948955	8.833243	O	5.345075	-3.421486	10.679969
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				O	-1.712290	-6.139643	4.157062
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				O	1.588713	-4.048746	7.464627
				C	-3.260550	-10.082460	10.295864

H	-3.338827	-10.194478	11.391452	C	-4.159260	-2.277456	7.129630
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N	-1.204736	-8.622530	10.652397	C	-2.070440	-0.435178	7.439161
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C	-4.973793	-1.732449	9.478522	H	-5.619592	-3.227443	5.960518
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C	-3.008276	-6.083425	13.602204	H	-6.087436	-2.335293	11.728416
C	-3.756346	-7.069235	12.932178	h	-4.674184	-7.224864	4.987369
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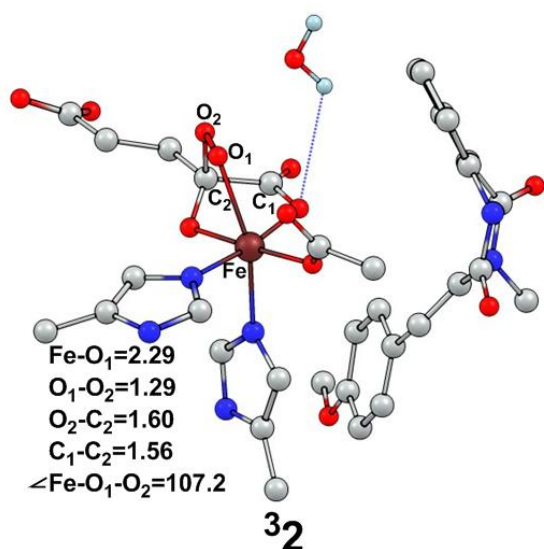


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Fe	-0.646323	-6.083511	7.526152
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O	-0.958403	-4.295203	8.318498
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O	1.113803	-5.888434	8.588057
C	2.637061	-4.034036	9.229602
C	3.971922	-4.664224	8.838400
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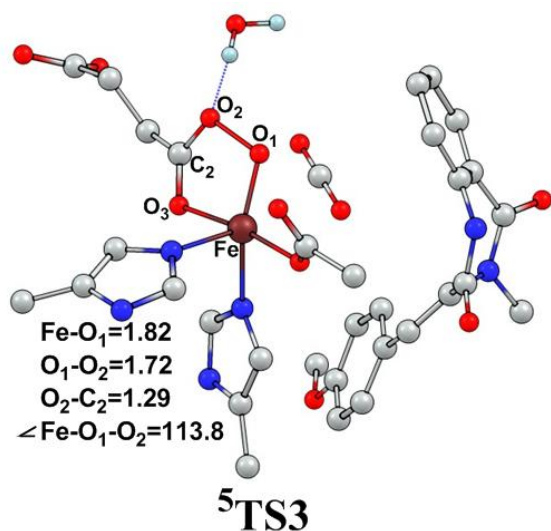
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C	-1.991133	-5.344368	15.598998	h	-2.959969	-11.177350	9.974889
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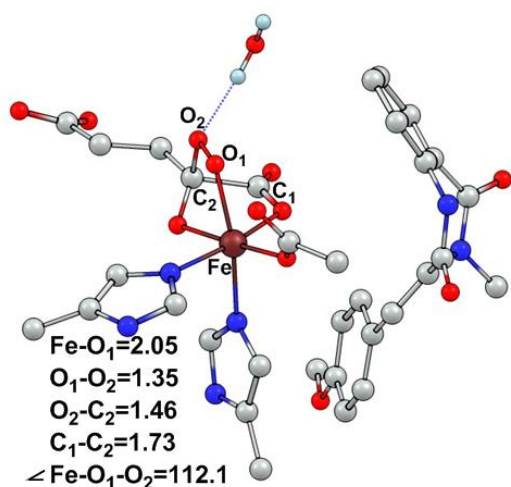
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H	2.230764	-2.465561	7.598528	O	1.327040	-6.016046	8.458652
Fe	-0.541462	-6.080874	7.188194	C	3.152121	-4.629472	9.182076
C	-0.842875	-3.328459	9.299380	C	4.482223	-4.212608	8.541404
O	0.102128	-2.776000	9.701161	C	5.603178	-4.067783	9.592320
				O	6.717378	-4.576352	9.318429
				O	5.353693	-3.454295	10.666748
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				H	3.287612	-5.508285	9.822312
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				H	4.811831	-4.942211	7.784194
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				H	-4.009186	-6.696063	3.424499
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				C	-2.562101	-6.324516	4.986393
				O	-2.351117	-6.328782	6.258488
				O	-1.688468	-6.158749	4.127444
				O	0.077108	-4.407694	6.809159

O	1.678029 -4.118364 7.360009	N	-5.197371 -3.172359 6.912184
C	-3.244389 -10.049675 10.289931	C	-4.140298 -2.264738 7.129465
H	-3.321484 -10.158494 11.385942	C	-3.251269 -2.004248 6.073730
H	-4.257464 -9.824153 9.914881	C	-2.061085 -0.413330 7.453541
N	-1.185185 -8.592989 10.642653	C	-2.956339 -0.648303 8.494155
H	-0.859043 -9.064910 11.488974	C	-3.991904 -1.588850 8.354119
C	-2.312234 -8.938781 9.916672	N	-5.355609 -2.979243 9.859157
C	-0.574577 -7.561320 10.014456	C	-4.659677 -5.330784 9.702128
H	0.339014 -7.082109 10.363523	C	-1.948522 -5.374892 15.628664
N	-1.248579 -7.217173 8.924003	O	-2.565538 -6.382496 14.846166
C	-2.334430 -8.062571 8.856167	O	-6.287863 -5.111838 7.272728
H	-3.050756 -7.980386 8.041930	O	-5.380295 -0.726817 10.076663
C	2.569417 -10.683986 6.374801	C	-6.330804 -3.074001 10.945870
H	2.708080 -11.340841 5.496192	H	-4.740892 -6.219265 9.069508
H	3.539660 -10.206242 6.582602	H	-4.862740 -7.579205 11.167603
N	0.303150 -9.844002 5.552852	H	-2.186176 -4.069282 13.462375
H	-0.073901 -10.725059 5.188682	H	-1.524473 -0.900691 5.407756
C	1.534806 -9.639024 6.148566	H	-1.757768 -5.813849 16.620528
C	-0.403019 -8.699015 5.633368	H	-0.990575 -5.044310 15.191604
H	-1.403511 -8.593980 5.225460	H	-2.600983 -4.493063 15.745143
N	0.306809 -7.762992 6.239199	H	-3.935570 -8.019931 13.431457
C	1.516632 -8.330958 6.560085	H	-3.176838 -3.615424 11.255918
H	2.280893 -7.779795 7.101294	H	-5.598150 -3.216345 5.955636
C	-4.966037 -1.727891 9.476977	H	-3.377099 -2.532675 5.126009
C	-5.095666 -4.187013 9.130822	H	-1.267565 0.327211 7.571552
C	-4.283282 -6.804264 11.675033	H	-2.879431 -0.088975 9.430288
C	-2.789194 -4.838698 12.977728	H	-7.353833 -2.874671 10.575894
C	-5.571108 -4.214245 7.708562	H	-6.306361 -4.081456 11.377147
C	-2.212177 -1.091771 6.236529	H	-6.080703 -2.339544 11.725033
C	-3.008357 -6.076906 13.605094	h	-4.657488 -7.224608 4.981898
C	-3.759711 -7.061270 12.936271	h	-2.941298 -11.029405 9.920700
C	-3.352890 -4.583670 11.727192	h	2.320720 -11.349935 7.201074
C	-4.112422 -5.550594 11.045018		

⁷TS2



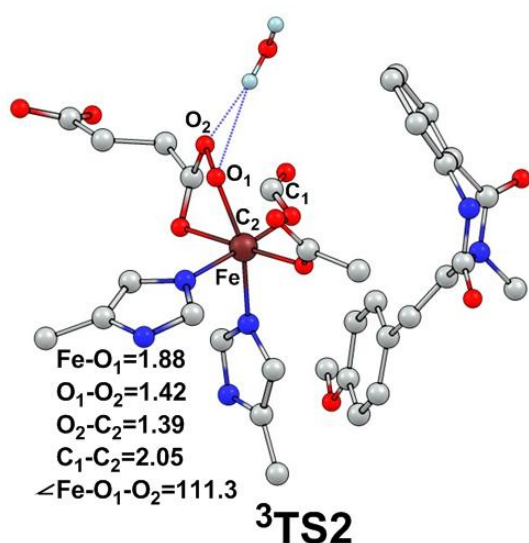
⁷TS2

O	1.003738	-1.275217	6.596736
H	0.846226	-0.983165	5.675774
H	1.001911	-2.247229	6.590169
Fe	-0.688171	-6.043390	7.433853
C	-0.123869	-3.805517	9.116869
O	-0.015737	-2.999643	10.012780
O	-1.113316	-4.345635	8.552904
C	1.321735	-4.504800	8.473252
O	1.087107	-5.789428	8.518950
C	2.564911	-3.888489	9.116836
C	3.895630	-4.553554	8.754276
C	5.127157	-4.086258	9.570676
O	6.252007	-4.440584	9.145318
O	4.956501	-3.431511	10.636058
H	2.566030	-2.822532	8.830420
H	2.418459	-3.926252	10.205859
H	4.131433	-4.428851	7.683175
H	3.813488	-5.644380	8.921312
C	-4.018780	-6.417917	4.607359
H	-4.008182	-6.586263	3.519694
H	-4.506611	-5.437825	4.768035
C	-2.564346	-6.263219	5.082875
O	-2.359704	-6.212943	6.369661
O	-1.679687	-6.140483	4.238529
O	0.392880	-4.700541	6.334389
O	1.275325	-4.012661	7.096353
C	-3.268742	-10.188328	10.374433
H	-3.337864	-10.337556	11.465786

H	-4.285397	-9.959868	10.011554
N	-1.225492	-8.701767	10.760314
H	-0.895218	-9.171311	11.609825
C	-2.345756	-9.062715	10.029887
C	-0.622260	-7.666924	10.131394
H	0.276006	-7.157053	10.480712
N	-1.297098	-7.344854	9.035088
C	-2.371449	-8.198511	8.962844
H	-3.093181	-8.130194	8.152403
C	2.539327	-10.560566	6.397016
H	2.669156	-11.175484	5.487645
H	3.502847	-10.066540	6.600197
N	0.233011	-9.777465	5.656145
H	-0.093403	-10.651091	5.230377
C	1.463216	-9.540890	6.246040
C	-0.538578	-8.688798	5.828329
H	-1.551534	-8.620523	5.444182
N	0.129614	-7.756103	6.484546
C	1.379147	-8.264504	6.745295
H	2.114768	-7.685647	7.299685
C	-4.920075	-1.719949	9.505107
C	-5.044202	-4.155581	9.084134
C	-4.313104	-6.756308	11.615895
C	-2.687434	-4.868091	12.871511
C	-5.559822	-4.140471	7.675626
C	-2.206152	-1.043369	6.254792
C	-3.024662	-6.054117	13.544189
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C	-3.187170	-4.622824	11.590983
C	-4.028416	-5.545987	10.945571
N	-5.239554	-3.058675	6.913036
C	-4.159742	-2.172776	7.130714
C	-3.299037	-1.882738	6.061071
C	-1.967781	-0.466135	7.508360
C	-2.855309	-0.703758	8.552545
C	-3.948920	-1.570298	8.382313
N	-5.307819	-2.979382	9.859902
C	-4.577314	-5.309818	9.605125
C	-1.985195	-5.348762	15.577583
O	-2.639654	-6.343573	14.810593
O	-6.267946	-5.042215	7.228604
O	-5.342002	-0.729038	10.114133

