

Supplementary material to accompany the manuscript:

Density functional theory studies on the conversion of hydroxyheme to iron-verdoheme in the presence of dioxygen.

Compounds	Stabilization Energy (kcal.mol ⁻¹)					
	B3LYP*			OPBE		
	Low	Intermediate	High	Low	Intermediate	High
2,4,6(1)	0.00	0.32	7.10	0.00	0.00	8.90
2,4,6(TS1)	12.15	14.77	29.50	10.35	10.88	---
2,4,6(2)	7.02	10.25	18.46	6.28	6.70	15.43
2,4,6(TS2)	9.87	11.00	25.02	7.69	7.85	---
2,4,6(3)	3.44	2.05	12.38	3.01	2.22	9.74
2,4,6(TS3)	10.95	10.60	19.00	9.61	8.92	---
2,4,6(4)	-14.56	-14.82	-3.55	-12.80	-13.68	-7.21
1,3,5(1)	1.05	0.00	9.07	0.97	0.00	8.25
1,3,5(TS1)	24.50	22.55	---	17.94	16.02	---
1,3,5(2)	20.37	17.26	26.50	12.00	10.35	22.06
1,3,5(TS2)	26.85	21.00	---	16.23	15.18	---
1,3,5(3)	9.84	9.14	15.72	8.22	7.00	12.45
1,3,5(TS3)	20.03	18.95	---	14.98	14.35	---
1,3,5(4)	6.21	5.46	8.95	6.80	4.00	8.21

Table S1. Calculated relative energies for species 1-4 using the B3LYP* and OPBE/6-311+G** methods

Table S2. Calculated Mulliken charges and spin densities for the Fe, O1, O2 atoms and the ring macrocycle (values in parentheses are charge densities)

Compound	Fe	O1	O2	ring
² (1)	1.03 (1.47)	-0.37 (-0.30)	-0.64 (-0.18)	0.98 (-0.99)
² (TS1)	0.97 (1.46)	0.10 (-0.34)	0.00 (-0.27)	0.08 (-0.87)
² (2)	0.92 (1.46)	0.14 (-0.35)	0.00 (-0.29)	0.14 (-0.84)
² (TS2)	1.30 (1.44)	0.57 (-0.38)	-0.63 (-0.37)	0.13 (-0.79)
² (3)	1.21 (1.42)	0.84 (-0.43)	-0.80 (-0.50)	-0.24 (-0.49)
² (TS3)	1.21 (1.41)	0.84 (-0.43)	0.09 (-0.52)	-0.96 (-0.46)
² (4)	1.19 (1.39)	0.84 (-0.43)	---	-0.98 (-0.96)
³ (1)	1.06 (1.45)	0.37 (-0.31)	0.61 (-0.22)	-0.04 (-1.92)
³ (TS1)	0.88 (1.43)	0.23 (-0.36)	0.33 (-0.26)	0.56 (-1.81)
³ (2)	0.96 (1.43)	0.13 (-0.36)	0.03 (-0.31)	0.88 (-1.76)
³ (TS2)	1.24 (1.41)	0.36 (-0.36)	-0.46 (-0.33)	0.86 (-1.72)
³ (3)	1.22 (1.35)	0.86 (-0.41)	0.01 (-0.53)	-0.09 (-1.41)
³ (TS3)	1.29 (1.34)	0.79 (-0.45)	-0.10 (-0.52)	0.02 (-1.37)
³ (4)	1.28 (1.34)	0.78 (-0.46)	---	-0.06 (-1.28)

Table S3. Calculated selected bond distances for all of the species in the doublet, quartet and sextet spin

Compound	Fe-O1	Fe-N3	Fe-N _{ave.ring}	O1-O2	O2-C7	C7-C6	C6-C8	C6-O5
^{2,4,6}(1)								
Doublet	1.86	2.06	2.02	1.35	2.96	1.44	1.44	1.27
Quartet	1.88	2.07	2.01	1.35	3.18	1.44	1.44	1.27
Sextet	2.36	2.20	1.99	1.22	3.68	1.45	1.45	1.24
^{2,4,6}(TS1)								
Doublet	1.90	2.06	2.00	1.48	1.77	1.52	1.44	1.25
Quartet	2.05	2.04	2.01	1.48	1.65	1.54	1.44	1.25
^{2,4,6}(2)								
Doublet	1.90	2.06	1.97	1.55	1.50	1.54	1.45	1.22
Quartet	1.96	2.50	1.96	1.44	1.46	1.55	1.46	1.22
Sextet	2.01	2.38	1.97	1.44	1.47	1.54	1.46	1.23
^{2,4,6}(TS2)								
Doublet	1.66	2.12	1.96	2.20	1.45	1.58	1.45	1.25
Quartet	1.73	2.41	1.96	2.05	1.44	1.55	1.46	1.24
^{2,4,6}(3)								
Doublet	1.62	2.22	1.99	3.10	1.31	1.78	1.40	1.21
Quartet	1.62	2.23	1.98	3.10	1.32	1.80	1.39	1.21
Sextet	1.62	2.21	2.00	3.01	1.31	1.80	1.41	1.21
^{2,4,6}(TS3)								
Doublet	1.62	2.13	2.01	---	1.30	3.02	1.50	1.21
Quartet	1.62	2.10	2.02	---	1.29	3.03	1.51	1.21
Sextet	1.62	2.10	2.07	---	1.30	3.15	1.50	1.21
^{2,4,6}(4)								
Doublet	1.62	2.20	2.00	---	---	---	---	1.14
Quartet	1.62	2.20	2.00	---	---	---	---	1.14
Sextet	1.61	2.24	2.05	---	---	---	---	1.14

stat
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Table S4. Calculated relative energies in the solvent

Relative Energies (kcal.mol ⁻¹)

Compounds	$\Delta(E_{\text{gas}})$		$\Delta(E+\text{protein})$		$\Delta(E+\text{ethanol})$	
	Low	Intermediate	Low	Intermediate	Low	Intermediate
^{2,4} (1)	0.00	0.32	-1.14	-1.08	-2.20	-2.34
^{2,4} TS1	12.15	14.77	9.36	11.08	5.05	7.24

Table S5. Calculated energies for all of the species using the CASSCF(7e, 7o) level and the MP2 corrected energies.

Compounds	Total energy (a.u.)	
	CASSCF	CASSCF/MP2

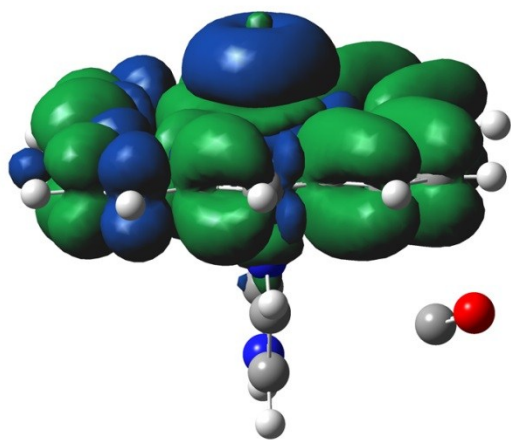
	Low	Intermediate	High	Low	Intermediate	High
2,4,6(1)	-2694.7862	-2694.7180	---	-2695.8351	-2695.7993	---
2,4,6(TS1)	-2694.5314	-2694.5280	---	-2695.6852	-2695.6530	---
2,4,6(2)	-2694.6608	-2694.6145	---	-2695.7553	-2695.7367	---
2,4,6(TS2)	-2694.5795	---	---	-2695.7125	---	---
2,4,6(3)	-2694.7235	-2694.6994	-	-2695.8110	-2695.7984	-2695.6813
2,4,6(TS3)	-2694.5826	-2694.5411	2694.5108	-2695.7068	-2695.7189	---
2,4,6(4)	-2695.1475	-2695.1475	---	-2696.3861	-2696.3414	-2696.1595
			2694.9067			
1,3,5(1)	-2696.4989	-2696.4552	-	-2697.5714	-2697.5825	-2697.3861
			2696.3395			
1,3,5(TS1)	-2695.6218	-2695.7164	---	-2697.3249	-2697.3401	---
1,3,5(2)	-2695.7809	-2695.8429	---	-2697.3526	-2697.3890	-2697.2739
1,3,5(TS2)	-2695.5740	-2695.5843	---	-2697.3335	-2697.3398	---
1,3,5(3)	-2696.3166	-2696.3082	-	-2697.4987	-2697.5068	-2697.3584
			2696.1835			
1,3,5(TS3)	-2695.5879	-2695.5822	---	-2697.3702	-2697.3764	---
1,3,5(4)	-2696.3942	-2696.4244	-	-2697.4930	-2697.5012	-2697.4198
			2696.3877			

Table S6. Calculated Mullikan spin densities for the iron atom and the ring macrocycle using the CASSCF(7e, 7o) level.

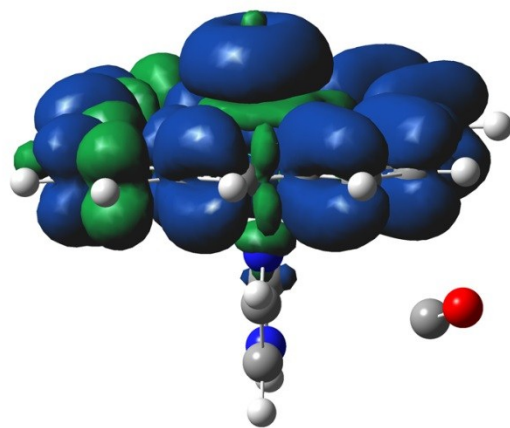
Compounds	Fe	Ring
² (1)	0.055	0.963
² (TS1)	1.163	-0.125
² (2)	1.068	-0.077
² (TS2)	0.972	0.008
² (3)	0.964	0.012
² (TS3)	0.885	0.157
² (4)	0.860	0.149

Table S7. Calculated selected bond distances for all of the species in the singlet, triplet and quintet spin states using B3LYP*/6-31+G* method.

Compound	Fe-O1	Fe-N3	Fe-N _{ave.ring}	O1-O2	O2-C7	C7-C6	C6-C8	C6-O5
^{1,3,5} (1)								
Singlet	1.89	2.08	2.01	1.36	3.34	1.45	1.45	1.25
Triplet	1.89	2.09	2.02	1.36	3.34	1.45	1.45	1.25
Quintet	2.48	2.17	1.99	1.25	3.59	1.45	1.45	1.24
^{1,3} (TS1)								
Singlet	1.93	2.07	2.00	1.50	1.62	1.52	1.44	1.24
Triplet	2.05	2.04	2.01	1.48	1.65	1.54	1.44	1.25
^{1,3,5} (2)								
Singlet	1.93	2.07	1.99	1.57	1.50	1.53	1.44	1.24
Triplet	2.07	2.45	2.00	1.48	1.49	1.55	1.44	1.25
^{1,3} (TS2)								
Singlet	1.70	2.08	2.00	1.96	1.47	1.58	1.45	1.24
Triplet	1.70	2.41	1.98	1.97	1.47	1.59	1.45	1.24
^{1,3,5} (3)								
Singlet	1.64	2.26	2.01	3.02	1.32	1.68	1.47	1.23
Triplet	1.64	2.26	2.00	3.03	1.32	1.70	1.47	1.23
Quintet	1.64	2.21	2.00	3.41	1.31	1.72	1.45	1.23
^{1,3} (TS3)								
Singlet	1.62	2.13	2.01	---	1.30	3.02	1.50	1.21
Triplet	1.62	2.10	2.02	---	1.29	3.03	1.51	1.21
^{1,3,5} (4)								
Singlet	1.64	2.17	2.00	---	---	---	---	1.16
Triplet	1.64	2.17	2.00	---	---	---	---	1.16
Quintet	1.63	2.30	2.08	---	---	---	---	1.15



doublet spin state



quartet spin state

Figure S1. ^{2,4}: spin-density plot (majority spin in blue; minority spin in green)

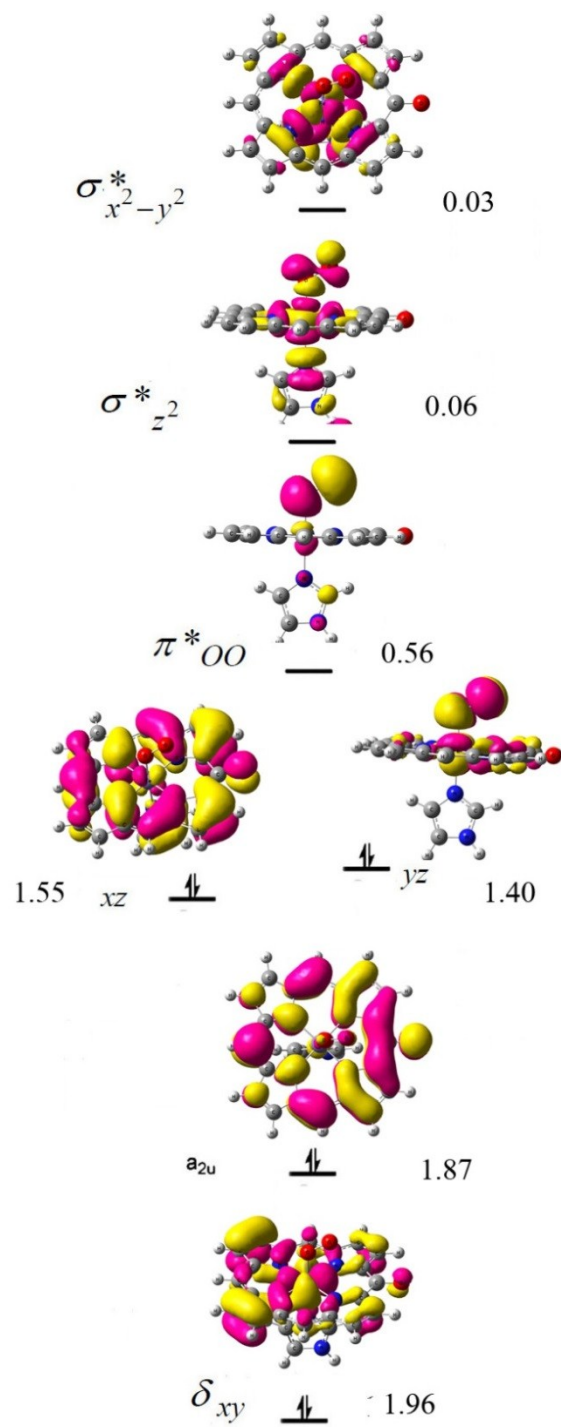
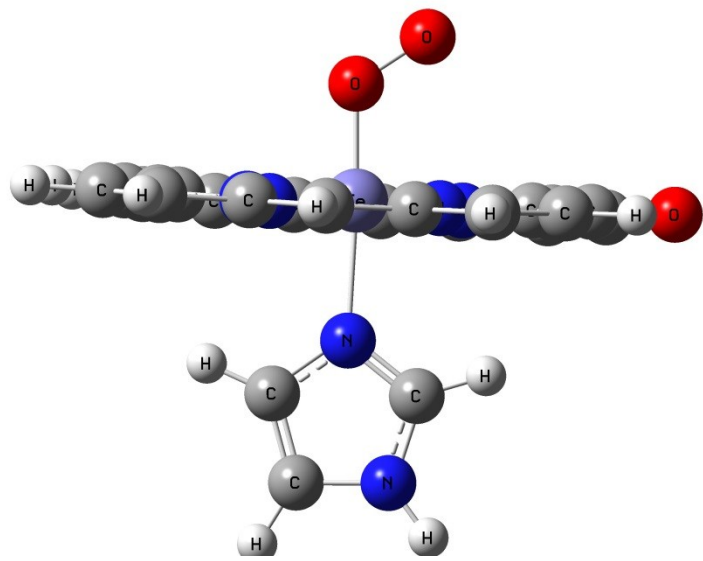


