Electronic Supplementary Information for

Which is the real oxidant in the competitive ligand self-hydroxylation and substrate oxidations, a biomimetic iron(II)-hydroperoxo species or an oxo-iron(IV)-hydroxy one?

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Scheme S1 Possible reaction pathways of (a) sulfoxidation of thioanisole and (b) hydroxylation of cyclohexane mediated by Fe^{II}-OOH species (**1**).

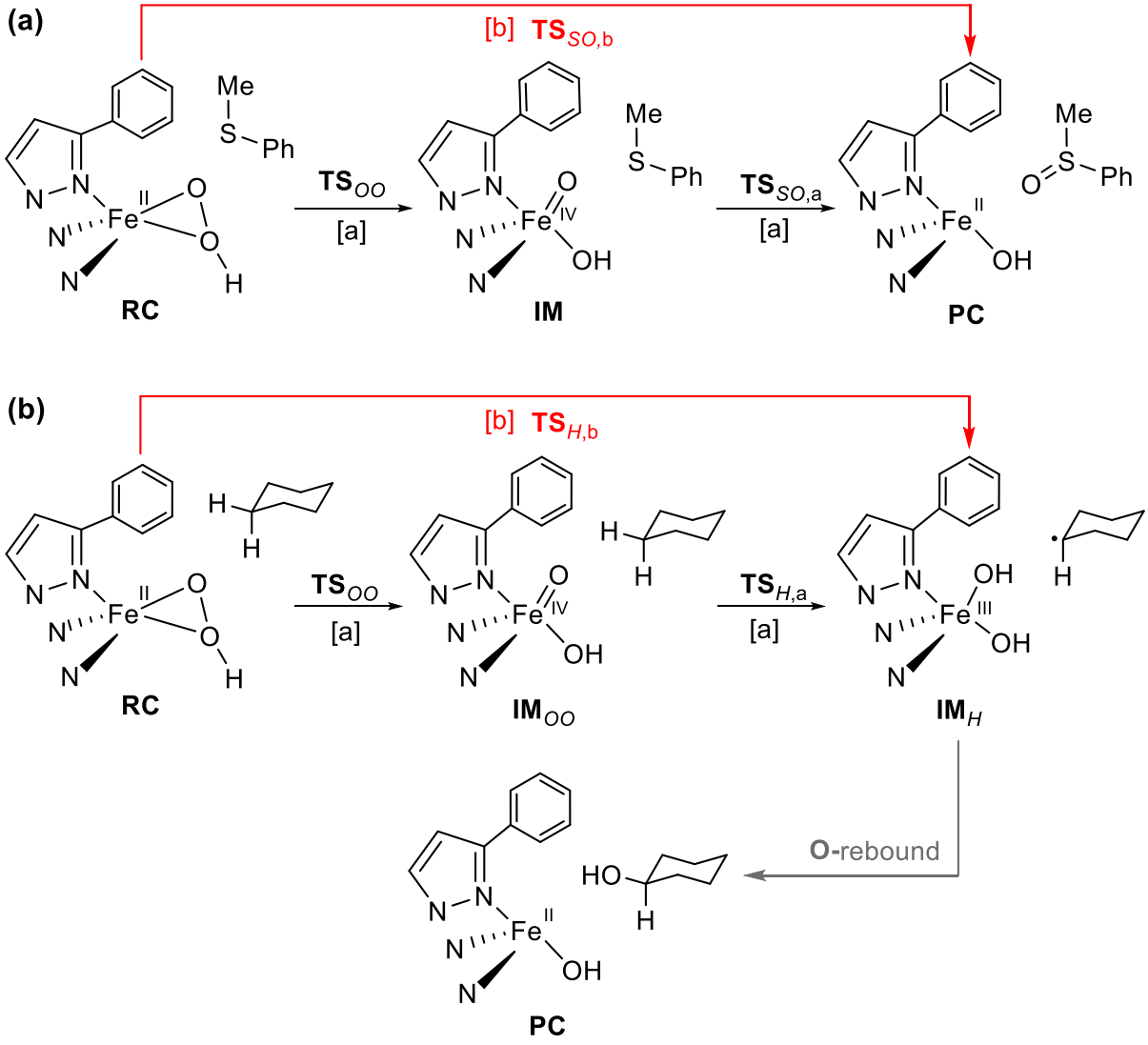

Table S1 Relative energies (in kcal/mol) of the ligand self-hydroxylation of **1** in the absence of any external substrate calculated using UB3LYP functional in solvent