C	-6.283589	-3.109886	10.941464	H	-5.655602	-3.083394	5.962320
H	-4.662533	-6.181785	8.949478	H	-3.482121	-2.340312	5.086096
H	-4.947625	-7.499243	11.125909	H	-1.083590	0.152954	7.658338
H	-2.030013	-4.131655	13.335247	H	-2.708019	-0.227485	9.524859
H	-1.523555	-0.846362	5.425387	H	-7.312101	-2.930779	10.574835
H	-1.861888	-5.759204	16.592206	H	-6.233740	-4.121033	11.363353
H	-0.990793	-5.100163	15.167976	H	-6.051289	-2.377152	11.727503
H	-2.578667	-4.420170	15.634880	h	-4.646623	-7.189207	5.053444
H	-4.092109	-7.928903	13.422928	h	-2.946709	-11.144274	9.961483
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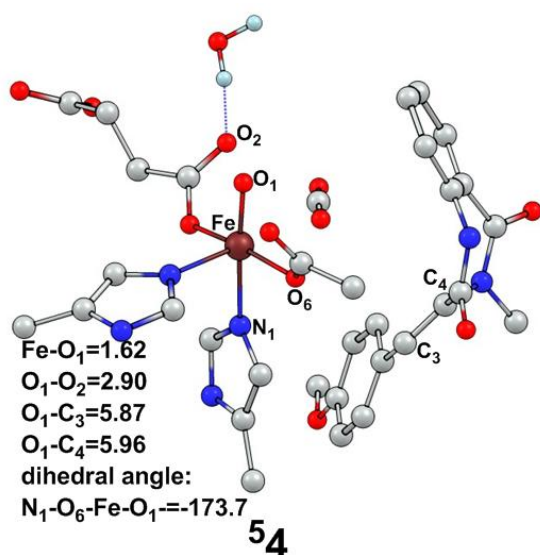
³TS2



O	0.966990	-1.430172	6.594315	H	3.980493	-5.627021	8.862063
H	0.856209	-1.098713	5.680345	C	-4.021710	-6.445237	4.556656
H	0.981311	-2.403962	6.544908	H	-4.018352	-6.626498	3.470925
Fe	-0.590001	-6.115338	7.318209	H	-4.499142	-5.458547	4.708064
C	-0.180843	-3.889579	9.008045	C	-2.560359	-6.304474	5.030563
O	-0.110021	-3.052667	9.861090	O	-2.356489	-6.268357	6.309494
O	-1.051655	-4.533526	8.399013	O	-1.682510	-6.189403	4.172940
C	1.565588	-4.663791	8.264282	O	0.565134	-5.120034	6.210945
O	1.303176	-5.878027	8.495177	O	1.347377	-4.204452	6.970661
C	2.691281	-3.895463	8.939373	C	-3.243098	-10.099626	10.309374
C	4.062708	-4.538299	8.683323	H	-3.298224	-10.206199	11.406331
C	5.241003	-4.064134	9.567595	H	-4.261843	-9.872406	9.951472
O	6.380222	-4.449113	9.210074	N	-1.191590	-8.617919	10.630901
O	5.019336	-3.393576	10.610979	H	-0.876995	-9.046568	11.504727
H	2.656441	-2.856133	8.571061	C	-2.309215	-9.000308	9.909347
H	2.488553	-3.881882	10.020689	C	-0.565824	-7.624546	9.959480
H	4.362833	-4.426769	7.627088	H	0.336880	-7.112672	10.293637
				N	-1.225367	-7.355070	8.838937
				C	-2.312372	-8.193189	8.796507
				H	-3.023007	-8.142951	7.976204
				C	2.532449	-10.579109	6.352708
				H	2.659158	-11.206171	5.451233
				H	3.496833	-10.082859	6.546562
				N	0.214251	-9.798718	5.633436
				H	-0.121648	-10.672605	5.215216
				C	1.456616	-9.559751	6.194138
				C	-0.558190	-8.712370	5.820187
				H	-1.580140	-8.641960	5.463824
				N	0.129315	-7.781115	6.455918
				C	1.387124	-8.280142	6.686289
				H	2.133616	-7.698522	7.220939

C	-4.926887	-1.723791	9.497301	O	-5.349408	-0.734986	10.109573
C	-5.035323	-4.158662	9.073512	C	-6.284566	-3.121208	10.932574
C	-4.279393	-6.758250	11.597280	H	-4.619893	-6.177791	8.930596
C	-2.682511	-4.856783	12.870255	H	-4.904736	-7.505283	11.101948
C	-5.557220	-4.146453	7.666182	H	-2.037352	-4.114389	13.342084
C	-2.215494	-1.035086	6.245724	H	-1.533931	-0.835033	5.416353
C	-3.009824	-6.049360	13.536322	H	-1.856176	-5.759444	16.588263
C	-3.804241	-7.007585	12.879468	H	-0.986525	-5.089812	15.168230
C	-3.179893	-4.611836	11.588467	H	-2.578876	-4.420058	15.636252
C	-4.004650	-5.542305	10.932671	H	-4.057703	-7.934005	13.402100
N	-5.239766	-3.064346	6.902727	H	-2.889538	-3.690569	11.077191
C	-4.164036	-2.174793	7.121498	H	-5.658432	-3.088181	5.953090
C	-3.303142	-1.881187	6.052520	H	-3.482222	-2.342165	5.078429
C	-1.982188	-0.454910	7.499014	H	-1.105626	0.175009	7.649529
C	-2.868218	-0.697253	8.543105	H	-2.725995	-0.217147	9.514429
C	-3.957073	-1.570518	8.373494	H	-7.313011	-2.936028	10.568999
N	-5.309966	-2.985199	9.850526	H	-6.237019	-4.135980	11.346077
C	-4.551879	-5.307463	9.590496	H	-6.049493	-2.395350	11.724314
C	-1.980239	-5.345109	15.575377	h	-4.654382	-7.205668	5.014409
O	-2.628378	-6.340008	14.803024	h	-2.940206	-11.075382	9.929605
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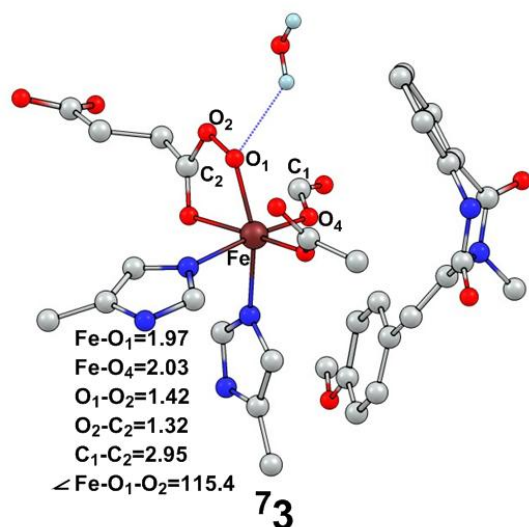
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O	2.910820	-1.472368	8.129527	O	-1.516923	-4.024951	8.450245
H	2.381549	-0.671233	7.983117	C	1.765675	-4.715985	8.449493
H	2.272731	-2.231140	8.081382	O	1.057535	-5.789836	8.284526
Fe	-0.531697	-6.033544	7.136517	C	3.091395	-4.909658	9.191374
C	-1.029232	-3.394296	9.296918	C	4.343999	-4.226918	8.615431
O	-0.621208	-2.771359	10.191021	C	5.495761	-4.121942	9.637980
				O	6.618412	-4.577408	9.308902
				O	5.267623	-3.569015	10.752376
				H	2.917557	-4.493698	10.201463
				H	3.263375	-5.990102	9.313043
				H	4.100374	-3.196460	8.309616
				H	4.714263	-4.763181	7.726249
				C	-4.039965	-6.400388	4.636507
				H	-4.084372	-6.481511	3.539647
				H	-4.483118	-5.423931	4.906697
				C	-2.557179	-6.363736	5.047324
				O	-2.311255	-6.322769	6.328679
				O	-1.705829	-6.354908	4.164696
				O	-0.045120	-4.976074	6.012139
				O	1.364838	-3.592705	8.130387

C	-3.216345 -10.008368 10.258050	N	-5.200276 -3.137064 6.911448
H	-3.269384 -10.088536 11.357636	C	-4.140068 -2.231706 7.123973
H	-4.235847 -9.786168 9.898891	C	-3.273795 -1.949574 6.055493
N	-1.152060 -8.541141 10.536439	C	-2.051885 -0.392176 7.445056
H	-0.826419 -8.972029 11.402993	C	-2.925172 -0.646872 8.499338
C	-2.285792 -8.913862 9.833951	C	-3.967198 -1.580704 8.359316
C	-0.541145 -7.540853 9.862827	N	-5.325918 -2.976406 9.861851
H	0.369518 -7.041170 10.188845	C	-4.614959 -5.321086 9.672978
N	-1.222206 -7.244276 8.762254	C	-1.959023 -5.374927 15.623925
C	-2.310982 -8.085879 8.736075	O	-2.584140 -6.377288 14.839487
H	-3.032144 -8.032093 7.925538	O	-6.277647 -5.084815 7.268941
C	2.599265 -10.675144 6.400279	O	-5.356073 -0.724622 10.085764
H	2.745086 -11.322529 5.515884	C	-6.303284 -3.081429 10.945986
H	3.566001 -10.195927 6.619079	H	-4.695776 -6.204033 9.032227
N	0.340627 -9.852387 5.563497	H	-4.847636 -7.566481 11.139092
H	-0.014359 -10.733011 5.177186	H	-2.149733 -4.078996 13.443178
C	1.558780 -9.635541 6.180978	H	-1.561888 -0.830437 5.377707
C	-0.394461 -8.727783 5.666866	H	-1.795947 -5.808423 16.623014
H	-1.387277 -8.632557 5.239718	H	-0.986518 -5.070020 15.200999
N	0.288310 -7.797672 6.306870	H	-2.593949 -4.478040 15.720229
C	1.506935 -8.338178 6.628307	H	-3.951081 -8.007558 13.415022
H	2.250573 -7.770448 7.182026	H	-3.102921 -3.622153 11.231378
C	-4.939039 -1.722497 9.485039	H	-5.611301 -3.175059 5.958608
C	-5.062207 -4.173358 9.118213	H	-3.420204 -2.456200 5.099024
C	-4.262052 -6.797297 11.648235	H	-1.252457 0.340971 7.563108
C	-2.759044 -4.843227 12.958836	H	-2.824159 -0.110149 9.445822
C	-5.558497 -4.187889 7.702596	H	-7.326271 -2.881439 10.576101
C	-2.231128 -1.041419 6.216688	H	-6.277171 -4.092100 11.369889
C	-3.003739 -6.073939 13.591175	H	-6.055977 -2.351830 11.730566
C	-3.756969 -7.053911 12.916775	h	-4.666946 -7.190784 5.049104
C	-3.301733 -4.588610 11.698955	h	-2.928012 -10.999090 9.906769
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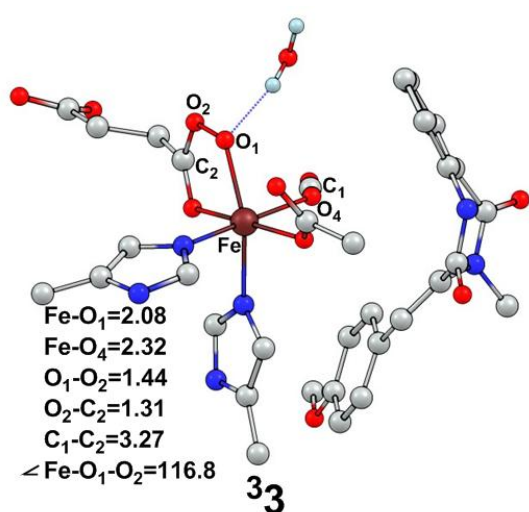


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H	0.588349	-1.052790	5.592146
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Fe	-0.739337	-5.900411	7.432940
C	-0.710866	-3.645552	9.361719
O	-0.965489	-2.939097	10.313099
O	-1.425822	-4.441612	8.671796
C	1.781848	-4.727301	8.207814
O	1.204767	-5.768837	8.530694
C	2.889288	-4.047243	8.972504
C	4.268664	-4.664678	8.713915
C	5.418602	-4.143241	9.608991
O	6.565878	-4.541620	9.295494
O	5.160134	-3.424230	10.607990
H	2.879287	-2.985347	8.680519
H	2.637235	-4.122193	10.041463
H	4.571969	-4.531293	7.660656
H	4.224081	-5.756901	8.883900
C	-4.018031	-6.403963	4.583966
H	-4.015072	-6.577859	3.497137
H	-4.512421	-5.427407	4.745746
C	-2.560057	-6.231136	5.040781
O	-2.348419	-6.137031	6.326416
O	-1.680560	-6.132168	4.190684
O	0.384164	-4.663606	6.389500
O	1.480098	-4.098976	7.089450
C	-3.238102	-10.129185	10.359771
H	-3.313864	-10.267880	11.452103

