

Supplementary Information

Mechanistic Insights into the Non-Heme 2-Oxoglutarate-Dependent Ethylene-Forming Enzyme: Ethylene-Formation versus L-Arg Hydroxylation

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Part I. MD Simulations.

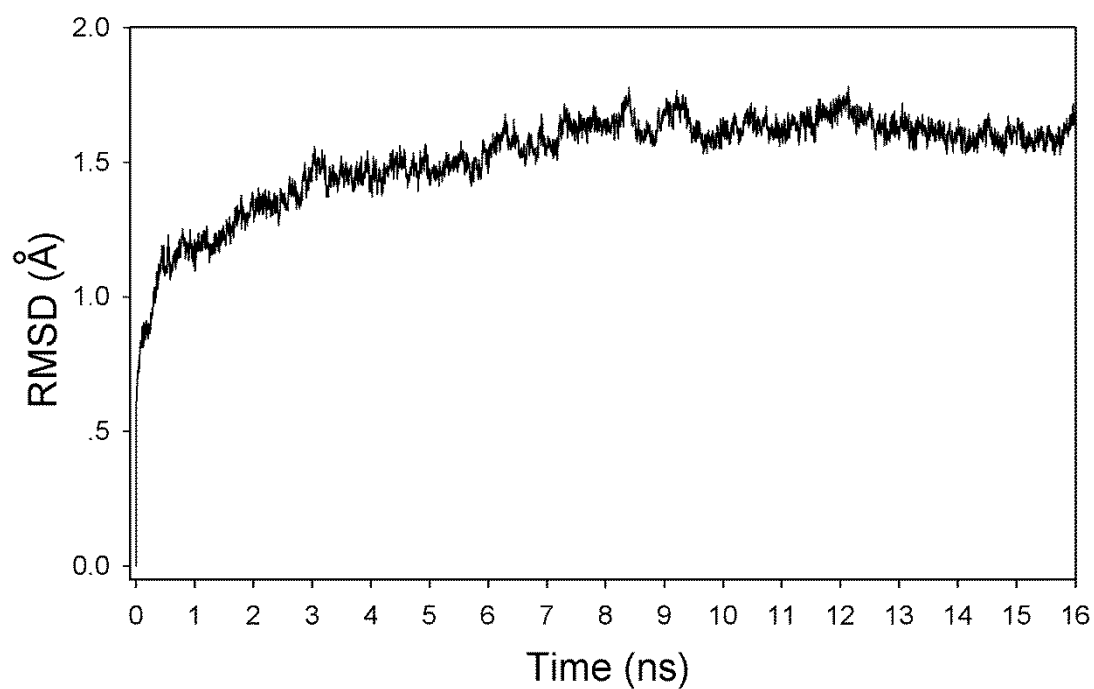


Fig. S1 The RMSD plot of backbone during MD simulations.

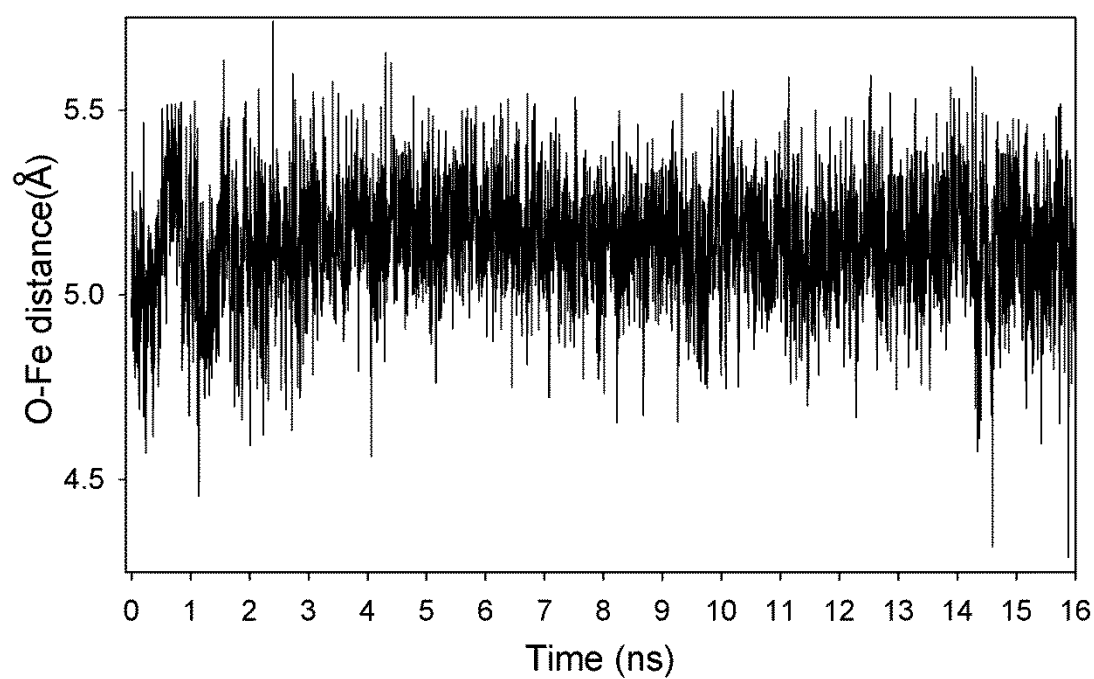


Fig. S2 The distance between the oxygen atom of the nearby water molecule and the iron center during MD simulations.

Part II. Residues Included in the QM/MM Optimization.

QM/MM optimized region included the following set of residues: substrate EFE and ASU, Fe, dioxygen, Thr86, Asp91, Pro93, Ile95, Hsd169, Arg171, Leu173, Phe175, Ile186, Gly187, Ala188, Hsd189, Thr190, Asp191, Tyr192, Gly193, Val196, Ala198, Gln200, Leu206, Tyr207, Ile208, Arg209, Asn220, Trp221, Leu222, Pro223, Gly224, Glu225, Ser226, Ser227, Ala228, Gly229, Trp237, Val240, Phe250, Pro251, Gly252, Asp253, Thr266, Pro267, Hsd268, Lys269, Val270, Arg277, Ala279, Gys280, Ala281, Phe283, Glu285; some crystal waters: Wat537, Wat561, Wat567, Wat585, Wat590, Wat597, Wat639, Wat674, Wat692, Wat695, Wat734, Wat785; and some solvent waters: Wat1936, Wat2455, Wat6338, Wat6673, Wat7693, Wat7769.

Part III. Energies and Spin Densities for the Key Species.

Table S1. Absolute energies (in a.u.) for the key species.

	B3LYP/B1		B3LYP/B2	
	QM	QM/MM	QM	QM/MM
⁷ 1	-3746.310560	-3876.020118	-3749.509072	-3879.218513
³ 1	-3746.307842	-3876.018287	-3749.507189	-3879.217626
¹ 1	-3746.287140	-3876.002144	-3749.490419	-3879.205431
³ TS1	-3746.272326	-3875.980039	-3749.471893	-3879.179224
³ A	-3746.277914	-3875.987727	-3749.477246	-3879.187002
¹ A	-3746.280175	-3875.990835	-3749.480416	-3879.191075
³ TS2	-3746.265011	-3875.974607	-3749.467001	-3879.176605
¹ TS1	-3746.266209	-3875.983764	-3749.470168	-3879.187611
³ 2	-3746.265945	-3875.975327	-3749.469362	-3879.178609
¹ 2	-3746.306255	-3876.010093	-3749.480416	-3879.197905
⁵ 1	-3746.295149	-3876.004476	-3749.495418	-3879.204501
⁵ TS1	-3746.279325	-3875.990088	-3749.480574	-3879.191238
⁵ 2	-3746.351990	-3876.054624	-3749.559178	-3879.262120
⁵ TS2	-3746.340721	-3876.044188	-3749.550395	-3879.253712
⁵ 3	-3746.371267	-3876.072507	-3749.585341	-3879.286410
⁵ TS3	-3746.375744	-3876.070239	-3749.587650	-3879.282146
⁵ 4	-3746.385287	-3876.117043	-3749.588224	-3879.319900
⁵ TS4	-3746.355349	-3876.088321	-3749.555647	-3879.288562
⁵ 5	-3746.393498	-3876.123306	-3749.599644	-3879.329375
⁵ TS5	-3746.383579	-3876.109457	-3749.591359	-3879.317173
⁵ 6	-3746.476707	-3876.199739	-3749.679363	-3879.402253
⁵ TS6	-3746.352974	-3876.053341	-3749.558912	-3879.259150
⁵ 7	-3746.378356	-3876.075235	-3749.584793	-3879.281511
⁵ 8	-3746.382541	-3876.101184	-3749.579185	-3879.297852
⁵ TS7	-3746.379306	-3876.080973	-3749.579499	-3879.281191
⁵ 9	-3746.391655	-3876.092586	-3749.595193	-3879.295932
⁵ TS8	-3746.391198	-3876.090629	-3749.593957	-3879.293298
⁵ 10	-3746.401712	-3876.113589	-3749.605216	-3879.316957
⁵ TS9	-3746.400558	-3876.112236	-3749.604483	-3879.315962
⁵ 11	-3746.424290	-3876.134340	-3749.618820	-3879.328825
⁵ TS10	-3746.397866	-3876.110463	-3749.612074	-3879.324671
⁵ 12	-3746.391198	-3876.090629	-3749.630962	-3879.334712

Table S2. The dispersion, ZPE, thermal, and entropy correction as well as the total correction to Gibbs free energy (G_{corr}) at the B3LYP-D3 level.

	E_{disp} (a.u.)	ZPE (a.u.)	E_{int} (J/mol)	S (J/mol/K)	G_{corr}
⁷ 1	-0.117538	0.767617	111767.2290	616.03762	0.735120
³ 1	-0.115858	0.766986	111122.5280	656.35169	0.735127
¹ 1	-0.115797	0.756507	116441.0920	693.28981	0.722473
³ TS1	-0.114537	0.759915	114381.5647	679.42387	0.726326
³ A	-0.117230	0.762637	113216.1666	670.73215	0.729227
¹ A	-0.116347	0.759829	114562.7908	682.83269	0.725922
³ TS2	-0.115380	0.767143	113406.2512	668.94837	0.727711
¹ TS1	-0.115465	0.767166	114335.6391	672.17340	0.727416
³ 2	-0.117473	0.755915	114956.1583	680.59864	0.722412
¹ 2	-0.116475	0.761040	112719.2764	667.30945	0.728193
⁵ 1	-0.116783	0.755692	119024.4013	702.46109	0.721255
⁵ TS1	-0.115998	0.756422	114760.9734	679.72293	0.722943
⁵ 2	-0.116270	0.768021	115384.0151	690.22662	0.733586
⁵ TS2	-0.116424	0.766212	122861.8796	700.04682	0.733511
⁵ 3	-0.119825	0.750714	123657.4554	752.08216	0.712406
⁵ TS3	-0.122353	0.752256	121155.1056	743.73905	0.713943
⁵ 4	-0.123284	0.752283	121147.5356	750.38188	0.713212
⁵ TS4	-0.125587	0.749197	117544.7298	706.03248	0.713791
⁵ 5	-0.122739	0.759651	114652.3249	692.01754	0.724734
⁵ TS5	-0.124597	0.747573	122041.6861	746.44268	0.709290
⁵ 6	-0.124087	0.772558	107971.7273	640.17059	0.740985
⁵ TS6	-0.115568	0.769734	110605.8018	643.01590	0.737706
⁵ 7	-0.112003	0.773727	109819.7939	652.43166	0.741465
⁵ 8	-0.115552	0.773613	108896.9770	638.96291	0.742530
⁵ TS7	-0.114781	0.774823	114186.1217	680.16442	0.741076
⁵ 9	-0.117623	0.761789	113452.8153	671.16240	0.728784
⁵ TS8	-0.114900	0.758695	115010.4898	689.64266	0.724185
⁵ 10	-0.120229	0.759986	116843.2820	708.86147	0.723992
⁵ TS9	-0.120490	0.758111	115107.1981	688.59455	0.723757
⁵ 11	-0.116932	0.758837	117770.1943	717.10893	0.722259
⁵ TS10	-0.117933	0.766417	113436.3698	679.98281	0.732404
⁵ 12	-0.116385	0.769130	116325.2344	701.90286	0.733729

Table S3. Relative energies (in kcal/mol) for the key species.

	B3LYP/B1		B3LYP/B2		B3LYP-D3	B3LYP-D3	B3LYP-D3
	QM	QM/MM	QM	QM/MM		+ZPE	ΔG
⁷ 1	0.0	0.0	0.0	0.0	0.0	0.0	0.0
³ 1	1.7	1.1	1.2	0.6	1.6	1.2	1.4
¹ 1	14.7	11.3	11.7	8.2	9.3	2.3	1.1
³ TS1	24.0	25.1	23.3	24.7	26.5	21.7	21.0
³ A	20.5	20.3	20.0	19.8	20.0	16.8	16.3
¹ A	19.1	18.4	18.0	17.2	18.0	13.1	12.2
³ TS2	28.6	28.6	26.4	26.3	27.7	27.4	23.0
¹ TS1	27.8	22.8	24.4	19.4	20.7	20.4	15.9
³ 2	28.0	28.1	25.0	25.0	25.1	17.7	17.1
¹ 2	2.7	6.3	18.0	12.9	13.6	9.5	9.2
⁵ 1	9.7	9.8	8.6	8.8	9.3	1.8	0.6
⁵ TS1	19.6	18.8	17.9	17.1	18.1	11.1	10.4
⁵ 2	-26.0	-21.7	-31.2	-27.4	-26.6	-26.3	-27.5
⁵ TS2	-18.9	-15.1	-25.9	-22.1	-21.4	-22.3	-22.4
⁵ 3	-38.1	-32.9	-47.9	-42.6	-44.0	-54.6	-58.3
⁵ TS3	-40.9	-31.5	-49.3	-39.9	-42.0	-51.7	-55.8
⁵ 4	-46.9	-60.8	-50.0	-63.6	-67.2	-76.8	-81.0
⁵ TS4	-28.1	-42.8	-29.2	-44.0	-49.0	-60.6	-62.4
⁵ 5	-52.0	-64.8	-56.8	-69.6	-72.8	-77.8	-79.4
⁵ TS5	-45.8	-56.1	-51.6	-61.9	-66.3	-78.9	-82.6
⁵ 6	-104.3	-112.7	-106.9	-115.3	-119.4	-116.3	-115.7
⁵ TS6	-26.6	-20.8	-31.3	-25.5	-24.3	-22.9	-22.6
⁵ 7	-42.5	-34.6	-47.5	-39.5	-36.1	-32.2	-32.1
⁵ 8	-45.2	-50.9	-44.0	-49.8	-48.5	-44.8	-43.9
⁵ TS7	-43.1	-38.2	-44.2	-39.3	-37.6	-33.1	-33.9
⁵ 9	-50.9	-45.5	-54.0	-48.6	-48.6	-52.2	-52.6
⁵ TS8	-50.6	-44.2	-53.3	-46.9	-45.3	-50.9	-56.2
⁵ 10	-57.2	-58.7	-60.3	-61.8	-63.5	-68.3	-70.4
⁵ TS9	-56.5	-57.8	-59.9	-61.2	-63.0	-69.0	-70.1
⁵ 11	-71.4	-71.7	-68.9	-69.2	-68.8	-74.4	-76.9
⁵ TS10	-54.8	-56.7	-64.6	-66.6	-66.9	-67.6	-68.6
⁵ 12	-50.6	-44.2	-76.5	-72.9	-72.2	-71.2	-72.0

Table S4. Spin density distribution for the key species using B3LYP /B1 level.