	ΔE(B1)	$\Delta\Delta$**BS**	ΔE(B2)	ΔZ_0(B1)	ΔE(Thermal)[a]	$-T\Delta S$[a]	ΔDisp[b]	ΔG(B2)[c]
^{5}**1**	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
^{3}**1**	17.82	+1.16	**18.98**	+0.50	-0.37	+0.99	-1.30	**18.80**
^{5}**TS**$_{12}$	18.97	+0.07	**19.04**	-1.24	-0.24	+0.35	-1.09	**16.83**
^{3}**TS**$_{12}$	25.84	+0.78	**26.62**	-0.50	-0.51	+1.36	-1.40	**25.57**
^{5}**2**	-16.17	-0.53	**-16.70**	+0.44	-0.40	+0.56	-1.09	**-17.20**
^{3}**2**	-3.37	-0.24	**-3.61**	+0.69	-0.55	+1.52	-2.57	**-4.51**
^{5}**TS**$_{23}$	1.16	-1.83	**-0.66**	-0.88	-0.74	+2.42	-2.88	**-2.75**
^{3}**TS**$_{23}$	4.89	-1.52	**3.36**	-0.92	-0.69	+2.64	-3.17	**1.23**
^{5}**3**	-8.70	-5.27	**-13.97**	-0.37	-0.70	+2.47	-2.82	**-15.39**
^{3}**3**	-8.85	-5.45	**-14.30**	-0.36	-0.72	+2.81	-2.83	**-15.39**
^{5}**TS**$_{34}$	5.89	-10.62	**-4.73**	-3.93	-0.19	+0.65	-0.33	**-8.52**
^{3}**TS**$_{34}$	19.66	-10.82	**8.84**	-3.15	-0.75	+2.43	-1.75	**5.62**
^{5}**TS**$_{N\text{-}proton}$	25.13	-7.81	**17.32**	-4.88	+0.13	+0.69	-3.95	**9.05**
^{3}**TS**$_{N\text{-}proton}$	53.68	-7.24	**46.44**	-4.47	-0.93	+3.48	-4.45	**40.08**
^{5}**4**	-37.90	-6.85	**-44.75**	-1.07	+0.18	-0.30	+0.17	**-45.78**
^{3}**4**	-22.79	-6.73	**-29.52**	-0.86	-0.51	+2.07	-1.92	**-30.74**
^{5}**TS**$_{4'5}$	-29.59	-7.44	**-37.03**	-4.25	-1.09	+3.40	-1.35	**-40.31**
^{3}**TS**$_{4'5}$	-12.92	-6.60	**-19.52**	-3.45	-1.45	+4.61	-3.02	**-22.81**
^{5}**5**	-66.69	-9.02	**-75.72**	+0.73	-0.41	+1.44	-1.81	**-75.76**
^{3}**5**	-53.83	-8.28	**-62.11**	+1.59	-0.77	+3.00	-3.72	**-62.02**

Note: B1 represents a small basis set of LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H); B2 represents a larger basis set of LACV3P(Fe), 6-311+G**(others). [a] Temperature is 298.15 K. [b] Grimme's D3-BJ corrections on the optimized structures. [c] Sum of the previous five columns.

Table S2 Mulliken spin densities of various species involved the ligand self-hydroxylation of **1** in the absence of any external substrate calculated at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent

	Fe	**O_p**	**O_dH**	**H**	**C**	**$Tp^{Ph,Me}$**		
^{5}**1**	3.78	0.12	0.01	0.00	0.00	0.10		
^{3}**1**	2.02	-0.01	-0.03	0.00	0.00	0.01		
^{5}**TS**$_{12}$	3.51	0.32	0.07	0.00	0.00	0.11		
^{3}**TS**$_{12}$	2.22	0.04	-0.28	0.00	0.00	0.02		
^{5}**2**	3.15	0.62	0.10	0.00	0.00	0.13		
^{3}**2**	1.40	0.61	0.03	0.00	0.00	-0.03		
^{5}**TS**$_{23}$	2.90	0.47	0.05	0.03	-0.15	0.69		
^{3}**TS**$_{23}$	2.79	-0.46	0.03	-0.03	0.15	-0.48		
^{5}**3**	2.85	0.07	0.05	0.06	-0.08	1.05		
^{3}**3**	2.76	0.05	0.05	-0.05	0.06	-0.87		
^{5}**TS**$_{34}$	3.78	0.03	0.14	0.01	0.00	0.03		
^{3}**TS**$_{34}$	2.18	0.00	0.00	-0.03	0.01	-0.15		
^{5}**TS**$_{N\text{-}proton}$	3.73	0.04	0.13	0.00	0.00	0.09		
^{3}**TS**$_{N\text{-}proton}$	1.98	-0.02	-0.01	0.00	0.00	0.04		
^{5}**4**	3.79	-0.01	0.14	0.00	-0.01	0.09		
^{3}**4**	2.50	0.06	0.04	-0.04	-0.23	-0.33		
	Fe	**O_p**	**O_dH**	**H**	**C**	**$Tp^{Ph,Me}$**	**H(H_2O)**	**OH(H_2O)**
^{5}**TS**$_{4'5}$	3.80	0.02	0.05	0.00	0.00	0.12	0.00	0.01
^{3}**TS**$_{4'5}$	2.00	-0.03	0.01	0.00	0.00	0.01	0.00	0.00
^{5}**5**	3.78	0.06	0.01	0.00	-0.01	0.16	0.00	0.00
^{3}**5**	1.97	0.03	-0.02	0.00	-0.01	0.04	0.00	0.00