H	-4.250948	-9.892937	9.991036
N	-1.192562	-8.649636	10.754968
H	-0.873092	-9.116918	11.608847
C	-2.303309	-9.013207	10.012772
C	-0.585855	-7.611137	10.132157
H	0.301554	-7.095955	10.500211
N	-1.245926	-7.292779	9.027660
C	-2.317433	-8.149167	8.944593
H	-3.034394	-8.082036	8.129567
C	2.504456	-10.514454	6.392268
H	2.624775	-11.116965	5.473272
H	3.469841	-10.021070	6.590253
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H	-0.141050	-10.589377	5.252235
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C	-0.573145	-8.625030	5.865953
H	-1.588113	-8.555128	5.488362
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H	2.098170	-7.662796	7.324953
C	-4.934155	-1.742747	9.527843
C	-5.100840	-4.184047	9.120920
C	-4.376957	-6.822024	11.650437
C	-2.778877	-4.916147	12.912423
C	-5.601743	-4.172174	7.709993
C	-2.325503	-1.011313	6.209258
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C	-4.225295	-2.188227	7.140910
C	-3.408919	-1.868893	6.044890
C	-2.044099	-0.455992	7.464809
C	-2.888134	-0.724892	8.537214
C	-3.979859	-1.597039	8.390722
N	-5.337147	-2.995386	9.887000
C	-4.675109	-5.349620	9.656745
C	-2.017849	-5.408210	15.591867
O	-2.662973	-6.412751	14.829060
O	-6.287127	-5.085955	7.250743
O	-5.343165	-0.743137	10.132188

C	-6.312997	-3.103988	10.970219	H	-5.715054	-3.120228	5.995554
H	-4.786021	-6.221903	9.005853	H	-3.621989	-2.310073	5.068836
H	-4.997023	-7.575144	11.156960	H	-1.164570	0.175266	7.595898
H	-2.127985	-4.171280	13.371417	H	-2.707739	-0.268757	9.512825
H	-1.695992	-0.777167	5.347357	H	-7.338933	-2.913933	10.601709
H	-1.872129	-5.820526	16.602934	H	-6.277977	-4.111927	11.400257
H	-1.033790	-5.137196	15.170383	H	-6.069974	-2.368591	11.750307
H	-2.628321	-4.491714	15.661784	h	-4.636586	-7.177745	5.038629
H	-4.107162	-8.014982	13.438009	h	-2.928561	-11.094000	9.958047
H	-3.014136	-3.740307	11.139150	h	2.306998	-11.231851	7.188773

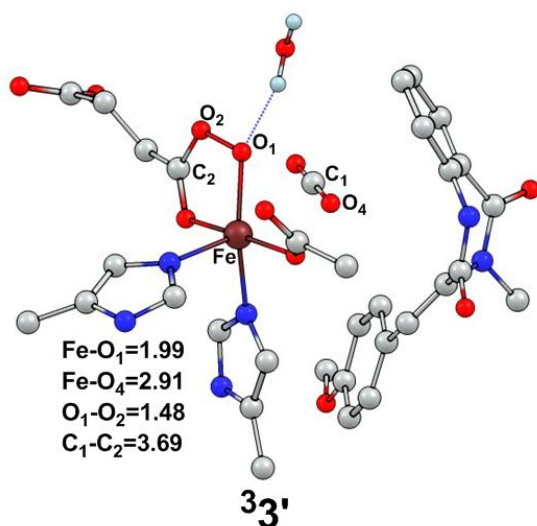
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O	0.527243	-1.749875	6.447950	C	-4.056328	-6.456997	4.480567
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H	0.408508	-2.705866	6.247437	H	-4.562360	-5.476458	4.562365
Fe	-0.603015	-5.958539	7.188856	C	-2.605958	-6.246312	4.970744
C	-0.987437	-3.441934	9.137441	O	-2.421982	-6.120616	6.235953
O	-0.594252	-2.854507	10.059546	O	-1.721288	-6.157828	4.107909
O	-1.399139	-4.044311	8.231092	O	0.686970	-4.609647	6.272788
C	1.906903	-4.669224	8.247456	O	1.816046	-4.169597	7.040756
O	1.152813	-5.548244	8.663439	C	-3.210676	-10.036490	10.294652
C	3.013468	-4.013308	9.044494	H	-3.278146	-10.146562	11.391200
C	4.387984	-4.631701	8.781725	H	-4.226303	-9.805270	9.929281
C	5.541308	-4.120629	9.672582	N	-1.167470	-8.558439	10.654238
O	6.682251	-4.537641	9.360096	H	-0.843688	-9.026245	11.503279
O	5.294380	-3.388278	10.667239	C	-2.277505	-8.927312	9.916262
H	3.024768	-2.946838	8.765749	C	-0.568039	-7.515279	10.024457
H	2.756420	-4.097264	10.111403	H	0.324046	-7.005506	10.389154
H	4.686651	-4.496877	7.727607	N	-1.228686	-7.195104	8.920866
H	4.337803	-5.724981	8.944937	C	-2.295087	-8.061030	8.846040
				H	-3.007734	-7.996134	8.026046
				C	2.517415	-10.489817	6.387791
				H	2.643948	-11.094168	5.470488
				H	3.485445	-10.004738	6.594301
				N	0.219667	-9.683934	5.649263
				H	-0.119871	-10.560958	5.244120
				C	1.449103	-9.459344	6.239688
				C	-0.528818	-8.569490	5.783959
				H	-1.535797	-8.487718	5.389679
				N	0.152853	-7.633383	6.421099
				C	1.387023	-8.167213	6.705085
				H	2.142507	-7.600968	7.244579
				C	-4.992810	-1.744039	9.527338

C	-5.101849	-4.185477	9.129522	C	-6.354639	-3.126621	10.971760
C	-4.273815	-6.803472	11.645730	H	-4.689653	-6.206827	9.021116
C	-2.773814	-4.849857	12.959018	H	-4.857975	-7.572514	11.135135
C	-5.616225	-4.195991	7.718662	H	-2.169029	-4.084764	13.447475
C	-2.368795	-1.004179	6.222171	H	-1.723768	-0.781613	5.371336
C	-3.018737	-6.080619	13.590295	H	-1.811849	-5.822240	16.624232
C	-3.770973	-7.060009	12.915137	H	-0.998017	-5.086103	15.203886
C	-3.312316	-4.595476	11.696532	H	-2.603382	-4.487114	15.722966
C	-4.077727	-5.555315	11.012033	H	-3.964523	-8.014392	13.411980
N	-5.317512	-3.112486	6.945872	H	-3.111706	-3.629470	11.227430
C	-4.260713	-2.201568	7.146013	H	-5.729239	-3.155815	5.993773
C	-3.438036	-1.875732	6.055417	H	-3.630175	-2.334740	5.083410
C	-2.111248	-0.428151	7.474736	H	-1.249802	0.228351	7.606311
C	-2.963045	-0.696057	8.539386	H	-2.815051	-0.208535	9.506519
C	-4.035978	-1.597027	8.394488	H	-7.381859	-2.942972	10.605105
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C	-4.626028	-5.328273	9.669752	H	-6.118968	-2.394038	11.757042
C	-1.972886	-5.387077	15.625373	h	-4.674241	-7.205593	4.976404
O	-2.600728	-6.385582	14.840541	h	-2.917756	-11.018381	9.922960
O	-6.308371	-5.110971	7.280175	h	2.310324	-11.208146	7.181003
O	-5.403599	-0.748717	10.136824				

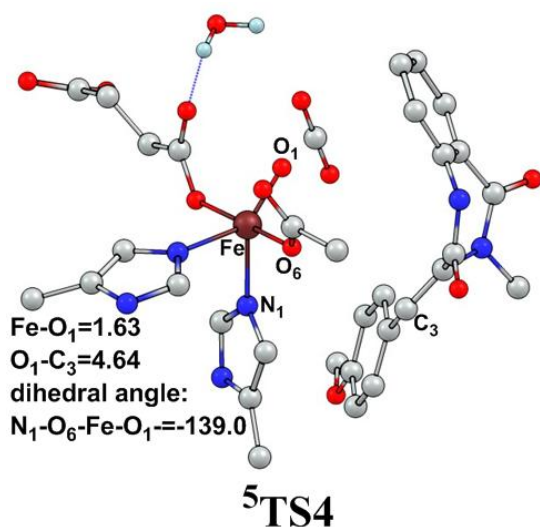
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O	0.654592	-1.508542	6.487407	C	1.840440	-4.886202	8.200995
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H	0.325403	-2.430627	6.417564	C	3.012541	-4.539757	9.090021
Fe	-0.535441	-6.009356	7.276472	C	4.340331	-4.137777	8.437336
C	-0.899817	-3.290850	9.395199	C	5.461765	-3.976821	9.491889
O	-0.093969	-2.823870	10.097475	O	6.578287	-4.482165	9.227416
O	-1.711932	-3.772927	8.724075	O	5.200245	-3.359811	10.559956
				H	2.668403	-3.725456	9.753054
				H	3.150046	-5.415422	9.737980
				H	4.223854	-3.182086	7.891870
				H	4.668426	-4.885218	7.697169
				C	-3.963306	-6.379625	4.593908
				H	-3.969698	-6.540379	3.504942
				H	-4.446842	-5.399709	4.768049
				C	-2.489595	-6.236941	5.051533
				O	-2.277916	-6.140887	6.317028
				O	-1.623721	-6.176438	4.169163
				O	0.267863	-4.322062	6.593905
				O	1.586882	-4.081133	7.215325
				C	-3.271716	-10.030842	10.260159

H	-3.361626 -10.128972 11.356170	C	-4.254951 -2.184087 7.154349
H	-4.282856 -9.821664 9.870332	C	-3.411143 -1.878055 6.074762
N	-1.241746 -8.542850 10.628074	C	-2.113774 -0.403355 7.494305
H	-0.922655 -9.002391 11.482737	C	-2.987232 -0.653817 8.546428
C	-2.349461 -8.912118 9.885183	C	-4.054011 -1.559925 8.395776
C	-0.639364 -7.503507 10.003092	N	-5.383592 -2.979502 9.894529
H	0.256186 -7.004952 10.371986	C	-4.639711 -5.309318 9.677419
N	-1.298213 -7.179318 8.897479	C	-1.950418 -5.360654 15.614691
C	-2.366708 -8.041859 8.817901	O	-2.572102 -6.364750 14.832444
H	-3.068642 -7.977393 7.990184	O	-6.309952 -5.090335 7.287608
C	2.569333 -10.653270 6.398349	O	-5.427192 -0.728156 10.138966
H	2.692128 -11.301665 5.511137	C	-6.355070 -3.107459 10.979504
H	3.545118 -10.183153 6.597974	H	-4.705821 -6.187984 9.029670
N	0.305207 -9.791160 5.602063	H	-4.859981 -7.554387 11.145713
H	-0.069178 -10.664739 5.219464	H	-2.158370 -4.062039 13.437197
C	1.536478 -9.601086 6.200714	H	-1.681480 -0.794287 5.408155
C	-0.399326 -8.644182 5.715601	H	-1.780496 -5.793857 16.612862
H	-1.394311 -8.525553 5.297857	H	-0.980587 -5.050082 15.188559
N	0.307654 -7.725641 6.346501	H	-2.589459 -4.466949 15.715067
C	1.513463 -8.303879 6.649871	H	-3.947964 -7.994268 13.416706
H	2.286336 -7.768392 7.197158	H	-3.130188 -3.608393 11.223425
C	-5.009510 -1.719560 9.527434	H	-5.719461 -3.139585 5.996126
C	-5.109885 -4.165182 9.136870	H	-3.584331 -2.353991 5.107002
C	-4.273416 -6.784335 11.652011	H	-1.253464 0.253457 7.627940
C	-2.765403 -4.828397 12.953205	H	-2.859805 -0.148136 9.507619
C	-5.617486 -4.174849 7.725675	H	-7.383671 -2.929385 10.614072
C	-2.345182 -1.003348 6.248151	H	-6.305757 -4.117687 11.402510
C	-3.002356 -6.060166 13.585934	H	-6.121231 -2.373075 11.763551
C	-3.759080 -7.040237 12.917299	h	-4.593458 -7.153103 5.032891
C	-3.316129 -4.575238 11.695876	h	-2.953722 -11.010935 9.904683
C	-4.085330 -5.535983 11.017009	h	2.326683 -11.325539 7.221296
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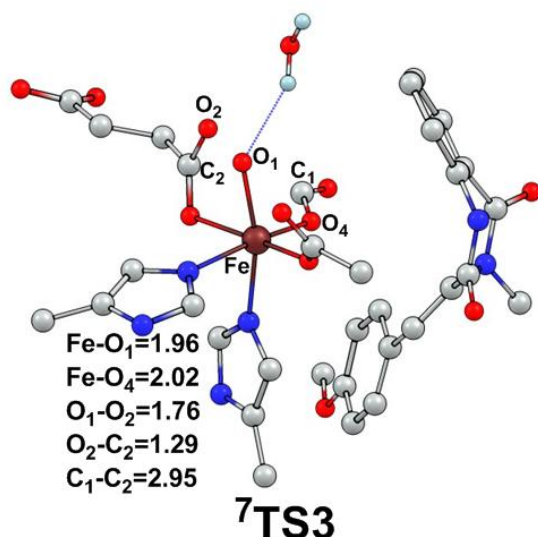
⁵TS4