species	Fe	O ₁	O ₂	C ^a	2OG ^b	Sub	L ^c	C ^d	other
⁷ 1	3.84	0.99	0.98	0.05	0.06	0.00	0.08	0.00	0.00
³ 1	3.79	-1.00	-0.94	0.04	0.05	0.00	0.07	0.00	0.00
¹ 1	1.14	-0.59	-0.49	-0.01	-0.01	0.00	-0.07	0.01	0.02
³ TS1	2.95	-0.43	-0.55	0.05	-0.01	0.00	0.02	0.00	-0.02
³ A	2.90	-0.39	-0.52	-0.04	-0.04	0.00	0.02	0.01	0.07
¹ A	1.07	-0.44	-0.55	-0.03	-0.02	0.00	-0.07	0.00	0.03
³ TS2	2.82	-0.23	-0.09	-0.35	-0.57	-0.01	0.03	-0.11	0.51
¹ TS1	0.96	-0.18	0.00	-0.42	-0.73	-0.01	-0.07	-0.13	0.58
³ 2	2.74	-0.15	0.02	-0.37	-0.67	-0.01	0.04	-0.22	0.61
¹ 2	-0.05	0.01	0.00	0.00	-0.01	0.00	0.05	0.00	0.00
⁵ 1	4.18	-0.46	-0.20	0.12	0.20	0.00	0.22	0.00	-0.08
⁵ TS1	4.18	-0.17	0.12	-0.26	-0.38	-0.01	0.22	-0.11	0.41
⁵ 2	3.80	0.01	0.07	0.00	0.02	0.00	0.06	0.00	0.04
⁵ TS2	3.94	-0.17	0.05	0.00	0.04	0.00	0.12	-0.01	0.03
⁵ 3	3.12	0.02	0.67	0.00	0.08	0.00	0.09	0.00	0.03
⁵ TS3	3.12	0.01	0.68	0.00	0.05	0.00	0.09	0.00	0.05
⁵ 4	3.16	0.00	0.63	0.00	0.05	0.00	0.07	0.00	0.08
⁵ TS4	4.06	0.00	-0.03	0.00	0.08	-0.38	0.16	0.01	0.09
⁵ 5	4.24	0.01	0.36	0.00	0.10	-0.99	0.18	0.01	0.09
⁵ TS5	3.84	0.00	0.07	0.00	0.03	-0.05	0.05	0.01	0.05
⁵ 6	3.82	0.00	0.00	0.00	0.04	0.00	0.07	0.01	0.06
⁵ TS6	3.82	0.01	0.04	0.00	0.02	0.00	0.07	0.00	0.03
⁵ 7	3.82	0.00	0.00	0.04	0.04	0.00	0.07	0.00	0.03
⁵ 8	3.83	0.00	0.00	0.02	0.02	0.00	0.07	0.00	0.06
⁵ TS7	4.03	-0.35	-0.06	0.16	0.14	0.00	0.09	-0.01	0.01
⁵ 9	4.20	-0.68	-0.20	0.31	0.25	0.00	0.21	-0.04	-0.04
⁵ TS8	4.22	-0.73	-0.16	0.23	0.15	0.00	0.22	-0.05	0.10
⁵ 10	4.24	-0.24	0.01	0.17	-0.56	0.00	0.14	-0.41	0.66
⁵ TS9	4.24	-0.21	0.09	0.17	-0.60	0.00	0.14	-0.52	0.76
⁵ 11	4.23	0.00	0.01	0.18	-0.80	0.00	0.14	-1.01	1.25
⁵ TS10	3.82	0.00	0.00	0.04	0.04	0.00	0.04	0.00	0.05
⁵ 12	3.80	0.00	0.00	0.05	0.05	0.00	0.03	0.00	0.07

O₁ represents the distal oxygen atom. O₂ represents the proximal oxygen atom.

^a The spin density for C2, O5, O7.

^b The spin density for C1, C2, O5, O7, C3, C4, C5 is also included.

^c The ligated N atoms of His189, His268 and ligated O atom of Asp191.

^d The spin density for C1, C3, C4, C5.

Part IV. Yamaguchi Spin Projection.

Due to the spin contamination of the quintet state, we applied the Yamaguchi's spin projected correction for the calculated energy of the symmetry-broken quintet state as shown below:

$$E_s = (E_c - aE_{s+1}) / (1 - a), \quad a = [\langle S^2 \rangle_c - s(s+1)] / 2(s+1)$$

E_c is the spin-contaminated energy for the quintet state (B3LYP(B2)/MM values), E_{s+1} is the energy for the septet state, $\langle S^2 \rangle_c$ is the calculated spin expectation value of the quintet state. The results are listed in Table S4. It should be pointed out that in the reaction ${}^5\mathbf{2} \rightarrow {}^5\mathbf{3}$, the reactant and product are both spin pure states. The spin density distribution (see Table S3) suggested that ${}^5\mathbf{TS2}$ is mainly an Fe^{II} species with four unpaired electrons on the iron. As such, the Yamaguchi spin projection may not be suitable to correct its energy.

Table S4. $\langle S^2 \rangle_c$, E_c , E_{s+1} , spin projection corrected energy for the symmetry-broken quintet state, and the energy difference upon Yamaguchi correction ($\Delta E_s = E_s - E_c$).

	$\langle S^2 \rangle_c$	E_c (a.u.)	E_{s+1} (a.u.)	E_s (a.u.)	ΔE (kcal/mol)
${}^5\mathbf{1}$	6.94	-3879.204501	-3879.205326	-3879.204348	0.1
${}^5\mathbf{TS1}$	6.73	-3879.191238	-3879.186759	-3879.191857	-0.4
${}^5\mathbf{2}$	6.01	-3879.261735	-	-	-
${}^5\mathbf{TS2}$	6.24	-3879.253712	-	-	-
${}^5\mathbf{3}$	6.05	-3879.286410	-	-	-
${}^5\mathbf{TS3}$	6.05	-3879.282146	-	-	-
${}^5\mathbf{4}$	6.06	-3879.319900	-	-	-
${}^5\mathbf{TS4}$	6.67	-3879.288562	-3879.273969	-3879.290395	-1.2
${}^5\mathbf{5}$	7.00	-3879.329375	-3879.329106	-3879.329429	-0.03
${}^5\mathbf{TS5}$	6.06	-3879.317173	-	-	-
${}^5\mathbf{6}$	6.00	-3879.402253	-	-	-
${}^5\mathbf{TS6}$	6.01	-3879.259150	-	-	-
${}^5\mathbf{7}$	6.01	-3879.281511	-	-	-
${}^5\mathbf{8}$	6.00	-3879.297852	-	-	-
${}^5\mathbf{TS7}$	6.98	-3879.281191	-3879.294894	-3879.278514	1.7
${}^5\mathbf{9}$	6.98	-3879.292668	-3879.295505	-3879.296016	-0.05
${}^5\mathbf{TS8}$	7.01	-3879.293298	-3879.293198	-3879.293318	-0.01
${}^5\mathbf{10}$	7.00	-3879.316957	-3879.317104	-3879.316927	0.02
${}^5\mathbf{TS9}$	7.01	-3879.315962	-3879.316046	-3879.315945	0.01
${}^5\mathbf{11}$	7.01	-3879.328825	-3879.343948	-3879.325763	1.9
${}^5\mathbf{TS10}$	6.01	-3879.324671	-	-	-
${}^5\mathbf{12}$	6.01	-3879.334712	-	-	-

Part V. Discard Pathways.

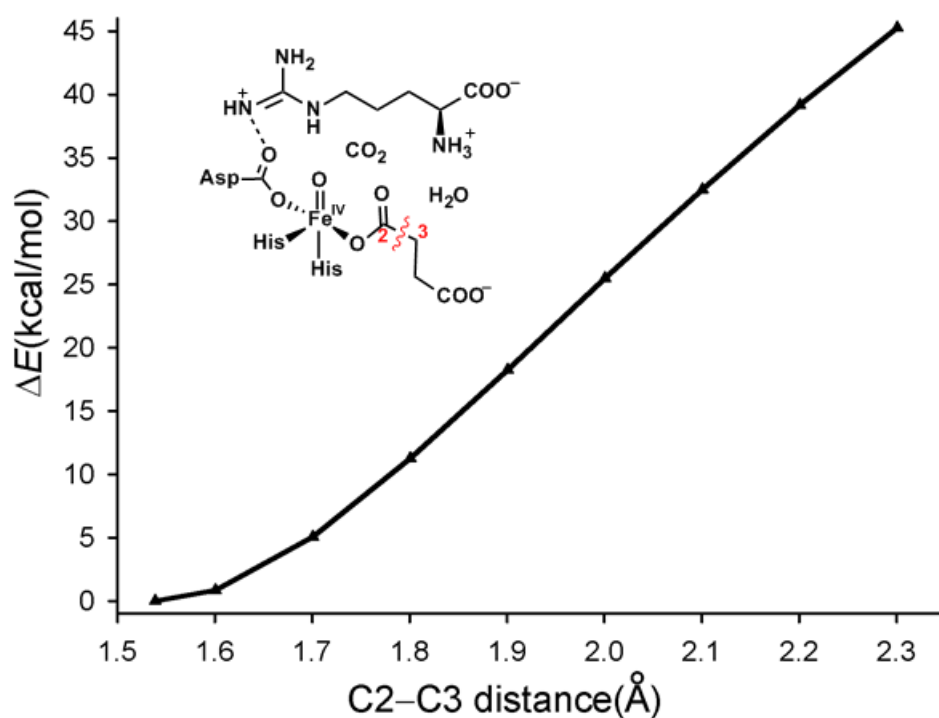


Fig. S3 Energy profile along the breaking C2-C3 bond starting from $^5\mathbf{3}$ at the B3LYP(def-SV(P))/MM level.

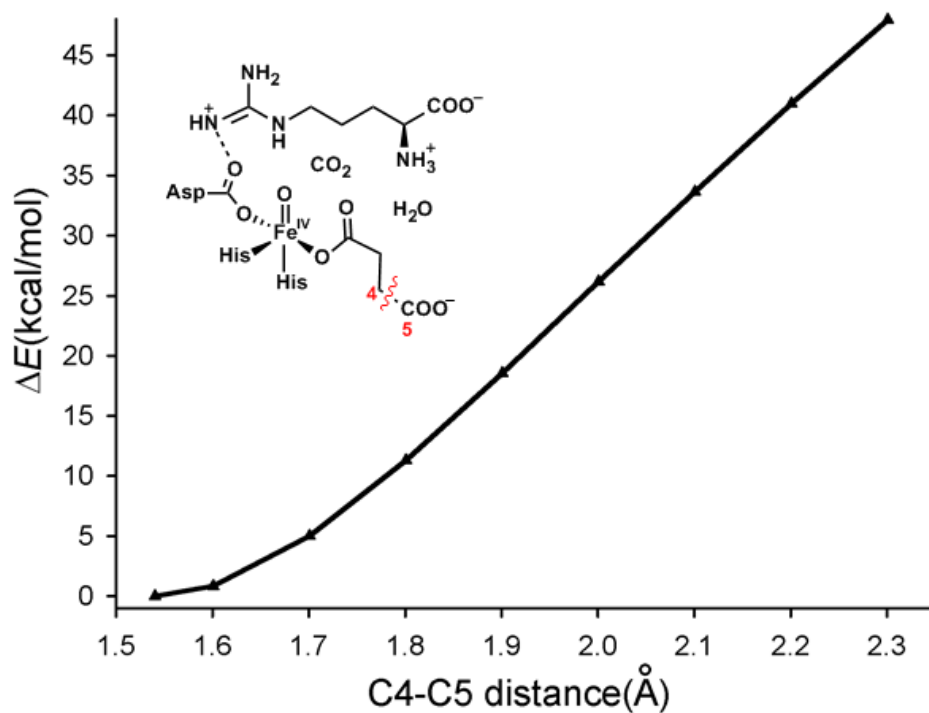


Fig. S4 Energy profile along the breaking C4-C5 bond starting from quintet $^5\mathbf{3}$ at the B3LYP(def-SV(P))/MM level.

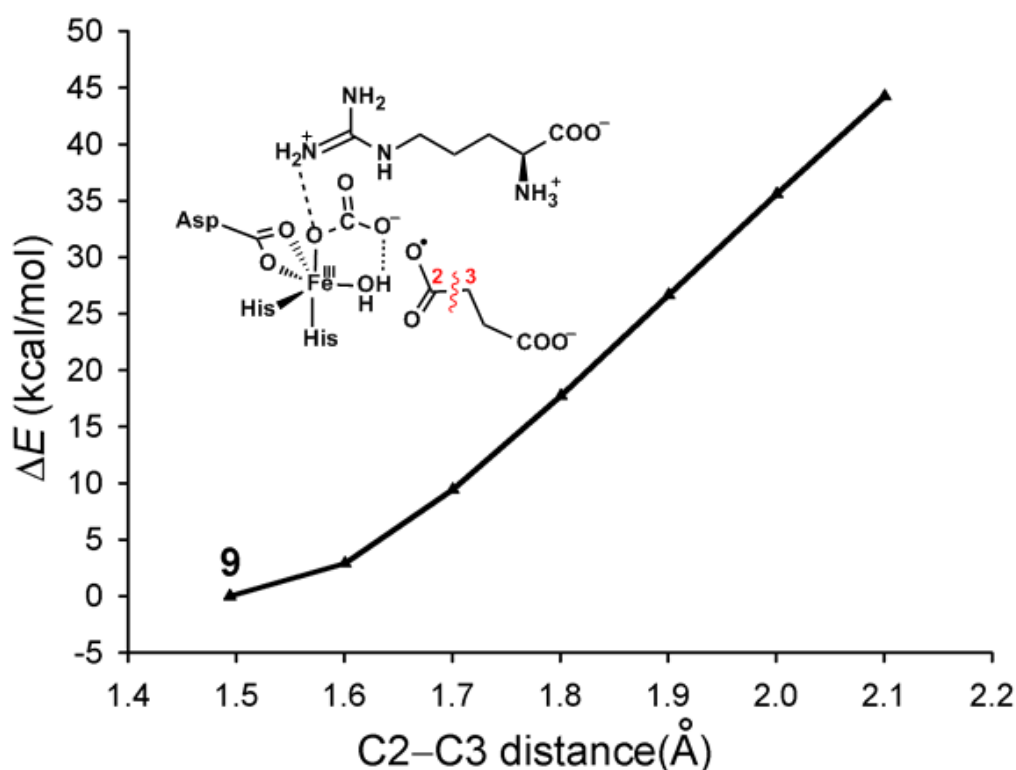


Fig. S5 Energy profile along the breaking C2–C3 bond starting from ⁵**9** at the B3LYP(def-SV(P))/MM level.

Part VI. Thermodynamics of the CO₂ Insertion

Table S5. Calculated reaction energies (at the B2 level) for the CO₂ insertion in EFE using different models

Models	⁵ 2	⁵ 7	ΔE (⁵ 2 → ⁵ 7)
Gas-phase	-3749.046109	-3749.044546	1.0
Gas-phase(QM2) ^a	-2743.626003	-2743.625333	0.4
QM/PC(4 Å) ^b	-3749.016033	-3749.043778	-17.4
QM/PC(full)	-3749.559178	-3749.584793	-16.1
Solvent (chlorobenzene)	-3749.171965	-3749.173979	-1.3

^a Gas-phase optimizations (B1) were performed using a small model including the first-sphere residues only. Then single-point calculations were carried out to correct energies by using larger basis set B2.

^b Residues within a radius of 4 Å around the reaction center included the following set of residues: Thr86, Arg171, Leu173, Phe175, Ile186, Gly187, Ala188, His189, Thr190, Asp191, Thr192, Val196, Gln200, Leu206, Tyr207, Ile208, Arg209, Ala228, Thr237, Phe250, Thr266, Pro267, His268, Lys269, Val270, Arg279, Ala281, Phe283.

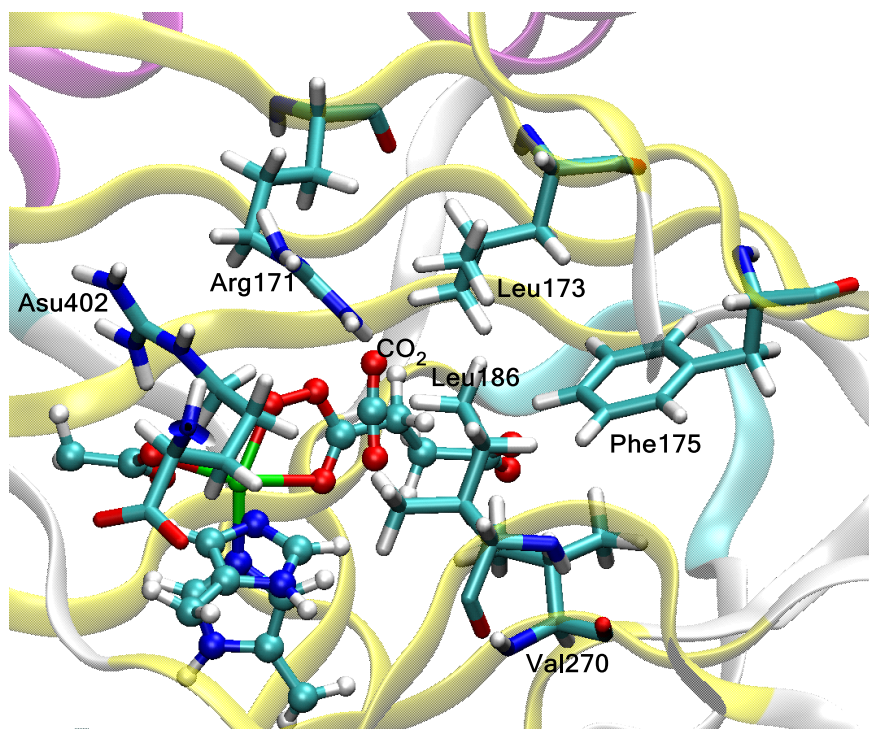


Fig. S5 QM/MM-optimized geometries of $^5\mathbf{2}$.