Table S3 APT charges of various species involved the ligand self-hydroxylation of **1** in the absence of any external substrate calculated at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent

	Fe	**O_p**	**O_dH**	**H**	**C**	**$Tp^{Ph,Me}$**		
^{5}**1**	1.74	-0.65	-0.22	0.06	-0.08	-0.85		
^{3}**1**	1.24	-0.43	-0.17	0.04	-0.06	-0.62		
^{5}**TS**$_{12}$	0.99	0.16	-0.12	0.06	-0.11	-0.98		
^{3}**TS**$_{12}$	0.71	0.30	-0.30	0.07	-0.09	-0.68		
^{5}**2**	2.07	-0.70	-0.56	0.07	-0.06	-0.82		
^{3}**2**	1.91	-0.76	-0.59	0.09	-0.07	-0.59		
^{5}**TS**$_{23}$	1.67	-0.20	-0.61	0.10	-0.23	-0.73		
^{3}**TS**$_{23}$	2.03	-0.54	-0.65	0.11	-0.23	-0.72		
^{5}**3**	2.05	-0.90	-0.64	-0.06	0.50	-0.94		
^{3}**3**	2.10	-0.92	-0.64	-0.06	0.48	-0.95		
^{5}**TS**$_{34}$	1.56	-0.79	-0.90	0.23	0.56	-0.66		
^{3}**TS**$_{34}$	1.10	-0.09	-0.92	0.58	0.00	-0.66		
^{5}**TS**$_{N\text{-}proton}$	1.72	-1.13	-0.83	0.69	0.25	-0.70		
^{3}**TS**$_{N\text{-}proton}$	1.66	-1.00	-0.79	0.66	0.20	-0.73		
^{5}**4**	1.74	-0.87	-0.86	0.10	0.85	-0.96		
^{3}**4**	1.29	1.02	-0.78	0.05	-0.75	-0.84		
	Fe	**O_p**	**O_dH**	**H**	**C**	**$Tp^{Ph,Me}$**	**H(H_2O)**	**OH(H_2O)**
^{5}**TS**$_{4'5}$	1.77	-1.17	-0.84	0.81	0.85	-1.30	0.77	-0.90
^{3}**TS**$_{4'5}$	1.35	-1.06	-0.77	0.76	0.82	-0.98	0.73	-0.85
^{5}**5**	1.79	-1.38	-0.53	0.62	0.71	-1.16	0.54	-0.60
^{3}**5**	1.41	-1.32	-0.46	0.62	0.68	-0.87	0.54	-0.59

Table S4 Relative energies (in kcal/mol) of sulfide oxidation by **1** through both routes a and b calculated using UB3LYP functional in solvent

	ΔE(B1)	$\Delta\Delta$BS	ΔE(B2)	ΔZ_0(B1)	ΔE(Thermal)[a]	$-T\Delta S$[a]	ΔDisp[b]	ΔG(B2)[c]
^{5}**RC**	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
^{3}**RC**	18.22	+2.01	**20.23**	+0.90	-0.54	+3.75	-1.86	**22.48**
^{5}**TS**$_{OO}$	13.94	-0.46	**13.48**	-1.02	-0.35	+2.49	-1.11	**13.49**
^{3}**TS**$_{OO}$	25.13	+1.84	**26.97**	+0.05	-0.77	+4.31	-2.09	**28.48**
^{5}**IM**	-16.32	+0.94	**-15.38**	+0.78	-0.62	+3.72	-3.24	**-14.76**
^{3}**IM**	-1.43	+0.53	**-0.90**	-0.03	-0.38	+3.61	-4.55	**-2.26**
^{5}**TS**$_{SO,a}$	-4.05	+1.22	**-2.83**	-1.01	-0.70	+5.88	-10.02	**-8.68**
^{3}**TS**$_{SO,a}$	2.80	+2.41	**5.21**	+0.16	-1.27	8.91	-12.27	**0.74**
^{5}**TS**$_{SO,b}$	19.52	+0.63	**20.15**	-0.49	-0.85	+6.50	-10.50	**14.82**
^{3}**TS**$_{SO,b}$	36.52	+1.15	**37.68**	+0.05	-1.21	+8.67	-12.99	**32.20**
^{5}**PC**	-36.60	+3.00	**-33.60**	+0.23	-0.63	+6.36	-10.07	**-37.70**
^{3}**PC**	-12.80	+3.22	**-9.58**	+0.88	-1.02	+8.05	-12.79	**-14.47**

Note: B1 represents a small basis set of LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H); B2 represents a larger basis set of LACV3P(Fe), 6-311+G**(others). [a] Temperature is 298.15 K. [b] Grimme's D3-BJ corrections on the optimized structures. [c] Sum of the previous five columns.