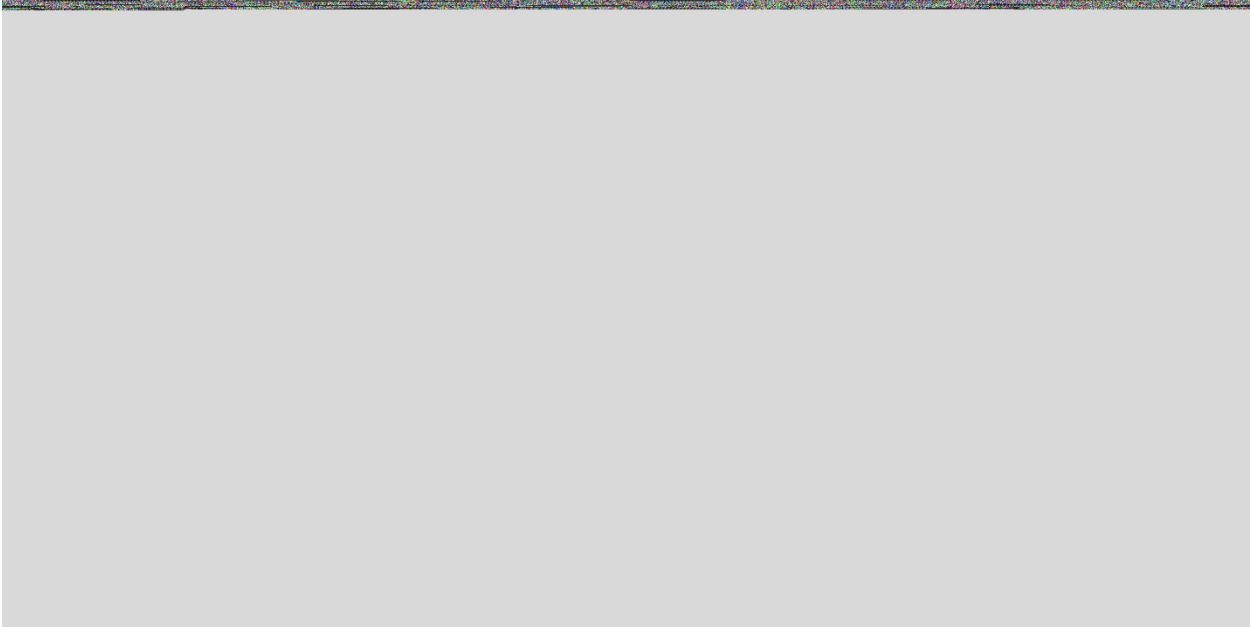
Figure S2. Natural orbitals and occupation numbers for CAS(7e, 7o) calculations of the singlet state configuration of complexes 1.

**Tables include the species optimized xyz Cartesian coordinates data in different spin states.
For each table, the corresponding figure is accompanied.**

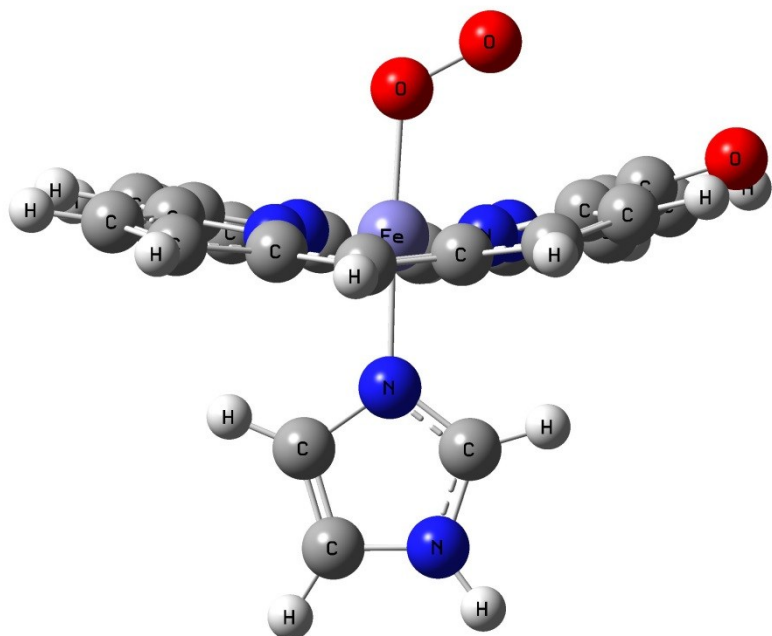
Fe	0.13721600	0.00000600	-0.39454600
N	-1.28744600	-1.41097700	-0.27479500
N	1.60411800	-1.41428300	-0.39593300
N	-1.28743300	1.41099700	-0.27479700
N	1.60412700	1.41427900	-0.39593700
C	-2.65069500	-1.25125700	-0.25297100
C	2.95760500	-1.23148200	-0.48223300
C	-1.07537000	-2.77476100	-0.24359400
C	1.40237300	-2.78336300	-0.35670300
C	-2.65068300	1.25128700	-0.25295300
C	2.95761400	1.23146700	-0.48223400
C	-1.07534800	2.77478000	-0.24357700
C	1.40239500	2.78336000	-0.35670000
C	-3.30786100	-2.50767300	-0.19889400
C	3.63375000	-2.51075200	-0.49739200
C	-2.32151500	-3.46697100	-0.19109800
C	2.66969100	-3.46884300	-0.41666600
C	-3.30783900	2.50770700	-0.19884000
C	3.63376800	2.51073100	-0.49740100
C	-2.32148600	3.46699800	-0.19105700
C	2.66971900	3.46882900	-0.41664400
H	-4.38243600	-2.62056900	-0.17415000
H	4.70855400	-2.63657900	-0.56189700
H	-2.42818300	-4.54580800	-0.16468200
H	2.78747600	-4.54650900	-0.40372700
H	-4.38241300	2.62061000	-0.17407500
H	4.70857300	2.63654900	-0.56191500
H	-2.42814600	4.54583500	-0.16462800
H	2.78751500	4.54649400	-0.40368900
C	3.60860600	-0.00001000	-0.52229200
C	0.17671500	3.40628200	-0.27705800
C	0.17668700	-3.40627400	-0.27706800
H	4.69269400	-0.00001400	-0.59146100
H	0.17300000	4.49356400	-0.25266600
H	0.17296200	-4.49355600	-0.25268600
H	2.35686100	0.00008000	2.03345400
C	1.37186300	0.00003200	2.47357700
C	1.00499700	-0.00004500	3.79134600
C	-0.79416400	-0.00004300	2.49628400
N	-0.38019500	-0.00005500	3.78858900
H	1.57833300	-0.00006900	4.70534800
H	-1.82913900	-0.00006300	2.19065800
H	-0.98438400	-0.00008600	4.59602800
N	0.24302400	0.00000500	1.68103800
C	-3.38711800	0.00001800	-0.25187100
O	-4.63856200	0.00002400	-0.21660900
O	0.15179400	-0.00000800	-2.12775600
O	-0.91504200	-0.00000400	-2.82846200



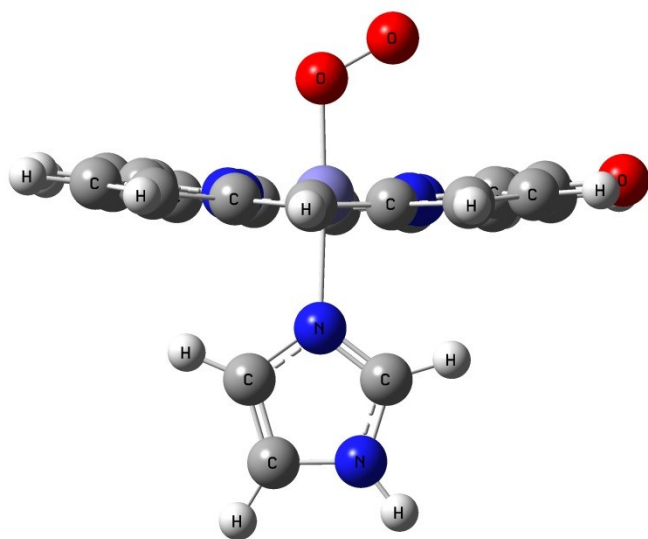
Fe	0.16658600	0.00000100	-0.36638500
N	-1.26060600	-1.42835100	-0.26618000
N	1.59806700	-1.41673600	-0.39890700
N	-1.26042300	1.42852600	-0.26611600
N	1.59825000	1.41656500	-0.39885600
C	-2.62002600	-1.25616900	-0.24639700
C	2.95347300	-1.23066500	-0.49240100
C	-1.06238200	-2.79261200	-0.24134900
C	1.40569800	-2.79263300	-0.36984200
C	-2.61986100	1.25651500	-0.24634300
C	2.95363200	1.23032900	-0.49237300
C	-1.06202600	2.79276100	-0.24123900
C	1.40605300	2.79248500	-0.36975500
C	-3.28962100	-2.50618300	-0.19557300
C	3.63362000	-2.50588600	-0.52083900
C	-2.31183900	-3.47507300	-0.19184200
C	2.67458000	-3.46895300	-0.44256700
C	-3.28930100	2.50661200	-0.19547900
C	3.63393700	2.50546600	-0.52078400
C	-2.31139800	3.47537800	-0.19171000
C	2.67501600	3.46864900	-0.44247600
H	-4.36511400	-2.60932100	-0.17235400
H	4.70838900	-2.62571900	-0.59509900
H	-2.42791500	-4.55298000	-0.17054600
H	2.79703000	-4.54610500	-0.43921400
H	-4.36478000	2.60988400	-0.17225800
H	4.70872000	2.62516700	-0.59505300
H	-2.42733700	4.55329900	-0.17037700
H	2.79760000	4.54578700	-0.43909700
C	3.60329500	-0.00021100	-0.53199100
C	0.18848000	3.42480400	-0.28414900
C	0.18805000	-3.42480700	-0.28426700
H	4.68685600	-0.00028100	-0.60752100
H	0.19012000	4.51210600	-0.26692600
H	0.18955700	-4.51211000	-0.26707600
H	2.34381400	0.00056800	2.07465200
C	1.35812900	0.00024800	2.51360100
C	0.98859800	0.00008700	3.83106200
C	-0.80837700	-0.00043100	2.53266300
N	-0.39561000	-0.00038100	3.82638000
H	1.56108500	0.00023100	4.74558500
H	-1.84278800	-0.00074900	2.22511300
H	-1.00080100	-0.00061500	4.63314600
N	0.23035500	-0.00006100	1.72022600
C	-3.35129100	0.00022100	-0.24726200
O	-4.60149500	0.00030100	-0.21252200
O	0.04735600	0.00005400	-2.23584200
O	-1.08018000	0.00017900	-2.86975200



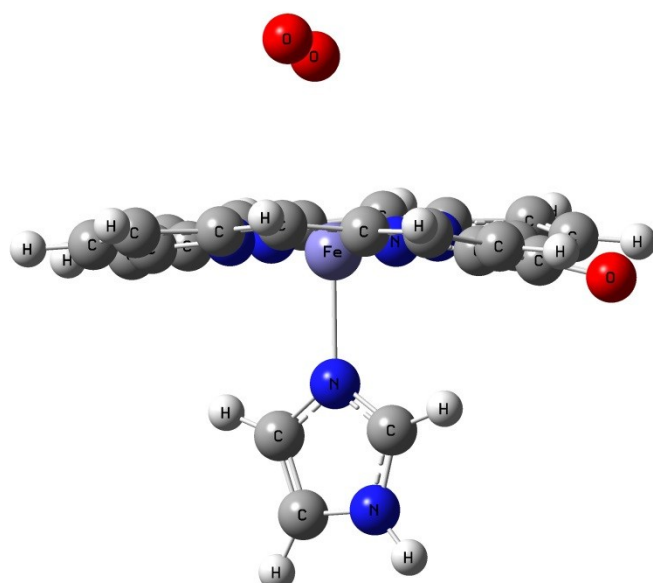
Fe	0.13941200	0.00000200	-0.34417000
N	-1.28709700	-1.41259000	-0.23134600
N	1.58580300	-1.41298800	-0.40924800
N	-1.28712300	1.41256600	-0.23133900
N	1.58577600	1.41302000	-0.40924600
C	-2.63266300	-1.26284600	-0.28660600
C	2.93274200	-1.23595300	-0.60918100
C	-1.07376000	-2.78070900	-0.14459400
C	1.40031500	-2.76807000	-0.31001600
C	-2.63268600	1.26279700	-0.28660100
C	2.93271800	1.23601100	-0.60918100
C	-1.07381200	2.78068900	-0.14458400
C	1.40026300	2.76809700	-0.31001100
C	-3.30745200	-2.52025000	-0.22039400
C	3.61002100	-2.50616600	-0.63459100
C	-2.33081500	-3.47300000	-0.12075900
C	2.65568000	-3.46003900	-0.43719000
C	-3.30749900	2.52018900	-0.22038900
C	3.60997400	2.50623600	-0.63458700
C	-2.33088000	3.47295600	-0.12074500
C	2.65561400	3.46009100	-0.43718800
H	-4.38120000	-2.63302500	-0.24909000
H	4.67471400	-2.63642300	-0.78111600
H	-2.44210000	-4.54845600	-0.05982800
H	2.77583200	-4.53524000	-0.39507100
H	-4.38125000	2.63294400	-0.24908800
H	4.67466500	2.63651400	-0.78111000
H	-2.44218600	4.54841000	-0.05981000
H	2.77574600	4.53529400	-0.39506800
C	3.56497400	0.00003500	-0.72178000
C	0.16625600	3.39843800	-0.15908600
C	0.16632000	-3.39843400	-0.15909500
H	4.63906100	0.00004500	-0.88122200
H	0.17473900	4.48306200	-0.09620600
H	0.17482400	-4.48305800	-0.09621700
H	2.39789800	0.00008600	2.05457600
C	1.42056700	0.00005000	2.51004200
C	1.08312600	-0.00019500	3.83471000
C	-0.74545700	-0.00001600	2.58525900
N	-0.29937900	0.00013500	3.86307300
H	1.67766500	-0.00034300	4.73470400
H	-1.78900100	-0.00000600	2.31216800
H	-0.88180300	0.00024500	4.68802900
N	0.27307300	-0.00000100	1.74222500
C	-3.35622400	-0.00003100	-0.35575700
O	-4.59783800	-0.00004300	-0.41870300
O	0.11426900	0.00000500	-2.18787300
O	-1.03063300	-0.00000700	-2.78243800