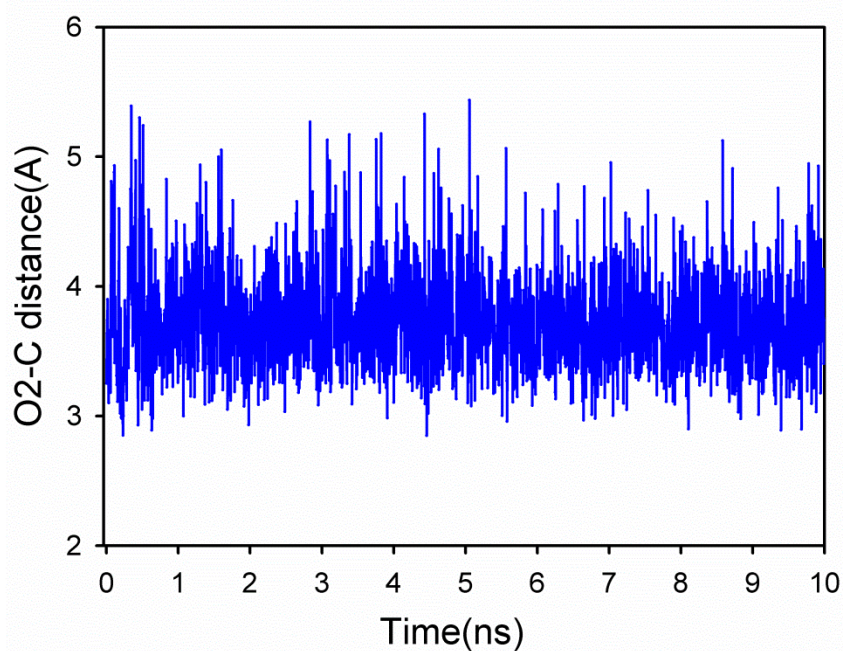
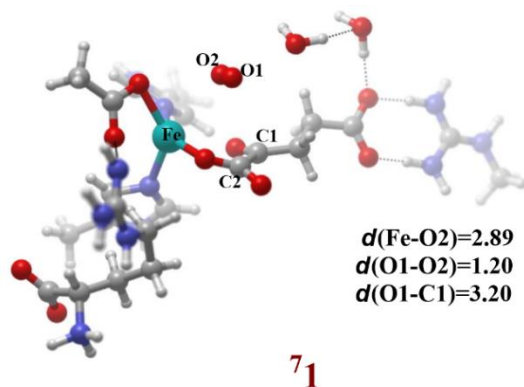


Fig. S6 The distance between the proximal oxygen atom (O2) and the C atom of CO_2 during MD simulations.

Part VII. Cartesian Coordinates of the QM Region of Key Species.

⁷1

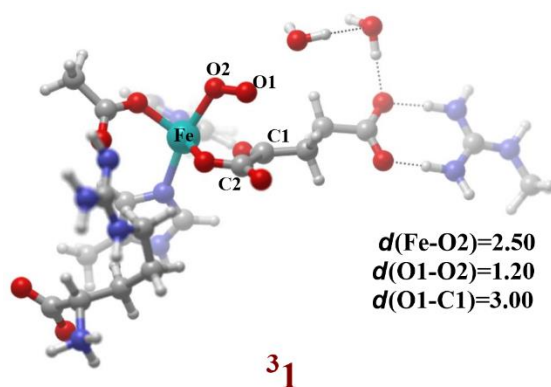


C	9.527016	12.888043	-2.592191
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H	6.456015	11.280306	-4.665662
H	6.447992	9.735809	-3.755137
Fe	5.663691	0.664223	-2.130340
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O	5.634632	1.688203	-0.356594
O	6.142770	3.437091	0.958365
C	6.344016	3.705691	-1.411616
O	6.667857	3.071980	-2.402647
C	6.297491	5.207112	-1.341125
C	6.201290	5.903771	-2.695585
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O	5.959481	8.143977	-3.512931
O	7.407061	7.793871	-1.848642
H	7.203398	5.543052	-0.797410
H	5.455942	5.484805	-0.683739
H	5.195671	5.755755	-3.117764
H	6.924163	5.436449	-3.388366
C	2.785350	-2.330718	-2.093053
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O	3.700739	-0.199655	-2.710257
O	3.233031	2.963434	-1.606685
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H	10.738009	-0.371150	-2.874504
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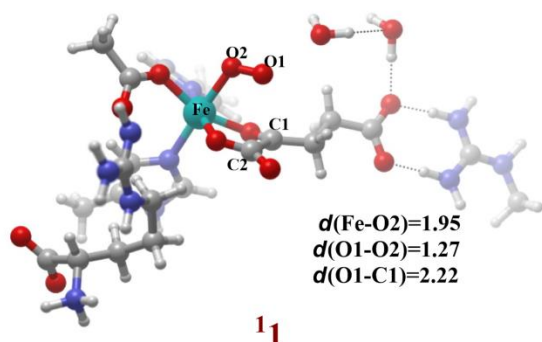


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Fe	5.677334	0.902918	-2.270404	O	4.078913	-0.357625	-2.676696
C	6.047914	2.947174	-0.162419	O	3.412175	3.153479	-1.537688
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O	6.214211	3.484430	0.940889	C	9.680375	-3.069057	-2.812011
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O	3.315421	8.104944	-4.122003
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H	2.921849	5.239433	-4.178424
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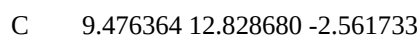
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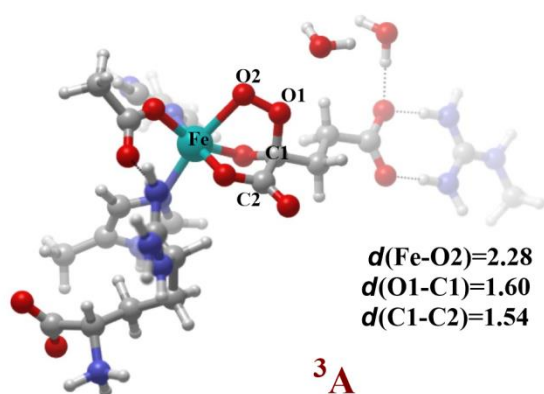
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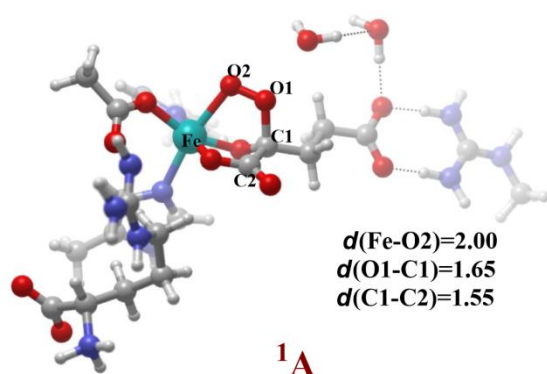
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H 6.637175 -1.185259 0.659542
H 6.518738 0.268780 1.646724
N 6.359813 -1.532450 2.715503
H 6.943790 -1.726663 3.527580
C 5.057056 -1.828814 2.798614
N 4.564225 -2.368516 3.930272
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H	3.653839	-2.818993	3.884905
N	4.207661	-1.518828	1.815522
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H	3.243967	-1.890048	1.912630
C	9.771094	-4.262638	0.572208
O	9.020215	-5.175973	0.192508
O	10.942700	-3.983781	0.217670
H	10.216538	-4.386417	3.128341
O	3.331875	8.171493	-4.236882

H	3.218872	7.502804	-4.948814
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O	3.010365	5.499883	-3.346771
H	2.859266	5.359073	-4.304839
H	2.947928	6.478770	-3.288543
h	3.173377	-3.249726	-2.578578
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¹A



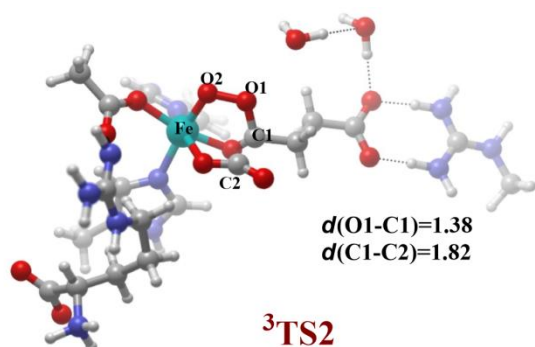
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H	6.397665	9.653263	-3.731184
Fe	5.683262	1.139542	-2.394493
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O	5.664117	1.484895	-0.462214
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C	5.943069	3.551473	-1.515214
O	6.551479	2.837231	-2.447077
C	6.235134	5.034518	-1.411899
C	6.110931	5.798103	-2.732603
C	6.487567	7.286823	-2.667216
O	5.922068	8.055971	-3.507308
O	7.357918	7.659367	-1.845344

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H	5.548813	5.446239	-0.654596
H	5.088603	5.702391	-3.131935
H	6.792790	5.337265	-3.470862
C	2.926777	-2.192710	-2.379728
H	2.158412	-2.187709	-1.583897
H	2.476331	-1.781423	-3.296269
C	4.104800	-1.323809	-1.896463
O	4.712824	-1.632251	-0.865021
O	4.374182	-0.304295	-2.621093
O	4.335152	3.473006	-1.878186
C	4.087968	2.337861	-2.440183
C	9.547634	-2.891687	-2.749447
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H	8.928553	-3.665610	-2.263889
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H	10.537477	-0.182368	-2.829453
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C	8.617151	0.651352	-2.499934
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H	5.631191	-0.436462	-7.184829
C	6.672794	1.297711	-6.410915
C	5.347329	0.033810	-5.159327
H	4.656963	-0.754810	-4.872781
N	5.821018	0.984992	-4.367640
C	6.635970	1.785309	-5.130829

H	7.139738	2.647540	-4.703506
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H	8.186263	-3.587759	1.922671
C	9.222296	-1.856698	1.035215
H	8.811572	-1.968690	0.019093
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N	4.200619	-1.500088	1.838323
H	4.523571	-1.366127	0.872605
H	3.236565	-1.870550	1.937705
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O	9.042497	-5.195681	0.211447
O	10.945522	-3.972472	0.198212
H	10.226793	-4.385897	3.121784
O	3.328296	8.141503	-4.233067
H	3.207340	7.472543	-4.944751
H	4.295188	8.103705	-3.994954
O	3.008570	5.482854	-3.309385
H	2.850271	5.315214	-4.261163
H	2.957980	6.464517	-3.280230
h	3.191970	-3.230280	-2.582674
h	9.711183	-3.148707	-3.795993
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³TS2

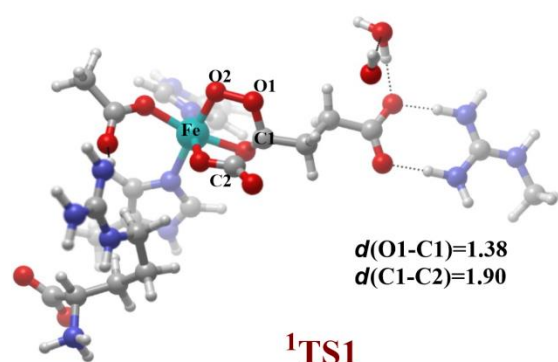


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C	7.818000	11.044000	-3.159000
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H	9.014000	10.492000	-1.602000
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Fe	5.629000	1.118000	-2.386000
C	6.013000	2.838000	0.101000

O	5.874000	1.631000	-0.045000
O	6.236000	3.613000	1.019000
C	5.827000	3.607000	-1.539000
O	6.555000	2.791000	-2.286000
C	6.191000	5.084000	-1.455000
C	6.109000	5.808000	-2.804000
C	6.498000	7.295000	-2.746000
O	5.937000	8.067000	-3.585000
O	7.371000	7.661000	-1.924000
H	7.203000	5.161000	-1.030000
H	5.503000	5.547000	-0.732000
H	5.092000	5.716000	-3.215000
H	6.808000	5.324000	-3.511000
C	2.911000	-2.238000	-2.411000
H	2.141000	-2.233000	-1.617000
H	2.460000	-1.839000	-3.333000
C	4.077000	-1.355000	-1.934000
O	4.660000	-1.614000	-0.874000
O	4.366000	-0.361000	-2.685000
O	4.461000	3.445000	-1.665000
O	4.127000	2.140000	-2.036000
C	9.551000	-2.926000	-2.769000
H	10.533000	-2.964000	-2.268000

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C	8.870000	-1.600000	-2.592000	H	6.609000	-1.200000	0.689000
C	8.560000	0.598000	-2.490000	H	6.493000	0.220000	1.721000
H	8.762000	1.666000	-2.502000	N	6.347000	-1.610000	2.733000
N	7.357000	0.049000	-2.335000	H	6.928000	-1.818000	3.544000
C	7.538000	-1.316000	-2.396000	C	5.038000	-1.880000	2.823000
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H	7.823000	2.833000	-7.603000	H	3.628000	-2.858000	3.914000
H	7.003000	1.639000	-8.634000	N	4.187000	-1.546000	1.849000
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H	5.677000	-0.396000	-7.308000	H	3.219000	-1.906000	1.953000
C	6.705000	1.347000	-6.531000	C	9.777000	-4.266000	0.551000
C	5.324000	0.123000	-5.305000	O	9.029000	-5.181000	0.167000
H	4.618000	-0.658000	-5.029000	O	10.945000	-3.977000	0.193000
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C	6.625000	1.856000	-5.260000	O	3.326000	8.128000	-4.262000
H	7.131000	2.720000	-4.833000	H	3.188000	7.454000	-4.968000
N	10.075000	-3.389000	2.848000	H	4.299000	8.098000	-4.051000
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H	9.704000	-2.879000	3.670000	H	2.826000	5.210000	-4.106000
C	9.189000	-3.281000	1.623000	H	2.973000	6.491000	-3.294000
H	8.187000	-3.611000	1.924000	h	3.191247	-3.273667	-2.603150
C	9.203000	-1.869000	1.035000	h	9.719023	-3.175257	-3.816714
H	8.783000	-1.978000	0.023000	h	8.447632	1.168213	-7.794927
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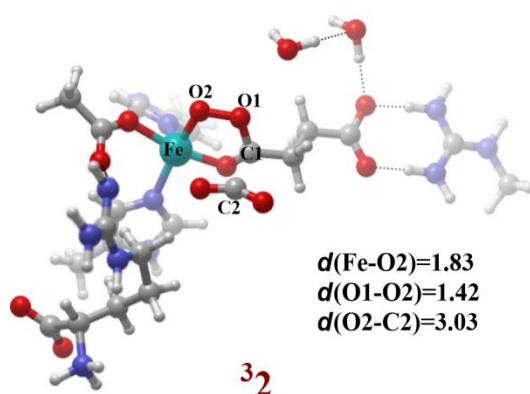
¹TS1



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H	10.076000	13.503000	-3.219000	C	7.831000	11.072000	-3.206000
				N	8.350000	10.172000	-2.360000
				H	8.990000	10.475000	-1.635000
				H	7.933000	9.202000	-2.261000
				N	6.803000	10.709000	-3.970000
				H	6.447000	11.314000	-4.715000
				H	6.405000	9.735000	-3.857000
				Fe	5.584000	1.175000	-2.481000
				C	5.709000	2.704000	-0.145000
				O	5.568000	1.515000	-0.469000
				O	5.881000	3.323000	0.884000