Table S5 Mulliken spin densities and APT charges of various species involved in the sulfoxidation by **1** through both routes a and b calculated at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent

	Spin densities						APT charges					
	Fe	**O_p**	**O_dH**	**$Tp^{Ph,Me}$**	**S**	**Sub-S**	**Fe**	**O_p**	**O_dH**	**$Tp^{Ph,Me}$**	**S**	**Sub-S**
^{5}**RC**	3.79	0.10	0.00	0.10	0.00	0.00	1.84	-0.68	-0.25	-0.94	-0.25	0.28
^{3}**RC**	2.02	-0.01	-0.03	0.01	0.00	0.00	1.31	-0.48	-0.18	-0.66	-0.25	0.26
^{5}**TS**$_{OO}$	3.95	0.22	-0.36	0.19	0.00	0.00	1.35	-0.13	-0.30	-0.95	-0.25	0.28
^{3}**TS**$_{OO}$	2.22	0.04	-0.28	0.02	0.00	0.00	0.68	0.37	-0.43	-0.65	-0.24	0.26
^{5}**IM**	3.16	0.61	0.11	0.12	0.00	0.00	2.09	-0.70	-0.52	-0.86	-0.22	0.22
^{3}**IM**	2.77	-0.83	0.03	0.05	-0.01	0.00	2.05	-0.51	-0.57	-0.97	-0.22	0.20
^{5}**TS**$_{SO,a}$	3.99	0.07	0.23	0.14	-0.37	-0.07	1.92	0.10	-0.63	-1.19	-0.31	0.12
^{3}**TS**$_{SO,a}$	2.46	-0.06	-0.03	0.01	-0.30	-0.08	0.91	0.78	-0.20	-0.83	-0.54	-0.11
^{5}**TS**$_{SO,b}$	3.79	0.10	0.04	0.08	-0.01	0.00	1.66	0.51	-1.15	-0.87	-0.22	0.07
^{3}**TS**$_{SO,b}$	2.06	-0.07	0.01	0.00	0.00	0.00	1.25	0.69	-1.19	-0.57	-0.21	0.04
^{5}**PC**	3.80	-0.01	0.13	0.07	0.01	0.00	1.76	-1.01	-0.84	-0.90	1.13	-0.14
^{3}**PC**	2.04	-0.02	-0.02	-0.01	0.00	0.00	1.38	-0.98	-0.75	-0.69	1.14	-0.10

Table S6 Relative energies (in kcal/mol) of cyclohexane hydroxylation by **1** through both routes a and b calculated using UB3LYP functional in solvent

	Δ***E*****(**B1**)**	ΔΔ**BS**	Δ***E*****(**B2**)**	Δ**Z**$_0$**(B1)**	Δ***E*****(Thermal)**[a]	-***T*****Δ*****S***[a]	ΔDisp[b]	Δ***G*****(**B2**)**[c]
^{5}**RC**	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
^{3}**RC**	17.56	+1.42	**19.06**	+0.78	-1.07	+4.03	-1.69	**21.12**
^{5}**TS**$_{OO}$	14.05	-0.65	**13.40**	-1.16	-0.26	+0.44	-0.65	**11.782**
^{3}**TS**$_{OO}$	24.62	+1.34	**25.96**	-0.21	-0.65	+1.85	-1.95	**25.00**
^{5}**IM**$_{OO}$	-16.33	-0.37	**-16.70**	+0.66	-0.49	+0.34	-1.57	**-17.76**
^{3}**IM**$_{OO}$	-3.66	+0.30	**-3.36**	+0.98	-0.70	+2.92	-4.55	**-4.72**
^{5}**TS**$_{H,a}$	7.56	-2.09	**5.47**	-3.43	-1.05	+5.51	-7.13	**-0.63**
^{3}**TS**$_{H,a}$	9.74	-1.82	**7.92**	-3.66	-0.95	+5.36	-7.36	**1.32**
^{5}**TS**$_{H,b}$	44.15	-0.42	**43.73**	-1.93	-2.10	+8.91	-9.07	**39.54**
^{3}**TS**$_{H,b}$	30.79	-2.04	**28.75**	-2.73	-1.81	+7.94	-6.54	**25.61**
^{5}**IM**$_H$	-3.15	-4.16	**-7.31**	-1.56	-0.22	+2.26	-4.87	**-11.69**
^{3}**IM**$_H$	-3.04	-4.19	**-7.23**	-1.62	-0.18	+2.14	-4.81	**-11.69**
^{5}**PC**	-55.18	-6.34	**-61.52**	+0.92	-0.57	+4.44	-8.22	**-64.95**
^{3}**PC**	-36.96	-5.84	**-42.80**	+2.28	-1.22	+6.96	-0.91	**-45.68**