O	2.705881	-1.751415	7.499900
H	1.848490	-1.302354	7.553833
H	2.489894	-2.628684	7.103977
Fe	-0.773849	-6.029194	7.377016
C	-0.365473	-2.555368	9.417085
O	0.131014	-2.197858	8.436960
O	-0.857989	-2.879840	10.424447
C	1.895858	-4.928673	7.908405
O	0.947902	-5.778326	8.220275
C	2.977122	-4.783711	8.987845
C	4.354175	-4.353438	8.465521
C	5.437344	-4.165109	9.546279
O	6.574167	-4.650019	9.313419
O	5.158450	-3.516534	10.592399
H	2.611891	-4.038055	9.718222
H	3.030373	-5.731436	9.544357
H	4.250122	-3.379708	7.957184
H	4.731146	-5.067606	7.715809
C	-3.969849	-6.549202	4.482899
H	-3.909214	-6.834442	3.421569
H	-4.440106	-5.548306	4.502473
C	-2.534692	-6.350079	5.009494
O	-2.380717	-6.385859	6.299131
O	-1.643120	-6.112010	4.198875
O	-0.849440	-4.454304	6.981625
O	1.935402	-4.303017	6.857940
C	-3.279157	-10.191643	10.371988
H	-3.340033	-10.334903	11.464823
H	-4.299177	-9.968814	10.015067

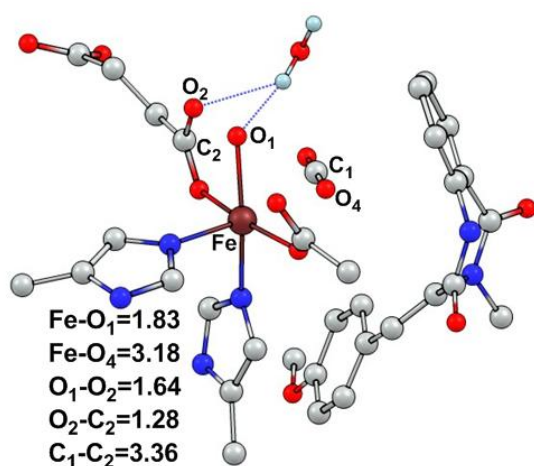
N	-1.246960	-8.682148	10.737808
H	-0.904982	-9.145728	11.584852
C	-2.366059	-9.061742	10.014260
C	-0.668192	-7.632615	10.106894
H	0.217296	-7.102893	10.459018
N	-1.352154	-7.326299	9.012295
C	-2.412105	-8.197519	8.947981
H	-3.138974	-8.140580	8.140921
C	2.494610	-10.552553	6.399637
H	2.628910	-11.161867	5.487037
H	3.453269	-10.047338	6.600759
N	0.171911	-9.796256	5.675423
H	-0.152454	-10.673682	5.257731
C	1.405543	-9.545745	6.251075
C	-0.607569	-8.715149	5.853994
H	-1.629383	-8.664065	5.492605
N	0.054630	-7.771420	6.499392
C	1.312500	-8.268706	6.744487
H	2.054225	-7.692384	7.289421
C	-4.953050	-1.730272	9.475902
C	-5.039992	-4.183706	9.096544
C	-4.312030	-6.800488	11.655218
C	-2.772224	-4.864188	12.947042
C	-5.509312	-4.195194	7.670175
C	-2.212801	-0.962206	6.256052
C	-3.042078	-6.081966	13.592778
C	-3.816769	-7.053001	12.929229
C	-3.297168	-4.614881	11.679031
C	-4.083136	-5.565738	11.006704
N	-5.128156	-3.151254	6.884200
C	-4.096012	-2.221064	7.126052
C	-3.215839	-1.910127	6.076152
C	-2.086734	-0.299082	7.484037
C	-2.970723	-0.586034	8.519205
C	-3.972760	-1.561180	8.362928
N	-5.327129	-2.992019	9.839949
C	-4.603040	-5.334820	9.653898
C	-1.975001	-5.383081	15.614919
O	-2.625988	-6.380077	14.845900
O	-6.230175	-5.086962	7.227062
O	-5.392095	-0.742920	10.080195
C	-6.307964	-3.109950	10.920922

⁷TS3

S39

C	1.328999	-8.224780	6.789375	O	-6.290853	-5.089461	7.251347
H	2.079042	-7.665898	7.342515	O	-5.360958	-0.745475	10.135227
C	-4.949750	-1.743325	9.529518	C	-6.323034	-3.110212	10.972779
C	-5.107123	-4.185005	9.122352	H	-4.785251	-6.221693	9.006669
C	-4.375709	-6.822387	11.650211	H	-4.994553	-7.576161	11.156233
C	-2.781784	-4.914297	12.914343	H	-2.132850	-4.168356	13.374460
C	-5.606454	-4.174420	7.710392	H	-1.680656	-0.793686	5.370561
C	-2.323291	-1.018629	6.224438	H	-1.871639	-5.824594	16.603533
C	-3.077356	-6.118627	13.572338	H	-1.034054	-5.137824	15.172208
C	-3.872903	-7.080272	12.920996	H	-2.628882	-4.494372	15.665173
C	-3.310316	-4.658640	11.649239	H	-4.102689	-8.016875	13.436190
C	-4.131717	-5.593978	10.996340	H	-3.023393	-3.735510	11.143430
N	-5.304377	-3.085862	6.947111	H	-5.717911	-3.122714	5.995962
C	-4.231324	-2.189035	7.145878	H	-3.614300	-2.318340	5.078448
C	-3.407695	-1.873387	6.054290	H	-1.168634	0.167690	7.614926
C	-2.050169	-0.459626	7.479919	H	-2.727449	-0.264835	9.522553
C	-2.902001	-0.723195	8.546841	H	-7.350311	-2.924384	10.605943
C	-3.992750	-1.596041	8.395824	H	-6.283174	-4.117816	11.403178
N	-5.349341	-2.997640	9.888231	H	-6.081958	-2.373315	11.752038
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C	-2.017848	-5.410319	15.593324	h	-2.932068	-11.108109	9.961857
O	-2.662643	-6.413821	14.829035	h	2.302576	-11.232011	7.189222

³TS3

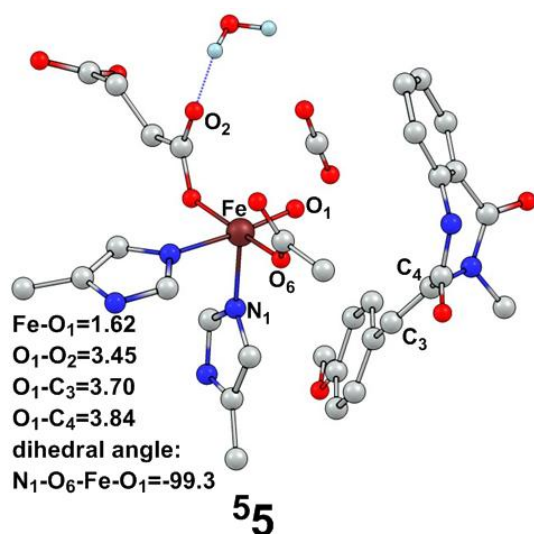


³TS3

O	0.639565	-1.758433	6.610107	O	-0.339035	-2.729325	10.093491
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H	0.482322	-2.707373	6.391971	C	1.922285	-4.713933	8.205662
Fe	-0.616197	-5.958203	7.136292	O	0.989472	-5.414751	8.629546
C	-0.925461	-3.218827	9.213395	C	3.041426	-4.257283	9.111095
				C	4.433909	-4.100855	8.494275
				C	5.544487	-3.931739	9.553060
				O	6.645454	-4.482510	9.311340
				O	5.299963	-3.264536	10.594678
				H	2.701969	-3.300409	9.546745
				H	3.052924	-4.970404	9.948584
				H	4.455621	-3.225125	7.818309
				H	4.692979	-4.971267	7.871221
				C	-4.007996	-6.475843	4.412454
				H	-3.994354	-6.748855	3.346183
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				C	-2.550350	-6.255344	4.880877
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O	-1.676159 -6.157782 4.012366	C	-4.074538 -5.530926 10.993895
O	0.544707 -4.551207 6.251738	N	-5.285300 -3.089440 6.922646
O	1.960635 -4.328990 6.958496	C	-4.231798 -2.175639 7.133452
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H	-3.321857 -10.031350 11.326255	C	-2.097264 -0.388708 7.481914
H	-4.286971 -9.773189 9.859906	C	-2.969453 -0.647185 8.533066
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H	-0.928121 -8.845057 11.387361	N	-5.370856 -2.977424 9.868603
C	-2.373962 -8.826815 9.807448	C	-4.623186 -5.304782 9.651265
C	-0.712400 -7.354224 9.893353	C	-1.957428 -5.354006 15.599743
H	0.167990 -6.818840 10.248476	O	-2.588598 -6.355283 14.820940
N	-1.400078 -7.060540 8.795023	O	-6.282818 -5.085891 7.251332
C	-2.435812 -7.964100 8.734697	O	-5.409589 -0.727587 10.123738
H	-3.152873 -7.928284 7.918217	C	-6.341588 -3.107586 10.954721
C	2.579400 -10.632130 6.401348	H	-4.691134 -6.184030 9.004657
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H	3.554346 -10.160801 6.602132	H	-2.128994 -4.071303 13.406842
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H	-0.054522 -10.664200 5.231608	H	-1.795186 -5.784139 16.600490
C	1.540902 -9.583526 6.210913	H	-0.983150 -5.056139 15.174943
C	-0.413223 -8.654701 5.746364	H	-2.587026 -4.452840 15.693764
H	-1.418265 -8.550728 5.347234	H	-3.986106 -7.973005 13.412777
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C	1.503910 -8.286728 6.664965	H	-5.691613 -3.132315 5.968205
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C	-5.594011 -4.170175 7.694341	H	-6.102879 -2.379614 11.743369
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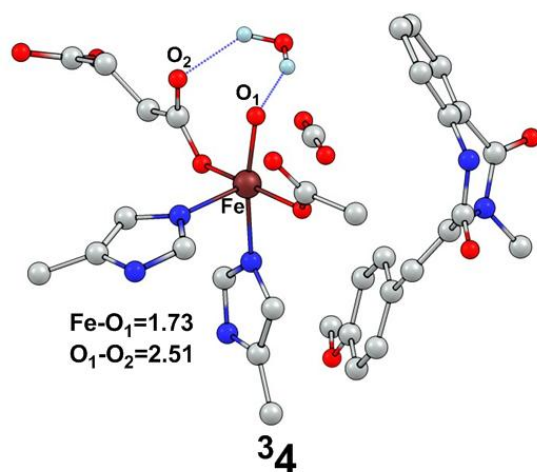