C	5.650000	3.673000	-1.779000	C	6.610000	1.797000	-5.164000
O	6.475000	2.909000	-2.447000	H	7.114000	2.657000	-4.731000
C	5.948000	5.145000	-1.560000	N	10.060000	-3.374000	2.873000
C	5.785000	5.956000	-2.851000	H	11.026000	-3.055000	2.683000
C	6.358000	7.384000	-2.810000	H	9.688000	-2.854000	3.689000
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O	7.284000	7.658000	-2.017000	H	8.181000	-3.571000	1.927000
H	6.978000	5.233000	-1.181000	C	9.230000	-1.848000	1.041000
H	5.262000	5.541000	-0.795000	H	8.829000	-1.959000	0.020000
H	4.726000	6.015000	-3.139000	H	10.292000	-1.573000	0.911000
H	6.308000	5.437000	-3.675000	C	8.470000	-0.683000	1.692000
C	2.919000	-2.223000	-2.349000	H	8.760000	0.225000	1.131000
H	2.182000	-2.233000	-1.524000	H	8.789000	-0.498000	2.732000
H	2.430000	-1.816000	-3.246000	C	6.940000	-0.755000	1.620000
C	4.103000	-1.337000	-1.909000	H	6.637000	-1.188000	0.656000
O	4.708000	-1.600000	-0.860000	H	6.515000	0.264000	1.646000
O	4.372000	-0.362000	-2.685000	N	6.358000	-1.534000	2.713000
O	4.310000	3.484000	-2.039000	H	6.946000	-1.740000	3.520000
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C	9.514000	-2.861000	-2.742000	N	4.560000	-2.337000	3.948000
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H	8.895000	-3.635000	-2.256000	H	3.647000	-2.784000	3.908000
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H	6.684000	-1.924000	-2.296000	O	3.283000	8.115000	-4.196000
C	7.479000	1.762000	-7.602000	H	3.059000	7.317000	-4.737000
H	7.740000	2.828000	-7.511000	H	4.279000	8.135000	-4.125000
H	6.918000	1.638000	-8.545000	O	3.359000	7.679000	-1.407000
N	5.822000	0.208000	-6.447000	H	2.466000	7.842000	-1.048000
H	5.630000	-0.427000	-7.228000	H	3.264000	7.827000	-2.380000
C	6.667000	1.306000	-6.442000	h	3.193822	-3.254275	-2.570384
C	5.312000	0.049000	-5.212000	h	9.688282	-3.128326	-3.784223
H	4.610000	-0.732000	-4.933000	h	8.388793	1.179229	-7.745946
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³2



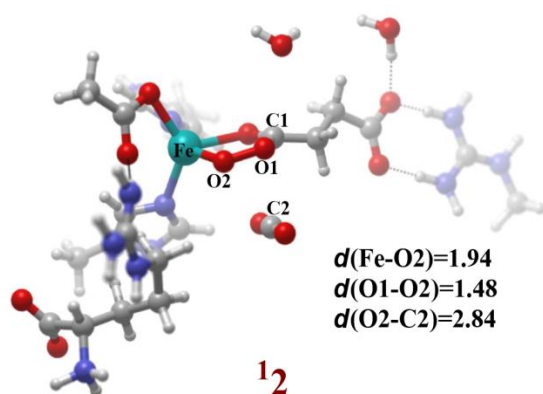
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C	5.797442	3.629299	-1.632122
O	6.544383	2.783133	-2.288740
C	6.172014	5.093427	-1.506453
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C	6.494584	7.323568	-2.766176
O	5.935065	8.103836	-3.598410
O	7.365055	7.677759	-1.937060
H	7.184214	5.155620	-1.078741
H	5.480865	5.549239	-0.782128
H	5.084865	5.755542	-3.257339
H	6.802389	5.361487	-3.553518
C	2.904316	-2.248059	-2.409174
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H	2.450967	-1.851563	-3.330782
C	4.066693	-1.357976	-1.934865
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O	4.456911	3.438873	-1.694974
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H	4.492237	-1.426576	0.885579
H	3.212471	-1.910740	1.961926
C	9.779428	-4.271667	0.543528
O	9.035930	-5.188494	0.159944
O	10.947183	-3.977634	0.187059
H	10.259697	-4.404942	3.089958
O	3.322575	8.136311	-4.255877

H	3.177190	7.448251	-4.948452
H	4.298575	8.118235	-4.058333
O	3.027317	5.552588	-3.138379
H	2.830742	5.222050	-4.035437
H	2.971789	6.528158	-3.261289
h	3.189949	-3.281823	-2.603631
h	9.719942	-3.179362	-3.819287
h	8.451891	1.165153	-7.801408
h	9.221558	13.384094	-1.659689

¹₂



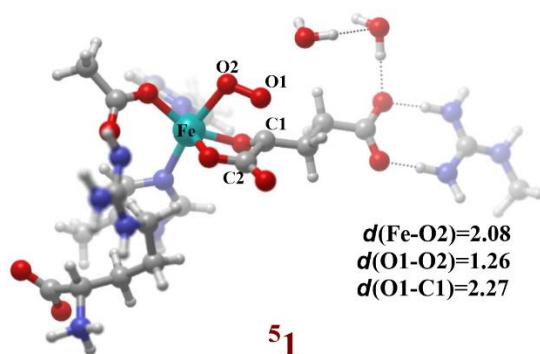
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H	7.810720	13.093232	-3.741942
C	7.846316	11.120898	-3.292695
N	8.314673	10.171005	-2.465728
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H	6.501450	11.473215	-4.812252
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Fe	5.461281	1.249616	-2.501001
C	7.363093	3.467586	0.026356
O	7.886248	3.342587	-0.996906
O	6.926892	3.665089	1.092064
C	5.177093	3.933408	-1.888200
O	5.542474	3.279515	-2.873244
C	5.322918	5.429369	-1.723394
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H	6.351627	5.585714	-1.340239
H	4.643279	5.754240	-0.919798
H	4.132513	6.584219	-3.123583
H	5.480052	5.719980	-3.862581
C	2.769154	-2.154091	-2.268882
H	2.131939	-2.231942	-1.367028
H	2.141868	-1.801614	-3.099304
C	3.902389	-1.149031	-1.970286
O	4.715424	-1.396397	-1.054076
O	3.931472	-0.096796	-2.681270
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C	9.508229	-2.784761	-2.764940
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H	8.780570	-2.039721	-0.069713
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C	8.543123	-0.763953	1.624339
H	8.877350	0.142043	1.086321
H	8.884353	-0.629437	2.666970
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H	6.637568	0.287088	1.650679
N	6.414989	-1.568512	2.623230
H	6.977289	-1.737605	3.456174
C	5.111559	-1.881741	2.687328
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C	9.769668	-4.352356	0.441657
O	8.995686	-5.242216	0.031439
O	10.949838	-4.101695	0.109004
H	10.317604	-4.489494	2.966756
O	2.996651	8.514454	-4.108480
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H	2.096600	3.896149	-3.774366
h	3.098915	-3.156605	-2.541442
h	9.675468	-3.078375	-3.801226
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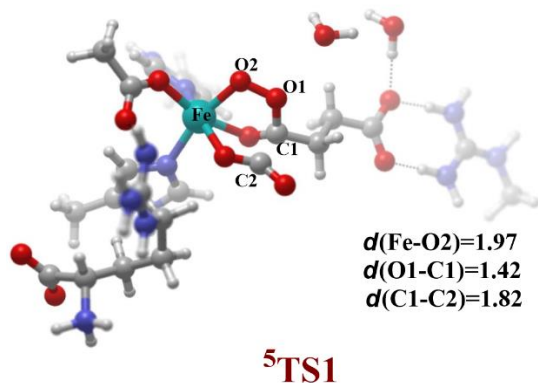
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Fe	5.527418	1.076506	-2.293782

C	6.011226	2.884935	-0.131375
O	5.748349	1.651080	-0.350577
O	6.150332	3.429834	0.968623
C	6.215454	3.699033	-1.420547
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C	6.330785	5.192074	-1.357204
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O	5.927620	8.143863	-3.513502
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H	5.606281	5.547704	-0.608576
H	5.120201	5.766282	-3.066314
H	6.819949	5.429009	-3.438490
C	2.817223	-2.308086	-2.418662
H	2.034177	-2.336288	-1.637636
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C	3.943049	-1.394013	-1.920445
O	4.602871	-1.694709	-0.919119
O	4.124515	-0.309351	-2.582765
O	3.964200	3.430623	-1.554485
O	3.920413	2.404690	-2.279571
C	9.579546	-2.939317	-2.769455

H	10.563984	-3.006395	-2.276981
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C	9.248570	-1.826943	1.066691
H	8.871656	-1.934642	0.037254
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C	8.481048	-0.658720	1.702008

H	8.769572	0.246057	1.136587
H	8.792517	-0.464402	2.743190
C	6.952739	-0.739515	1.621672
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H	6.519967	0.275303	1.624328
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H	6.951397	-1.697149	3.536279
C	5.063648	-1.794247	2.807597
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H	3.650981	-2.764747	3.898134
N	4.217289	-1.483514	1.821670
H	4.546225	-1.357920	0.859273
H	3.252192	-1.853477	1.914876
C	9.757665	-4.253753	0.612647
O	9.007796	-5.186118	0.278500
O	10.918832	-3.975142	0.226416
H	10.158213	-4.370212	3.176269
O	3.323905	8.156879	-4.223759
H	3.210937	7.483792	-4.933030
H	4.293067	8.145259	-3.995641
O	3.067211	5.471870	-3.324100
H	2.921671	5.307164	-4.278313
H	2.985134	6.450677	-3.282704
h	3.145325	-3.328509	-2.616530
h	9.732050	-3.182293	-3.821012
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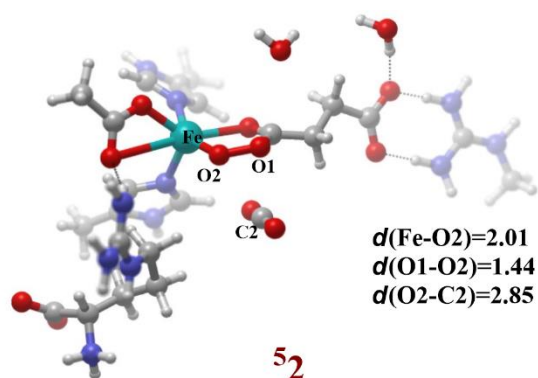
⁵TS1



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N	8.395438	10.240988	-2.318193
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H	7.982052	9.269097	-2.176410
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H	6.454074	11.305540	-4.678739
H	6.429195	9.753163	-3.776904
Fe	5.529156	1.118009	-2.373631
C	6.027969	2.835173	0.001038

O	5.851550	1.636463	-0.224617	C	6.608060	1.795535	-5.203722
O	6.275159	3.525004	0.975085	H	7.105467	2.657281	-4.765089
C	5.840069	3.717347	-1.584640	N	10.068730	-3.386021	2.853321
O	6.473186	2.954449	-2.412491	H	11.026153	-3.053030	2.645996
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C	6.494413	7.410949	-2.708927	H	8.176414	-3.597146	1.934397
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O	7.381159	7.770155	-1.898969	H	8.786538	-1.977271	0.022402
H	7.211260	5.259512	-1.009103	H	10.264087	-1.590306	0.887532
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H	2.344578	-1.912660	-3.327016	H	6.503694	0.245275	1.693129
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N	9.546396	-0.357141	-2.633717	H	3.228809	-1.908912	1.931818
H	10.543522	-0.201016	-2.846453	C	9.758477	-4.268406	0.560709
C	8.911311	-1.586971	-2.576555	O	9.003089	-5.177254	0.179061
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H	8.841700	1.677890	-2.463713	H	10.240930	-4.394504	3.106866
N	7.421434	0.078745	-2.263710	O	3.311424	8.162666	-4.206539
C	7.588535	-1.286628	-2.342797	H	3.191013	7.483464	-4.910930
H	6.761160	-1.974228	-2.200587	H	4.285538	8.165965	-3.998432
C	7.516125	1.753316	-7.629120	O	3.027339	5.515242	-3.198183
H	7.781315	2.817861	-7.533875	H	2.862343	5.257715	-4.126091
H	6.964791	1.633751	-8.579243	H	2.965319	6.496184	-3.249291
N	5.839086	0.205602	-6.497327	h	3.143435	-3.314501	-2.606245
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C	6.688695	1.300887	-6.479135	h	8.424283	1.165977	-7.764573
C	5.302988	0.061749	-5.270926	h	9.247373	13.406631	-1.672569
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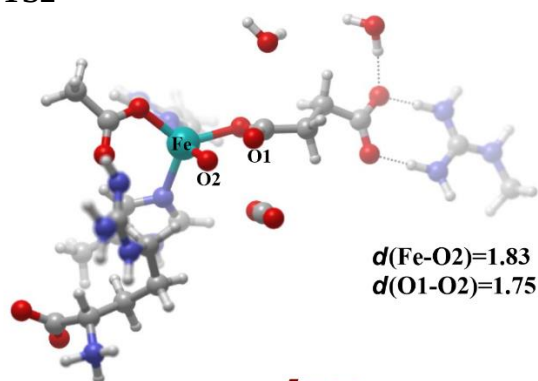
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Fe	5.409818	0.944345	-2.240568
C	7.388431	3.467094	0.041030
O	7.901521	3.273378	-0.976479/
O	6.965964	3.728056	1.098833
C	5.196424	3.937565	-1.855513
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H	4.689190	5.782760	-0.910356
H	4.162837	6.572228	-3.124063
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C	2.702864	-2.238197	-2.080178
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C	3.724477	-1.097180	-2.062184
O	4.734320	-1.143109	-1.287049

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C	5.279520	-0.114716	-5.221770
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H	10.353142	-1.650516	0.831304
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H	3.714753	-2.791517	3.726407
N	4.294173	-1.486082	1.671040
H	4.623504	-1.336963	0.709723
H	3.328501	-1.846761	1.772269
C	9.752288	-4.301782	0.466625
O	8.951086	-5.161533	0.042253
O	10.939380	-4.082843	0.141070
H	10.263681	-4.467308	3.007294
O	3.002446	8.506556	-4.106566

H	2.845763	7.660175	-4.578484
H	3.989514	8.562679	-4.048994
O	2.709754	4.585020	-3.402203
H	2.781218	5.188118	-4.174528
H	2.270974	3.792696	-3.756981
h	3.073567	-3.183890	-2.475539
h	9.737910	-3.151542	-3.856485
h	8.365669	1.173629	-7.713820
h	9.256338	13.385642	-1.659316

⁵TS2



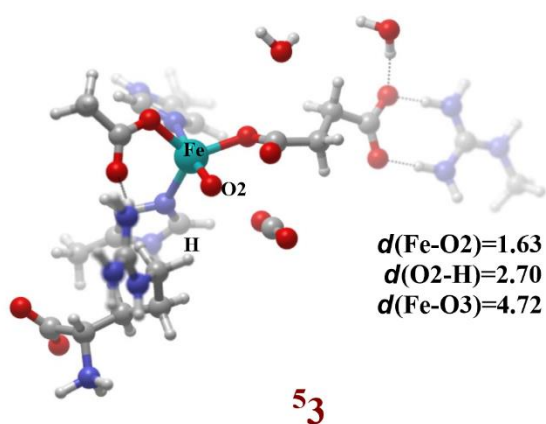
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H	7.811005	13.103968	-3.740636
C	7.851515	11.128799	-3.304089
N	8.322334	10.174629	-2.484800
H	8.942760	10.428001	-1.725740
H	7.852182	9.230071	-2.433654
N	6.841915	10.830131	-4.112635
H	6.504165	11.491183	-4.818011
H	6.364017	9.884576	-4.018298
Fe	5.462074	1.197880	-2.279348
C	7.384872	3.490899	-0.000726
O	7.885701	3.368460	-1.037357
O	7.002749	3.705609	1.082267
C	5.105207	3.996689	-1.764800
O	5.433842	3.307419	-2.749870
C	5.292203	5.506285	-1.692919
C	5.186168	6.308655	-2.979636
C	6.024959	7.600408	-2.987907
O	5.646979	8.479519	-3.823184

O	7.015200	7.718258	-2.229003
H	6.319047	5.647976	-1.301055
H	4.614707	5.898430	-0.917913
H	4.143784	6.589782	-3.176261
H	5.515625	5.694115	-3.836743
C	2.764051	-2.194789	-2.403980
H	2.027596	-2.241732	-1.578786
H	2.240772	-1.831749	-3.300629
C	3.873963	-1.212334	-1.989743
O	4.676968	-1.514216	-1.086299
O	3.891254	-0.088835	-2.596237
O	4.759706	3.487798	-0.631470
O	5.326250	1.828682	-0.567870
C	9.526069	-2.848218	-2.789987
H	10.508297	-2.920692	-2.293165
H	8.887333	-3.610218	-2.311684
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H	10.556258	-0.154529	-2.942395
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C	8.675469	0.706635	-2.467682
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N	7.467192	0.214937	-2.225050
C	7.594716	-1.156038	-2.318122
H	6.751102	-1.817510	-2.146606
C	7.478978	1.746434	-7.594255
H	7.724405	2.815180	-7.486233
H	6.914702	1.631565	-8.537882
N	5.869683	0.136913	-6.447491
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C	6.678554	1.261125	-6.437257
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H	4.655614	-0.816565	-4.951505

N	5.763672	0.947684	-4.412675
C	6.582024	1.755041	-5.161044
H	7.038914	2.648750	-4.740952
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H	9.757652	-3.015403	3.548526
C	9.198630	-3.401575	1.508860
H	8.205383	-3.729279	1.839034
C	9.200013	-1.991256	0.911467
H	8.725989	-2.097720	-0.076072
H	10.253603	-1.730130	0.706774
C	8.510878	-0.808756	1.610941
H	8.834669	0.098863	1.069740
H	8.859505	-0.670741	2.650653
C	6.978541	-0.806730	1.568392
H	6.642304	-1.172267	0.588462
H	6.598687	0.229260	1.655422
N	6.398423	-1.632575	2.624494
H	6.962447	-1.786100	3.459217
C	5.102837	-1.976497	2.688057