Note: B1 represents a small basis set of LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H); B2 represents a larger basis set of LACV3P(Fe), 6-311+G**(others). [a] Temperature is 298.15 K. [b] Grimme's D3-BJ corrections on the optimized structures. [c] Sum of the previous five columns.

Table S7 Mulliken spin densities and APT charges of cyclohexane hydroxylation by **1** through both routes a and b calculated at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent

	Spin densities						APT charges					
	Fe	**O_p**	**O_dH**	**$Tp^{Ph,Me}$**	**H**	**Sub-H**	**Fe**	**O_p**	**O_dH**	**$Tp^{Ph,Me}$**	**H**	**Sub-H**
^{5}**RC**	3.79	0.11	0.01	0.10	0.00	0.00	1.79	-0.68	-0.22	-0.91	-0.03	0.04
^{3}**RC**	2.03	-0.01	-0.03	0.01	0.00	0.00	1.28	-0.47	-0.16	-0.67	-0.04	0.06
^{5}**TS**$_{OO}$	3.94	0.23	-0.36	0.18	0.00	0.00	1.34	-0.09	-0.31	-0.97	-0.02	0.04
^{3}**TS**$_{OO}$	2.23	0.03	-0.28	0.02	0.00	0.00	0.71	0.36	-0.41	-0.68	-0.04	0.06
^{5}**IM1**	3.16	0.61	0.10	0.13	0.00	0.00	2.07	-0.71	-0.55	-0.82	-0.03	0.05
^{3}**IM1**	1.40	0.61	0.02	-0.03	0.00	0.00	1.91	-0.76	-0.58	-0.58	-0.04	0.06
^{5}**TS**$_{H,a}$	2.90	0.46	0.04	0.09	-0.04	0.55	1.76	-0.19	-0.53	-0.91	-0.49	0.36
^{3}**TS**$_{H,a}$	2.84	-0.49	0.05	0.07	0.04	-0.51	2.21	-0.53	-0.59	-1.03	-0.42	0.36
^{5}**TS**$_{H,b}$	3.79	0.07	0.06	0.09	0.00	-0.02	1.70	0.44	-0.98	-0.93	-0.51	0.27
^{3}**TS**$_{H,b}$	2.05	0.01	-0.07	0.00	0.00	0.02	1.06	0.72	-0.88	-0.63	-0.53	0.26
^{5}**IM2**	2.86	0.05	0.04	0.08	0.01	0.96	2.04	-0.94	-0.57	-0.86	0.33	0.01
^{3}**IM2**	2.84	0.01	0.04	0.08	-0.02	-0.96	2.06	-0.96	-0.59	-0.85	0.34	0.00
^{5}**PC**	3.80	-0.01	0.13	0.07	0.00	0.00	1.72	-0.82	-0.83	-0.90	0.29	0.54
^{3}**PC**	2.00	-0.02	0.03	-0.01	0.00	0.00	1.35	-0.77	-0.77	-0.66	0.30	0.55