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Fe	-0.777549	-6.081594	7.417450
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C	2.997630	-4.793067	8.962958
C	4.367440	-4.338260	8.443369
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C	-3.951562	-6.562029	4.461835
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C	-3.301904	-10.199095	10.384621
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H	-4.322303	-9.980584	10.026222
N	-1.277607	-8.685170	10.766215
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H	-0.152184	-10.661033	5.246254
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O	-2.627709	-6.377756	14.845609
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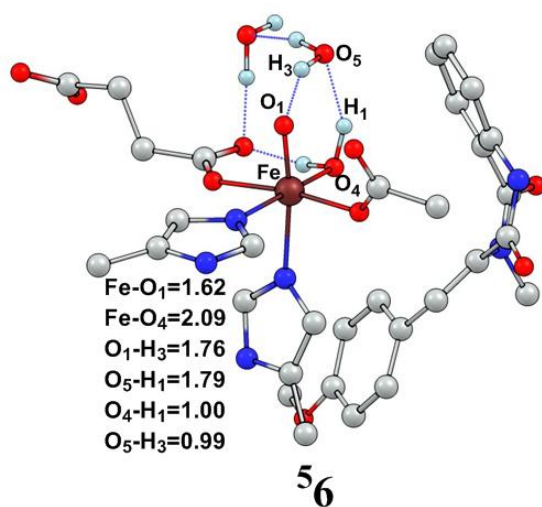
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Fe	-0.603939	-5.975799	7.178878	C	4.384190	-4.224028	8.556027
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				H	-4.500237	-5.438127	4.797548
				C	-2.563148	-6.315885	5.034805
				O	-2.348686	-6.274106	6.322100
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				O	-0.232943	-4.684528	6.090462
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C	-3.191232 -9.968753 10.264436	N	-5.195555 -3.092051 6.908927
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N	0.232741 -7.749802 6.338691	H	-2.601182 -4.484042 15.705455
C	1.457433 -8.285060 6.648466	H	-3.972409 -7.997499 13.394144
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C	-4.973946 -1.711053 9.501942	H	-5.597399 -3.123652 5.952216
C	-5.070619 -4.156209 9.104427	H	-3.400565 -2.357101 5.125316
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C	-2.761289 -4.840927 12.937221	H	-2.855036 -0.109952 9.530468
C	-5.551145 -4.155145 7.682251	H	-7.354564 -2.897334 10.572177
C	-2.215922 -0.978849 6.295748	H	-6.302050 -4.116695 11.348920
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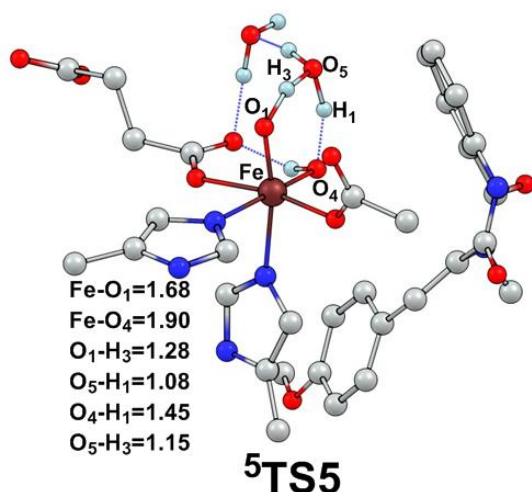


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C	3.208076	-5.010682	9.344279
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C	5.515390	-4.013342	9.612272
O	6.613922	-4.509873	9.271516
O	5.322923	-3.404700	10.704262
H	3.181927	-4.710261	10.404832
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H	-1.635020	-0.717598	5.362485	H	-6.243562	-4.134698	11.347602
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H	-2.578790	-4.408195	15.643913	h	-2.940334	-10.935503	9.900196
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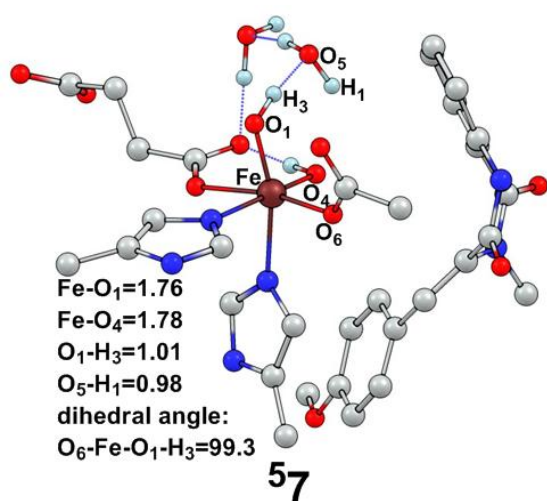
⁵TS5



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Fe	-0.580059	-5.963382	7.018703	H	0.801183	-2.437230	6.688332
C	1.811143	-4.920468	8.885363	C	-4.062181	-6.549757	4.368966
O	1.331876	-5.875310	8.220765	H	-4.083139	-6.810756	3.299390
C	3.255073	-5.027885	9.363039	H	-4.528162	-5.549201	4.451443
C	4.328636	-4.170173	8.665560	C	-2.590004	-6.373892	4.794571
C	5.530619	-3.982889	9.616739	O	-2.340994	-6.398135	6.066895
O	6.625439	-4.510830	9.310774	O	-1.762121	-6.174523	3.907657
O	5.330792	-3.331330	10.681459	O	0.232396	-5.196506	5.770698
H	3.233984	-4.720190	10.421480	O	1.148538	-3.895462	9.243670
H	3.555401	-6.085501	9.307450	C	-3.244515	-9.922921	10.206258
H	3.914296	-3.179411	8.416606	H	-3.297337	-9.965763	11.308016
H	4.662999	-4.634733	7.724376	H	-4.265124	-9.717671	9.840279
O	-1.108598	-4.339392	7.849618	N	-1.167290	-8.477091	10.419517
H	-0.480637	-4.206937	8.610079	H	-0.825728	-8.900713	11.281955
				C	-2.321908	-8.836050	9.746523
				C	-0.562120	-7.485731	9.731444
				H	0.376684	-7.028267	10.024318
				N	-1.266140	-7.176848	8.652058
				C	-2.366429	-8.005372	8.648864
				H	-3.104388	-7.941582	7.853971
				C	2.539447	-10.623718	6.368486
				H	2.679261	-11.256521	5.472542
				H	3.502094	-10.128599	6.572981
				N	0.232144	-9.844168	5.617749
				H	-0.115296	-10.727588	5.230685
				C	1.470594	-9.603835	6.186430
				C	-0.526479	-8.741773	5.766420

H	-1.547269	-8.668817	5.406649	O	-2.584709	-6.310573	14.788642
N	0.163708	-7.803322	6.386472	O	-6.234399	-5.053991	7.199305
C	1.410997	-8.312029	6.645361	O	-5.341857	-0.732314	10.105825
H	2.156650	-7.721211	7.169151	C	-6.276046	-3.117526	10.918065
C	-4.922938	-1.718138	9.484659	H	-4.609043	-6.174830	8.931683
C	-5.024198	-4.155208	9.059857	H	-4.896766	-7.486680	11.114840
C	-4.264745	-6.739015	11.600511	H	-1.982482	-4.099365	13.305981
C	-2.642764	-4.837706	12.847286	H	-1.626657	-0.677142	5.355711
C	-5.531795	-4.150739	7.647674	H	-1.832674	-5.716635	16.578130
C	-2.278731	-0.917336	6.198174	H	-0.970895	-5.026280	15.164277
C	-2.973470	-6.024098	13.523756	H	-2.579221	-4.392257	15.622469
C	-3.779049	-6.982003	12.879602	H	-4.031381	-7.903992	13.410396
C	-3.156189	-4.598161	11.570350	H	-2.875793	-3.679466	11.048701
C	-3.991470	-5.527728	10.927237	H	-5.615529	-3.107943	5.925624
N	-5.206231	-3.072536	6.878967	H	-3.486186	-2.292893	5.051934
C	-4.156423	-2.158099	7.100757	H	-1.266190	0.407671	7.578637
C	-3.321435	-1.821994	6.023650	H	-2.803712	-0.118899	9.473625
C	-2.068037	-0.322534	7.449050	H	-7.303969	-2.923173	10.558190
C	-2.918670	-0.620457	8.509274	H	-6.233660	-4.135653	11.323418
C	-3.962704	-1.548552	8.354415	H	-6.034371	-2.399177	11.714653
N	-5.304097	-2.979791	9.832715	h	-4.686575	-7.267809	4.900567
C	-4.542235	-5.300377	9.585354	h	-2.955050	-10.925017	9.889904
C	-1.960183	-5.304071	15.565022	h	2.316991	-11.314121	7.182073

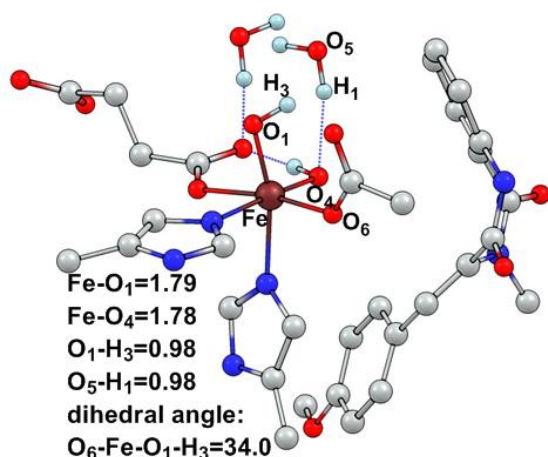
57



O	2.096608	-1.773018	7.839954	O	1.329886	-5.919523	8.307057
H	1.707714	-0.940573	8.171388	C	3.241358	-4.967280	9.379871
H	1.753983	-2.498602	8.449278	C	4.332549	-4.145907	8.669030
Fe	-0.611231	-5.984248	7.071327	C	5.538841	-3.976028	9.617544
C	1.809731	-4.903091	8.866792	O	6.632818	-4.497143	9.298231
				O	5.344808	-3.339179	10.692918
				H	3.198293	-4.613714	10.423823
				H	3.543244	-6.024835	9.379658
				H	3.946184	-3.147595	8.405905
				H	4.656756	-4.633532	7.735893
				O	-1.096689	-4.471031	7.869517
				H	-0.330826	-4.173218	8.463204
				H	-0.562034	-2.754595	6.751594
				O	0.166679	-2.628098	6.111647
				H	0.329023	-4.209752	5.862812
				H	0.938026	-2.255507	6.617755
				C	-4.067941	-6.551611	4.390932
				H	-4.085458	-6.802448	3.318942

H	-4.528523	-5.549473	4.482676	C	-3.780939	-6.985456	12.882162
C	-2.597952	-6.395184	4.827381	C	-3.159489	-4.601438	11.572305
O	-2.363503	-6.408845	6.104656	C	-3.993311	-5.532180	10.928987
O	-1.754960	-6.223490	3.950416	N	-5.225171	-3.080633	6.881018
O	0.335990	-5.221131	5.805399	C	-4.172503	-2.168265	7.095242
O	1.140316	-3.841748	9.097462	C	-3.342969	-1.836011	6.011944
C	-3.260458	-9.970840	10.232499	C	-2.072774	-0.343317	7.429107
H	-3.314614	-10.025945	11.333629	C	-2.918454	-0.635803	8.494769
H	-4.280638	-9.763518	9.866742	C	-3.968588	-1.558604	8.347020
N	-1.177975	-8.530915	10.455646	N	-5.306276	-2.984451	9.833211
H	-0.836964	-8.959203	11.316607	C	-4.545640	-5.306054	9.587685
C	-2.334943	-8.882671	9.782718	C	-1.961965	-5.305843	15.566941
C	-0.562602	-7.547756	9.764359	O	-2.588789	-6.311843	14.791590
H	0.379003	-7.092607	10.054008	O	-6.242643	-5.066752	7.206197
N	-1.265295	-7.239028	8.684252	O	-5.338012	-0.736018	10.103471
C	-2.372702	-8.056621	8.681852	C	-6.275771	-3.119555	10.921177
H	-3.111064	-7.988562	7.887733	H	-4.614305	-6.181373	8.935185
C	2.528319	-10.598832	6.383265	H	-4.896637	-7.492083	11.116766
H	2.674722	-11.226040	5.484414	H	-1.988495	-4.100531	13.309239
H	3.486744	-10.096977	6.591430	H	-1.648022	-0.697246	5.331128
N	0.216342	-9.832735	5.627415	H	-1.834063	-5.718191	16.580058
H	-0.121667	-10.715963	5.231692	H	-0.972603	-5.030026	15.164939
C	1.451738	-9.585546	6.201975	H	-2.579512	-4.393079	15.624576
C	-0.550699	-8.736916	5.773000	H	-4.032992	-7.907322	13.413268
H	-1.569488	-8.672429	5.406989	H	-2.879737	-3.682423	11.050949
N	0.131249	-7.793645	6.396370	H	-5.634484	-3.120224	5.927575
C	1.381827	-8.294410	6.660932	H	-3.517834	-2.303598	5.040607
H	2.120163	-7.699726	7.190586	H	-1.264722	0.380688	7.552776
C	-4.923976	-1.723840	9.482496	H	-2.794072	-0.134596	9.458171
C	-5.029166	-4.161512	9.061568	H	-7.304067	-2.922906	10.563727
C	-4.265770	-6.743593	11.602641	H	-6.234795	-4.137751	11.326501
C	-2.646978	-4.839936	12.849708	H	-6.030403	-2.401800	11.717182
C	-5.542749	-4.160398	7.651728	h	-4.696713	-7.272111	4.913992
C	-2.296358	-0.933648	6.177263	h	-2.963923	-10.966561	9.902844
C	-2.976781	-6.026476	13.526455	h	2.311487	-11.295125	7.193344