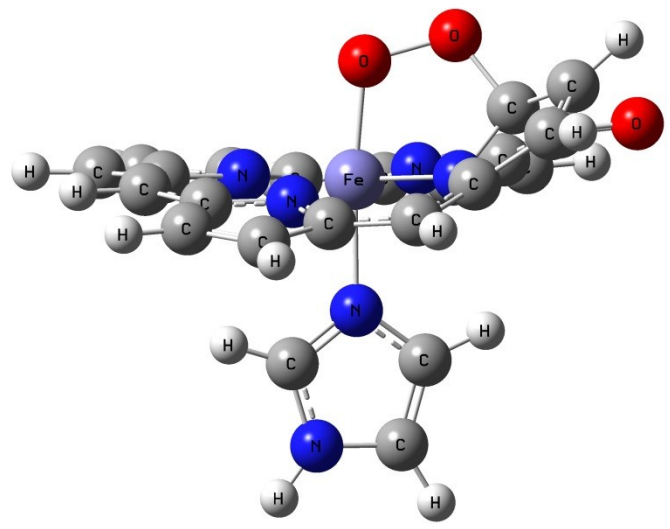
Fe	0.13401600	0.01749200	-0.31533000
N	-1.32204700	-1.37612200	-0.22887300
N	1.56580600	-1.39228300	-0.25451600
N	-1.29931800	1.44380600	-0.38053800
N	1.58398600	1.42609400	-0.41161300
C	-2.66840800	-1.22023600	-0.27907400
C	2.92762500	-1.22883700	-0.34383800
C	-1.11872800	-2.74521800	-0.13915600
C	1.36207700	-2.74490500	-0.17145200
C	-2.64936200	1.30035100	-0.41379500
C	2.94268200	1.23790200	-0.48484500
C	-1.08075000	2.81353400	-0.41733000
C	1.39918600	2.78503500	-0.45381000
C	-3.34992100	-2.47480300	-0.21118300
C	3.59380900	-2.50446700	-0.30011700
C	-2.37806500	-3.43240100	-0.11992000
C	2.61746500	-3.44876800	-0.18853000
C	-3.31580700	2.56195300	-0.46532300
C	3.62628900	2.50150400	-0.56884700
C	-2.33235900	3.51302300	-0.46476900
C	2.66294100	3.46648200	-0.54524300
H	-4.42433100	-2.58173400	-0.23883700
H	4.66596600	-2.64383600	-0.35514200
H	-2.49391300	-4.50727900	-0.05838900
H	2.72277600	-4.52496000	-0.13483900
H	-4.38894200	2.67832600	-0.50050200
H	4.70006900	2.62042100	-0.63875600
H	-2.43622400	4.59022900	-0.50459000
H	2.78352800	4.54126900	-0.59566800
C	3.57611300	-0.00260400	-0.45449600
C	0.16213500	3.42581900	-0.43978300
C	0.11773900	-3.36784900	-0.10435300
H	4.65987200	-0.01339900	-0.52185900
H	0.17273300	4.51165800	-0.47595400
H	0.11769200	-4.45263300	-0.04330800
H	2.25972300	0.25056000	2.15285700
C	1.26089800	0.22105900	2.55741600
C	0.85331900	0.28459800	3.86030300
C	-0.90371400	0.09374100	2.52549800
N	-0.52619200	0.20226300	3.82021900
H	1.39861100	0.37765700	4.78622200
H	-1.92923500	0.00928200	2.20266500
H	-1.15133400	0.21988300	4.61302400
N	0.15714400	0.10255400	1.73515600
C	-3.38452400	0.04325900	-0.37387300
O	-4.62909900	0.05319900	-0.39391600
O	0.11643400	-0.16069100	-2.18699700
O	0.16505100	-1.24793900	-2.85259600



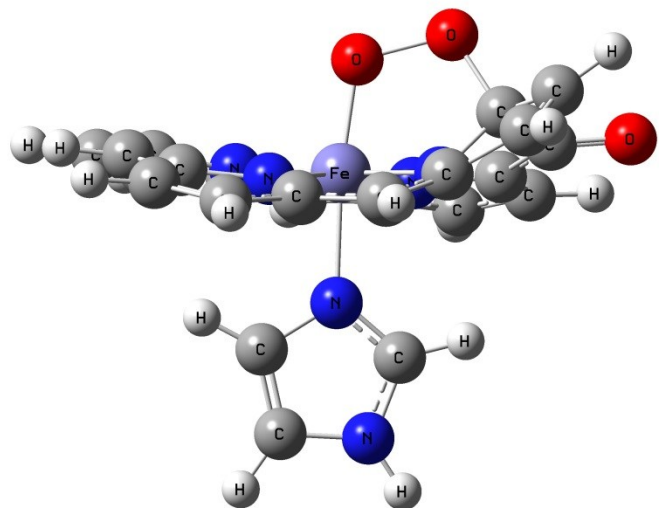
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N	-1.57337400	1.30728300	-0.04382100
N	1.27968000	-1.37355400	-0.65492700
N	-1.53462100	-1.43859200	-0.45791700
C	2.61523800	1.23583200	-0.14577800
C	-2.92649900	1.08912400	0.13625000
C	1.02773300	2.75183600	-0.16531400
C	-1.42164000	2.69477300	-0.02290100
C	2.64618700	-1.21667800	-0.55978300
C	-2.89317900	-1.32168400	-0.23117100
C	1.10031900	-2.69142600	-1.05283800
C	-1.34473200	-2.76255300	-0.86182200
C	3.25734500	2.48884900	-0.09072700
C	-3.62342300	2.33914500	0.28248000
C	2.26234900	3.44489400	-0.12121200
C	-2.69713100	3.32788400	0.16130500
C	3.32275000	-2.40402900	-0.90606100
C	-3.55343100	-2.57578400	-0.46879300
C	2.35373400	-3.32840800	-1.23433700
C	-2.59888500	-3.45689700	-0.87802500
H	4.32997500	2.61258700	-0.05524300
H	-4.69201200	2.42842700	0.43129000
H	2.36441400	4.52288200	-0.10370600
H	-2.84601200	4.39977500	0.20076500
H	4.39842000	-2.50293600	-0.90843700
H	-4.61859000	-2.73582700	-0.36010600
H	2.48304400	-4.35527300	-1.55303600
H	-2.71859100	-4.49417700	-1.16511300
C	-3.54915700	-0.14756700	0.10926300
C	-0.13452500	-3.33227600	-1.16586600
C	-0.22790700	3.36369500	-0.11056200
H	-4.62298400	-0.18497400	0.25856200
H	-0.12878300	-4.37316500	-1.47478900
H	-0.25236200	4.44883700	-0.08607800
H	-1.94621100	-1.09915200	2.50076500
C	-0.96030300	-0.84591200	2.85936500
C	-0.45404300	-0.91141200	4.12784900
C	1.09264600	-0.15171700	2.73498000
N	0.85117000	-0.46668100	4.02854500
H	-0.88596400	-1.22375900	5.06561500
H	2.03605900	0.22702500	2.37022800
H	1.51786000	-0.39193400	4.78366800
N	0.01313100	-0.37150000	2.00210200
C	3.36099300	-0.00745300	-0.19773800
O	4.58782000	-0.02566500	0.00638200
O	-0.49143400	1.01098900	-3.20622100
O	-0.69016900	2.20594200	-3.32527200



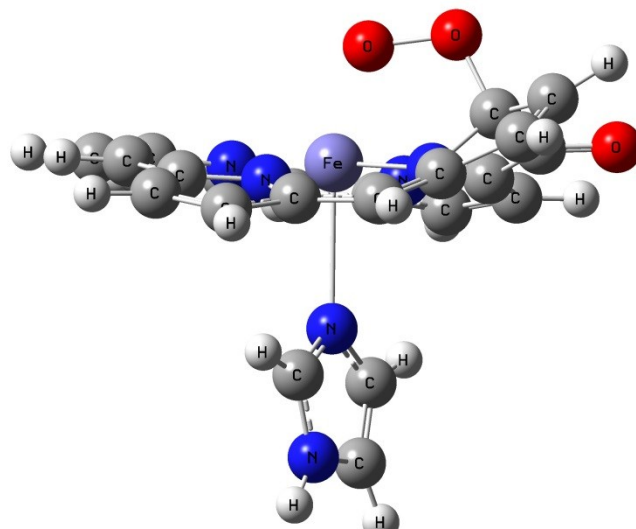
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N	-0.55641000	-0.26943700	1.65542000
C	-1.76994400	-0.33755900	2.16844800
C	0.32439900	-0.41944200	2.70620600
C	-0.37193300	-0.58024300	3.87273000
N	-1.70826700	-0.52609300	3.51467500
H	-2.68945500	-0.25438900	1.60931800
H	1.38978200	-0.40889700	2.53588000
H	-0.05518700	-0.72482300	4.89404800
H	-2.50004400	-0.60795800	4.13326800
C	2.41586600	1.12795600	-0.72488300
N	1.21848500	1.37598900	0.05793100
C	3.10583000	2.46111700	-0.82737600
C	2.63662200	-1.24034300	0.08905700
Fe	-0.07449600	0.02301200	-0.31976200
C	1.09016500	2.70009700	0.19265900
C	2.31953900	3.37955100	-0.24350200
H	4.07124600	2.59614200	-1.29598300
N	1.30427300	-1.41045900	-0.15600500
N	-1.44403500	-1.31725400	-0.82744400
C	3.27488600	-2.48364000	0.34904400
N	-1.49847500	1.46624000	-0.31297900
C	-0.12541500	3.35184800	0.45156100
H	2.47508000	4.45226100	-0.18305100
C	-1.27524800	-2.69882100	-0.86395000
C	1.08884200	-2.76847800	-0.11216600
C	2.30075900	-3.45143200	0.21973300
C	-2.74988700	-1.09251700	-1.16780500
H	4.33147700	-2.60239800	0.54984400
C	-2.82027900	1.32787400	-0.65494400
C	-1.34384000	2.75179700	0.13962100
H	-0.11620000	4.41398500	0.68005900
C	-0.12890300	-3.36387300	-0.48139100
C	-2.50026200	-3.33434300	-1.28348600
C	-3.41176700	-2.34084600	-1.48039000
H	2.40631900	-4.52695700	0.30901200
C	-3.40029500	0.15047500	-1.10454800
C	-3.52883800	2.56934100	-0.40721300
C	-2.62086500	3.44455400	0.10401300
H	-0.15897900	-4.45165500	-0.49947700
H	-2.63200500	-4.40403100	-1.40093500
H	-4.44630500	-2.42808200	-1.79340900
H	-4.45524900	0.17340000	-1.36701500
H	-4.58226100	2.73170900	-0.60776400
H	-2.77351400	4.47425300	0.40708700
O	4.49908000	0.21794100	0.09224300
C	3.29782500	0.02845600	-0.12340100



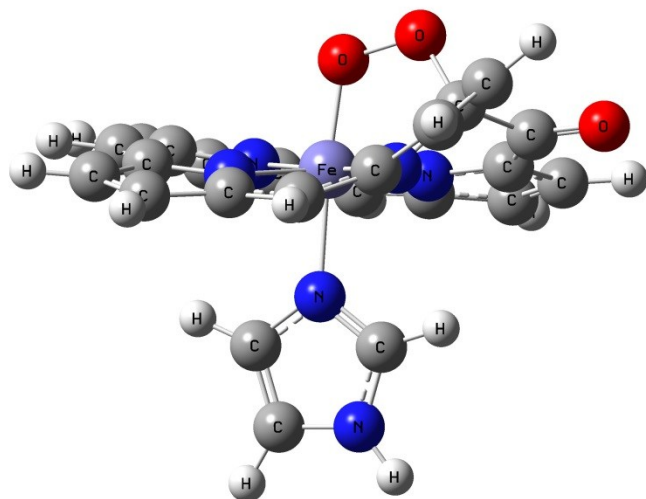
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O	0.54261500	0.29229300	-1.99776200
N	-0.60174000	-0.27253500	1.64286700
C	-1.82355400	-0.39330700	2.12186200
C	0.26200700	-0.37722400	2.71088300
C	-0.45601800	-0.56514200	3.85957700
N	-1.78525600	-0.57191900	3.46714400
H	-2.72936000	-0.34926100	1.53663200
H	1.32810200	-0.31324800	2.55986700
H	-0.16005000	-0.69307200	4.88913700
H	-2.58775900	-0.68959400	4.06621800
C	2.48880600	0.98938800	-0.71275600
N	1.34479300	1.28580500	0.11755300
C	3.27501600	2.27628100	-0.77094700
C	2.55932000	-1.40658000	0.05077900
Fe	-0.06519200	0.05362600	-0.32835600
C	1.28753800	2.62687600	0.27964200
C	2.56797500	3.22173400	-0.13221200
H	4.24175900	2.36049500	-1.24831700
N	1.19983100	-1.48426200	-0.11880700
N	-1.54906700	-1.21022600	-0.84691900
C	3.10544200	-2.69376700	0.27994400
N	-1.37227000	1.57168800	-0.29691800
C	0.13013300	3.34597500	0.53565700
H	2.81389600	4.27296900	-0.01865200
C	-1.48661100	-2.58828200	-0.83085600
C	0.87695500	-2.81693200	-0.07198200
C	2.05013900	-3.58371100	0.20674800
C	-2.82273700	-0.87937100	-1.23958300
H	4.15813600	-2.89625200	0.42622000
C	-2.70228600	1.53581600	-0.69073500
C	-1.13849500	2.83220600	0.19112300
H	0.20413900	4.40753200	0.75434400
C	-0.39221200	-3.33365100	-0.40352900
C	-2.74564100	-3.13393000	-1.27046500
C	-3.56956200	-2.07449300	-1.53732300
H	2.07999900	-4.66471300	0.28848700
C	-3.35768600	0.41270200	-1.18632500
C	-3.31181700	2.80923900	-0.43423900
C	-2.35097300	3.60588400	0.13458400
H	-0.50078900	-4.41571100	-0.39556100
H	-2.96352500	-4.19250100	-1.35754800
H	-4.59781100	-2.09269800	-1.88119300
H	-4.39690500	0.53391600	-1.48322900
H	-4.34492400	3.05522600	-0.65360600
H	-2.43866000	4.63781900	0.45510300
O	4.53185600	-0.10523400	-0.02991600
C	3.30673300	-0.19386800	-0.18370700



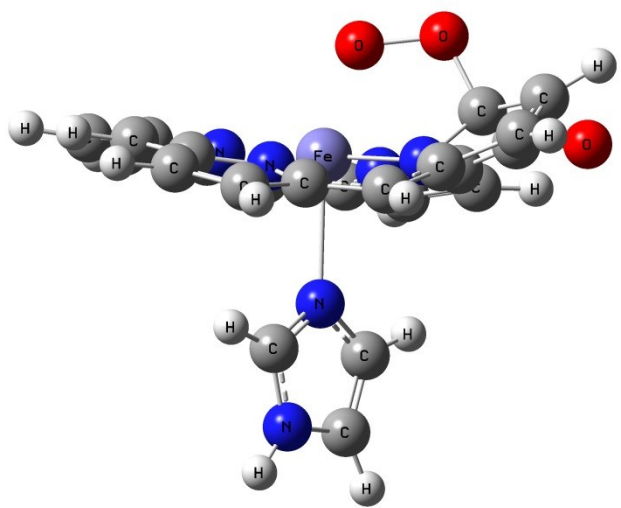
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N	0.63944200	0.29969100	2.02134900
C	1.51698600	-0.41910400	2.68574700
C	0.01873800	1.10266100	2.95286800
C	0.53316400	0.86372200	4.20094800
N	1.49526000	-0.11470600	4.01630400
H	2.17069200	-1.16510400	2.25634400
H	-0.75578800	1.79532700	2.65598300
H	0.31649400	1.27819800	5.17413900
H	2.06562300	-0.53750900	4.73294000
C	-2.42566300	-1.20718600	-0.74163900
N	-1.16311600	-1.40467300	-0.07061100
C	-3.09632700	-2.56034600	-0.70168800
C	-2.62728500	1.17187300	0.11014900
Fe	0.09223400	-0.03112200	-0.56972100
C	-0.98094400	-2.73155800	0.12021000
C	-2.24185500	-3.43629300	-0.15185000
H	-4.09976500	-2.73232800	-1.06616100
N	-1.30046000	1.39811900	-0.13873200
N	1.42313800	1.40232200	-0.94052700
C	-3.28925400	2.38422600	0.43078200
N	1.55285900	-1.39535300	-0.43506000
C	0.24070300	-3.33687900	0.35237600
H	-2.38440900	-4.50193700	-0.00379500
C	1.22423700	2.77058500	-0.88625900
C	-1.11739600	2.75714500	-0.05404300
C	-2.34172200	3.38587700	0.32926000
C	2.73442500	1.21023800	-1.31367400
H	-4.34429800	2.46501000	0.65545400
C	2.88028300	-1.20490400	-0.79354500
C	1.45124300	-2.68877700	0.02881900
H	0.27348700	-4.39888300	0.57613700
C	0.07563500	3.40237900	-0.42536700
C	2.42311500	3.44367600	-1.30143300
C	3.35303300	2.47790400	-1.58032300
H	-2.47860900	4.45328400	0.46292400
C	3.40927100	-0.01249600	-1.27543800
C	3.62253700	-2.40071200	-0.53036000
C	2.74301400	-3.31369100	0.00186200
H	0.08682400	4.48893800	-0.39097200
H	2.53796700	4.52027400	-1.35328100
H	4.37923700	2.60782500	-1.90442300
H	4.46004900	-0.00821200	-1.55361900
H	4.68259800	-2.52414500	-0.72135700
H	2.94169000	-4.33242900	0.31432500
O	-4.47842700	-0.29139600	0.12866900
C	-3.27856500	-0.10285200	-0.10664700