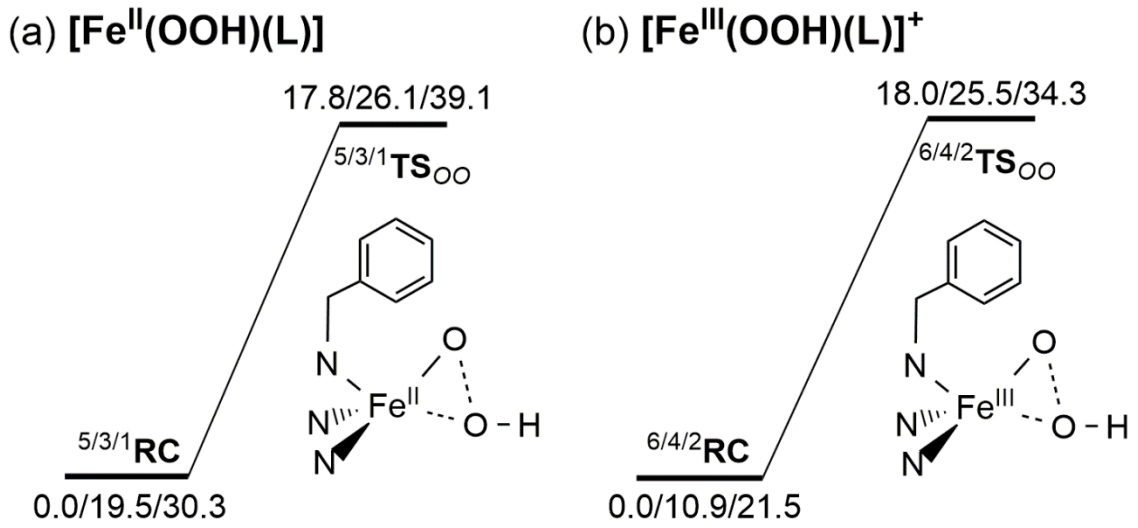

Figure S1 Energy profiles for the O−O bond cleavage of (a) Fe^{II}-OOH and (b) Fe^{III}-OOH species with the same ligand framework.

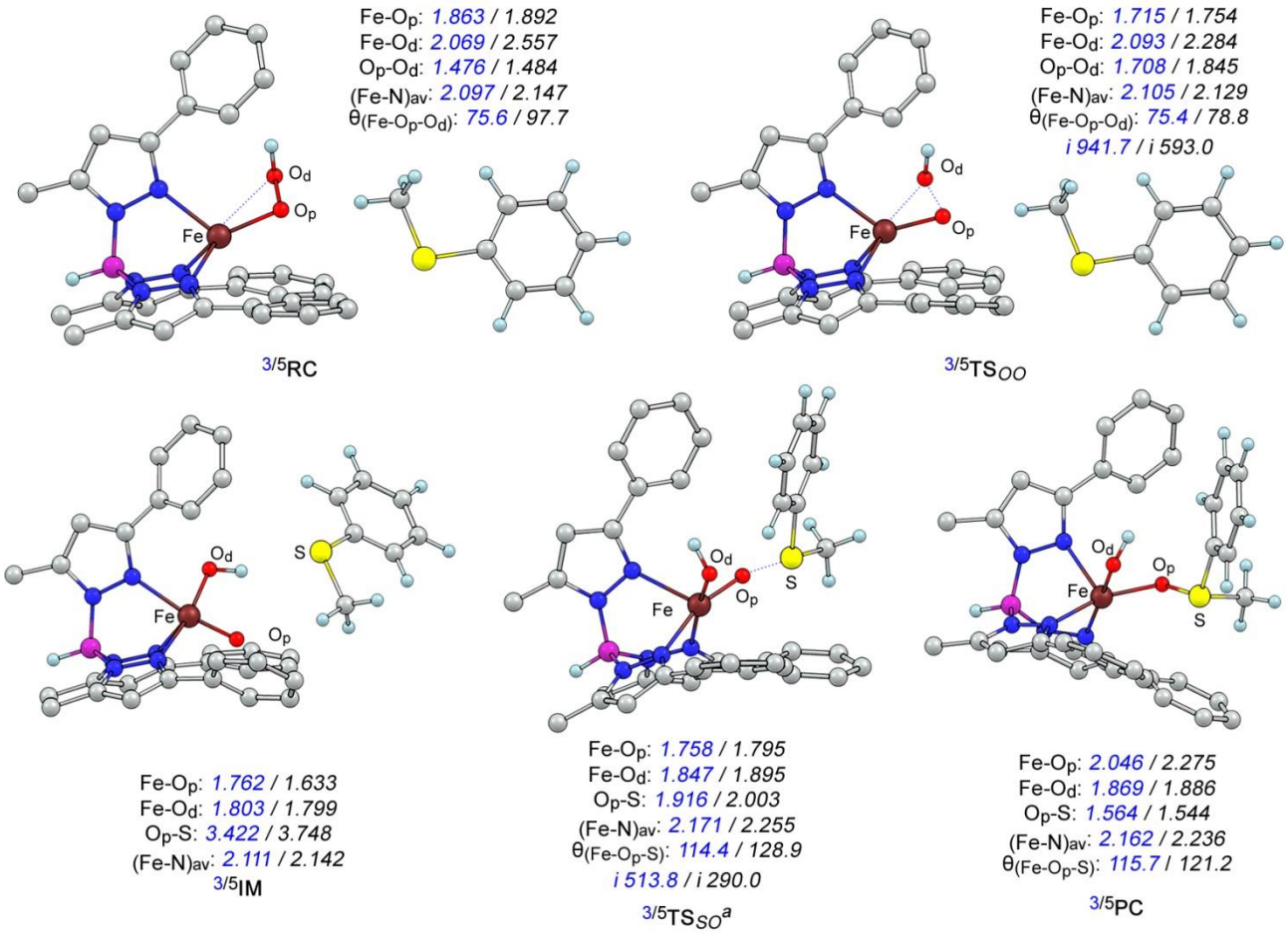

Figure S2 Key geometric information for sulfoxidation by **1** through the preferred route a as shown in Scheme S1. Bond length is in Å, bond angle is in ° and imaginary frequency is in cm^{-1} unit. All hydrogen atoms in the ligand except that attached to B and O atoms have been omitted for clarity. Calculations were done at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent.