N	4.627353	-2.544691	3.810489
H	5.280527	-2.755269	4.583806
H	3.713536	-2.989354	3.776174
N	4.250308	-1.699351	1.699628
H	4.557550	-1.526072	0.734473
H	3.290035	-2.069322	1.816084
C	9.769363	-4.382416	0.425094
O	8.996914	-5.270250	0.007108
O	10.947499	-4.124357	0.090413
H	10.347882	-4.502252	2.951663
O	2.981141	8.547873	-4.089748
H	2.808154	7.702279	-4.557347
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O	2.634799	4.621565	-3.398461
H	2.775352	5.218343	-4.165840
H	1.962972	3.992179	-3.713283
h	3.099832	-3.207864	-2.625335
h	9.691716	-3.119544	-3.832584
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⁵3

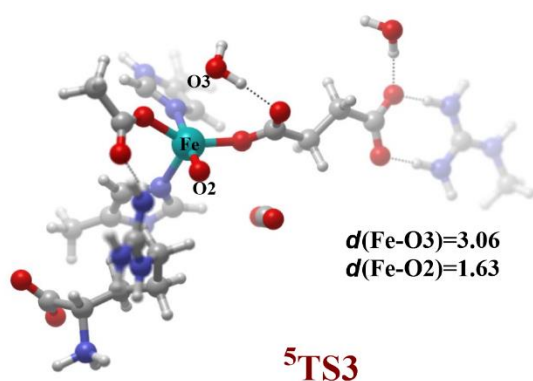


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H	7.761130	13.038855	-3.719775
C	7.813265	11.067347	-3.246538
N	8.299608	10.130427	-2.417107
H	8.919706	10.401986	-1.663966
H	7.850980	9.173228	-2.354368
N	6.801938	10.743553	-4.044434
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H	6.352634	9.783680	-3.939565
Fe	5.615734	1.137394	-2.261389
C	7.611955	3.407641	-0.307542
O	8.297460	3.340702	-1.238106
O	7.000108	3.512256	0.680743
C	4.957142	3.867130	-1.640078
O	5.625357	3.053287	-2.451569
C	5.465033	5.319430	-1.621328
C	5.314881	6.152750	-2.893518
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O	5.698944	8.344664	-3.729407
O	7.082894	7.636100	-2.127509
H	6.540074	5.327879	-1.368348
H	4.931525	5.811784	-0.793554
H	4.258161	6.389116	-3.075677
H	5.653222	5.572448	-3.772045
C	2.831719	-2.180397	-2.455194
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C	3.980571	-1.292490	-1.941446
O	4.663742	-1.662565	-0.981022
O	4.148015	-0.180843	-2.565150
O	4.081446	3.492081	-0.888139

O	5.660535	1.154614	-0.636444	C	8.513151	-0.841761	1.630523
C	9.574928	-2.936203	-2.820028	H	8.821607	0.070125	1.087093
H	10.558848	-3.010331	-2.327581	H	8.875782	-0.702351	2.664584
H	8.936570	-3.698236	-2.341786	C	6.981019	-0.846318	1.606552
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C	8.948993	-1.582646	-2.646152	N	6.402012	-1.671690	2.664070
C	8.720949	0.624947	-2.630273	H	6.973352	-1.856789	3.487313
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N	7.512876	0.135327	-2.386143	N	4.616912	-2.575070	3.840593
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H	7.716991	2.855405	-7.444601	H	4.556634	-1.460912	0.804647
H	6.875171	1.672840	-8.470139	H	3.281936	-2.018208	1.864490
N	5.860406	0.196892	-6.360639	C	9.780978	-4.405320	0.423535
H	5.687983	-0.444393	-7.139356	O	9.017912	-5.307724	0.020487
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C	5.339519	0.051819	-5.126518	H	10.366547	-4.523037	2.950400
H	4.658833	-0.749908	-4.849244	O	3.050190	8.440636	-4.133362
N	5.750871	1.033726	-4.340982	H	2.874898	7.595513	-4.599600
C	6.566830	1.839283	-5.095998	H	4.034933	8.452878	-4.027190
H	7.015884	2.737269	-4.676867	O	2.760332	4.656488	-3.564077
N	10.136583	-3.517649	2.707953	H	2.810013	5.222833	-4.367543
H	11.067979	-3.126940	2.486796	H	1.930099	4.161854	-3.672892
H	9.771550	-3.038943	3.547970	h	3.123155	-3.209655	-2.664378
C	9.211246	-3.426619	1.509610	h	9.729020	-3.191126	-3.868520
H	8.220299	-3.758194	1.842312	h	8.365055	1.212300	-7.715203
C	9.204465	-2.014335	0.917710	h	9.228234	13.366491	-1.650765
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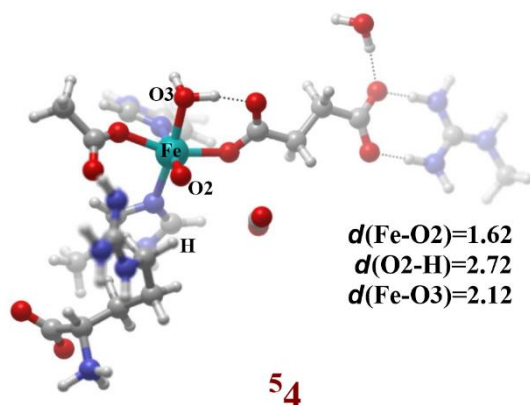
⁵TS3



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N	6.894000	10.896000	-4.120000

H	6.544000	11.555000	-4.821000	C	5.401000	-0.055000	-5.203000
H	6.391000	9.970000	-3.980000	H	4.720000	-0.859000	-4.936000
Fe	5.668000	0.920000	-2.313000	N	5.860000	0.877000	-4.381000
C	7.740000	3.353000	-0.424000	C	6.668000	1.705000	-5.120000
O	8.532000	3.362000	-1.267000	H	7.163000	2.562000	-4.672000
O	7.012000	3.378000	0.489000	N	10.131000	-3.503000	2.710000
C	5.298000	3.929000	-2.171000	H	11.055000	-3.112000	2.461000
O	5.966000	2.852000	-2.488000	H	9.781000	-3.015000	3.552000
C	6.102000	5.222000	-2.317000	C	9.183000	-3.430000	1.529000
C	5.301000	6.403000	-2.854000	H	8.203000	-3.778000	1.879000
C	6.109000	7.708000	-2.915000	C	9.142000	-2.021000	0.930000
O	5.667000	8.590000	-3.710000	H	8.650000	-2.141000	-0.047000
O	7.127000	7.838000	-2.193000	H	10.187000	-1.740000	0.704000
H	6.985000	5.031000	-2.946000	C	8.448000	-0.852000	1.645000
H	6.488000	5.501000	-1.318000	H	8.746000	0.058000	1.093000
H	4.404000	6.581000	-2.235000	H	8.818000	-0.703000	2.675000
H	4.914000	6.193000	-3.865000	C	6.915000	-0.861000	1.634000
C	2.846000	-2.312000	-2.535000	H	6.559000	-1.240000	0.666000
H	2.012000	-2.319000	-1.810000	H	6.537000	0.175000	1.710000
H	2.491000	-1.865000	-3.476000	N	6.340000	-1.661000	2.712000
C	3.996000	-1.499000	-1.918000	H	6.938000	-1.919000	3.495000
O	4.364000	-1.759000	-0.772000	C	5.029000	-1.922000	2.821000
O	4.520000	-0.609000	-2.683000	N	4.564000	-2.562000	3.905000
O	4.141000	3.962000	-1.764000	H	5.225000	-2.823000	4.654000
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C	9.653000	-3.058000	-2.873000	N	4.154000	-1.486000	1.909000
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H	9.023000	-3.837000	-2.411000	H	3.200000	-1.882000	1.995000
N	9.691000	-0.502000	-2.716000	C	9.753000	-4.400000	0.435000
H	10.685000	-0.354000	-2.949000	O	8.993000	-5.302000	0.026000
C	9.028000	-1.713000	-2.645000	O	10.921000	-4.119000	0.082000
C	8.799000	0.492000	-2.531000	H	10.370000	-4.505000	2.959000
H	9.058000	1.546000	-2.566000	O	3.002000	8.430000	-4.096000
N	7.590000	-0.011000	-2.318000	H	2.875000	7.583000	-4.585000
C	7.716000	-1.380000	-2.391000	H	3.980000	8.533000	-4.025000
H	6.870000	-2.044000	-2.250000	O	2.818000	1.900000	-2.849000
C	7.493000	1.763000	-7.578000	H	2.594000	2.268000	-3.721000
H	7.741000	2.830000	-7.461000	H	3.149000	2.663000	-2.316000
H	6.917000	1.657000	-8.514000	h	3.139744	-3.343228	-2.730829
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H	5.680000	-0.459000	-7.242000	h	8.405203	1.191912	-7.750655
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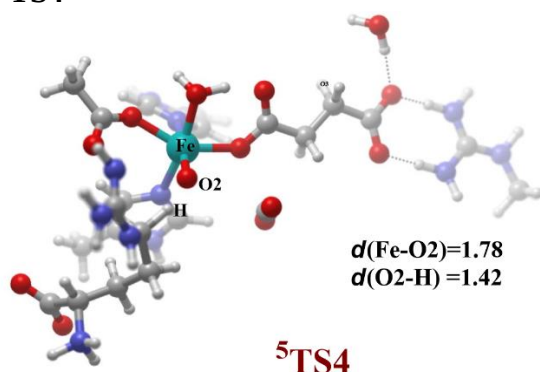
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C	7.962512	11.247477	-3.371616
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H	7.956913	9.357868	-2.474397
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H	6.583673	11.630584	-4.848505
H	6.408015	10.048451	-4.009078
Fe	5.430886	0.952822	-2.267191
C	7.729281	3.414957	-0.439370
O	8.547038	3.486808	-1.255876
O	6.991250	3.380158	0.466684
C	5.282427	4.030794	-2.243557
O	5.980523	2.950882	-2.369220
C	6.064551	5.337871	-2.290116
C	5.292940	6.507808	-2.887827
C	6.100869	7.808667	-2.939982
O	5.639359	8.708612	-3.703977
O	7.141406	7.916748	-2.247462
H	7.005714	5.168996	-2.835080
H	6.357099	5.597916	-1.254995
H	4.359744	6.700572	-2.330279
H	4.958240	6.275071	-3.912793
C	2.793415	-2.457626	-2.477276
H	1.989235	-2.494276	-1.721042
H	2.393493	-2.023033	-3.406930
C	3.953211	-1.625684	-1.907510
O	4.354821	-1.871194	-0.766713
O	4.444444	-0.745247	-2.695867

O	4.052632	4.070079	-2.072036
O	5.363791	0.952002	-0.647938
C	9.559579	-2.937972	-2.824622
H	10.543196	-2.996074	-2.329299
H	8.934139	-3.713549	-2.350768
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H	10.528432	-0.216994	-2.988616
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H	8.842067	1.661259	-2.660060
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C	7.585605	-1.292906	-2.390103
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H	7.686993	2.855242	-7.378086
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N	5.827825	0.155620	-6.400465
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C	6.622816	1.290286	-6.361353
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N	5.654602	0.947703	-4.365741
C	6.485845	1.774910	-5.084931
H	6.934641	2.655678	-4.632633
N	10.136977	-3.509084	2.704752
H	11.061196	-3.118919	2.454707
H	9.786344	-3.019100	3.544499
C	9.191977	-3.442189	1.521334
H	8.213648	-3.796223	1.868597
C	9.147152	-2.034592	0.920861
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H	10.190825	-1.749594	0.696771
C	8.446368	-0.866784	1.633182
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C	6.913530	-0.878453	1.614354
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C	5.024868	-1.920043	2.814603
N	4.559721	-2.535712	3.914119
H	5.225629	-2.794549	4.660366

H	3.620428	-2.923702	3.894191
N	4.151101	-1.498881	1.895074
H	4.440910	-1.347652	0.920094
H	3.194411	-1.889980	1.986284
C	9.772372	-4.409325	0.429311
O	9.018308	-5.312078	0.015391
O	10.942975	-4.123232	0.087100
H	10.378179	-4.509377	2.956988
O	2.964684	8.534348	-4.018310

H	2.851890	7.684027	-4.503782
H	3.942477	8.654767	-3.966976
O	3.448760	1.668517	-2.450962
H	3.130248	1.574114	-3.365694
H	3.520732	2.677184	-2.249587
h	3.115781	-3.475473	-2.696672
h	9.722672	-3.190797	-3.872261
h	8.344820	1.221582	-7.689658
h	9.325626	13.437841	-1.688536

5TS4



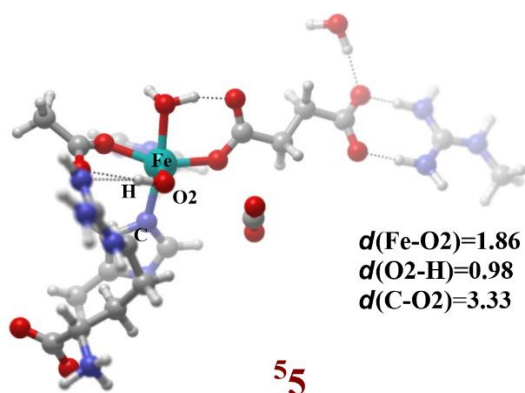
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C	7.972534	11.253031	-3.380213
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H	7.971482	9.359815	-2.489741
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H	6.589981	11.639822	-4.852739
H	6.422169	10.051473	-4.022850
Fe	5.546288	0.969977	-1.765223
C	7.780692	3.572583	-0.368403
O	8.591001	3.533094	-1.197685
O	7.093875	3.664128	0.573817
C	5.287893	4.046738	-2.179168
O	5.988229	2.981273	-1.946787
C	6.072031	5.346975	-2.281296
C	5.307882	6.509424	-2.897646
C	6.119705	7.807631	-2.958213
O	5.661134	8.704983	-3.726848
O	7.159441	7.918107	-2.264348
H	7.003572	5.148948	-2.836602

H	6.397018	5.630291	-1.263112
H	4.372511	6.715251	-2.348229
H	4.973348	6.263387	-3.919114
C	2.859676	-2.499836	-2.444942
H	2.018004	-2.551146	-1.729470
H	2.504293	-2.013701	-3.367284
C	3.992756	-1.705318	-1.777573
O	4.461254	-2.122056	-0.706433
O	4.368335	-0.645784	-2.373060
O	4.052744	4.067962	-2.292792
O	5.794609	0.867585	-0.009476
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H	10.570352	-3.096327	-2.379246
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H	10.589725	-0.302033	-2.910106
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H	7.630372	2.890629	-7.172318
H	6.735225	1.750761	-8.197427
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C	6.628707	1.319276	-6.103345
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H	4.664892	-0.806605	-4.609952
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H	6.982652	2.697798	-4.396658

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C	9.218004	-3.399548	1.500845
H	8.224376	-3.751047	1.805583
C	9.204616	-1.985776	0.909616
H	8.825224	-2.107249	-0.115495
H	10.253618	-1.660124	0.794424
C	8.387156	-0.846377	1.551334
H	8.667335	0.071848	1.005927
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C	4.962005	-1.739599	2.828727
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H	3.630306	-2.627885	4.065615
N	4.097558	-1.595809	1.840860
H	4.395195	-1.478976	0.856501
H	3.159645	-2.029774	1.966081
C	9.831974	-4.367934	0.421939
O	9.101803	-5.287571	0.010918
O	10.999029	-4.059415	0.089939
H	10.337158	-4.495512	2.965169
O	2.991153	8.497031	-4.034131
H	2.878282	7.646111	-4.520179
H	3.968055	8.627907	-3.992254
O	3.560929	1.680872	-1.793489
H	3.123384	1.162264	-2.490402
H	3.579656	2.682826	-2.041648
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h	9.735162	-3.226068	-3.921088
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⁵5