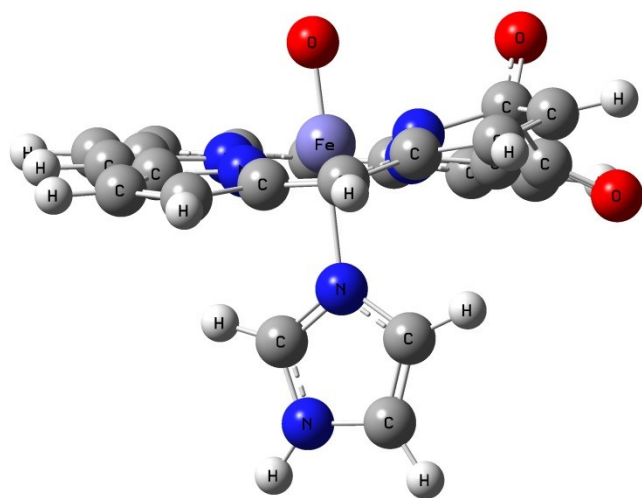
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O	0.51118900	0.26051600	-1.97251000
N	-0.58272200	-0.27494200	1.67277800
C	-1.78382500	-0.51505200	2.16982100
C	0.29225100	-0.25215700	2.73988100
C	-0.39672800	-0.48300300	3.89755300
N	-1.71576200	-0.64686000	3.51590700
H	-2.69583700	-0.59091600	1.59878700
H	1.34508300	-0.07361300	2.59115000
H	-0.08254800	-0.54580900	4.92742900
H	-2.49651300	-0.83531100	4.12758000
C	2.45275300	1.02401300	-0.73463400
N	1.30396000	1.31113700	0.10300300
C	3.22253000	2.31908700	-0.80122500
C	2.55870200	-1.39658100	0.00612000
Fe	-0.07995500	0.04800000	-0.29517400
C	1.25026800	2.63035700	0.28517700
C	2.51740600	3.25082400	-0.14386100
H	4.18021100	2.41672400	-1.29299500
N	1.21119800	-1.47116200	-0.11407400
N	-1.53566500	-1.21598800	-0.82237200
C	3.12963400	-2.67764100	0.23509200
N	-1.38085500	1.54558800	-0.28502600
C	0.07051400	3.33292100	0.57764500
H	2.75436000	4.30097700	-0.01870800
C	-1.45846000	-2.60256100	-0.81408300
C	0.89623500	-2.81211100	-0.04265700
C	2.08165500	-3.57186200	0.20466600
C	-2.78616500	-0.90799800	-1.24495300
H	4.18671100	-2.86993500	0.35231200
C	-2.69453000	1.50585400	-0.72035400
C	-1.16197800	2.80592900	0.20103100
H	0.12694600	4.38223500	0.84513300
C	-0.35903900	-3.32728300	-0.38706400
C	-2.70023300	-3.15885600	-1.27762600
C	-3.52390500	-2.10584300	-1.56088500
H	2.12195600	-4.65056300	0.29252100
C	-3.33436300	0.40023100	-1.22251900
C	-3.31846500	2.80035400	-0.49016800
C	-2.39266200	3.58647700	0.10657000
H	-0.45855100	-4.41005900	-0.38245500
H	-2.90671900	-4.21731200	-1.37643700
H	-4.54082500	-2.12874100	-1.93178600
H	-4.36317900	0.51368400	-1.55023800
H	-4.34132600	3.04329700	-0.75028200
H	-2.48961900	4.61603200	0.42766700
O	4.50906700	-0.07279600	-0.12597800
C	3.29118700	-0.15990600	-0.23471800



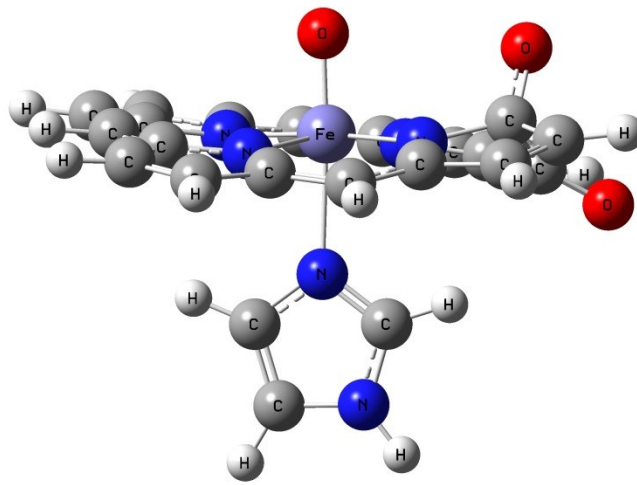
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N	0.52474500	0.30651900	1.95533100
C	1.61462600	-0.05148800	2.60559400
C	-0.31793700	0.85733500	2.89889100
C	0.27584800	0.82820800	4.13263500
N	1.51181500	0.24473700	3.92899200
H	2.48329000	-0.52133600	2.16840000
H	-1.29126100	1.23708700	2.62617600
H	-0.05201100	1.15567600	5.10717100
H	2.21262800	0.06781500	4.63389900
C	-2.36321100	-1.28642800	-0.74602400
N	-1.10502000	-1.45497800	-0.05589700
C	-3.00357100	-2.65266600	-0.71659100
C	-2.65190500	1.12815200	0.01418300
Fe	0.12704000	-0.03345700	-0.48131100
C	-0.91305500	-2.75348000	0.17094900
C	-2.15027600	-3.49978200	-0.12458400
H	-3.99243500	-2.85143100	-1.10546200
N	-1.33361100	1.36006800	-0.16583600
N	1.42079500	1.40259200	-0.87932300
C	-3.36156400	2.33585900	0.28147500
N	1.59327100	-1.37114000	-0.36689400
C	0.33659300	-3.32670900	0.44163500
H	-2.27415100	-4.56314900	0.04303700
C	1.18363500	2.77151400	-0.86992100
C	-1.17677900	2.73268600	-0.09713400
C	-2.43308000	3.34818300	0.20693400
C	2.72155600	1.24315200	-1.25452900
H	-4.42675800	2.39821300	0.45322200
C	2.91174000	-1.16860900	-0.75004300
C	1.50764100	-2.66094400	0.09133600
H	0.39356000	-4.37516900	0.71079800
C	0.00460900	3.37768400	-0.45266900
C	2.36110300	3.46408200	-1.29023700
C	3.31646800	2.51273300	-1.54378900
H	-2.59675900	4.41396400	0.30737700
C	3.42490600	0.01237300	-1.21962100
C	3.67305200	-2.38222300	-0.51015000
C	2.82295900	-3.28667300	0.03330200
H	-0.00642800	4.46468300	-0.44627100
H	2.44928700	4.53987500	-1.37538400
H	4.33704200	2.65911300	-1.87353700
H	4.47100100	0.03395800	-1.50872700
H	4.72715900	-2.49874600	-0.72973900
H	3.03054100	-4.30277700	0.34427800
O	-4.45886400	-0.38462200	0.02024700
C	-3.26419300	-0.18588400	-0.16899100



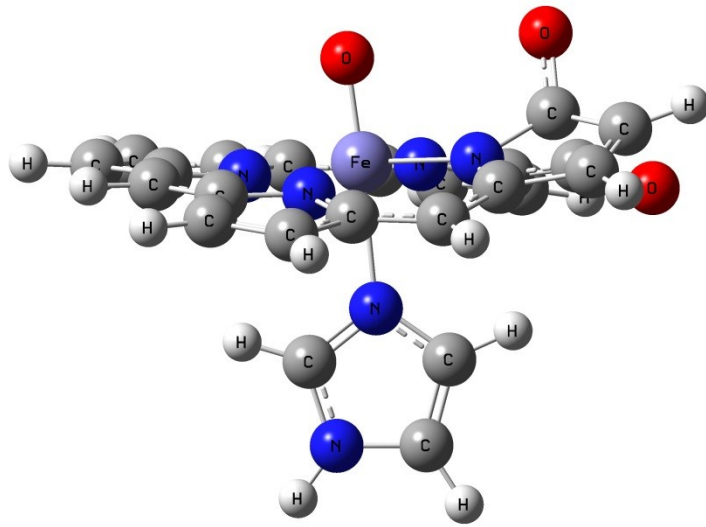
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N	-0.17267000	0.09466900	1.66700100
C	-1.22771200	-0.14170800	2.41713500
C	0.86899400	0.36034400	2.52927400
C	0.43029200	0.28251200	3.82402800
N	-0.91367000	-0.03740000	3.73775100
H	-2.21253500	-0.38246500	2.04618000
H	1.86090100	0.57457400	2.16060000
H	0.93040600	0.41635400	4.77095600
H	-1.54741900	-0.17946500	4.50933300
C	2.78696900	0.61869300	-0.97383100
N	1.40435900	1.13982500	-0.67177500
C	3.65834300	1.84596200	-0.83298600
C	2.22507100	-1.65037200	-0.05689200
Fe	-0.22997800	0.02109700	-0.62204600
C	1.50582500	2.43027600	-0.40787600
C	2.90122400	2.89782400	-0.51126500
H	4.72908700	1.79544700	-0.98199300
N	0.89108000	-1.59543300	-0.25784700
N	-1.92897600	-1.12592400	-0.50200600
C	2.65151800	-2.98283900	0.21714600
N	-1.34842100	1.63106000	-0.34904500
C	0.43521400	3.29586200	-0.09030400
H	3.20050800	3.92776500	-0.34003700
C	-1.98307600	-2.50304600	-0.52058200
C	0.43717300	-2.91211100	-0.17998900
C	1.53844800	-3.77782900	0.10574700
C	-3.21493800	-0.69723100	-0.63759200
H	3.67628200	-3.25284900	0.42851300
C	-2.72914900	1.71128300	-0.42526000
C	-0.88763700	2.91005600	-0.14398700
H	0.65854900	4.34472700	0.08137400
C	-0.87355700	-3.32509400	-0.34851300
C	-3.33671200	-2.94440700	-0.66939100
C	-4.11183200	-1.81390700	-0.74363400
H	1.46527400	-4.85540200	0.20050000
C	-3.59855400	0.65968800	-0.59368000
C	-3.13959300	3.08982100	-0.24307100
C	-2.01483300	3.82231800	-0.04970200
H	-1.05251000	-4.39801100	-0.32409000
H	-3.65294400	-3.98068600	-0.70714100
H	-5.18759200	-1.74050600	-0.85441800
H	-4.65950800	0.88590600	-0.65829200
H	-4.16985600	3.42661800	-0.26151800
H	-1.92326000	4.88902700	0.11792000
O	4.23825800	-0.60973900	0.59464900
C	3.16660400	-0.50890300	-0.00535000



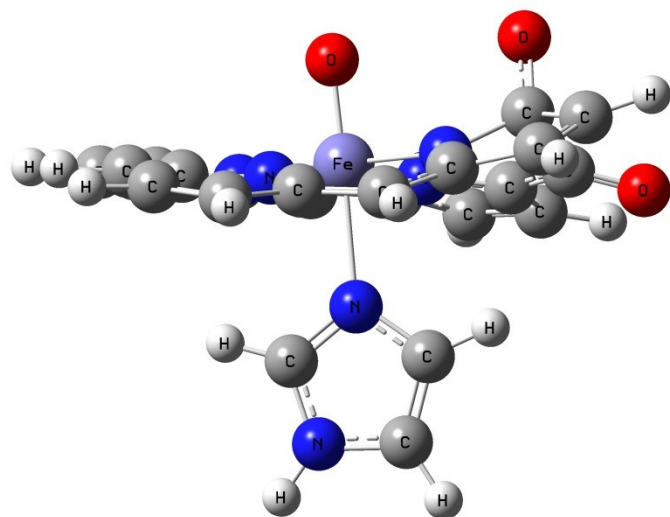
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C	1.29566600	0.02491500	2.39740900
C	-0.84819500	-0.20424000	2.53711700
C	-0.38387700	-0.19964200	3.82464000
N	0.98896900	-0.05277700	3.72028100
H	2.29886800	0.13966000	2.01563100
H	-1.86398800	-0.29369900	2.18256600
H	-0.88332400	-0.28189500	4.77767500
H	1.64753400	-0.00666700	4.48272300
C	-2.73686500	-0.84646000	-0.89826200
N	-1.30851900	-1.24113300	-0.57442100
C	-3.49616100	-2.13897200	-0.69913100
C	-2.39081100	1.51806100	-0.12356800
Fe	0.22348500	-0.00070300	-0.59536000
C	-1.28910300	-2.54261700	-0.33004400
C	-2.64555300	-3.12038400	-0.39187100
H	-4.56990200	-2.18178100	-0.82718700
N	-1.05769600	1.55268800	-0.30472700
N	1.81948000	1.26528200	-0.45158800
C	-2.92040000	2.82528400	0.11427600
N	1.49246800	-1.54682900	-0.40682300
C	-0.14751900	-3.33427300	-0.08721100
H	-2.85138000	-4.17196200	-0.21455700
C	1.76112900	2.64420400	-0.46165800
C	-0.69917100	2.89751900	-0.23258000
C	-1.86568600	3.69382600	0.01071400
C	3.13874400	0.94088600	-0.59737000
H	-3.96549400	3.02555400	0.30312700
C	2.87003300	-1.51181600	-0.50235700
C	1.14336200	-2.85607500	-0.21004100
H	-0.29072400	-4.39826900	0.07634800
C	0.58863300	3.38854400	-0.33891500
C	3.07500800	3.19106900	-0.59350600
C	3.93932800	2.12717900	-0.67984900
H	-1.86825700	4.77472800	0.09550800
C	3.64078500	-0.37809200	-0.61201500
C	3.39871400	-2.85759300	-0.37322200
C	2.34078400	-3.68269000	-0.17461000
H	0.70038700	4.47064400	-0.31315800
H	3.30635900	4.24975800	-0.62062900
H	5.01726600	2.14197700	-0.79180000
H	4.71771500	-0.50139300	-0.69046300
H	4.45231500	-3.10897800	-0.41896700
H	2.33882900	-4.75692000	-0.03106200
O	-4.32150900	0.34659100	0.55225500
C	-3.23212500	0.30504400	-0.02600600