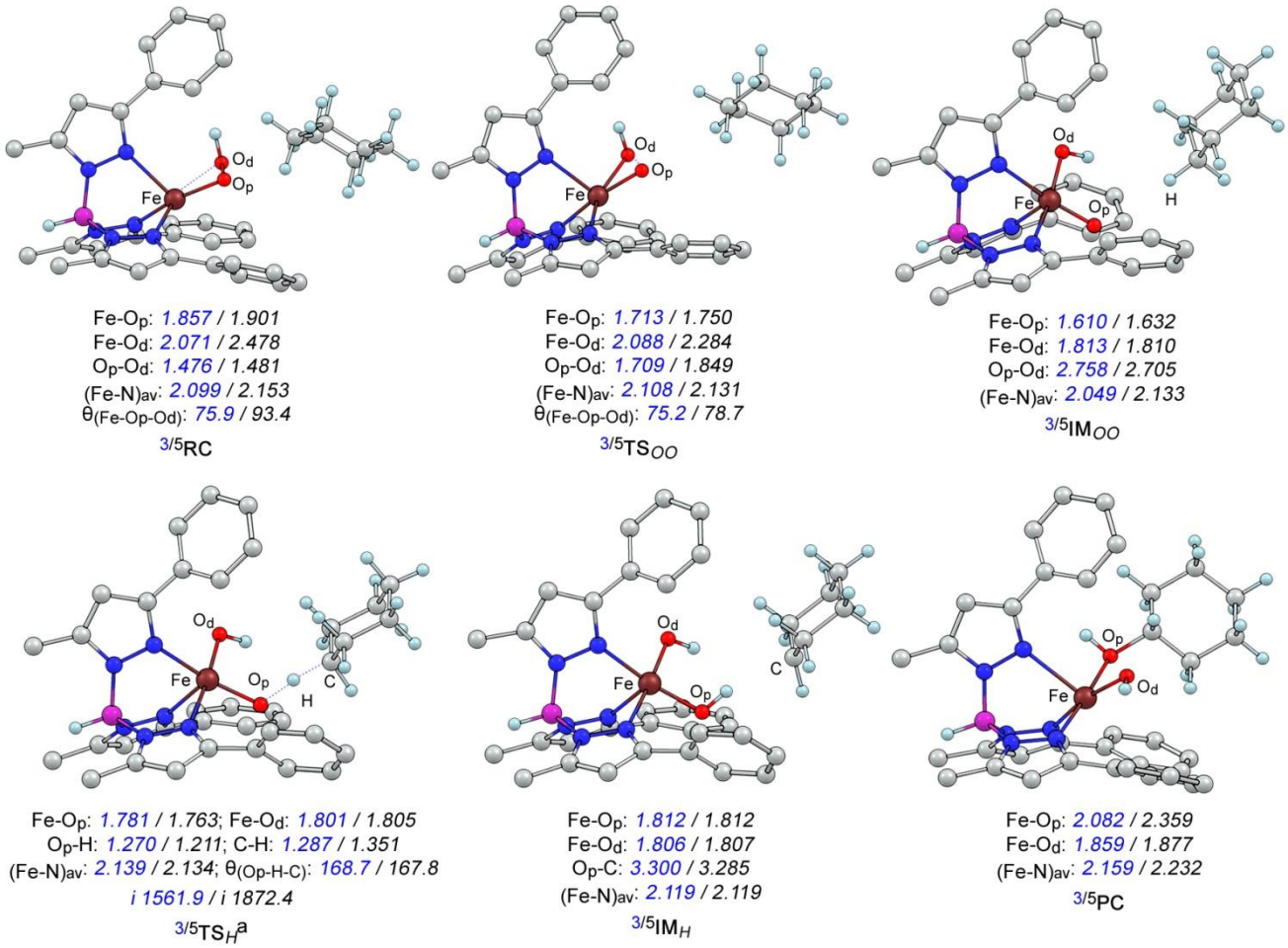

Figure S3 Key geometric information for cyclohexane oxidation by **1** through the preferred route a as shown in Scheme S1. Bond length is in Å, bond angle is in ° and imaginary frequency is in cm^{-1} unit. All hydrogen atoms in the ligand except that attached to B and O atoms have been omitted for clarity. Calculations were done at the UB3LYP/LACVP(Fe), 6-31+G*(O), 6-31G*(B,N), 6-31G(C,H) level in solvent.