⁵TS6



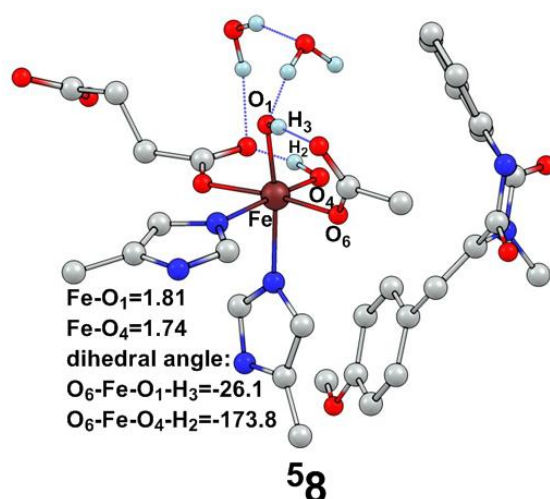
⁵TS6

O	2.280561	-1.825492	7.778376
H	1.691941	-1.053060	7.699628
H	1.781874	-2.478580	8.338304
Fe	-0.558815	-6.053682	7.114842
C	1.750648	-4.908467	8.824643
O	1.287407	-5.952869	8.274702
C	3.168900	-4.967359	9.375595
C	4.292146	-4.195126	8.658239
C	5.496018	-4.024947	9.611427
O	6.600049	-4.518405	9.280545
O	5.296561	-3.404128	10.693963
H	3.107564	-4.568401	10.401964
H	3.451384	-6.028919	9.427768
H	3.938525	-3.193404	8.364928
H	4.614380	-4.715761	7.742376
O	-1.143518	-4.523229	7.805536
H	-0.380613	-4.156084	8.375285
H	-0.450085	-3.063209	6.606530
O	0.076919	-2.476312	6.027505
H	-0.219829	-4.843906	5.162761
H	0.995579	-2.542185	6.356150
C	-4.031613	-6.578528	4.376085
H	-3.974333	-6.912573	3.327725
H	-4.531895	-5.592181	4.338694
C	-2.600598	-6.290015	4.867465
O	-2.324427	-6.486110	6.111949
O	-1.813820	-5.828075	4.030838
O	0.375995	-5.336837	5.767903
O	1.071579	-3.855846	9.005285

C	-3.259466	-9.996047	10.253711
H	-3.319350	-10.063571	11.353759
H	-4.276160	-9.777338	9.885096
N	-1.171087	-8.566997	10.506140
H	-0.842170	-9.001550	11.369940
C	-2.324044	-8.909746	9.821687
C	-0.544505	-7.584535	9.824250
H	0.395638	-7.132088	10.123014
N	-1.236844	-7.269380	8.738922
C	-2.349354	-8.080393	8.723736
H	-3.082542	-8.006830	7.925402
C	2.535034	-10.658335	6.365596
H	2.670673	-11.292342	5.470332
H	3.495837	-10.157221	6.563278
N	0.215162	-9.890457	5.635724
H	-0.125424	-10.768052	5.228279
C	1.456334	-9.646890	6.196604
C	-0.560857	-8.807607	5.825196
H	-1.588943	-8.735310	5.485789
N	0.125517	-7.878734	6.464017
C	1.384843	-8.370147	6.692478
H	2.128321	-7.780633	7.221033
C	-4.954251	-1.728778	9.492330
C	-5.045544	-4.167902	9.069835
C	-4.268360	-6.750955	11.609842
C	-2.662870	-4.838180	12.859108
C	-5.552192	-4.168511	7.656717
C	-2.310296	-0.930573	6.205503
C	-2.979053	-6.030306	13.532348
C	-3.777873	-6.993198	12.887354
C	-3.180255	-4.599832	11.583703
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N	-5.236684	-3.088346	6.890059
C	-4.189189	-2.168164	7.110554
C	-3.354333	-1.833859	6.032698
C	-2.099174	-0.337098	7.457299
C	-2.951152	-0.629053	8.516111
C	-3.996912	-1.557227	8.362572
N	-5.331168	-2.993419	9.841003
C	-4.558893	-5.310838	9.596705
C	-1.956251	-5.309501	15.568681
O	-2.582798	-6.317059	14.794740

O	-6.245635	-5.080354	7.208664	H	-2.911878	-3.675364	11.065996
O	-5.375085	-0.745756	10.116344	H	-5.647810	-3.122584	5.937664
C	-6.299847	-3.134253	10.928358	H	-3.519435	-2.305729	5.061336
H	-4.623611	-6.186228	8.943826	H	-1.287053	0.380679	7.588196
H	-4.895799	-7.502556	11.124201	H	-2.832758	-0.128843	9.480838
H	-2.012018	-4.093419	13.320635	H	-7.328817	-2.937526	10.572904
H	-1.648708	-0.701123	5.369601	H	-6.257342	-4.153638	11.330464
H	-1.818422	-5.724014	16.579615	H	-6.055614	-2.418603	11.726594
H	-0.971523	-5.026776	15.159784	h	-4.671871	-7.278768	4.912556
H	-2.578722	-4.400642	15.633860	h	-2.965787	-10.988928	9.913115
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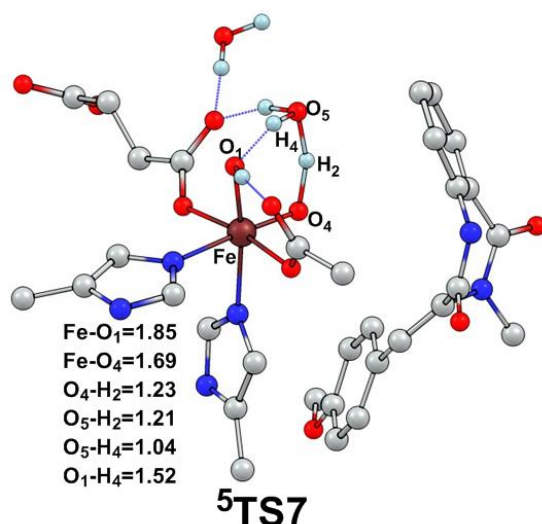
⁵8



H	-0.328783	-4.162563	8.618632	H	-0.328783	-4.162563	8.618632
H	-0.476522	-2.367313	6.763793	H	-0.476522	-2.367313	6.763793
O	0.260999	-2.517356	6.149063	O	0.260999	-2.517356	6.149063
H	-0.419504	-5.564512	5.031152	H	-0.419504	-5.564512	5.031152
H	0.255542	-3.501297	6.000421	H	0.255542	-3.501297	6.000421
C	-4.037088	-6.579432	4.417858	C	-4.037088	-6.579432	4.417858
H	-3.983673	-6.859722	3.354345	H	-3.983673	-6.859722	3.354345
H	-4.505066	-5.577144	4.447313	H	-4.505066	-5.577144	4.447313
C	-2.613236	-6.401484	4.959563	C	-2.613236	-6.401484	4.959563
O	-2.429148	-6.454942	6.225374	O	-2.429148	-6.454942	6.225374
O	-1.713153	-6.164926	4.124522	O	-1.713153	-6.164926	4.124522
O	0.035954	-5.150835	5.825893	O	0.035954	-5.150835	5.825893
O	1.007550	-3.898858	9.241151	O	1.007550	-3.898858	9.241151
C	-3.277068	-10.049291	10.290750	C	-3.277068	-10.049291	10.290750
H	-3.336264	-10.137970	11.389342	H	-3.336264	-10.137970	11.389342
H	-4.293878	-9.825621	9.925780	H	-4.293878	-9.825621	9.925780
N	-1.184914	-8.623462	10.560688	N	-1.184914	-8.623462	10.560688
H	-0.850216	-9.070427	11.417290	H	-0.850216	-9.070427	11.417290
C	-2.341435	-8.956712	9.877635	C	-2.341435	-8.956712	9.877635
C	-0.560253	-7.634755	9.885799	C	-0.560253	-7.634755	9.885799
H	0.378588	-7.181055	10.187264	H	0.378588	-7.181055	10.187264
N	-1.258248	-7.309789	8.807492	N	-1.258248	-7.309789	8.807492
C	-2.371680	-8.117258	8.788504	C	-2.371680	-8.117258	8.788504
H	-3.110343	-8.032674	7.996288	H	-3.110343	-8.032674	7.996288
C	2.507707	-10.564079	6.382467	C	2.507707	-10.564079	6.382467
H	2.647679	-11.177441	5.473337	H	2.647679	-11.177441	5.473337
H	3.465042	-10.058632	6.587454	H	3.465042	-10.058632	6.587454
N	0.173624	-9.814629	5.685050	N	0.173624	-9.814629	5.685050
H	-0.159629	-10.696765	5.281850	H	-0.159629	-10.696765	5.281850

C	1.420192	-9.556819	6.228579	C	-1.964771	-5.299297	15.543578
C	-0.604828	-8.733459	5.864265	O	-2.591587	-6.309356	14.772243
H	-1.637425	-8.687904	5.537445	O	-6.235271	-5.064578	7.176279
N	0.081707	-7.782679	6.474806	O	-5.348845	-0.737213	10.095874
C	1.347380	-8.270176	6.699631	C	-6.287222	-3.119096	10.908486
H	2.093015	-7.667385	7.209717	H	-4.643061	-6.183300	8.922900
C	-4.932588	-1.722750	9.473723	H	-4.923645	-7.491238	11.112961
C	-5.043772	-4.160166	9.046868	H	-1.994684	-4.102216	13.281872
C	-4.288249	-6.743227	11.593781	H	-1.636454	-0.685763	5.340207
C	-2.658215	-4.840733	12.828394	H	-1.826462	-5.711412	16.555327
C	-5.544667	-4.155000	7.632734	H	-0.980842	-5.016267	15.133896
C	-2.288887	-0.926023	6.182528	H	-2.588172	-4.390945	15.606673
C	-2.987003	-6.025212	13.509442	H	-4.049586	-7.903239	13.405927
C	-3.797388	-6.983314	12.871507	H	-2.894973	-3.687256	11.028972
C	-3.176298	-4.603874	11.553383	H	-5.620067	-3.118074	5.907424
C	-4.015500	-5.534243	10.915831	H	-3.517128	-2.280733	5.033716
N	-5.225417	-3.072521	6.866877	H	-1.241337	0.358390	7.574766
C	-4.173273	-2.159045	7.087761	H	-2.786953	-0.149356	9.466965
C	-3.340604	-1.822356	6.009065	H	-7.314933	-2.915576	10.553194
C	-2.062619	-0.347425	7.439425	H	-6.250839	-4.139025	11.309773
C	-2.915867	-0.641352	8.499679	H	-6.037486	-2.406256	11.707493
C	-3.971582	-1.555628	8.342945	h	-4.693027	-7.286859	4.925162
N	-5.318366	-2.984084	9.819683	h	-2.976765	-11.032696	9.929089
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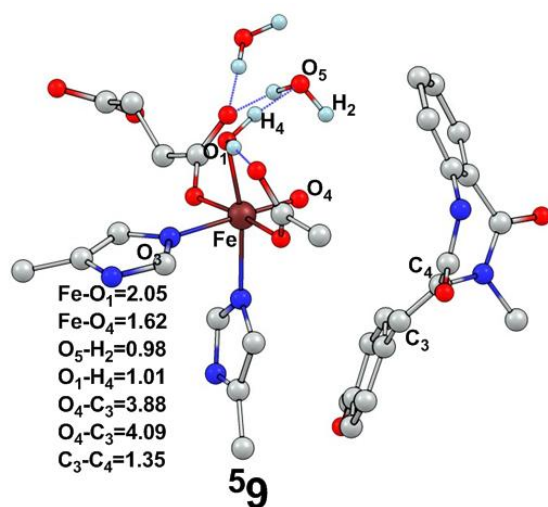
⁵TS7



O	3.120813	-1.445260	8.281512	C	2.040885	-4.769962	8.255062
H	2.524204	-0.702243	8.094178	O	1.303640	-5.794795	8.113379
H	2.619255	-2.268675	8.054938	C	3.235403	-4.881625	9.202057
Fe	-0.574220	-6.004296	7.075538	C	4.545898	-4.267082	8.688841
				C	5.644966	-4.177942	9.761190
				O	6.763890	-4.679449	9.485383
				O	5.386524	-3.601441	10.855589
				H	2.949245	-4.362129	10.136039
				H	3.371928	-5.942899	9.455644
				H	4.362483	-3.239057	8.337704
				H	4.938803	-4.843169	7.835217
				O	-1.198420	-4.554238	7.673784
				H	0.745056	-3.062008	6.777012
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				O	-0.115918	-2.947163	6.248300
				H	-0.465103	-5.714718	4.755053
				H	-0.018909	-3.772484	5.624438