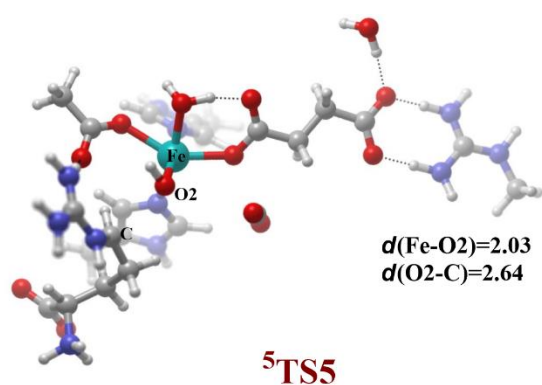


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C	7.996458	11.279688	-3.402516
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N	6.973340	10.998988	-4.199280
H	6.616417	11.684622	-4.870249
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Fe	5.436730	1.044169	-2.164404
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O	8.569081	3.558626	-1.307467
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C	5.235305	4.116656	-2.281524
O	5.936813	3.027141	-2.240532
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O	5.611559	8.800639	-3.701912
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C	3.992383	-1.592421	-1.897068
O	4.505889	-1.795138	-0.774317
O	4.385649	-0.689275	-2.690074
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O	5.329113	0.931471	-0.315864	H	10.143608	-1.705124	0.705913
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H	6.893097	1.714545	-8.479553	H	4.337238	-2.118984	0.864626
N	5.845369	0.193777	-6.421161	H	3.101288	-2.555799	2.024225
H	5.713031	-0.451303	-7.204574	C	9.866584	-4.422960	0.318650
C	6.638695	1.328926	-6.388588	O	9.137935	-5.319358	-0.146326
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C	6.489537	1.826786	-5.117170	H	2.836007	7.737692	-4.479724
H	6.940350	2.713163	-4.675358	H	3.911241	8.728902	-3.948998
N	10.190241	-3.562111	2.613336	O	3.438059	1.710848	-2.405693
H	11.101962	-3.148438	2.355417	H	3.099401	1.476576	-3.286641
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C	9.243640	-3.513058	1.432208	h	3.153018	-3.476767	-2.633678
H	8.281128	-3.918774	1.768187	h	9.727564	-3.177714	-3.897509
C	9.122111	-2.091648	0.879014	h	8.364899	1.231352	-7.709284
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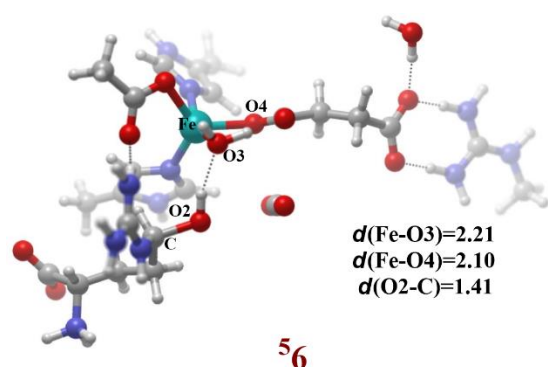
⁵TS5



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				N	8.554000	12.498000	-3.449000
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				C	7.980000	11.270000	-3.377000
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				H	6.595000	11.653000	-4.846000
				H	6.403000	10.081000	-3.988000
				Fe	5.639000	0.953000	-1.690000

C	7.867000	3.574000	-0.495000	N	5.773000	0.991000	-4.026000
O	8.691000	3.588000	-1.317000	C	6.580000	1.809000	-4.782000
O	7.243000	3.612000	0.497000	H	7.052000	2.689000	-4.349000
C	5.341000	4.104000	-2.073000	N	10.199000	-3.544000	2.629000
O	6.082000	3.071000	-1.882000	H	11.106000	-3.133000	2.347000
C	6.072000	5.438000	-2.187000	H	9.855000	-3.053000	3.470000
C	5.263000	6.589000	-2.766000	C	9.247000	-3.534000	1.455000
C	6.067000	7.888000	-2.869000	H	8.303000	-3.983000	1.791000
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H	6.429000	5.719000	-1.179000	C	8.183000	-1.064000	1.547000
H	4.356000	6.788000	-2.167000	H	8.288000	-0.143000	0.949000
H	4.879000	6.339000	-3.769000	H	8.507000	-0.844000	2.580000
C	2.854000	-2.582000	-2.263000	C	6.745000	-1.412000	1.506000
H	2.101000	-2.683000	-1.460000	H	6.218000	-1.560000	0.560000
H	2.381000	-2.091000	-3.127000	H	4.789000	0.383000	0.473000
C	4.030000	-1.751000	-1.736000	N	6.134000	-1.752000	2.641000
O	4.613000	-2.149000	-0.680000	H	6.675000	-1.672000	3.509000
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O	4.097000	4.087000	-2.148000	N	4.501000	-2.621000	4.032000
O	5.696000	0.706000	0.326000	H	5.243000	-2.730000	4.755000
C	9.644000	-3.046000	-2.899000	H	3.620000	-3.112000	4.166000
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H	9.032000	-3.845000	-2.448000	H	4.238000	-2.199000	0.757000
N	9.687000	-0.503000	-2.622000	H	3.061000	-2.717000	2.009000
H	10.662000	-0.339000	-2.917000	C	9.911000	-4.426000	0.339000
C	9.020000	-1.713000	-2.606000	O	9.212000	-5.329000	-0.148000
C	8.814000	0.469000	-2.271000	O	11.076000	-4.067000	0.058000
H	9.078000	1.524000	-2.234000	H	10.473000	-4.536000	2.893000
N	7.620000	-0.039000	-2.009000	O	2.936000	8.580000	-4.003000
C	7.733000	-1.395000	-2.227000	H	2.838000	7.727000	-4.489000
H	6.895000	-2.072000	-2.082000	H	3.912000	8.705000	-3.932000
C	7.386000	1.842000	-7.274000	O	3.602000	1.662000	-1.685000
H	7.652000	2.905000	-7.153000	H	3.174000	1.206000	-2.429000
H	6.736000	1.769000	-8.165000	H	3.648000	2.669000	-1.892000
N	5.869000	0.199000	-6.080000	h	3.169317	-3.574586	-2.584581
H	5.694000	-0.418000	-6.873000	h	9.772741	-3.244331	-3.963029
C	6.666000	1.332000	-6.070000	h	8.278773	1.281308	-7.550851
C	5.367000	0.029000	-4.838000	h	9.339718	13.445927	-1.696745
H	4.711000	-0.793000	-4.565000				

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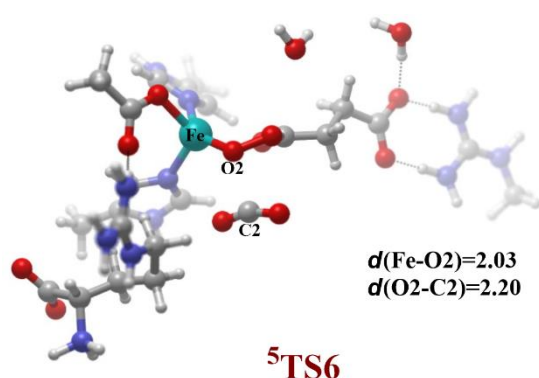
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C	7.837342	11.075094	-3.215660
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H	6.350769	9.779907	-3.814530
Fe	5.493405	0.785558	-2.331242
C	7.436082	3.648821	-0.221257
O	8.203377	3.600056	-1.092335
O	6.699754	3.704961	0.677115
C	5.112335	3.865086	-2.149230
O	5.670006	2.851168	-2.675137
C	5.453741	5.208714	-2.794637
C	5.071795	6.486749	-2.027291
C	5.990132	7.657751	-2.422202
O	5.624448	8.377016	-3.401301
O	7.056424	7.820879	-1.779659
H	5.009721	5.216309	-3.807320
H	6.546892	5.176018	-2.954016
H	5.180723	6.307606	-0.946837
H	4.027121	6.766008	-2.239725
C	2.684489	-2.317983	-2.277343
H	2.154229	-2.433355	-1.312378
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C	3.734446	-1.218034	-2.119399
O	4.761862	-1.392362	-1.391785
O	3.539946	-0.118812	-2.698060

O	4.376781	3.799427	-1.128593
O	6.784299	0.684990	1.166917
C	9.657591	-2.992988	-2.862872
H	10.661336	-3.054365	-2.410797
H	9.055958	-3.783895	-2.383565
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H	10.600790	-0.243796	-2.902719
C	8.999731	-1.665978	-2.619704
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H	8.899018	1.587251	-2.377628
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C	5.306489	-0.218317	-5.315814
H	4.587601	-1.016878	-5.132797
N	5.749112	0.659426	-4.435640
C	6.585852	1.511852	-5.112487
H	7.056470	2.353516	-4.611866
N	10.114295	-3.512782	2.727969
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C	9.222168	-3.391485	1.506945
H	8.208071	-3.666397	1.824027
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N	6.482649	-1.299160	2.498379
H	7.043809	-1.388527	3.346646
C	5.201223	-1.701559	2.567739
N	4.725473	-2.179934	3.729090

H	5.381274	-2.421193	4.496844
H	3.819849	-2.646008	3.706360
N	4.353229	-1.551691	1.539166
H	4.694861	-1.565053	0.568855
H	3.411124	-1.960689	1.682653
C	9.757178	-4.406788	0.436807
O	8.944157	-5.259569	0.019139
O	10.944789	-4.200861	0.106750
H	10.320672	-4.524798	2.963092
O	3.010801	8.438198	-4.036697

H	2.891401	7.605538	-4.552626
H	3.978399	8.463870	-3.837651
O	4.692270	1.435140	-0.378329
H	3.859746	0.941373	-0.271384
H	4.473035	2.471634	-0.618456
h	3.076223	-3.287475	-2.585072
h	9.779129	-3.220030	-3.921998
h	8.382507	1.169046	-7.734347
h	9.239006	13.377567	-1.666035

⁵TS6



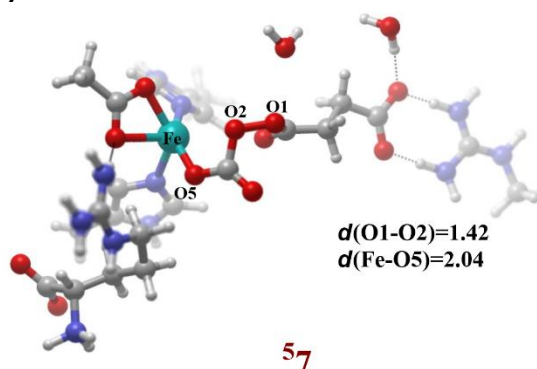
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H	10.265760	12.059575	-2.337009
H	10.214862	13.595584	-3.197938
N	8.482893	12.441932	-3.396329
H	7.872184	13.179463	-3.774450
C	7.921589	11.209693	-3.336356
N	8.399774	10.267175	-2.510827
H	9.038289	10.529982	-1.770279
H	7.918236	9.328118	-2.426072
N	6.899244	10.910298	-4.128109
H	6.552124	11.570144	-4.829510
H	6.418672	9.968598	-4.019932
Fe	5.507688	1.071989	-2.387098
C	6.926945	2.559104	0.343690
O	7.616998	1.712463	-0.065366
O	6.585211	3.503517	0.970240
C	5.458780	4.084351	-1.818727
O	6.212498	3.449967	-2.544487
C	5.433642	5.582051	-1.671301
C	5.352461	6.381484	-2.966005
C	6.123763	7.707263	-2.958240
O	5.718073	8.563805	-3.803342

O	7.096874	7.864990	-2.185491
H	6.391753	5.828248	-1.172996
H	4.625793	5.856740	-0.976785
H	4.305983	6.599213	-3.209561
H	5.756515	5.784805	-3.803242
C	2.758630	-2.278708	-2.282474
H	2.134283	-2.383685	-1.375277
H	2.119098	-1.922567	-3.102608
C	3.873670	-1.263196	-1.986475
O	4.670276	-1.460137	-1.042514
O	3.916190	-0.229944	-2.724235
O	4.666016	3.485776	-0.926390
O	5.041898	2.120664	-0.706871
C	9.588645	-2.902064	-2.834707
H	10.577540	-2.954870	-2.350062
H	8.966829	-3.671304	-2.345945
N	9.563693	-0.334059	-2.803931
H	10.558091	-0.180591	-3.028118
C	8.933637	-1.560507	-2.673660
C	8.635017	0.637292	-2.667925
H	8.863602	1.699774	-2.726107
N	7.439100	0.117430	-2.435051
C	7.612925	-1.249366	-2.438310
H	6.786036	-1.927915	-2.253178
C	7.493839	1.789509	-7.628507
H	7.764466	2.853142	-7.533527
H	6.947227	1.674316	-8.582528
N	5.821816	0.238422	-6.498401
H	5.683848	-0.428270	-7.262991
C	6.647455	1.351378	-6.486252
C	5.240749	0.129951	-5.286443
H	4.533576	-0.654862	-5.021571

N	5.627293	1.123143	-4.501773
C	6.498281	1.892471	-5.234263
H	6.958620	2.782521	-4.810365
N	10.169166	-3.550642	2.645467
H	11.083062	-3.152848	2.370546
H	9.836668	-3.059724	3.490882
C	9.196762	-3.491911	1.484420
H	8.227150	-3.843942	1.856263
C	9.135688	-2.083934	0.888878
H	8.596585	-2.188621	-0.065429
H	10.170385	-1.808310	0.616694
C	8.491895	-0.923104	1.658941
H	8.792731	0.001151	1.140180
H	8.888732	-0.829223	2.684299
C	6.961173	-0.901599	1.685600
H	6.578141	-1.139871	0.683473
H	6.615241	0.122413	1.922363
N	6.392539	-1.828118	2.658300
H	6.945163	-2.017123	3.493354
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N	4.623386	-2.771294	3.812021
H	5.260012	-2.924597	4.609855
H	3.705151	-3.205804	3.782319
N	4.242058	-1.874167	1.723975
H	4.542806	-1.717242	0.752492
H	3.278125	-2.230395	1.849660
C	9.754663	-4.458135	0.386345
O	8.978894	-5.344266	-0.030466
O	10.927436	-4.191922	0.038548
H	10.419819	-4.549249	2.899434
O	3.042413	8.531726	-4.108728
H	2.878740	7.680051	-4.567258
H	4.029454	8.600213	-4.068982
O	2.906922	4.654390	-3.418456
H	2.903547	5.218056	-4.225638
H	2.104882	4.111319	-3.504654
h	3.116470	-3.265401	-2.576502
h	9.740744	-3.170148	-3.880204
h	8.398820	1.198229	-7.768024
h	9.298274	13.425576	-1.677516

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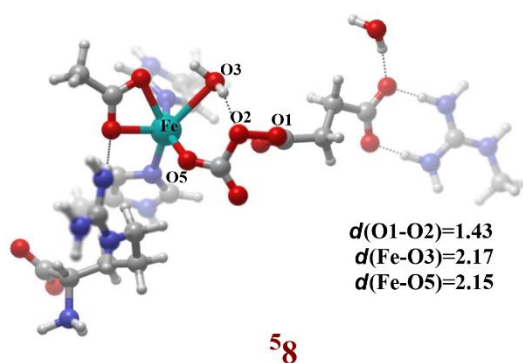
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H	10.418652	12.198121	-2.434630
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H	8.010060	13.364757	-3.816895
C	8.107249	11.384845	-3.511529
N	8.612442	10.406231	-2.753165
H	9.253365	10.641057	-2.005776
H	8.101845	9.473216	-2.696243
N	7.072740	11.128760	-4.303156
H	6.693870	11.844479	-4.928248
H	6.532654	10.221226	-4.198270
Fe	5.573462	0.402197	-2.122694

C	5.586068	2.318550	0.039305
O	5.853359	1.124047	-0.240223
O	6.079684	3.080301	0.860591
C	5.465801	4.593686	-1.699135
O	6.189565	3.848716	-2.308044
C	5.533230	6.088748	-1.659691
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C	6.165150	8.031698	-3.162192
O	5.688669	8.897413	-3.956420
O	7.235918	8.146348	-2.520204
H	6.540602	6.333028	-1.277408
H	4.787298	6.477413	-0.949523
H	4.316166	6.931002	-3.235281
H	5.738136	6.050055	-3.811590
C	2.671208	-2.456854	-2.201051
H	2.195716	-2.612838	-1.214524
H	1.895454	-2.137422	-2.910966
C	3.728482	-1.374406	-2.062545
O	4.734903	-1.527563	-1.301203
O	3.602856	-0.309569	-2.720659
O	4.498345	4.168451	-0.833211
O	4.509999	2.749731	-0.761179

C	9.792046	-3.215229	-2.932115
H	10.809050	-3.280490	-2.514407
H	9.216056	-4.031386	-2.464395
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H	10.709753	-0.448390	-2.839282
C	9.126470	-1.907438	-2.628215
C	8.772601	0.267132	-2.372622
H	8.973779	1.336517	-2.322305
N	7.589158	-0.309038	-2.221540
C	7.798426	-1.657818	-2.379317
H	6.989633	-2.373497	-2.289121
C	7.426350	1.781225	-7.358664
H	7.687094	2.837900	-7.191336
H	6.819602	1.736021	-8.281166
N	5.814632	0.129391	-6.307675
H	5.637119	-0.442411	-7.137190
C	6.652828	1.228756	-6.208849
C	5.266025	-0.096693	-5.098416
H	4.537095	-0.884143	-4.913169
N	5.696002	0.797929	-4.220540
C	6.557128	1.631579	-4.897647
H	7.025963	2.481873	-4.404413
N	10.173058	-3.555614	2.670788
H	11.088946	-3.154138	2.408263
H	9.832769	-3.068680	3.515776
C	9.208531	-3.492592	1.505656
H	8.236573	-3.846200	1.870852
C	9.153177	-2.083207	0.912452
H	8.626383	-2.195949	-0.047037
H	10.189828	-1.805812	0.650199