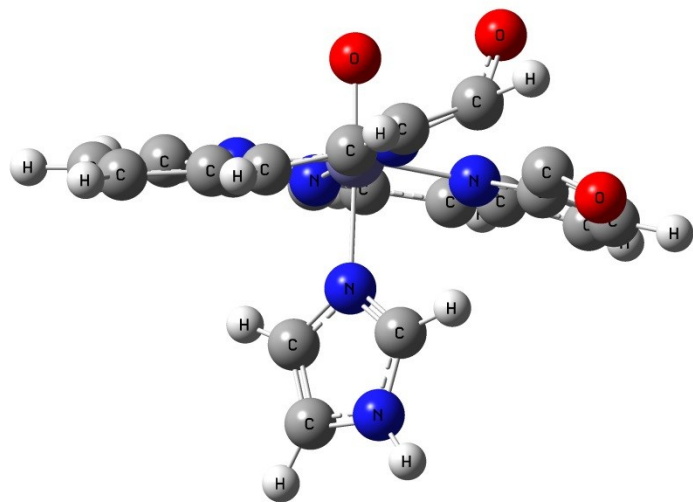
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N	0.23789900	-0.03690800	1.66032500
C	1.32958200	0.14373500	2.37348800
C	-0.78406800	-0.25589100	2.55729000
C	-0.29797100	-0.20542600	3.83603100
N	1.05623800	0.05012200	3.70286400
H	2.31135000	0.33560700	1.96821800
H	-1.79280000	-0.43130000	2.21753900
H	-0.76981200	-0.32127400	4.79967000
H	1.72416000	0.15402900	4.45129400
C	-2.72806100	-0.67916900	-1.06901900
N	-1.40999200	-1.10547500	-0.55055900
C	-3.63669200	-1.87252400	-0.81226100
C	-2.28135800	1.65142700	0.02706800
Fe	0.21711900	-0.00643700	-0.60779400
C	-1.50496600	-2.40592100	-0.20667500
C	-2.89808800	-2.86993100	-0.31931000
H	-4.68883600	-1.84451700	-1.06057800
N	-0.94591300	1.62814600	-0.30445600
N	1.88578500	1.12941300	-0.49989400
C	-2.68722400	2.96409400	0.38565000
N	1.34599200	-1.64477800	-0.38025700
C	-0.45017400	-3.25245900	0.10205100
H	-3.21186400	-3.87689700	-0.06246700
C	1.92668900	2.50802800	-0.53230300
C	-0.50403800	2.91789000	-0.16651900
C	-1.57695700	3.76749100	0.23997300
C	3.17187700	0.69324200	-0.71170000
H	-3.69647100	3.23733600	0.66417100
C	2.72136500	-1.72882500	-0.50824500
C	0.89881900	-2.89714300	-0.06839300
H	-0.67722600	-4.28400600	0.35506300
C	0.83159800	3.33799700	-0.34606700
C	3.28147600	2.94690600	-0.74658600
C	4.05175400	1.82223400	-0.86164200
H	-1.49530500	4.83556100	0.40655300
C	3.56871800	-0.64709700	-0.70737700
C	3.13958100	-3.08602600	-0.28738600
C	2.01380400	-3.80741600	0.00821900
H	1.01646100	4.40886200	-0.31192600
H	3.59283600	3.98375100	-0.80307300
H	5.12081700	1.75426200	-1.02918800
H	4.62931200	-0.85490300	-0.82621300
H	4.16695100	-3.42995900	-0.32982500
H	1.93199700	-4.86397800	0.23586500
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C	-3.21604400	0.57550400	-0.09480500



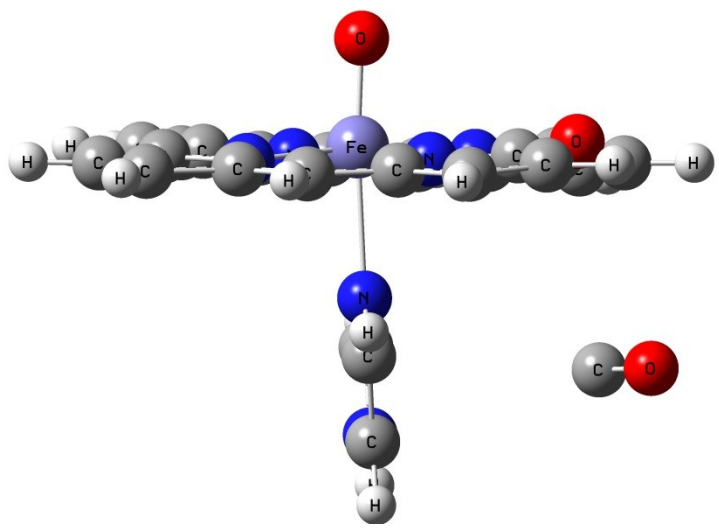
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N	-0.24414000	-0.00237000	1.66854800
C	-1.32349000	-0.20448900	2.40168800
C	0.79520900	0.18891300	2.55545000
C	0.33188900	0.10007600	3.83952200
N	-1.02174800	-0.15052300	3.72358700
H	-2.31603900	-0.38499400	2.01926600
H	1.80037000	0.37698100	2.21307800
H	0.82303700	0.18728800	4.79605400
H	-1.67377700	-0.27876600	4.48360100
C	2.69079900	0.77211700	-1.02250900
N	1.35813800	1.17436300	-0.50256500
C	3.57146800	1.98843800	-0.79374100
C	2.33451700	-1.61676800	-0.03826300
Fe	-0.22139100	0.01748500	-0.55614400
C	1.42829800	2.45982200	-0.18091400
C	2.80776600	2.97161200	-0.31441100
H	4.62221300	1.98453600	-1.04725400
N	0.99656600	-1.59098600	-0.30776400
N	-1.85380000	-1.15292800	-0.51720800
C	2.77458500	-2.92415200	0.29720400
N	-1.38730300	1.61227000	-0.34718000
C	0.33326600	3.28398400	0.14111800
H	3.09427100	3.98837000	-0.07165700
C	-1.85700400	-2.54272800	-0.55448300
C	0.57835100	-2.89297700	-0.17813100
C	1.66929800	-3.73714800	0.17977700
C	-3.13133000	-0.76409400	-0.73273600
H	3.79518600	-3.18885400	0.53537600
C	-2.75594500	1.66034100	-0.50171800
C	-0.97746800	2.87868200	-0.03831300
H	0.52750800	4.32084000	0.39215700
C	-0.74797200	-3.33053000	-0.36534600
C	-3.19852700	-3.01706700	-0.78549400
C	-3.99105600	-1.91515100	-0.90118100
H	1.60931800	-4.80906400	0.32039900
C	-3.57403000	0.57995600	-0.72107200
C	-3.21975400	3.02850200	-0.29731500
C	-2.13495300	3.77020500	0.01639800
H	-0.90430100	-4.40625300	-0.35216800
H	-3.48248600	-4.05981300	-0.85265800
H	-5.05749400	-1.86870200	-1.08170500
H	-4.63667400	0.75879300	-0.84971100
H	-4.25324500	3.34276200	-0.37364100
H	-2.08198600	4.82734100	0.24415900
O	4.38245500	-0.47012300	0.26746500
C	3.24273400	-0.49913900	-0.14340500



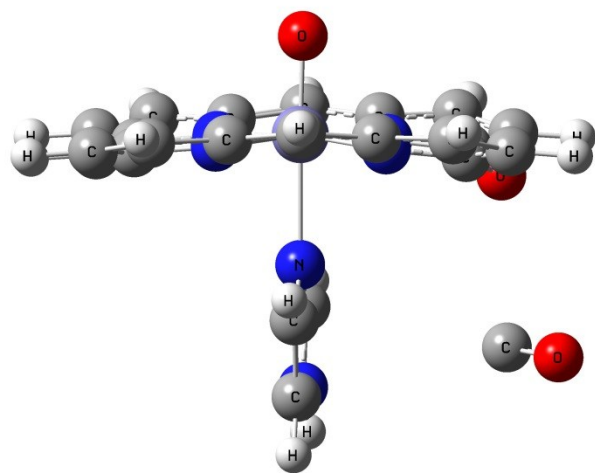
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C	-1.32355200	-0.20668100	2.40515000
C	0.79501300	0.18840800	2.55847100
C	0.33199500	0.09892400	3.84262900
N	-1.02147400	-0.15283400	3.72694200
H	-2.31593800	-0.38821900	2.02273800
H	1.79991600	0.37756200	2.21584900
H	0.82324700	0.18642600	4.79907900
H	-1.67319600	-0.28185200	4.48710100
C	2.69076400	0.77573900	-1.02112000
N	1.35694500	1.17528900	-0.50007200
C	3.56833200	1.99421700	-0.79252400
C	2.33741500	-1.61434500	-0.04106900
Fe	-0.22136600	0.01732800	-0.55695100
C	1.42400400	2.46207700	-0.18089600
C	2.80213100	2.97655000	-0.31538700
H	4.61899800	1.99285200	-1.04644400
N	0.99981000	-1.59027000	-0.31095000
N	-1.85242400	-1.15556700	-0.51356700
C	2.77947400	-2.92155800	0.29312500
N	-1.39073500	1.61121600	-0.34870100
C	0.32786400	3.28485100	0.13935000
H	3.08610600	3.99445000	-0.07446700
C	-1.85309700	-2.54538600	-0.55412200
C	0.58325700	-2.89309200	-0.18222000
C	1.67560100	-3.73608200	0.17480600
C	-3.13069000	-0.76841800	-0.73016900
H	3.80044600	-3.18463700	0.53153100
C	-2.75938800	1.65698800	-0.50245300
C	-0.98257200	2.87806500	-0.04075700
H	0.52073100	4.32229000	0.38904100
C	-0.74259000	-3.33196100	-0.36762700
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C	-3.98784000	-1.92059400	-0.90182200
H	1.61700000	-4.80813000	0.31495100
C	-3.57576700	0.57468500	-0.71890800
C	-3.22510700	3.02470800	-0.29928500
C	-2.14118200	3.76825300	0.01319800
H	-0.89754900	-4.40790100	-0.35591300
H	-3.47546300	-4.06451200	-0.85729800
H	-5.05410500	-1.87577700	-1.08377700
H	-4.63876700	0.75143700	-0.84752700
H	-4.25912200	3.33734300	-0.37506500
H	-2.08956900	4.82561600	0.24017600
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C	3.24378000	-0.49473800	-0.14262900



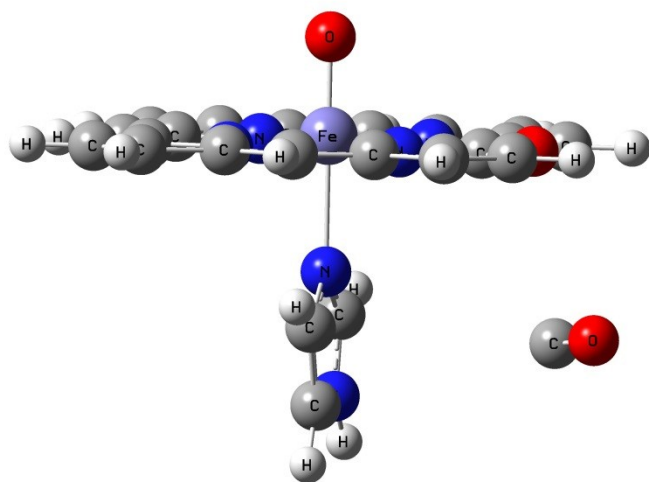
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N	0.09915000	-0.00938100	1.49847900
C	0.15697000	-1.09536800	2.24151500
C	0.45262100	1.04100400	2.31869300
C	0.72763100	0.57690200	3.57753500
N	0.52539200	-0.79095500	3.51504400
H	-0.05449600	-2.09746800	1.90028700
H	0.48674800	2.05066800	1.93891100
H	1.02852900	1.07304700	4.48763400
H	0.67594100	-1.45503900	4.25878600
C	2.10821300	1.59775400	-1.11581200
N	0.81119800	1.60675400	-0.78940700
C	2.69769800	2.87772100	-1.10080300
C	2.43113500	-0.76795400	-1.20047300
Fe	-0.46857500	0.02177000	-0.70792800
C	0.50868700	2.95044800	-0.56310000
C	1.66556300	3.74303100	-0.74554800
H	3.73403300	3.09461100	-1.32123800
N	1.18362900	-1.15341400	-0.90782300
N	-1.57203100	-1.57146200	-0.33931100
C	3.34576200	-1.83985000	-1.26121700
N	-1.94288000	1.21533500	-0.19141200
C	-0.78083600	3.39361800	-0.23477300
H	1.70784000	4.82122900	-0.64037700
C	-1.16123400	-2.90595400	-0.36415600
C	1.25453800	-2.54184000	-0.79346100
C	2.58177400	-2.97735000	-1.00355400
C	-2.92063800	-1.58591500	-0.11986100
H	4.40072900	-1.75306400	-1.48319800
C	-3.24274500	0.85198700	0.01949300
C	-1.89738100	2.60535300	-0.07147800
H	-0.91122700	4.46656300	-0.10656100
C	0.12924800	-3.34664700	-0.55380000
C	-2.29967300	-3.76014600	-0.13966700
C	-3.38696000	-2.95261600	0.00360300
H	2.91177500	-4.00982500	-0.98419000
C	-3.72734900	-0.45717200	0.01421500
C	-4.04704400	2.02537000	0.28972700
C	-3.21205100	3.10078600	0.23935600
H	0.29372800	-4.42231900	-0.53091500
H	-2.25609300	-4.84330200	-0.10445300
H	-4.41781400	-3.23466800	0.18465700
H	-4.78781500	-0.60740400	0.19442200
H	-5.11084200	2.00541500	0.49656300
H	-3.45215100	4.14743200	0.39132800
O	4.59269000	0.13397300	1.63282500
C	3.74606700	-0.60240300	1.83549500



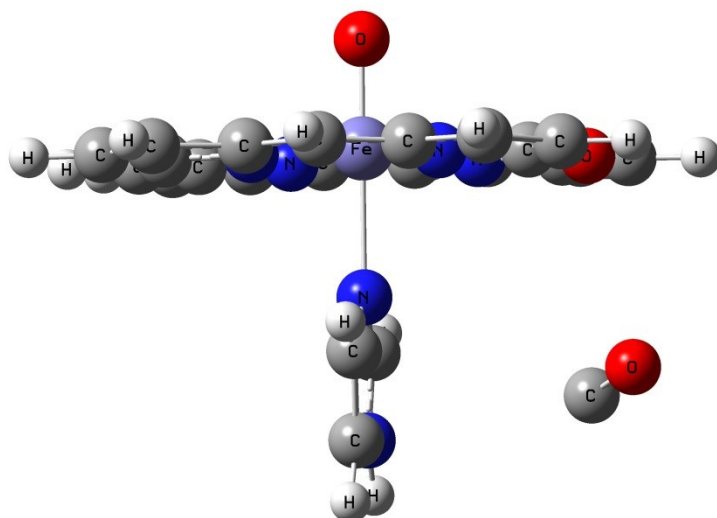
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O	-0.73082400	0.04255300	-2.24143300
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C	0.09765500	-1.08843000	2.27351700
C	0.42412500	1.04579500	2.34312100
C	0.64371800	0.58827400	3.61543600
N	0.42271200	-0.77772600	3.55656900
H	-0.12041200	-2.08742900	1.92718700
H	0.47916300	2.05048100	1.95243500
H	0.91811700	1.08677900	4.53250700
H	0.53191400	-1.43616800	4.31255400
C	2.54909500	0.53604000	-1.01336100
N	1.31801300	1.04165900	-0.84986700
C	3.49658500	1.50193100	-1.38520800
C	2.00379900	-1.77872500	-0.91570800
Fe	-0.40771100	0.02853100	-0.65477600
C	1.44395100	2.40592000	-1.12309900
C	2.78289500	2.70263600	-1.45078300
H	4.54869300	1.31855200	-1.55601000
N	0.67753600	-1.66517400	-0.74555400
N	-2.02247000	-1.02857500	-0.16575200
C	2.41270200	-3.09206400	-1.18787800
N	-1.36940200	1.72666800	-0.27053900
C	0.38204800	3.31523100	-0.96533000
H	3.16434200	3.68869800	-1.69023000
C	-2.17651800	-2.40458600	-0.34046000
C	0.17531600	-2.95899100	-0.90901400
C	1.23528500	-3.84848400	-1.17747200
C	-3.23525200	-0.53712800	0.21964800
H	3.43288300	-3.41330000	-1.34941300
C	-2.66691100	1.86086500	0.12664300
C	-0.89372200	3.00900700	-0.54997500
H	0.60422700	4.36328400	-1.15626600
C	-1.18108800	-3.28129700	-0.70483200
C	-3.53286700	-2.76950900	-0.02018800
C	-4.18393800	-1.62772600	0.34032900
H	1.13164800	-4.91648700	-1.33252200
C	-3.54148600	0.81036600	0.42015700
C	-3.02472300	3.26526900	0.14826000
C	-1.93659300	3.96460500	-0.28371600
H	-1.45547100	-4.32907300	-0.81072900
H	-3.92325300	-3.78058500	-0.06285800
H	-5.21810700	-1.50974100	0.64348100
H	-4.55493800	1.06216900	0.71867900
H	-3.99692700	3.64591600	0.44006100
H	-1.83328200	5.03715100	-0.40752900
O	4.46382900	0.32305700	1.95168600
C	3.72728300	-0.51891600	2.16572600