C	-4.061919 -6.697530 4.280945	C	-3.020440 -6.047452 13.498713
H	-4.030869 -7.049299 3.237796	C	-3.812008 -7.010878 12.845498
H	-4.509209 -5.686155 4.251011	C	-3.232480 -4.602302 11.561746
C	-2.627004 -6.517875 4.793195	C	-4.046119 -5.541832 10.905556
O	-2.413291 -6.553300 6.048042	N	-5.197771 -3.084314 6.846803
O	-1.750094 -6.295960 3.925798	C	-4.164248 -2.159039 7.101338
O	0.066988 -5.281782 5.493029	C	-3.307200 -1.808264 6.046446
O	1.852326 -3.661306 7.696330	C	-2.101914 -0.302887 7.505508
C	-3.195700 -9.948653 10.258382	C	-2.974833 -0.613159 8.542443
H	-3.238957 -10.015188 11.359214	C	-4.005890 -1.551525 8.361177
H	-4.216478 -9.719210 9.907051	N	-5.365629 -2.998587 9.806923
N	-1.132312 -8.469633 10.510380	C	-4.586148 -5.313310 9.559375
H	-0.805816 -8.882310 11.384681	C	-1.979032 -5.341332 15.530810
C	-2.262105 -8.864818 9.813873	O	-2.619064 -6.341232 14.757487
C	-0.531500 -7.469151 9.824177	O	-6.232096 -5.065787 7.141900
H	0.378047 -6.958669 10.137493	O	-5.406305 -0.753845 10.102754
N	-1.217810 -7.202270 8.722039	C	-6.336614 -3.145399 10.891943
C	-2.297961 -8.054075 8.703581	H	-4.636090 -6.184956 8.899975
H	-3.020220 -8.019847 7.892047	H	-4.920910 -7.515968 11.075765
C	2.537731 -10.627376 6.361410	H	-2.076812 -4.098253 13.307677
H	2.678780 -11.252637 5.460596	H	-1.603812 -0.645713 5.426397
H	3.498124 -10.129535 6.569585	H	-1.831009 -5.763572 16.537029
N	0.221442 -9.868130 5.631323	H	-0.997445 -5.061160 15.111303
H	-0.117183 -10.754168 5.241866	H	-2.596413 -4.430040 15.611591
C	1.461335 -9.613377 6.189799	H	-4.050003 -7.942202 13.366525
C	-0.555274 -8.783668 5.799895	H	-2.970641 -3.671858 11.051520
H	-1.584123 -8.733806 5.462365	H	-5.545691 -3.146020 5.869946
N	0.126788 -7.834001 6.415521	H	-3.446807 -2.274630 5.068776
C	1.385471 -8.326001 6.658876	H	-1.308596 0.430656 7.658071
H	2.127466 -7.728719 7.180879	H	-2.886356 -0.115200 9.511278
C	-4.981406 -1.733003 9.475045	H	-7.360883 -2.919030 10.541458
C	-5.068299 -4.168039 9.032661	H	-6.314018 -4.174469 11.269824
C	-4.301032 -6.762784 11.568468	H	-6.078569 -2.454306 11.707571
C	-2.716618 -4.846048 12.836350	h	-4.719629 -7.357840 4.846166
C	-5.543262 -4.160680 7.608697	h	-2.927341 -10.948587 9.917528
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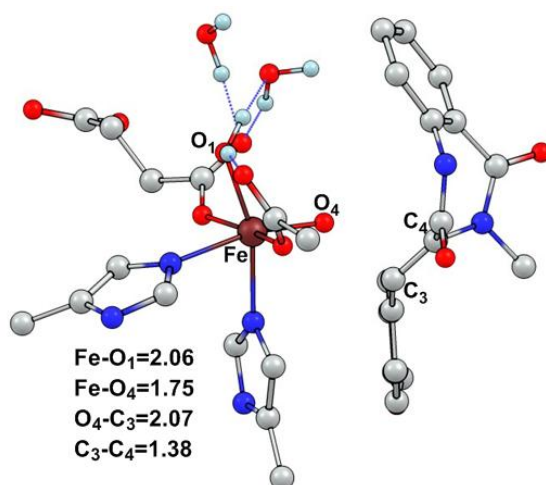


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Fe	-0.585232	-6.011387	7.235049
C	1.970677	-4.781661	8.297192
O	1.236795	-5.823099	8.187979
C	3.169249	-4.870788	9.241092
C	4.489772	-4.314266	8.688628
C	5.603023	-4.196117	9.745334
O	6.727893	-4.674985	9.454886
O	5.351837	-3.616852	10.839843
H	2.903254	-4.295399	10.147577
H	3.283144	-5.918964	9.550116
H	4.327915	-3.299837	8.288518
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O	-1.191462	-4.620426	7.807778
H	0.700901	-2.979518	6.700971
H	-0.826709	-2.815517	6.627401
O	-0.026695	-2.695709	6.081058
H	-0.456434	-5.603571	4.778264
H	0.078545	-4.240265	5.518972
C	-4.037214	-6.626380	4.375232
H	-3.993088	-6.954327	3.324896
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O	-2.378389	-6.470761	6.140009
O	-1.746736	-6.143557	4.015798
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O	1.765249	-3.703569	7.704962

C	-3.237122	-10.044935	10.297225
H	-3.298180	-10.142561	11.395024
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H	0.347430	-7.066221	10.277798
N	-1.243134	-7.263778	8.852724
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C	2.524381	-10.618596	6.365630
H	2.658363	-11.236102	5.458371
H	3.486540	-10.122937	6.571471
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C	-5.549435	-4.153390	7.634769
C	-2.311808	-0.885141	6.219835
C	-3.017887	-6.050681	13.516587
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C	-4.186627	-2.147232	7.106120
C	-3.351793	-1.791759	6.033411
C	-2.098607	-0.313436	7.481471
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C	-4.579096	-5.309253	9.578003
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O	-6.235041	-5.062629	7.172426	H	-2.967045	-3.667730	11.077245
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H	-4.638960	-6.181527	8.920298	H	-1.290197	0.405498	7.623588
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H	-1.656080	-0.632352	5.384051	H	-6.282613	-4.156754	11.306268
H	-1.837604	-5.773516	16.558971	H	-6.067580	-2.427745	11.718716
H	-0.995999	-5.072990	15.137105	h	-4.691650	-7.310343	4.915580
H	-2.594382	-4.436306	15.631603	h	-2.950234	-11.030544	9.930706
H	-4.041426	-7.947878	13.375915	h	2.309286	-11.321042	7.170845

⁵TS8

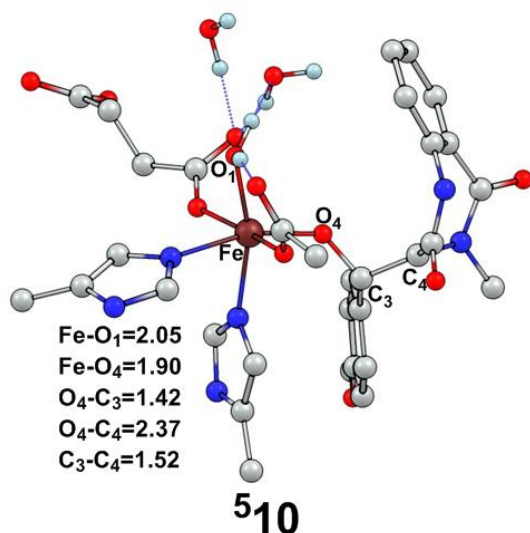


⁵TS8

O	0.633092	-2.672617	7.643823	H	-0.162832	-1.571654	6.837491
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O	0.526367	-2.250203	6.736153	H	-0.815475	-4.915691	5.229590
H	-0.815475	-4.915691	5.229590	H	-0.080980	-3.679437	6.123775
H	-0.080980	-3.679437	6.123775	C	-4.077497	-6.679102	4.351617
C	-4.077497	-6.679102	4.351617	H	-3.853979	-7.176853	3.394184
H	-3.853979	-7.176853	3.394184	H	-4.622171	-5.756412	4.075849
H	-4.622171	-5.756412	4.075849	C	-2.763613	-6.216693	5.000454
C	-2.763613	-6.216693	5.000454	O	-2.648785	-6.282422	6.265954
O	-2.648785	-6.282422	6.265954	O	-1.901928	-5.749719	4.216730
O	-1.901928	-5.749719	4.216730	O	-0.401092	-4.623027	6.088739
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H	-4.388449	-10.116800	10.032195	N	-1.355855	-8.812598	10.792435
N	-1.355855	-8.812598	10.792435	H	-1.005672	-9.282029	11.634419
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C	-2.460121	-9.197351	10.055087	C	-0.790137	-7.747455	10.173146
C	-0.790137	-7.747455	10.173146	H	0.087514	-7.218244	10.536675
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N	-1.468911	-7.431652	9.082820	C	-2.501083	-8.330431	8.990692
C	-2.501083	-8.330431	8.990692	H	-3.215897	-8.293526	8.171659
H	-3.215897	-8.293526	8.171659	C	2.401568	-10.373020	6.420372
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H	2.551970	-10.917845	5.469573	H	3.346665	-9.852153	6.647481
H	3.346665	-9.852153	6.647481	N	0.058683	-9.663288	5.736939
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H	-0.231669	-10.544262	5.304390	C	1.278797	-9.391498	6.329860
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H	-1.768396	-8.565403	5.555956	O	-5.822833	-5.065128	7.217504
N	-0.115498	-7.639040	6.578800	O	-5.120040	-0.859174	9.996836
C	1.146402	-8.118080	6.836939	C	-5.621651	-3.340280	10.882886
H	1.868326	-7.519361	7.388151	H	-4.035741	-6.272948	8.904894
C	-4.591612	-1.764502	9.348368	H	-4.755690	-7.270847	10.988575
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C	-4.069506	-6.618071	11.536153	H	-1.453178	-0.390027	5.199763
C	-2.320659	-4.956899	12.944956	H	-2.176286	-5.742178	16.781463
C	-5.031436	-4.180722	7.534456	H	-1.003291	-5.396735	15.472008
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C	-2.969773	-6.008388	13.611559	H	-4.349747	-7.658655	13.418365
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C	-2.540175	-4.758281	11.576765	H	-5.315611	-3.118120	5.838405
C	-3.422405	-5.571195	10.856728	H	-3.135941	-2.198127	4.898809
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C	-3.818500	-2.114243	6.942835	H	-2.652922	0.035440	9.325279
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C	-2.728824	-0.468505	8.358975	H	-5.176347	-2.909295	11.791676
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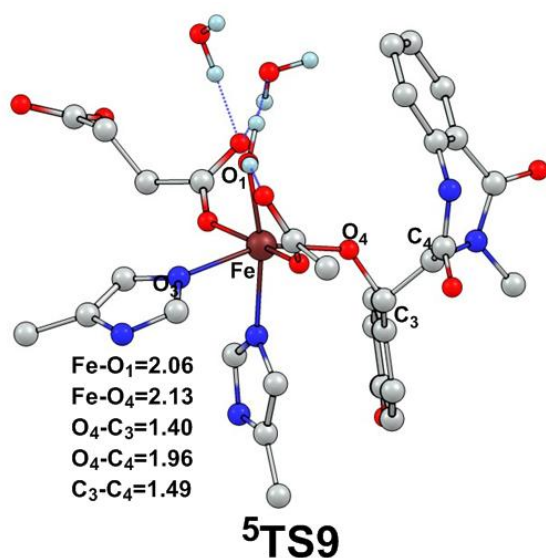
⁵10



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H	2.336106	-2.292142	8.537127	O	0.815481	-5.678022	8.521339
				C	2.951228	-5.057317	9.431008
				C	4.175823	-4.470955	8.698775
				C	5.376069	-4.209813	9.635749
				O	6.514049	-4.568708	9.249561
				O	5.167165	-3.625337	10.738049
				H	2.985684	-4.661967	10.461198
				H	3.030432	-6.152910	9.486596
				H	3.921825	-3.496805	8.244256
				H	4.506054	-5.129752	7.879279
				O	-2.256524	-4.807408	8.534672
				H	0.512177	-2.796834	7.654685
				H	-0.409881	-1.805657	6.839448
				O	0.351694	-2.405390	6.743702
				H	-0.715141	-5.129931	5.221522