C	8.488858	-0.925951	1.667857
H	8.754777	-0.002241	1.123048
H	8.894447	-0.794373	2.685470
C	6.961978	-0.950133	1.701457
H	6.596416	-1.219015	0.703282
H	6.582319	0.063400	1.905287
N	6.407990	-1.880113	2.680989
H	6.945524	-2.043349	3.531741
C	5.114109	-2.229105	2.709540
N	4.615328	-2.808370	3.812278
H	5.237168	-2.947020	4.623999
H	3.697504	-3.242642	3.772227
N	4.283272	-1.945699	1.697906
H	4.635563	-1.812767	0.746732
H	3.315537	-2.297585	1.798487
C	9.762022	-4.449642	0.398358
O	8.973934	-5.316198	-0.039179
O	10.938416	-4.193849	0.056806
H	10.424590	-4.555012	2.921007
O	3.001023	8.658402	-4.116185
H	2.870667	7.803715	-4.576417
H	3.980344	8.808480	-4.141308
O	3.128334	4.804439	-3.474566
H	3.011316	5.343325	-4.291647
H	2.343904	4.231460	-3.444005
h	3.077243	-3.402539	-2.560049
h	9.870518	-3.376537	-4.007238
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⁵8

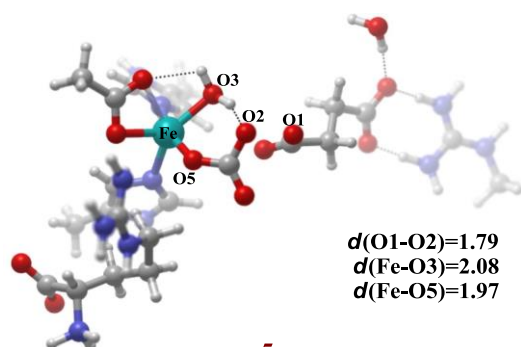


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N	8.693105	12.678061	-3.542848
H	8.016869	13.413030	-3.802290
C	8.196958	11.422329	-3.617825
N	8.770023	10.416495	-2.951204
H	9.408533	10.623241	-2.193945
H	8.307342	9.458800	-2.973811
N	7.149020	11.175672	-4.397499
H	6.730070	11.913139	-4.970314
H	6.622368	10.263175	-4.316717
Fe	5.430131	0.568127	-2.206155

C	5.486015	2.489964	0.179581	N	5.769543	0.504174	-4.323872
O	5.354099	1.314022	-0.194487	C	6.585584	1.398205	-4.972949
O	6.282015	3.069855	0.904097	H	7.064099	2.224188	-4.448506
C	5.688859	4.896394	-1.335443	N	10.151527	-3.533151	2.704433
O	6.266848	4.017822	-1.916876	H	11.079131	-3.140693	2.470563
C	5.884216	6.367896	-1.507824	H	9.799301	-3.056431	3.550739
C	5.483395	6.834411	-2.909808	C	9.207928	-3.437551	1.522968
C	6.294607	8.071639	-3.301093	H	8.219383	-3.756066	1.876143
O	5.728974	8.933418	-4.029648	C	9.210551	-2.030162	0.922032
O	7.474689	8.131265	-2.879811	H	8.699187	-2.131152	-0.047152
H	6.960660	6.570984	-1.386971	H	10.260105	-1.789930	0.676870
H	5.323537	6.923414	-0.740135	C	8.570943	-0.841566	1.651370
H	4.409632	7.059391	-2.986657	H	8.898921	0.067501	1.115973
H	5.714526	6.046775	-3.649586	H	8.945582	-0.724370	2.683253
C	2.632700	-2.478049	-2.212526	C	7.042083	-0.804767	1.636529
H	2.229245	-2.625777	-1.192849	H	6.690841	-1.120259	0.645249
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C	3.632948	-1.334592	-2.173942	N	6.440728	-1.660494	2.656757
O	4.697884	-1.408839	-1.479531	H	6.985988	-1.833050	3.501112
O	3.383763	-0.295621	-2.827604	C	5.140555	-1.983015	2.688541
O	4.707754	4.670839	-0.404530	N	4.626676	-2.545719	3.794766
O	4.386498	3.283608	-0.340013	H	5.257662	-2.755999	4.586147
C	9.684366	-3.056233	-2.865275	H	3.708953	-2.980486	3.736876
H	10.690043	-3.121890	-2.419305	N	4.313780	-1.681045	1.677046
H	9.090754	-3.858567	-2.395067	H	4.677287	-1.568726	0.728338
N	9.639233	-0.500132	-2.554275	H	3.348175	-2.043881	1.763876
H	10.625779	-0.305533	-2.784865	C	9.743435	-4.417938	0.424938
C	9.023184	-1.738156	-2.589856	O	8.938060	-5.272298	-0.005415
C	8.702254	0.433266	-2.261442	O	10.925029	-4.189583	0.084371
H	8.920477	1.498027	-2.184384	H	10.385970	-4.539434	2.941596
N	7.513222	-0.131320	-2.097256	O	3.030493	8.574695	-4.109196
C	7.703134	-1.478025	-2.308921	H	2.919158	7.742117	-4.628410
H	6.884031	-2.183838	-2.239291	H	3.996377	8.775216	-4.163384
C	7.419630	1.705822	-7.423875	O	4.146108	2.229045	-2.767752
H	7.644689	2.764178	-7.217513	H	3.366898	1.694392	-3.016049
H	6.832281	1.670168	-8.359159	H	3.947641	2.729415	-1.945272
N	5.828742	-0.022015	-6.448920	h	3.056708	-3.415416	-2.572564
H	5.644303	-0.563020	-7.299214	h	9.799070	-3.260035	-3.929875
C	6.651013	1.083118	-6.307529	h	8.342153	1.176145	-7.661488
C	5.327841	-0.338997	-5.237326	h	9.421285	13.509369	-1.724628
H	4.618378	-1.151328	-5.080720				

⁵TS7



⁵TS7

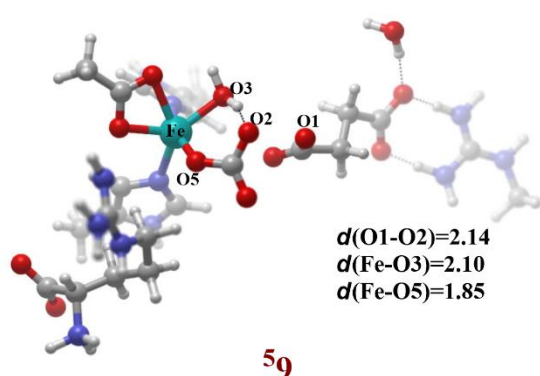
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N	8.740687	10.400299	-2.924481
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H	6.603553	10.240059	-4.298674
Fe	5.713513	0.487741	-2.107648
C	5.766260	2.417569	0.189711
O	5.884018	1.227000	-0.294889
O	6.588745	3.018780	0.871802
C	5.593745	4.877550	-1.281013
O	6.187249	4.031736	-1.918896
C	5.786798	6.371400	-1.498065
C	5.491187	6.785327	-2.935493
C	6.290652	8.037737	-3.297026
O	5.726815	8.909014	-4.018153
O	7.464864	8.107053	-2.858599
H	6.854847	6.561465	-1.296731
H	5.185375	6.956106	-0.784120
H	4.420590	6.970999	-3.100099
H	5.811509	5.980514	-3.620615
C	2.571008	-2.462262	-2.338466
H	2.271578	-2.572520	-1.277031
H	1.650623	-2.299102	-2.917680
C	3.426238	-1.205185	-2.445965
O	4.628996	-1.210666	-1.952030
O	2.908677	-0.208709	-2.951420

O	4.725722	4.688142	-0.312845
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C	9.803157	-3.269346	-2.962813
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H	9.214835	-4.090335	-2.519873
N	9.814759	-0.747820	-2.460216
H	10.807860	-0.550924	-2.662933
C	9.168339	-1.959184	-2.610763
C	8.893610	0.198828	-2.172971
H	9.135559	1.249347	-2.017397
N	7.682298	-0.335549	-2.125817
C	7.841845	-1.672068	-2.403252
H	6.999360	-2.350697	-2.443259
C	7.416624	1.704933	-7.398942
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H	6.804751	1.659198	-8.317619
N	5.905442	-0.057729	-6.360576
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H	4.801450	-1.229505	-4.946080
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C	9.183624	-3.462631	1.531353
H	8.240558	-3.832086	1.949860
C	9.058846	-2.062959	0.922103
H	8.494064	-2.206263	-0.012356
H	10.073641	-1.759991	0.608023
C	8.396600	-0.913932	1.692294
H	8.619197	0.014951	1.137409
H	8.835935	-0.770559	2.693715
C	6.872488	-0.962689	1.782405
H	6.461173	-1.179190	0.790536
H	6.498932	0.037927	2.058486
N	6.362745	-1.944840	2.743814
H	6.874798	-2.019672	3.623513
C	5.079090	-2.343565	2.781415
N	4.546431	-2.743665	3.943779

H	5.174352	-2.806486	4.763365
H	3.676506	-3.270048	3.927571
N	4.303488	-2.287425	1.690654
H	4.767877	-2.512153	0.790210
H	3.331294	-2.621374	1.815184
C	9.711087	-4.417188	0.409589
O	8.910127	-5.278893	-0.016652
O	10.878445	-4.161076	0.040872
H	10.462046	-4.489390	2.912287
O	3.024720	8.581684	-4.086512

H	2.913837	7.749739	-4.606935
H	3.992749	8.773620	-4.135391
O	4.285659	1.934186	-2.538308
H	3.539597	1.306372	-2.764613
H	4.103994	2.441224	-1.708090
h	3.021344	-3.390655	-2.689681
h	9.880112	-3.396323	-4.042638
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⁵9



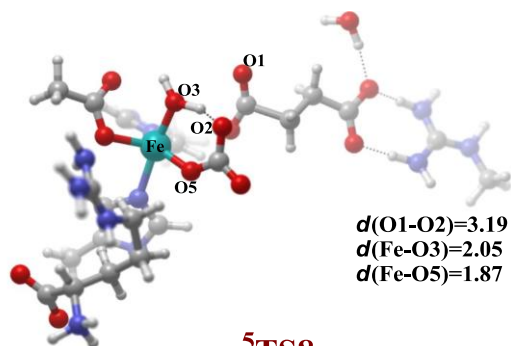
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H	8.003063	13.417074	-3.774106
C	8.211396	11.422580	-3.667809
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Fe	5.384305	0.530138	-2.264097
C	5.333217	2.296702	0.090391
O	5.496002	1.102491	-0.507292
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C	5.845166	4.948256	-1.298293
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C	6.385716	8.058472	-3.475389
O	5.722694	8.980934	-4.029944

O	7.629471	8.068365	-3.302238
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H	5.896456	7.079586	-0.832681
H	4.557375	7.050572	-2.900798
H	5.763609	6.023030	-3.712665
C	2.608880	-2.443682	-2.506177
H	2.092502	-2.490783	-1.527341
H	1.841932	-2.210391	-3.259396
C	3.601444	-1.301134	-2.442169
O	4.796346	-1.454850	-2.004208
O	3.258143	-0.152708	-2.790849
O	4.823900	4.962360	-0.506884
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H	9.121055	-3.856579	-2.416913
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H	4.603974	-1.153149	-5.138822

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H	6.891526	2.335568	-4.470422
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H	8.211664	-3.771047	1.931034
C	9.076278	-2.017828	0.909308
H	8.535800	-2.152182	-0.041861
H	10.103313	-1.727028	0.623586
C	8.403595	-0.860192	1.658585
H	8.650560	0.064275	1.106258
H	8.818657	-0.717242	2.671600
C	6.876715	-0.900092	1.714772
H	6.482931	-1.181018	0.730925
H	6.496100	0.116001	1.916217
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C	5.080027	-2.236748	2.775396

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N	4.316960	-2.241108	1.673375
H	4.797134	-2.520533	0.797777
H	3.345252	-2.575904	1.801725
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O	8.867364	-5.222005	-0.034762
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O	3.028586	8.587525	-4.045146
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H	3.483160	1.997479	-3.065100
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h	3.027844	-3.419897	-2.750184
h	9.815512	-3.267182	-3.962250
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⁵TS8

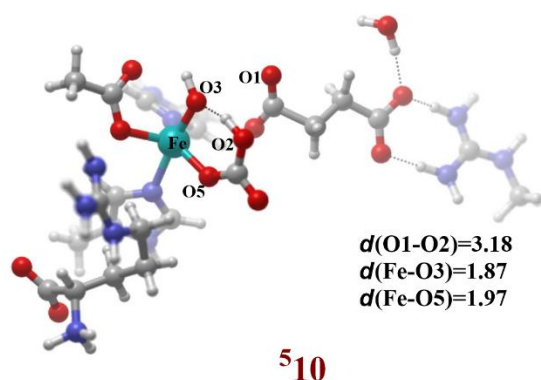


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C	8.231409	11.445920	-3.691088
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H	9.476522	10.559581	-2.344131
H	8.412774	9.436213	-3.255396
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Fe	5.391057	0.562007	-2.265893
C	5.406044	2.362191	0.079048
O	5.716748	1.222464	-0.513973
O	6.077904	2.827720	0.994145
C	5.885911	5.051442	-1.285966
O	6.561391	4.116006	-1.677354
C	6.219036	6.507478	-1.630642
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O	5.720548	9.020924	-4.087631
O	7.630314	8.101660	-3.374327
H	7.314700	6.572799	-1.683416
H	5.852696	7.197583	-0.852585
H	4.554474	7.104697	-2.933345
H	5.775429	6.057485	-3.701369
C	2.627557	-2.428810	-2.444204
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C	3.618727	-1.284254	-2.392194
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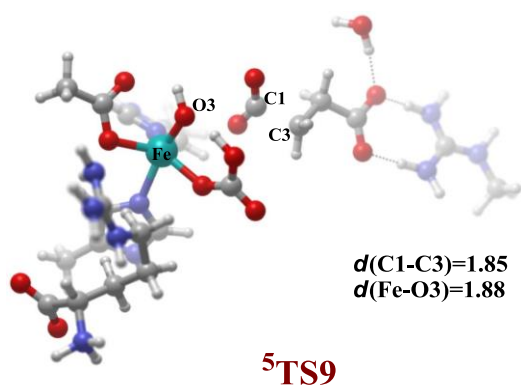
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H	10.711164	-3.107133	-2.45547	H	8.812796	-0.714699	2.668099
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C	9.023970	-1.747068	-2.657168	N	6.357965	-1.822475	2.725623
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H	8.828113	1.494757	-2.295393	C	5.083341	-2.240588	2.771472
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C	7.683420	-1.509099	-2.483025	H	5.181248	-2.668754	4.759263
H	6.877024	-2.230711	-2.466926	H	3.691454	-3.147278	3.938287
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H	7.649421	2.784087	-7.209229	H	4.805458	-2.541921	0.796465
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N	5.834037	-0.019735	-6.484188	C	9.694271	-4.385254	0.409234
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N	8.582883	12.519314	-3.456692
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H	7.957433	9.404230	-2.521245
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Fe	5.469745	0.551252	-2.176446	N	5.780091	0.747632	-4.256419
C	6.499384	2.503861	-0.126329	C	6.652986	1.589061	-4.912036
O	6.613777	1.920389	-1.282521	H	7.142445	2.410570	-4.398653
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C	5.061715	6.788690	-2.869667	H	8.231639	-3.317714	2.166846
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H	5.172527	5.730022	-0.948036	H	8.827980	0.304021	1.007804
H	4.026817	7.098304	-2.657313	H	8.851241	-0.348751	2.643122
H	5.050016	6.468706	-3.928260	C	7.023186	-0.692721	1.517338
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O	4.831296	-1.303382	-1.203410	C	5.134804	-1.738822	2.713491
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H	10.814565	-3.268697	-2.545817	H	4.620753	-1.312781	0.748510
H	9.252175	-4.106973	-2.498580	H	3.319418	-1.816651	1.814704
N	9.623081	-0.723364	-2.509333	C	9.861990	-4.225736	1.129797
H	10.610808	-0.480752	-2.683024	O	9.075634	-5.287324	1.136043
C	9.062751	-1.983891	-2.611239	O	10.911460	-4.140470	0.522825
C	8.632582	0.161658	-2.257215	H	9.464763	-6.045849	0.595990
H	8.777602	1.229089	-2.104816	O	2.834498	8.712041	-3.974517
N	7.459621	-0.458293	-2.196618	H	2.810231	7.868817	-4.482995
C	7.717202	-1.785073	-2.417285	H	3.793723	8.901266	-3.835853
H	6.926489	-2.523646	-2.423903	O	3.980602	1.400380	-1.382951
C	7.484538	1.802005	-7.378621	H	3.690867	2.263394	-1.793552
H	7.750475	2.856820	-7.203826	H	4.627280	1.978632	-0.170700
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H	5.646818	-0.381155	-7.207462	h	8.380089	1.230184	-7.621673
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⁵TS9