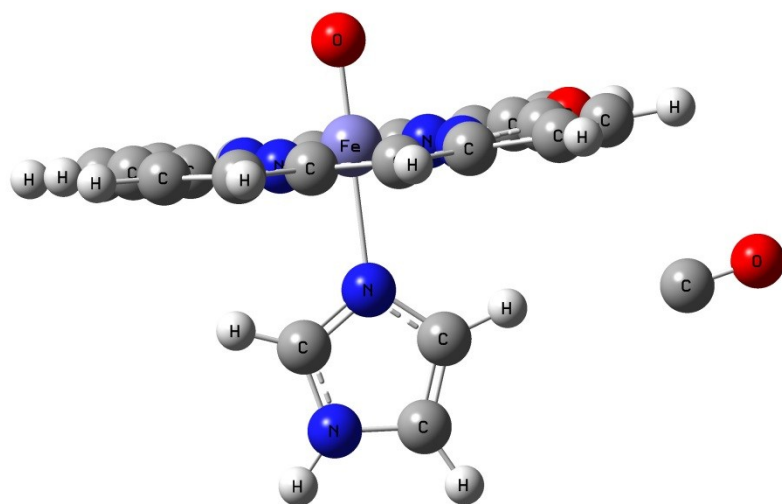
O	2.91401800	0.67476800	-1.14536800
O	-0.70914100	0.02624000	-2.26434900
N	0.01589000	-0.02164400	1.50517200
C	0.40853900	-1.08264800	2.17980900
C	-0.06132700	1.01584100	2.40857600
C	0.29348300	0.56990500	3.65327100
N	0.58735900	-0.77418400	3.49156600
H	0.57390500	-2.06379900	1.76013500
H	-0.36625200	2.00155600	2.09165400
H	0.36014300	1.06171500	4.61155000
H	0.90810500	-1.41018700	4.20536500
C	2.07645900	1.72195300	-0.97762500
N	0.75531700	1.65306200	-0.71670800
C	2.55955700	3.04062800	-1.05918900
C	2.53518100	-0.62005100	-1.07631900
Fe	-0.40336100	0.00833100	-0.67506100
C	0.33633000	2.98172400	-0.63605700
C	1.44806700	3.84578900	-0.83929100
H	3.58691000	3.31921600	-1.25080900
N	1.28582800	-1.07652800	-0.85109500
N	-1.45492700	-1.67717100	-0.33993600
C	3.47940300	-1.64944300	-1.25034700
N	-1.99969200	1.13573200	-0.20093800
C	-0.98037400	3.37231000	-0.38039800
H	1.40219300	4.92825800	-0.82263400
C	-1.00418900	-2.96868800	-0.45314700
C	1.39794900	-2.46736000	-0.89501500
C	2.75128600	-2.83016700	-1.13740400
C	-2.81402800	-1.75661300	-0.08349700
H	4.53231200	-1.50438300	-1.45146100
C	-3.28584300	0.67740400	0.03459600
C	-2.06603400	2.50623000	-0.18864200
H	-1.18243400	4.43963300	-0.34200600
C	0.32697200	-3.34412200	-0.69821600
C	-2.09071400	-3.88401500	-0.25053100
C	-3.21470300	-3.12597300	-0.02203800
H	3.11638600	-3.84750500	-1.21307200
C	-3.65731000	-0.66120700	0.09463000
C	-4.16907100	1.78895800	0.21205300
C	-3.41478500	2.92696500	0.07474800
H	0.54011000	-4.40832400	-0.75863700
H	-2.00166100	-4.96396700	-0.28294100
H	-4.22683500	-3.46503500	0.16866900
H	-4.70589000	-0.87375600	0.29087900
H	-5.23118600	1.70645500	0.41407900
H	-3.73561000	3.96026000	0.14210700
O	4.52841700	0.42592900	1.67939400
C	3.93222100	-0.52193800	1.89250800



O	3.00337100	-0.00424200	-1.10459200
O	-0.66946400	0.03880700	-2.24901600
N	0.03342500	-0.00977100	1.50733900
C	0.05779400	-1.08451700	2.27455000
C	0.26511600	1.06691900	2.33879500
C	0.43077400	0.62912200	3.62486800
N	0.28828900	-0.74383800	3.56618000
H	-0.08826700	-2.09930300	1.93820300
H	0.28986600	2.07443600	1.95424900
H	0.62078900	1.14995200	4.55029900
H	0.38058400	-1.38856000	4.33737900
C	2.38163600	1.19079200	-1.02481500
N	1.08404200	1.38974600	-0.78802100
C	3.11764300	2.39197200	-1.19701500
C	2.36392300	-1.19155200	-1.04507400
Fe	-0.37506100	0.01813000	-0.65756700
C	0.92696300	2.77821800	-0.81877400
C	2.18685100	3.39972900	-1.06718000
H	4.17890200	2.45167600	-1.39075100
N	1.06166300	-1.37573300	-0.82008400
N	-1.73159900	-1.39808600	-0.29024000
C	3.08347800	-2.40042800	-1.23043000
N	-1.70732400	1.44405200	-0.25363500
C	-0.28685300	3.42040100	-0.60948800
H	2.34891800	4.46778500	-1.13600900
C	-1.55042000	-2.76122400	-0.41456800
C	0.88477000	-2.76049000	-0.87399400
C	2.13640300	-3.39678800	-1.12336200
C	-3.05531800	-1.20759800	-0.01015100
H	4.14405600	-2.47306100	-1.42412100
C	-3.03291400	1.26885000	0.02549000
C	-1.50388500	2.80583800	-0.34265800
H	-0.28176200	4.50618600	-0.65398000
C	-0.34109700	-3.38863700	-0.68540100
C	-2.79883300	-3.44120300	-0.18561500
C	-3.73216000	-2.48054800	0.06912400
H	2.28297800	-4.46577400	-1.21052200
C	-3.67072000	0.03384800	0.15919600
C	-3.68796200	2.55010600	0.14133100
C	-2.73906800	3.50098400	-0.09167800
H	-0.35213100	-4.47323000	-0.75334600
H	-2.93158900	-4.51549800	-0.22033100
H	-4.78584000	-2.60583900	0.28409900
H	-4.73346100	0.04027100	0.37964000
H	-4.73844100	2.68731800	0.36436500
H	-2.85276300	4.57793800	-0.09649300
O	4.28953500	0.21626600	1.86243900
C	3.57767000	-0.51661500	2.36228700

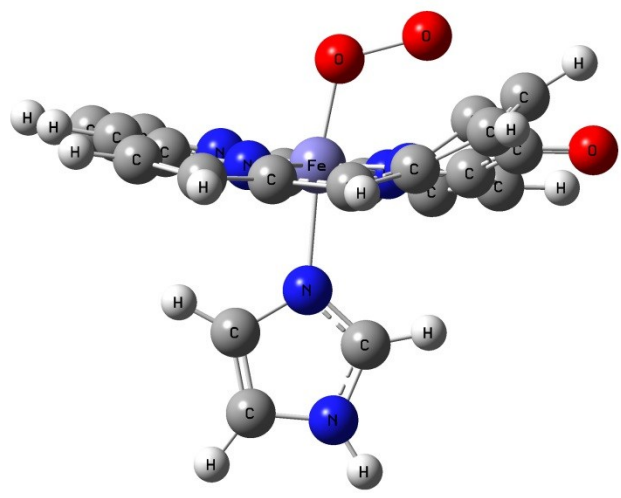


O	-2.93109200	0.26006600	-1.12626500
O	0.64276100	0.00780700	-2.21615200
N	0.12608900	-0.00694500	1.57140000
C	1.11018200	-0.05377400	2.45111200
C	-1.04579000	0.03257700	2.29992800
C	-0.75789000	0.00925300	3.63705000
N	0.62090700	-0.04600100	3.71572600
H	2.16243100	-0.09351400	2.21513500
H	-2.01335700	0.07196700	1.82475900
H	-1.38535200	0.02601700	4.51439400
H	1.17230900	-0.07524800	4.56078600
C	-2.40483700	-0.97591200	-0.97801400
N	-1.13015000	-1.25944000	-0.70417500
C	-3.23020700	-2.12458900	-1.08571700
C	-2.22821800	1.39887300	-0.94137000
Fe	0.42221400	0.00186000	-0.61236300
C	-1.08138300	-2.65362000	-0.64181800
C	-2.38259700	-3.19051300	-0.86618700
H	-4.28897700	-2.11702300	-1.30173100
N	-0.92569700	1.48199000	-0.66589800
N	1.89844900	1.30516000	-0.28043900
C	-2.87422900	2.66006200	-1.01350800
N	1.68765700	-1.51405800	-0.31817100
C	0.08792200	-3.37828200	-0.44598300
H	-2.62606500	-4.24520700	-0.87172600
C	1.78111500	2.67975900	-0.24474900
C	-0.67072200	2.85122700	-0.56387700
C	-1.87864900	3.58146300	-0.76768100
C	3.23452600	1.02854200	-0.19164800
H	-3.92299500	2.81530300	-1.22262700
C	3.04936800	-1.44091100	-0.22075800
C	1.36743200	-2.85634100	-0.31703100
H	-0.00581500	-4.46082200	-0.42741100
C	0.59242600	3.38878800	-0.35391400
C	3.08373100	3.27646200	-0.10986300
C	3.98752600	2.25538300	-0.08279900
H	-1.96305400	4.66030400	-0.74172400
C	3.78671200	-0.25517600	-0.16584400
C	3.61166500	-2.76854100	-0.14120100
C	2.56690100	-3.64300400	-0.19480000
H	0.66036200	4.47239500	-0.30669800
H	3.27127000	4.34168300	-0.05532500
H	5.06547000	2.31193900	0.00149300
H	4.86649100	-0.33708100	-0.09131300
H	4.66887000	-2.98623000	-0.05636500
H	2.59402000	-4.72525300	-0.16616800
O	-5.82122000	-0.06962000	1.06191100
C	-4.75457900	0.00851700	1.44882400



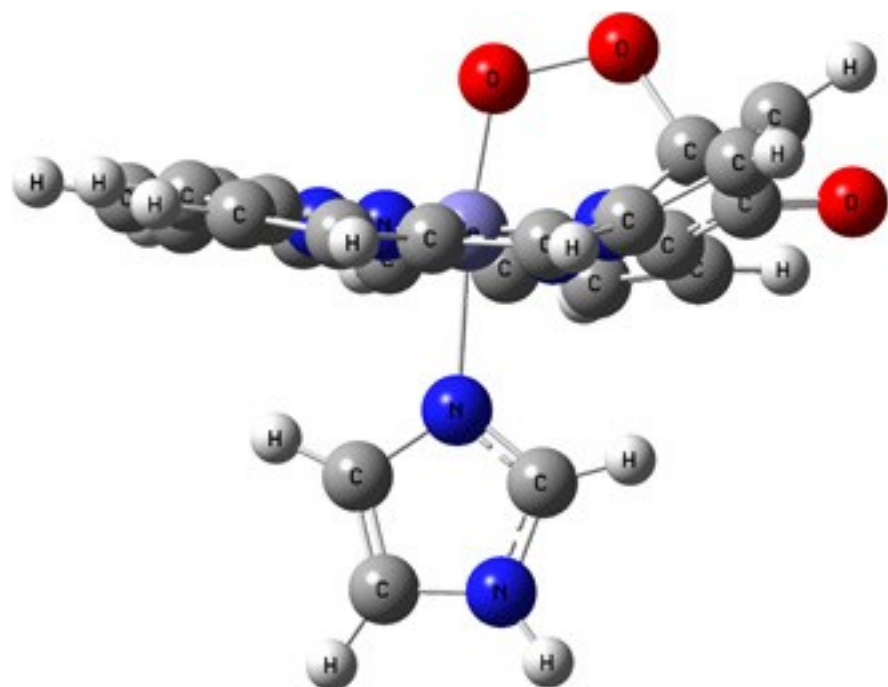
²TS1

1	8	0	1.880704	0.863709	-2.070745
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3	7	0	-0.555394	-0.306944	1.734483
4	6	0	-0.229950	-1.389766	2.446459
5	6	0	-1.179641	0.580890	2.616780
6	6	0	-1.227594	0.019181	3.867032
7	7	0	-0.624450	-1.228238	3.744205
8	1	0	0.276456	-2.260998	2.075562
9	1	0	-1.534389	1.539953	2.292689
10	1	0	-1.620003	0.385040	4.799395
11	1	0	-0.490183	-1.898821	4.483323
12	6	0	2.336768	1.318617	-0.714963
13	7	0	1.097187	1.494999	0.049196
14	6	0	2.937730	2.697798	-0.808595
15	6	0	2.717909	-1.048307	0.058615
16	26	0	-0.109372	0.031039	-0.282978
17	6	0	0.884313	2.815390	0.184841
18	6	0	2.087361	3.565979	-0.230234
19	1	0	3.898975	2.890593	-1.257441
20	7	0	1.384473	-1.316004	-0.104679
21	7	0	-1.384762	-1.435211	-0.785178
22	6	0	3.461145	-2.248909	0.237050
23	7	0	-1.595223	1.356497	-0.308709
24	6	0	-0.378762	3.386380	0.404378
25	1	0	2.190394	4.638607	-0.143840
26	6	0	-1.100746	-2.809851	-0.844158
27	6	0	1.271251	-2.704907	-0.123105
28	6	0	2.556266	-3.290165	0.120002
29	6	0	-2.690459	-1.299086	-1.162554
30	1	0	4.529997	-2.294447	0.373107
31	6	0	-2.916502	1.113827	-0.701190
32	6	0	-1.533508	2.686703	0.076640
33	1	0	-0.452726	4.446442	0.613193
34	6	0	0.101858	-3.385278	-0.491460
35	6	0	-2.274776	-3.521586	-1.295510
36	6	0	-3.254811	-2.589502	-1.501605
37	1	0	2.760070	-4.351157	0.148369
38	6	0	-3.415486	-0.087882	-1.132653
39	6	0	-3.696122	2.334994	-0.536635
40	6	0	-2.863074	3.286173	-0.038984
41	1	0	0.166182	-4.468279	-0.548703
42	1	0	-2.329944	-4.591439	-1.437163
43	1	0	-4.267858	-2.748176	-1.841146
44	1	0	-4.458255	-0.127834	-1.428135
45	1	0	-4.746271	2.424195	-0.774948
46	1	0	-3.089310	4.314293	0.203896
47	8	0	4.487570	0.527216	0.031421
48	6	0	3.274805	0.268969	-0.144507