H	-0.060059 -3.863414 6.131714	C	-2.934761 -5.888605 13.421159
C	-4.063037 -6.666682 4.384512	C	-3.811533 -6.686666 12.663530
H	-3.883803 -7.112499 3.393104	C	-2.429514 -4.605693 11.422767
H	-4.584342 -5.711236 4.185833	C	-3.296448 -5.393734 10.658936
C	-2.718617 -6.286854 5.017653	N	-4.957765 -2.966195 6.716340
O	-2.583809 -6.387950 6.280014	C	-3.951179 -2.007326 6.943164
O	-1.843859 -5.843904 4.234412	C	-3.126710 -1.614891 5.878790
O	-0.234032 -4.849817 6.057998	C	-1.923823 -0.115950 7.356809
O	1.171929 -3.520296 8.968997	C	-2.765209 -0.476613 8.407386
C	-3.378244 -10.345100 10.394479	C	-3.775554 -1.429496 8.217021
H	-3.445856 -10.506987 11.483848	N	-4.898533 -3.030400 9.684621
H	-4.395630 -10.121095 10.031367	C	-3.472667 -5.154623 9.163764
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C	-2.459519 -9.216690 10.060351	O	-5.905726 -4.982807 7.119778
C	-0.746348 -7.815298 10.157697	O	-5.216602 -0.802279 10.015201
H	0.143718 -7.302085 10.513842	C	-5.797434 -3.320546 10.809025
N	-1.419532 -7.499805 9.062864	H	-3.875592 -6.082474 8.717079
C	-2.483448 -8.361562 8.986523	H	-4.683592 -7.054578 10.730501
H	-3.201821 -8.309274 8.171786	H	-1.580235 -4.191454 13.363570
C	2.425203 -10.423544 6.415796	H	-1.484674 -0.373154 5.248594
H	2.575990 -10.980071 5.472056	H	-2.187450 -5.735886 16.610236
H	3.371115 -9.903602 6.640483	H	-1.006110 -5.322995 15.326687
N	0.081181 -9.716881 5.731777	H	-2.457856 -4.304593 15.562073
H	-0.209778 -10.596056 5.294441	H	-4.346292 -7.500948 13.161311
C	1.304994 -9.441485 6.316087	H	-1.854878 -3.816085 10.930687
C	-0.728220 -8.655035 5.926697	H	-5.460705 -2.966596 5.809116
H	-1.754637 -8.632697 5.573991	H	-3.282186 -2.057378 4.891999
N	-0.096122 -7.701937 6.585832	H	-1.149704 0.637429 7.513345
C	1.171882 -8.171999 6.829755	H	-2.658918 -0.009429 9.389313
H	1.894423 -7.571584 7.377173	H	-6.839306 -3.055699 10.549844
C	-4.698519 -1.715554 9.363902	H	-5.747011 -4.390803 11.043247
C	-4.495875 -4.084741 8.823129	H	-5.491217 -2.742072 11.693687
C	-3.991601 -6.431681 11.305815	h	-4.721177 -7.335241 4.939442
C	-2.256680 -4.831839 12.794701	h	-3.037734 -11.287499 9.965520
C	-5.158671 -4.076367 7.483137	h	2.255754 -11.186414 7.175653
C	-2.116029 -0.678057 6.085942		

⁵TS9

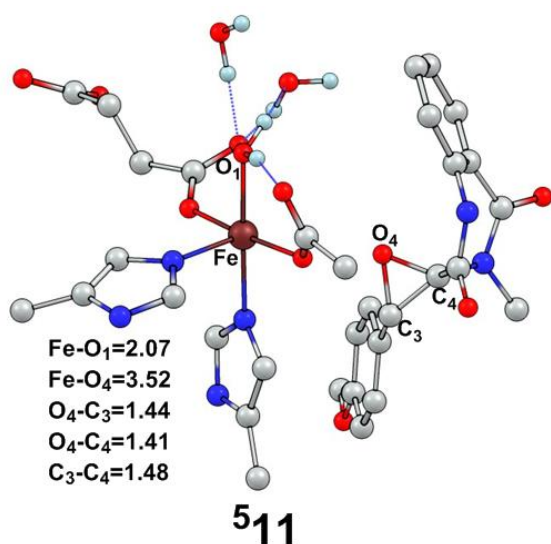


O	3.023117	-1.683550	8.044614
H	2.467466	-1.522164	7.259145
H	2.426197	-2.248738	8.592267
Fe	-1.073732	-5.849946	7.600737
C	1.527997	-4.631932	8.933889
O	0.757765	-5.563202	8.546391
C	2.915536	-5.013383	9.459449
C	4.163656	-4.479516	8.726006
C	5.367265	-4.216921	9.657526
O	6.503996	-4.572804	9.264035
O	5.167427	-3.630487	10.761127
H	2.959151	-4.606624	10.484940
H	2.955099	-6.110341	9.531280
H	3.941440	-3.508937	8.247488
H	4.483476	-5.166131	7.925464
O	-2.552325	-4.788800	8.699780
H	0.633092	-2.672617	7.643823
H	-0.162832	-1.571654	6.837491
O	0.526367	-2.250203	6.736153
H	-0.815475	-4.915691	5.229590
H	-0.080980	-3.679437	6.123775
C	-4.077497	-6.679102	4.351617
H	-3.853979	-7.176853	3.394184
H	-4.622171	-5.756412	4.075849
C	-2.763613	-6.216693	5.000454
O	-2.648785	-6.282422	6.265954
O	-1.901928	-5.749719	4.216730
O	-0.401092	-4.623027	6.088739

O	1.195539	-3.416951	8.975751
C	-3.367592	-10.334984	10.389563
H	-3.429344	-10.498200	11.479204
H	-4.388449	-10.116800	10.032195
N	-1.355855	-8.812598	10.792435
H	-1.005672	-9.282029	11.634419
C	-2.460121	-9.197351	10.055087
C	-0.790137	-7.747455	10.173146
H	0.087514	-7.218244	10.536675
N	-1.468911	-7.431652	9.082820
C	-2.501083	-8.330431	8.990692
H	-3.215897	-8.293526	8.171659
C	2.401568	-10.373020	6.420372
H	2.551970	-10.917845	5.469573
H	3.346665	-9.852153	6.647481
N	0.058683	-9.663288	5.736939
H	-0.231669	-10.544262	5.304390
C	1.278797	-9.391498	6.329860
C	-0.745237	-8.592508	5.919308
H	-1.768396	-8.565403	5.555956
N	-0.115498	-7.639040	6.578800
C	1.146402	-8.118080	6.836939
H	1.868326	-7.519361	7.388151
C	-4.591612	-1.764502	9.348368
C	-4.398383	-4.161510	8.894192
C	-4.069506	-6.618071	11.536153
C	-2.320659	-4.956899	12.944956
C	-5.031436	-4.180722	7.534456
C	-2.064813	-0.706309	6.046538
C	-2.969773	-6.008388	13.611559
C	-3.845334	-6.843356	12.892362
C	-2.540175	-4.758281	11.576765
C	-3.422405	-5.571195	10.856728
N	-4.789021	-3.111881	6.731155
C	-3.818500	-2.114243	6.942835
C	-3.012054	-1.712248	5.869394
C	-1.906904	-0.094705	7.298612
C	-2.728824	-0.468505	8.358975
C	-3.684980	-1.480930	8.195503
N	-4.764438	-3.086262	9.709928
C	-3.644920	-5.356957	9.374018
C	-2.073960	-5.389368	15.743328

O	-2.830193	-6.272576	14.936519	H	-1.996177	-3.969039	11.051248
O	-5.822833	-5.065128	7.217504	H	-5.315611	-3.118120	5.838405
O	-5.120040	-0.859174	9.996836	H	-3.135941	-2.198127	4.898809
C	-5.621651	-3.340280	10.882886	H	-1.181420	0.710362	7.433560
H	-4.035741	-6.272948	8.904894	H	-2.652922	0.035440	9.325279
H	-4.755690	-7.270847	10.988575	H	-6.612830	-2.886566	10.712687
H	-1.632235	-4.299593	13.479252	H	-5.739171	-4.421052	11.018987
H	-1.453178	-0.390027	5.199763	H	-5.176347	-2.909295	11.791676
H	-2.176286	-5.742178	16.781463	h	-4.728621	-7.339005	4.924881
H	-1.003291	-5.396735	15.472008	h	-3.027609	-11.277569	9.960597
H	-2.440366	-4.350326	15.677653	h	2.241072	-11.147194	7.17068
H	-4.349747	-7.658655	13.418365				

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O	2.884407	-1.700082	8.049343	O	-3.206578	-4.319456	8.884170
H	2.314537	-1.519035	7.279396	H	0.578309	-2.904760	7.622818
H	2.325084	-2.327559	8.568209	H	-0.376612	-1.844652	6.940018
Fe	-0.615467	-6.084665	7.292007	O	0.383730	-2.423260	6.758775
C	1.752881	-4.768789	8.848384	H	-0.584098	-5.055646	4.996492
O	1.180022	-5.780493	8.350997	H	0.070933	-3.851590	5.944028
C	3.139894	-4.968238	9.454212	C	-4.054674	-6.580152	4.400645
C	4.355457	-4.350653	8.736698	H	-3.914037	-7.013688	3.397337
C	5.548174	-4.152465	9.691219	H	-4.591322	-5.627729	4.228141
O	6.672075	-4.582146	9.333534	C	-2.680582	-6.189608	4.975542
O	5.346393	-3.554742	10.788037	O	-2.481710	-6.248515	6.227642
H	3.102876	-4.526291	10.464479	O	-1.850739	-5.767547	4.128824
H	3.292489	-6.051690	9.554312	O	0.011685	-4.832907	5.769482
H	4.094846	-3.358195	8.328802	O	1.228874	-3.620739	8.924171
H	4.679009	-4.977415	7.889541	C	-3.286045	-10.150463	10.327702
				H	-3.352047	-10.274354	11.422662
				H	-4.301697	-9.917037	9.964567
				N	-1.218430	-8.700472	10.677567
				H	-0.890599	-9.168300	11.527235
				C	-2.349344	-9.044353	9.957241
				C	-0.607323	-7.675942	10.037462
				H	0.310192	-7.199810	10.372859
				N	-1.282043	-7.336091	8.949640
				C	-2.364884	-8.183254	8.885631
				H	-3.078347	-8.120946	8.067085
				C	2.519866	-10.633904	6.354764
				H	2.671596	-11.264154	5.458625
				H	3.476577	-10.129921	6.566068
				N	0.205633	-9.874415	5.600958

H	-0.138687	-10.764472	5.227553	C	-2.020952	-5.397746	15.803766
C	1.444066	-9.622504	6.166134	O	-2.755872	-6.312399	15.009577
C	-0.552463	-8.765976	5.736589	O	-6.157739	-5.004630	7.337717
H	-1.578527	-8.701954	5.383314	O	-5.295218	-0.783811	10.060901
N	0.132863	-7.811805	6.332614	C	-6.065637	-3.272610	10.832906
C	1.377928	-8.321650	6.601046	H	-4.145630	-6.233465	8.983759
H	2.125938	-7.724363	7.118517	H	-4.831110	-7.345536	11.152319
C	-4.808329	-1.729000	9.433890	H	-1.775086	-4.224717	13.545957
C	-4.600717	-4.111280	8.975549	H	-1.561394	-0.530322	5.294712
C	-4.169369	-6.655140	11.681673	H	-2.057833	-5.774494	16.837965
C	-2.455396	-4.910271	13.037056	H	-0.965342	-5.335285	15.486551
C	-5.325514	-4.158361	7.634484	H	-2.453723	-4.383599	15.771495
C	-2.199410	-0.811150	6.136933	H	-4.245848	-7.772996	13.534058
C	-2.984605	-6.026574	13.704823	H	-2.353186	-3.823427	11.174691
C	-3.838054	-6.905333	13.009323	H	-5.487245	-3.140149	5.888853
C	-2.792301	-4.675318	11.699383	H	-3.320650	-2.266307	4.994173
C	-3.662850	-5.527833	11.009142	H	-1.262940	0.568760	7.522728
N	-5.007795	-3.123108	6.810379	H	-2.790344	-0.014899	9.401022
C	-4.019323	-2.142517	7.031821	H	-7.045983	-2.841792	10.564195
C	-3.188199	-1.776907	5.961959	H	-6.176136	-4.355391	10.972012
C	-2.027677	-0.198346	7.386726	H	-5.726085	-2.826630	11.781209
C	-2.877873	-0.527453	8.440157	h	-4.692152	-7.260802	4.964918
C	-3.875451	-1.501093	8.282319	h	-2.981195	-11.121466	9.937463
N	-5.082127	-3.021885	9.782039	h	2.300609	-11.328838	7.165356
C	-3.979290	-5.319593	9.563704				