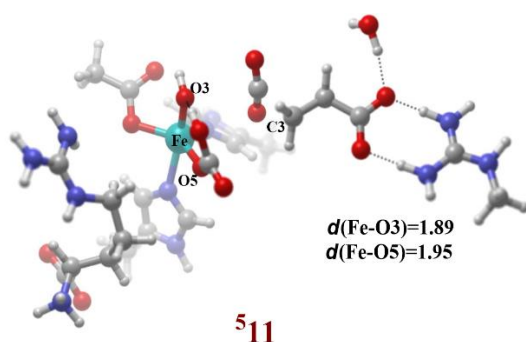
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C	4.709562	4.167106	-2.557362
O	5.633382	3.537151	-3.024362
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O	7.145527	7.963113	-2.295339
H	6.550363	5.433110	-1.762080
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H	1.779234	-2.432525	-2.348102
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O	3.194607	-0.587380	-3.151280

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C	8.795927	0.184666	-2.132336
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C	7.427656	1.734555	-7.339224
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N	10.173075	-3.486636	2.676041
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C	9.189376	-3.412965	1.528497
H	8.223585	-3.753335	1.920071
C	9.131983	-2.004874	0.926945
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C	8.461513	-0.843515	1.671069
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H	3.699013	-3.106223	3.887644
N	4.358465	-2.172004	1.646921
H	4.837075	-2.448911	0.770952
H	3.385500	-2.505573	1.769538
C	9.705872	-4.378020	0.410077
O	8.889651	-5.221780	-0.022621
O	10.881339	-4.146299	0.051676
H	10.420588	-4.488514	2.920969
O	2.942204	8.637025	-4.000526

H	2.859504	7.801582	-4.520550
H	3.911937	8.809369	-3.950632
O	4.023029	1.468433	-1.683746
H	3.277111	1.265592	-2.274558
H	4.279947	2.412219	-0.552536
h	3.155869	-3.525116	-2.496321
h	9.872355	-3.383425	-4.040903
h	8.339812	1.201368	-7.607085
h	9.357619	13.460762	-1.692312

⁵11

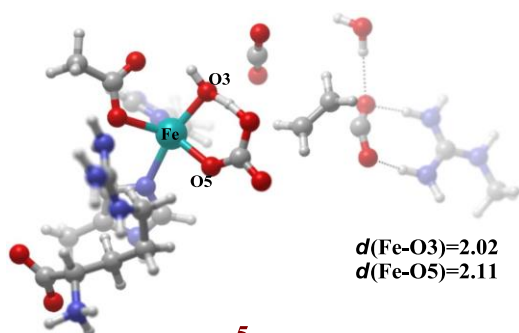


C	9.734130	13.047078	-2.650219
H	10.423163	12.212238	-2.445504
H	10.330217	13.792502	-3.206068
N	8.645947	12.593599	-3.509388
H	7.986862	13.321945	-3.821539
C	8.119661	11.343819	-3.477916
N	8.643631	10.398093	-2.690763
H	9.260212	10.674759	-1.936769
H	8.165014	9.446492	-2.599423
N	7.097829	11.038330	-4.270037
H	6.695945	11.731706	-4.906333
H	6.547521	10.150585	-4.067640
Fe	5.679539	0.628372	-2.097235
C	5.985429	2.702568	0.070709
O	6.469990	1.824518	-0.772410
O	6.673239	3.274632	0.911341
C	3.789294	4.230448	-3.421294
O	4.742759	4.041901	-4.062823
C	5.822173	5.900694	-1.459057
C	5.345828	6.816355	-2.523081
C	6.224004	8.035379	-2.808396
O	5.718946	8.889126	-3.600976
O	7.365616	8.103961	-2.301216

H	6.888077	5.841524	-1.222908
H	5.125125	5.257863	-0.913424
H	4.310009	7.166232	-2.361743
H	5.298657	6.305100	-3.510996
C	2.744658	-2.516369	-2.085605
H	2.677451	-2.643598	-0.988528
H	1.727778	-2.343822	-2.471014
C	3.574273	-1.284104	-2.419734
O	4.734617	-1.131558	-1.825673
O	3.128126	-0.467293	-3.215495
O	2.832278	4.440268	-2.798436
O	4.679487	2.956394	0.021609
C	9.775317	-3.258619	-2.950081
H	10.788359	-3.339657	-2.526945
H	9.194512	-4.086335	-2.509522
N	9.755247	-0.743698	-2.408920
H	10.751771	-0.542877	-2.590333
C	9.120964	-1.957927	-2.596574
C	8.823496	0.185508	-2.101938
H	9.045742	1.231556	-1.898311
N	7.614768	-0.361863	-2.084628
C	7.789306	-1.686492	-2.399126
H	6.953050	-2.367676	-2.467993
C	7.455795	1.732464	-7.396155
H	7.682104	2.798577	-7.235433
H	6.829816	1.659901	-8.303057
N	5.948170	0.015182	-6.282339
H	5.720728	-0.542252	-7.111455
C	6.746106	1.146673	-6.223871
C	5.501599	-0.258814	-5.044916
H	4.812800	-1.071025	-4.827462
N	5.959963	0.642558	-4.186507

C	6.733384	1.524518	-4.905086	H	5.200750	-2.650272	4.735797
H	7.215035	2.383200	-4.441142	H	3.694369	-3.058111	3.892580
N	10.175342	-3.476320	2.686289	N	4.340536	-2.090151	1.662393
H	11.092778	-3.083855	2.414475	H	4.807937	-2.368953	0.779707
H	9.851044	-2.992909	3.540390	H	3.368447	-2.427495	1.789268
C	9.191420	-3.392273	1.540371	C	9.698606	-4.356628	0.415713
H	8.224459	-3.726723	1.933644	O	8.876834	-5.195208	-0.016774
C	9.140700	-1.982527	0.941359	O	10.872062	-4.126782	0.050654
H	8.622582	-2.102382	-0.022874	H	10.418885	-4.480711	2.925560
H	10.178224	-1.705947	0.683305	O	3.052819	8.581414	-4.042046
C	8.468412	-0.818385	1.679932	H	2.974523	7.720945	-4.512542
H	8.733610	0.103039	1.132022	H	4.024401	8.737738	-3.941668
H	8.863545	-0.677937	2.700408	O	4.140959	1.720167	-2.095677
C	6.939899	-0.848599	1.706573	H	3.420216	1.273725	-2.587177
H	6.570840	-1.138011	0.715047	H	4.261999	2.513379	-0.795673
H	6.562315	0.171572	1.901044	h	3.111767	-3.429836	-2.553448
N	6.396466	-1.759438	2.718823	h	9.861863	-3.387543	-4.028948
H	6.923941	-1.825072	3.590389	h	8.370586	1.195415	-7.646756
C	5.111969	-2.150009	2.760350	h	9.387806	13.491761	-1.717276
N	4.568424	-2.537527	3.922470				

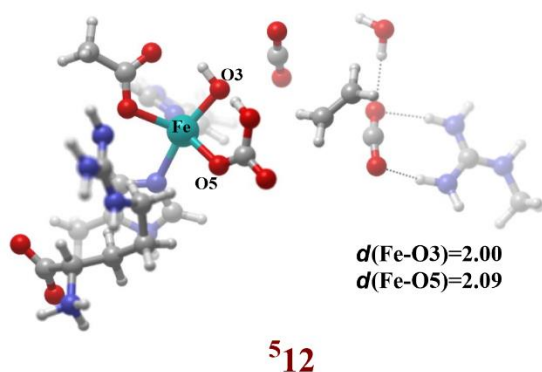
⁵TS10



C	9.668000	13.015000	-2.660000	Fe	5.695000	0.783000	-2.030000
H	10.402000	12.214000	-2.476000	C	6.022000	2.985000	0.143000
H	10.196000	13.761000	-3.278000	O	6.519000	1.992000	-0.511000
N	8.543000	12.498000	-3.446000	O	6.622000	3.580000	1.074000
H	7.890000	13.205000	-3.816000	C	3.574000	4.305000	-3.553000
C	8.086000	11.237000	-3.393000	O	4.586000	4.363000	-4.133000
N	8.688000	10.338000	-2.597000	C	5.755000	5.539000	-1.475000
H	9.339000	10.647000	-1.885000	C	4.987000	6.654000	-1.737000
H	8.310000	9.393000	-2.464000	C	6.411000	7.855000	-2.468000
N	7.050000	10.864000	-4.149000	O	5.959000	8.276000	-3.506000
H	6.614000	11.493000	-4.835000	O	7.346000	7.966000	-1.721000
H	6.652000	9.923000	-4.048000	H	5.881000	4.762000	-2.231000
				H	6.323000	5.427000	-0.546000
				H	4.725000	7.326000	-0.907000
				H	4.325000	6.691000	-2.609000
				C	2.700000	-2.424000	-2.197000
				H	2.526000	-2.575000	-1.114000
				H	1.723000	-2.229000	-2.660000
				C	3.594000	-1.182000	-2.383000
				O	4.753000	-1.160000	-1.816000
				O	3.130000	-0.233000	-3.024000
				O	2.542000	4.376000	-3.024000

O	4.817000	3.445000	-0.192000	C	8.499000	-0.788000	1.648000
C	9.752000	-3.229000	-2.927000	H	8.780000	0.125000	1.096000
H	10.759000	-3.319000	-2.488000	H	8.875000	-0.647000	2.677000
H	9.156000	-4.047000	-2.487000	C	6.970000	-0.804000	1.644000
N	9.796000	-0.719000	-2.376000	H	6.619000	-1.114000	0.653000
H	10.789000	-0.528000	-2.577000	H	6.594000	0.223000	1.799000
C	9.119000	-1.915000	-2.578000	N	6.409000	-1.688000	2.672000
C	8.877000	0.219000	-2.047000	H	6.939000	-1.761000	3.541000
H	9.115000	1.265000	-1.835000	C	5.121000	-2.062000	2.716000
N	7.663000	-0.298000	-2.018000	N	4.584000	-2.468000	3.879000
C	7.800000	-1.613000	-2.355000	H	5.224000	-2.624000	4.679000
H	6.940000	-2.262000	-2.421000	H	3.708000	-2.986000	3.836000
C	7.446000	1.706000	-7.412000	N	4.334000	-1.961000	1.635000
H	7.663000	2.776000	-7.247000	H	4.778000	-2.173000	0.726000
H	6.835000	1.630000	-8.326000	H	3.368000	-2.311000	1.760000
N	5.946000	-0.027000	-6.308000	C	9.713000	-4.355000	0.433000
H	5.730000	-0.592000	-7.133000	O	8.900000	-5.201000	-0.000000
C	6.730000	1.116000	-6.249000	O	10.897000	-4.140000	0.095000
C	5.498000	-0.290000	-5.057000	H	10.367000	-4.469000	2.949000
H	4.810000	-1.106000	-4.840000	O	3.126000	8.381000	-4.154000
N	5.947000	0.606000	-4.199000	H	2.868000	7.573000	-4.670000
C	6.710000	1.485000	-4.926000	H	4.098000	8.369000	-4.172000
H	7.201000	2.338000	-4.461000	O	4.273000	2.212000	-2.182000
N	10.140000	-3.464000	2.705000	H	3.454000	1.714000	-2.362000
H	11.067000	-3.083000	2.453000	H	4.413000	2.853000	-1.099000
H	9.798000	-2.973000	3.548000	h	3.083815	-3.354630	-2.614948
C	9.186000	-3.371000	1.531000	h	9.853824	-3.369182	-4.003126
H	8.204000	-3.689000	1.900000	h	8.364433	1.178076	-7.668600
C	9.172000	-1.963000	0.928000	h	9.352391	13.474133	-1.723168
H	8.673000	-2.076000	-0.047000				
H	10.219000	-1.704000	0.691000				

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C	9.616683	13.015409	-2.643733
H	10.354371	12.217998	-2.467481
H	10.128594	13.762916	-3.272094
N	8.474530	12.487761	-3.401312
H	7.812436	13.191946	-3.769319
C	8.075864	11.213595	-3.395568
N	8.714896	10.323461	-2.613355
H	9.308208	10.635501	-1.853013
H	8.484959	9.334799	-2.609812
N	7.064624	10.810477	-4.174322

H	6.614707	11.424884	-4.868342	C	5.521242	-0.344994	-5.030529
H	6.684005	9.869931	-4.092569	H	4.865590	-1.180277	-4.794066
Fe	5.767647	0.824595	-2.005483	N	5.968742	0.558493	-4.183669
C	5.965535	2.914728	0.217517	C	6.706926	1.447296	-4.919056
O	6.555587	2.001042	-0.467854	H	7.181199	2.313385	-4.459746
O	6.534697	3.591246	1.110124	N	10.123521	-3.455239	2.733549
C	3.728566	4.420704	-3.624291	H	11.058298	-3.078720	2.502898
O	4.779043	4.567176	-4.114397	H	9.766840	-2.965089	3.571509
C	5.220220	5.830060	-1.103500	C	9.190971	-3.352279	1.543010
C	4.411663	6.896600	-1.231897	H	8.201750	-3.666796	1.895456
C	6.715246	7.658581	-2.587501	C	9.190652	-1.940713	0.948899
O	6.097796	7.846574	-3.563847	H	8.717541	-2.046685	-0.039381
O	7.530279	7.652581	-1.752781	H	10.242906	-1.676845	0.739959
H	5.362626	5.108090	-1.912960	C	8.495032	-0.772268	1.660225
H	5.756622	5.589838	-0.177466	H	8.769556	0.143449	1.108840
H	4.229831	7.571105	-0.383074	H	8.861617	-0.625266	2.691792
H	3.839047	7.110551	-2.143285	C	6.966219	-0.805070	1.643946
C	2.664410	-2.336289	-2.274926	H	6.627340	-1.130667	0.653158
H	2.389540	-2.451496	-1.206972	H	6.576773	0.218416	1.782141
H	1.733341	-2.145186	-2.828664	N	6.404847	-1.683731	2.677246
C	3.565382	-1.089515	-2.409272	H	6.937133	-1.756552	3.544434
O	4.731266	-1.097771	-1.864165	C	5.115749	-2.052734	2.725550
O	3.086340	-0.115961	-2.998240	N	4.581575	-2.462956	3.889036
O	2.650364	4.399574	-3.194786	H	5.221979	-2.617683	4.687784
O	4.682073	3.168432	-0.019734	H	3.701392	-2.973094	3.848415
C	9.764002	-3.202376	-2.921602	N	4.324553	-1.946507	1.648231
H	10.772592	-3.304303	-2.490016	H	4.764226	-2.163093	0.736115
H	9.161807	-4.011832	-2.475707	H	3.358948	-2.296645	1.775799
N	9.824104	-0.689499	-2.408435	C	9.727879	-4.337792	0.450826
H	10.811942	-0.509548	-2.635501	O	8.922472	-5.194289	0.021869
C	9.143448	-1.881393	-2.579184	O	10.911172	-4.117335	0.112739
C	8.924367	0.265147	-2.066833	H	10.340386	-4.462076	2.975617
H	9.185453	1.303631	-1.869155	O	3.221086	8.211622	-4.255807
N	7.705967	-0.239749	-2.004120	H	2.915262	7.417843	-4.773476
C	7.827226	-1.566743	-2.333181	H	4.181092	8.090484	-4.208006
H	6.960851	-2.214700	-2.378430	O	4.370441	2.231095	-2.255575
C	7.409519	1.679101	-7.413507	H	3.617653	1.679675	-2.553961
H	7.616571	2.748203	-7.245240	H	4.395989	2.731967	-0.970320
H	6.783296	1.604089	-8.321754	h	3.066091	-3.278150	-2.648579
N	5.940713	-0.072902	-6.288310	h	9.861178	-3.354471	-3.996539
H	5.714875	-0.636288	-7.112306	h	8.335866	1.168396	-7.676427
C	6.714755	1.074925	-6.241049	h	9.313711	13.476837	-1.703862