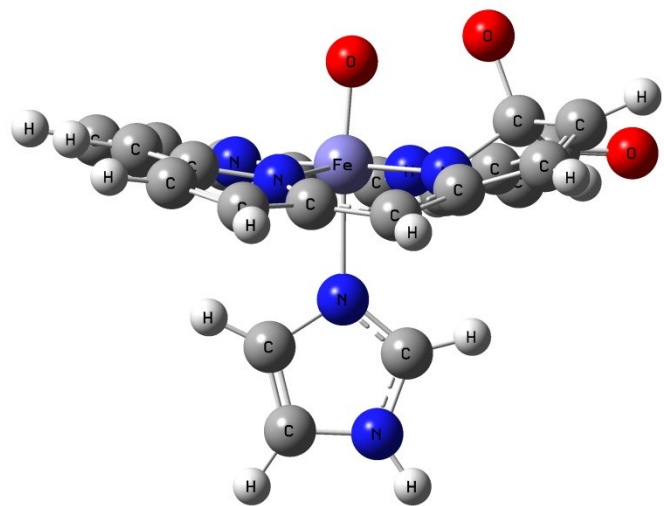
³TS1

1	8	0	1.916758	0.594810	-2.189289
2	8	0	0.497715	0.277549	-2.029704
3	7	0	-0.559969	-0.220253	1.661477
4	6	0	-1.777696	-0.399467	2.165740
5	6	0	0.338763	-0.218612	2.726208
6	6	0	-0.354308	-0.401310	3.896338
7	7	0	-1.697560	-0.514112	3.528297
8	1	0	-2.688019	-0.441452	1.595236
9	1	0	1.390857	-0.086551	2.551993
10	1	0	-0.030469	-0.460915	4.920660
11	1	0	-2.474597	-0.655444	4.151212
12	6	0	2.563170	1.106686	-0.494387
13	7	0	1.316525	1.348172	0.102568
14	6	0	3.283343	2.381331	-0.586029
15	6	0	2.608780	-1.346721	-0.011998
16	26	0	-0.082642	0.040675	-0.302242
17	6	0	1.186162	2.717649	0.227181
18	6	0	2.456406	3.351023	-0.108960
19	1	0	4.298929	2.463316	-0.938671
20	7	0	1.236698	-1.454984	-0.094828
21	7	0	-1.538844	-1.282752	-0.766305
22	6	0	3.198349	-2.628615	0.190409
23	7	0	-1.457272	1.515507	-0.333310
24	6	0	-0.014674	3.392556	0.384892
25	1	0	2.642349	4.415602	-0.050495
26	6	0	-1.428952	-2.672943	-0.716191
27	6	0	0.947991	-2.811862	-0.017591
28	6	0	2.163624	-3.545643	0.197537
29	6	0	-2.831646	-1.006246	-1.184991
30	1	0	4.260171	-2.800978	0.275668
31	6	0	-2.790940	1.422964	-0.729284
32	6	0	-1.260384	2.824198	0.086611
33	1	0	0.017658	4.463722	0.561533
34	6	0	-0.305883	-3.371549	-0.298727
35	6	0	-2.673577	-3.269227	-1.148789
36	6	0	-3.531926	-2.244531	-1.453166
37	1	0	2.227689	-4.621935	0.288787
38	6	0	-3.413161	0.262028	-1.181064
39	6	0	-3.438643	2.698068	-0.537975
40	6	0	-2.499883	3.556501	-0.017554
41	1	0	-0.378046	-4.455638	-0.268932
42	1	0	-2.854053	-4.333939	-1.215409
43	1	0	-4.552251	-2.309759	-1.807108
44	1	0	-4.451821	0.338205	-1.490140
45	1	0	-4.474613	2.903466	-0.773276
46	1	0	-2.620768	4.599875	0.241685
47	8	0	4.606876	-0.099308	-0.251805
48	6	0	3.336389	-0.129710	-0.238769



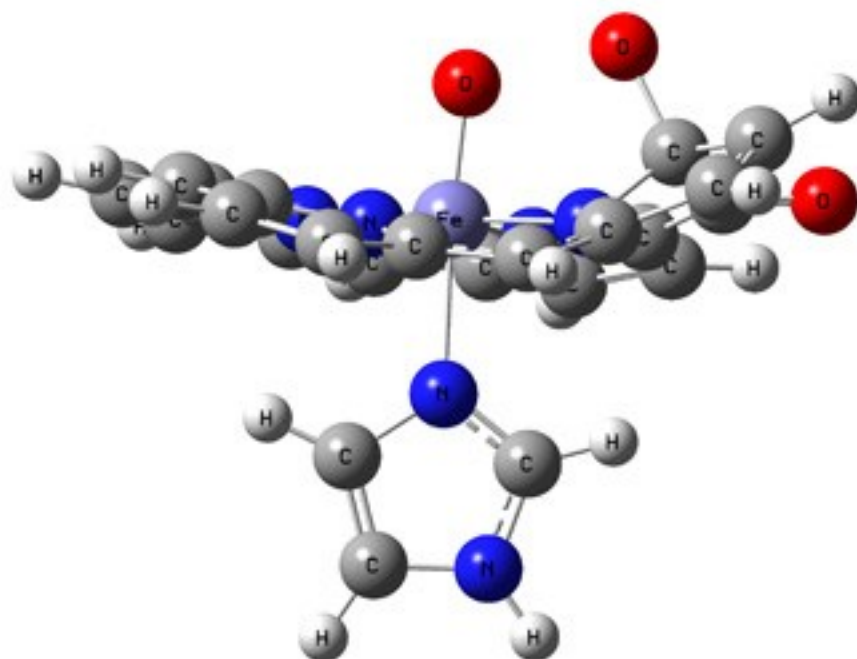
²TS2

1	8	0	2.136131	0.772023	-2.128026
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3	7	0	-0.502279	-0.213375	1.691708
4	6	0	-1.689386	-0.316686	2.261364
5	6	0	0.429268	-0.278501	2.707087
6	6	0	-0.210661	-0.423332	3.906877
7	7	0	-1.559614	-0.445252	3.604401
8	1	0	-2.636914	-0.299922	1.745462
9	1	0	1.485913	-0.221309	2.498984
10	1	0	0.154953	-0.511674	4.917855
11	1	0	-2.318786	-0.542892	4.262774
12	6	0	2.536792	0.978525	-0.808154
13	7	0	1.318483	1.264055	-0.017420
14	6	0	3.336192	2.259889	-0.706011
15	6	0	2.506739	-1.460064	-0.065200
16	26	0	-0.101898	0.042780	-0.411741
17	6	0	1.291479	2.568609	0.239750
18	6	0	2.595472	3.176098	-0.066939
19	1	0	4.329203	2.360800	-1.120904
20	7	0	1.157401	-1.504826	-0.176230
21	7	0	-1.631897	-1.208975	-0.740160
22	6	0	3.046046	-2.750874	0.182651
23	7	0	-1.381696	1.556413	-0.316118
24	6	0	0.124786	3.295419	0.541612
25	1	0	2.840087	4.213721	0.129687
26	6	0	-1.579900	-2.594837	-0.707421
27	6	0	0.808795	-2.837098	-0.065238
28	6	0	1.977549	-3.620087	0.180631
29	6	0	-2.887326	-0.880476	-1.135118
30	1	0	4.099057	-2.963002	0.301112
31	6	0	-2.705464	1.544030	-0.716812
32	6	0	-1.118909	2.813188	0.159814
33	1	0	0.212425	4.334020	0.839877
34	6	0	-0.470905	-3.332428	-0.332289
35	6	0	-2.849546	-3.132591	-1.107857
36	6	0	-3.660685	-2.068259	-1.388956
37	1	0	1.990554	-4.696732	0.296641
38	6	0	-3.396864	0.441932	-1.153452
39	6	0	-3.287464	2.859104	-0.490298
40	6	0	-2.330050	3.624983	0.081356
41	1	0	-0.590080	-4.412564	-0.299054
42	1	0	-3.082502	-4.188194	-1.171247
43	1	0	-4.690466	-2.077754	-1.722772
44	1	0	-4.431821	0.573997	-1.452650
45	1	0	-4.309717	3.125502	-0.728723
46	1	0	-2.393872	4.658070	0.399017
47	8	0	4.509773	-0.223602	-0.122494
48	6	0	3.293868	-0.245759	-0.276573



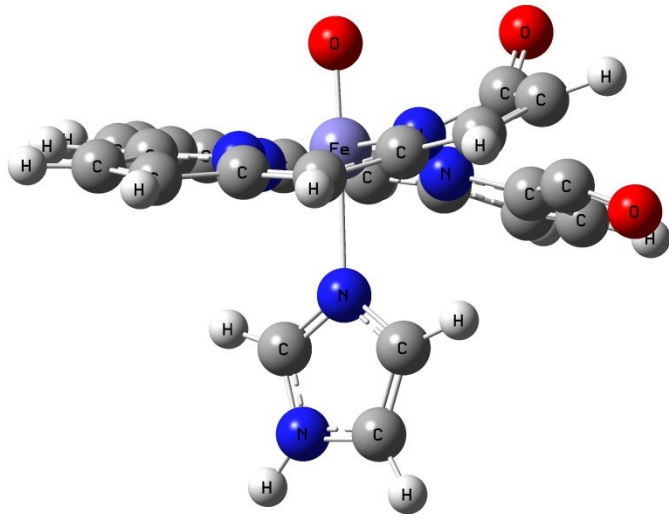
³TS2

1	8	0	2.171929	0.678414	-2.183997
2	8	0	0.320306	0.150904	-2.038835
3	7	0	-0.505080	-0.185485	1.655267
4	6	0	-1.699855	-0.350064	2.213402
5	6	0	0.437115	-0.175605	2.681079
6	6	0	-0.206160	-0.337867	3.882915
7	7	0	-1.564375	-0.446881	3.574185
8	1	0	-2.633461	-0.396379	1.682188
9	1	0	1.482203	-0.056024	2.459826
10	1	0	0.160846	-0.386677	4.893304
11	1	0	-2.314846	-0.575867	4.231609
12	6	0	2.583785	0.892411	-0.809950
13	7	0	1.363658	1.223007	-0.031822
14	6	0	3.413615	2.156383	-0.725234
15	6	0	2.489357	-1.499326	-0.018547
16	26	0	-0.101649	0.043055	-0.425678
17	6	0	1.365472	2.561856	0.213523
18	6	0	2.693540	3.111267	-0.104351
19	1	0	4.413137	2.217258	-1.126337
20	7	0	1.112041	-1.536232	-0.167072
21	7	0	-1.672499	-1.182288	-0.736886
22	6	0	2.982442	-2.806351	0.246608
23	7	0	-1.357303	1.601450	-0.312198
24	6	0	0.235710	3.320661	0.493386
25	1	0	2.974033	4.142325	0.072614
26	6	0	-1.651557	-2.575465	-0.702843
27	6	0	0.734432	-2.864911	-0.060134
28	6	0	1.891763	-3.661782	0.221459
29	6	0	-2.952590	-0.805885	-1.123292
30	1	0	4.025666	-3.044366	0.389105
31	6	0	-2.708862	1.614351	-0.678169
32	6	0	-1.053634	2.866619	0.163923
33	1	0	0.356356	4.367053	0.753093
34	6	0	-0.562369	-3.347862	-0.318153
35	6	0	-2.947058	-3.075953	-1.099136
36	6	0	-3.742500	-1.988417	-1.370681
37	1	0	1.886757	-4.736549	0.346307
38	6	0	-3.429431	0.507377	-1.111956
39	6	0	-3.250385	2.924249	-0.422662
40	6	0	-2.241139	3.687966	0.117767
41	1	0	-0.703473	-4.424424	-0.278147
42	1	0	-3.207303	-4.124116	-1.162869
43	1	0	-4.775415	-1.982156	-1.692747
44	1	0	-4.468043	0.664106	-1.389323
45	1	0	-4.274204	3.214847	-0.618059
46	1	0	-2.282134	4.723101	0.428771
47	8	0	4.547410	-0.324121	-0.077632
48	6	0	3.293393	-0.333344	-0.253673



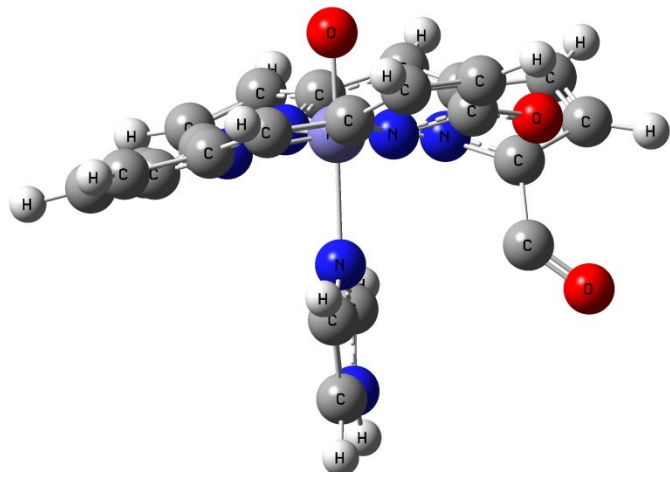
⁴TS2

O	-2.73343600	0.06987800	-2.24985900
O	0.31979300	0.11274600	-2.19259700
N	0.18155400	-0.10064400	1.65913200
C	1.22479600	0.16567400	2.42331500
C	-0.84922100	-0.43058500	2.51534500
C	-0.41688100	-0.36054300	3.81157000
N	0.90848100	0.02037000	3.73504800
H	2.20132800	0.45697600	2.06944300
H	-1.82707000	-0.69665000	2.14639700
H	-0.91290000	-0.53977000	4.75266400
H	1.53296900	0.17380400	4.51329000
C	-2.64032500	-0.71999400	-1.27946700
N	-1.36557400	-1.12828800	-0.67479600
C	-3.56847700	-1.88638400	-1.07907800
C	-2.27222800	1.66888700	0.09692500
Fe	0.23021500	0.00017400	-0.58109000
C	-1.48830800	-2.40817200	-0.32299600
C	-2.86837900	-2.88393700	-0.52682100
H	-4.60132000	-1.86074800	-1.39844800
N	-0.95341000	1.62416100	-0.25332700
N	1.88621400	1.13411100	-0.45537400
C	-2.68185600	2.98707200	0.43453100
N	1.35302100	-1.62480800	-0.37753900
C	-0.42774900	-3.24701400	0.06146400
H	-3.19690400	-3.88707400	-0.28107200
C	1.91437300	2.52200400	-0.52514700
C	-0.51451200	2.91929700	-0.15468100
C	-1.57424600	3.78349000	0.24645300
C	3.15980100	0.71694000	-0.65438400
H	-3.68333700	3.26793400	0.72990000
C	2.72395900	-1.70164700	-0.46248100
C	0.90165500	-2.87904900	-0.07304700
H	-0.65566400	-4.27801600	0.31026600
C	0.81862900	3.33333200	-0.36385200
C	3.26827600	2.96770900	-0.75005000
C	4.04225800	1.85078100	-0.83060200
H	-1.49147500	4.85488100	0.37897100
C	3.57363700	-0.63280900	-0.63690900
C	3.14823800	-3.07660000	-0.23338000
C	2.03271500	-3.79391400	0.03509900
H	0.99210900	4.40626900	-0.37488200
H	3.57139000	4.00363800	-0.83594700
H	5.10989700	1.78217300	-0.99649700
H	4.63635800	-0.83307300	-0.72837700
H	4.17678200	-3.41404800	-0.26133200
H	1.94772700	-4.84809300	0.26679300
O	-4.30117200	0.45705100	0.51096400
C	-3.19597900	0.57472200	0.07437300



²TS3

1	8	0	3.187730	0.917388	-0.625053
2	8	0	-0.180981	-0.016937	-2.142929
3	7	0	-0.279121	0.030492	1.630680
4	6	0	-0.246340	-1.036479	2.428198
5	6	0	-0.323730	1.156232	2.451955
6	6	0	-0.316361	0.756262	3.764558
7	7	0	-0.268590	-0.636081	3.735509
8	1	0	-0.203136	-2.059482	2.101885
9	1	0	-0.343339	2.147575	2.037958
10	1	0	-0.330841	1.314255	4.684190
11	1	0	-0.238587	-1.243620	4.538014
12	6	0	2.239731	1.790719	-0.852854
13	7	0	0.913918	1.694293	-0.547753
14	6	0	2.553727	3.108848	-1.417186
15	6	0	2.664036	-0.699798	0.141439
16	26	0	-0.210259	-0.010691	-0.496947
17	6	0	0.351192	2.946354	-0.884587
18	6	0	1.401683	3.826625	-1.386149
19	1	0	3.542248	3.401620	-1.732928
20	7	0	1.431497	-1.120881	-0.285983
21	7	0	-1.240942	-1.712069	-0.504792
22	6	0	3.695985	-1.640871	-0.361148
23	7	0	-1.894283	1.045015	-0.337747
24	6	0	-0.968977	3.282235	-0.784485
25	1	0	1.243948	4.852060	-1.688766
26	6	0	-0.769014	-2.912592	-0.964396
27	6	0	1.616961	-2.323377	-0.987204
28	6	0	3.048311	-2.609404	-1.054930
29	6	0	-2.605363	-1.871351	-0.263364
30	1	0	4.749354	-1.532522	-0.157158
31	6	0	-3.157221	0.535346	-0.043995
32	6	0	-2.028919	2.402187	-0.449088
33	1	0	-1.241162	4.309299	-1.007217
34	6	0	0.586953	-3.164970	-1.307698
35	6	0	-1.840794	-3.878018	-0.984023
36	6	0	-2.970922	-3.240536	-0.525903
37	1	0	3.477886	-3.472846	-1.542890
38	6	0	-3.473392	-0.821926	0.008329
39	6	0	-4.093278	1.623753	0.054301
40	6	0	-3.396545	2.781308	-0.210456
41	1	0	0.818203	-4.121639	-1.763014
42	1	0	-1.740664	-4.906395	-1.299343
43	1	0	-3.965211	-3.649088	-0.415793
44	1	0	-4.513948	-1.075050	0.190194
45	1	0	-5.146804	1.516798	0.269239
46	1	0	-3.774683	3.792723	-0.242791
47	8	0	3.730356	-0.140005	2.261921
48	6	0	2.798827	-0.041328	1.490042

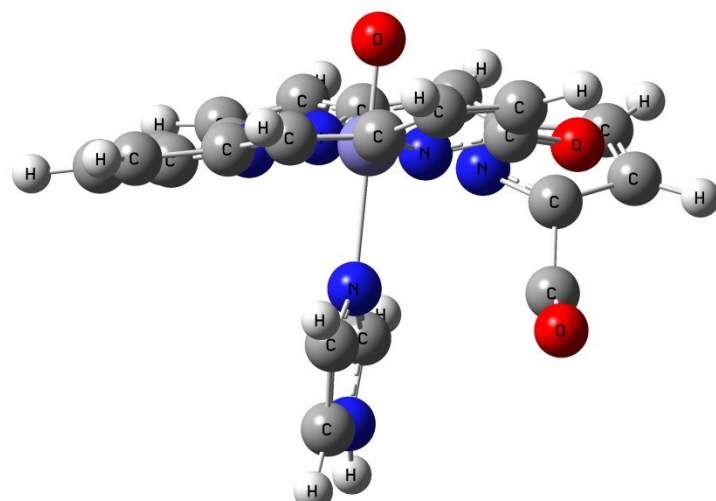


³TS3

1	8	0	-3.161691	-0.507372	-1.026601
2	8	0	0.225341	0.148011	-2.214925
3	7	0	0.245311	-0.133047	1.586429
4	6	0	0.338185	0.906933	2.407646
5	6	0	0.166526	-1.277800	2.376412
6	6	0	0.211894	-0.917002	3.700201
7	7	0	0.322354	0.475007	3.709126
8	1	0	0.414272	1.933262	2.098028
9	1	0	0.075824	-2.250655	1.928400
10	1	0	0.166824	-1.497103	4.605452
11	1	0	0.365764	1.062086	4.524757
12	6	0	-2.355835	-1.566978	-0.995077
13	7	0	-1.023438	-1.573741	-0.690642
14	6	0	-2.825731	-2.904964	-1.273481
15	6	0	-2.639615	0.838056	0.047841
16	26	0	0.223832	0.029321	-0.575102
17	6	0	-0.604024	-2.916543	-0.811875
18	6	0	-1.738017	-3.737480	-1.155831
19	1	0	-3.848875	-3.145240	-1.518728
20	7	0	-1.347119	1.239720	-0.265175
21	7	0	1.394029	1.656529	-0.421840
22	6	0	-3.563750	1.942740	-0.281935
23	7	0	1.825753	-1.173599	-0.407483
24	6	0	0.698064	-3.357929	-0.679821
25	1	0	-1.696914	-4.808468	-1.304551
26	6	0	1.003428	2.946901	-0.742400
27	6	0	-1.424233	2.542014	-0.772216
28	6	0	-2.815755	2.957114	-0.796603
29	6	0	2.774553	1.680700	-0.245780
30	1	0	-4.627277	1.900744	-0.103883
31	6	0	3.132246	-0.776216	-0.157164
32	6	0	1.829953	-2.559042	-0.465388
33	1	0	0.866149	-4.428284	-0.770585
34	6	0	-0.325867	3.343704	-0.992343
35	6	0	2.152385	3.809262	-0.725539
36	6	0	3.245468	3.031957	-0.397857
37	1	0	-3.158428	3.929084	-1.127106
38	6	0	3.570426	0.549547	-0.065986
39	6	0	3.971473	-1.941725	-0.053861
40	6	0	3.166463	-3.042520	-0.251967
41	1	0	-0.492571	4.369357	-1.307681
42	1	0	2.129421	4.871654	-0.929382
43	1	0	4.278331	3.340670	-0.305586
44	1	0	4.634518	0.708165	0.086857
45	1	0	5.037199	-1.919252	0.130573
46	1	0	3.452170	-4.086144	-0.249775
47	8	0	-3.799191	0.147911	2.093575
48	6	0	-2.876561	0.034818	1.300787

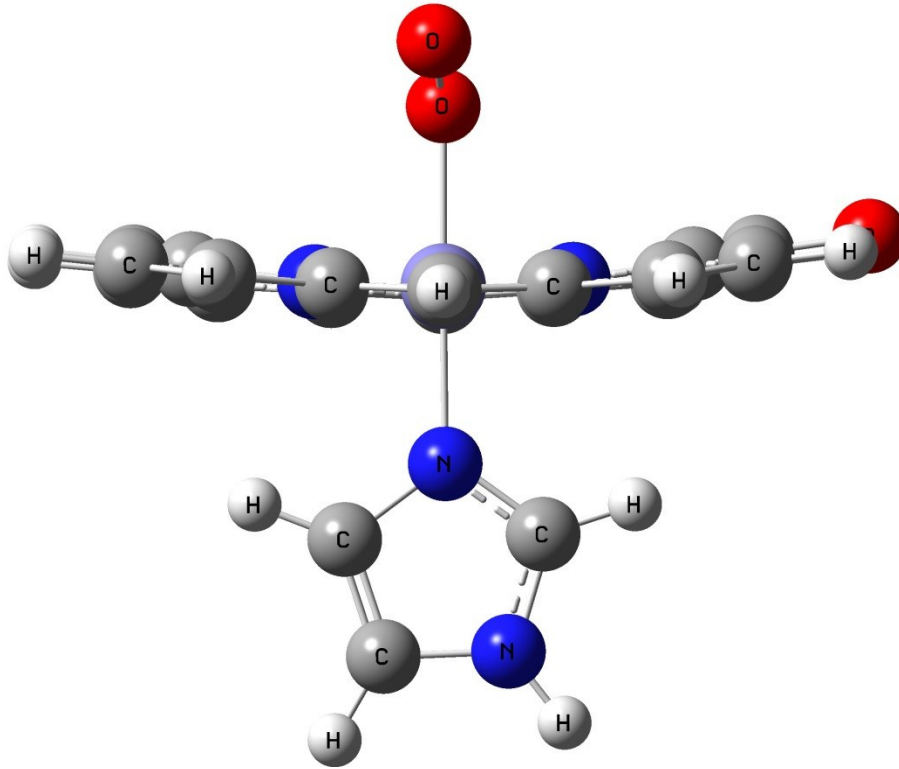
⁴TS3

O	-3.28263800	-0.13888400	-0.74709800
O	0.10559700	0.11336300	-2.15372100
N	0.27154900	-0.12822800	1.64974100
C	0.46723100	0.88830700	2.47061500
C	0.18749800	-1.25752400	2.43711800
C	0.33439900	-0.91257300	3.75232900
N	0.51502600	0.45835500	3.75538800
H	0.57880300	1.91889300	2.17153300
H	0.02107500	-2.22987800	2.00095600
H	0.32333300	-1.49380300	4.66101400
H	0.64868800	1.04195800	4.56821600
C	-2.58454400	-1.19558000	-0.90530400
N	-1.28230300	-1.39521600	-0.57422600
C	-3.18586000	-2.42750600	-1.43498400
C	-2.45177900	1.20991700	0.24493700
Fe	0.17419300	0.02439800	-0.53807300
C	-1.01493800	-2.73002800	-0.88738300
C	-2.22740600	-3.37597300	-1.36942600
H	-4.21718500	-2.50097400	-1.75090500
N	-1.17525900	1.43049300	-0.17979700
N	1.53368800	1.47765500	-0.49226100
C	-3.28403000	2.39630700	-0.08992000
N	1.60095900	-1.36433100	-0.44813100
C	0.20212000	-3.34385400	-0.82523600
H	-2.29315700	-4.42213300	-1.64266700
C	1.31126900	2.76708300	-0.85399600
C	-1.13884000	2.68679000	-0.76676900
C	-2.47596600	3.26272900	-0.73598900
C	2.89899100	1.33748000	-0.32568400
H	-4.33543000	2.48451000	0.14729400
C	2.94346000	-1.14104400	-0.21227700
C	1.44335000	-2.70721100	-0.55200200
H	0.23659800	-4.40750400	-1.04361500
C	0.02342900	3.32312900	-1.10137800
C	2.55246300	3.48975300	-0.88761500
C	3.53813400	2.60485400	-0.53329600
H	-2.73862800	4.23214900	-1.14143700
C	3.53853300	0.11840500	-0.14303400
C	3.63501000	-2.39365600	-0.15302300
C	2.69997700	-3.37305800	-0.37632400
H	-0.02434800	4.33939100	-1.47883900
H	2.65315800	4.53835100	-1.13782600
H	4.60341800	2.78424200	-0.45809900
H	4.61693900	0.14239000	-0.00812200
H	4.69889000	-2.50861300	0.01297400
H	2.84809400	-4.44472700	-0.41825800
O	-3.18053800	-0.30648300	2.08214500
C	-2.66821100	0.63930800	1.59565200



21b

Fe	0.13907400	0.00614700	-0.35375300
N	-1.34050600	-1.36095300	-0.25652100
N	1.51772200	-1.45456100	-0.28015300
N	-1.24541700	1.48799800	-0.36707200
N	1.61361800	1.39006200	-0.39807700
C	-2.68065700	-1.15668900	-0.30423100
C	2.88102600	-1.31609800	-0.35933200
C	-1.18499800	-2.73806800	-0.18431100
C	1.28793500	-2.80567500	-0.20545000
C	-2.59480100	1.37201800	-0.39075800
C	2.96509400	1.15576400	-0.46832300
C	-0.99788000	2.85412700	-0.38720100
C	1.47479700	2.75531500	-0.42564200
C	-3.40387800	-2.38764200	-0.25417500
C	3.52261600	-2.60501500	-0.32219500
C	-2.46537600	-3.38059800	-0.17612200
C	2.52905300	-3.53249900	-0.22236700
C	-3.23580400	2.64941900	-0.41903400
C	3.69059400	2.39792700	-0.53267600
C	-2.23394700	3.58023500	-0.41427500
C	2.76072100	3.39467400	-0.50218800
H	-4.48131800	-2.45735200	-0.28263000
H	4.59235800	-2.76374900	-0.37212800
H	-2.61899400	-4.45141400	-0.12896600
H	2.61414400	-4.61070500	-0.17485300
H	-4.30660000	2.78811300	-0.44356500
H	4.76819100	2.48130500	-0.59529400
H	-2.31563300	4.65973500	-0.43677400
H	2.91753100	4.46531400	-0.53702800
C	3.55980900	-0.10374200	-0.45253800
C	0.25896800	3.43401400	-0.40611900
C	0.03140400	-3.39947900	-0.14649300
H	4.64320400	-0.14366700	-0.51443900
H	0.30082700	4.51937700	-0.43005700
H	0.00114300	-4.48414500	-0.09287100
H	2.21970400	0.47087500	2.17176400
C	1.23371600	0.31148000	2.57788600
C	0.83147200	0.29103900	3.88479300
C	-0.89742700	-0.07324600	2.55006500
N	-0.52733700	0.04645500	3.84813800
H	1.36934600	0.42351700	4.81033700
H	-1.90854200	-0.27084200	2.23057200
H	-1.14487100	-0.02972800	4.64335000
N	0.14765600	0.08349400	1.75594800
C	-3.35948200	0.13114700	-0.37198700
O	-4.60282600	0.17310500	-0.38668600
O	0.12303200	0.03622800	-2.19470500
O	0.07175500	-1.09362900	-2.81481500



21c

Fe	-0.15823400	0.00436800	-0.39935200
N	1.26423800	1.46555400	-0.41628400
N	-1.60391900	1.42458100	-0.35560000
N	1.29276200	-1.39210000	-0.30582200
N	-1.56468100	-1.41957500	-0.27147600
C	2.62282500	1.31352300	-0.35635800
C	-2.95462500	1.22102000	-0.26553100
C	1.04808300	2.82330300	-0.52720900
C	-1.42834000	2.79486000	-0.46526300
C	2.64998500	-1.19764900	-0.25819400
C	-2.92140800	-1.24230600	-0.20115800
C	1.11525900	-2.76079900	-0.32295700
C	-1.35839600	-2.79131900	-0.29543200
C	3.27919500	2.57192700	-0.43190400
C	-3.65371000	2.48651300	-0.30337300
C	2.29238700	3.52300800	-0.54447400
C	-2.70808900	3.45777300	-0.43399300
C	3.33732500	-2.43853300	-0.23930400
C	-3.59092500	-2.52441500	-0.17231800
C	2.37585900	-3.42375000	-0.28208300
C	-2.62337200	-3.47970100	-0.23666000
H	4.35305100	2.69042300	-0.40421200
H	-4.73078600	2.59495300	-0.24692400
H	2.39653900	4.59925900	-0.62738100
H	-2.84645900	4.53097900	-0.50173300
H	4.41404100	-2.52560200	-0.20616800
H	-4.66603800	-2.65349100	-0.12140500
H	2.51051300	-4.49976200	-0.29140500
H	-2.73726000	-4.55786800	-0.24423200
C	-3.58339400	-0.01833400	-0.17721100
C	-0.12955000	-3.41017200	-0.32334400
C	-0.21210500	3.43749500	-0.55984700
H	-4.66817900	-0.03189000	-0.12049200
H	-0.11649500	-4.49759100	-0.33284000
H	-0.22690900	4.52182500	-0.64292300
H	-0.33213100	2.18966500	2.05663200
C	-0.18483500	1.21012300	2.48330800
C	-0.06340100	0.83920800	3.79407100
C	0.09451500	-0.93731700	2.47749400
N	0.11226300	-0.53444300	3.77366400
H	-0.07990900	1.40332400	4.71358300
H	0.22075100	-1.96007100	2.15710500
H	0.25360000	-1.13408100	4.57197100
N	-0.08532500	0.09576600	1.67745500
C	3.36376900	0.06921000	-0.23681800
O	4.61089200	0.08597400	-0.13564000
O	-0.16530200	0.02768800	-2.13228000
O	-0.21308100	-1.03918100	-2.83441000