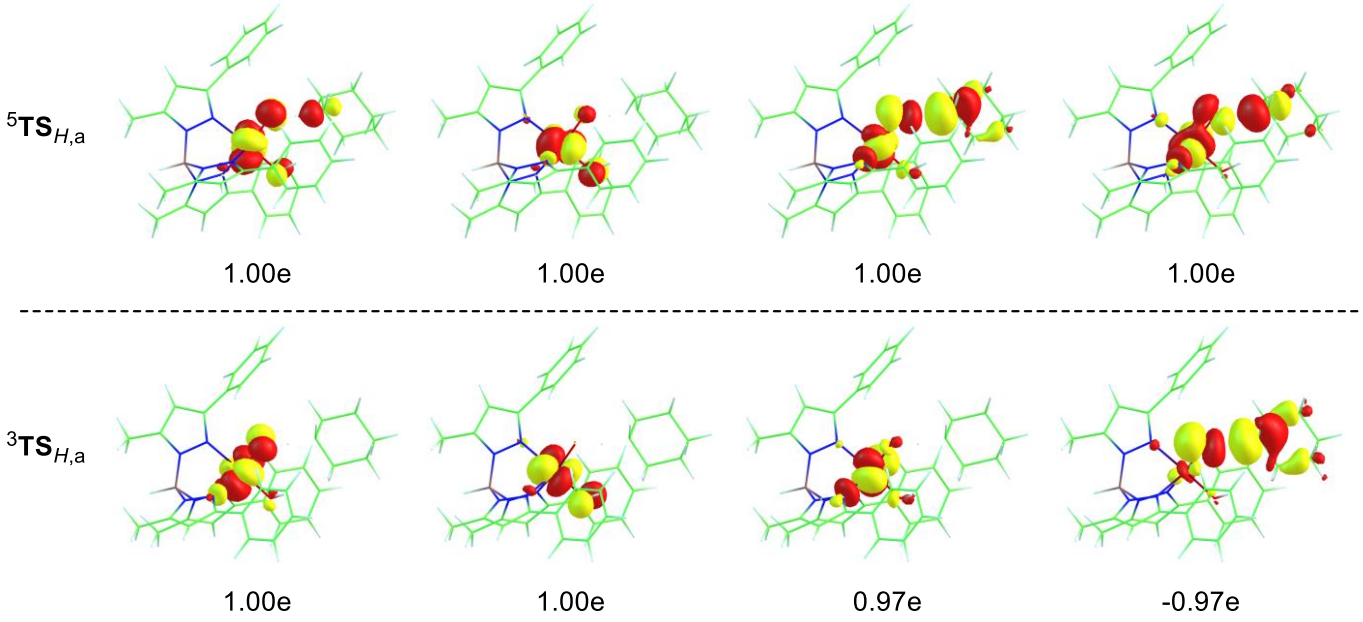

Figure S4 Singly occupied spin-natural bond orbitals (SNOs) of both ^{5}**TS**$_{H,a}$ (top) and ^{3}**TS**$_{H,a}$ (bottom). Positive value means a spin-up electron and negative value means a spin-down electron.

DFT Calculated Cartesian Coordinates

1. Ligand self-hydroxylation

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N 1.122585 0.554423 0.243644
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N 3.389398 1.756116 2.030860
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C 0.964116 4.083945 -4.544516
C 0.672930 3.048376 -3.651139
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C -0.148022 0.365082 -0.221287
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C 5.794456 3.574614 2.342690
C 6.720502 4.622154 2.374511
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C 5.316417 5.822578 3.938417
C 4.386127 4.780558 3.902265
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C 7.746246 -1.994629 -2.762247
C 6.599029 -2.183755 -1.988267
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H -1.337996 -0.405591 1.471549

^{5}TS$_{12}$

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^{3}TS$_{12}$

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H -1.233848 5.299882 2.354281
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^{5}2

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C 2.526382 1.671056 -2.227262
C 3.234000 1.599923 -3.430402
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^{3}2

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C -4.324190 -0.580977 -1.809287
C -2.668372 2.054993 -2.236321
C -1.699091 2.929370 -1.756978
C 3.051256 0.094339 -0.833050
C 3.562471 -1.291564 -0.845453
C 2.996527 -2.303576 -1.642689
C 3.557468 -3.585426 -1.657978
C 4.690702 -3.873555 -0.887677
C 5.266759 -2.868926 -0.100147
C 4.710169 -1.586892 -0.082420
C 3.834255 1.251927 -1.007870
C 2.972340 2.342111 -0.902818
H 1.139862 -2.399450 0.679274
H 0.606459 3.777971 -0.305412
H -2.391381 -1.051661 1.579535
H -3.331343 -3.078657 2.639135
H -2.691222 -3.687627 4.967631
H -1.094190 -2.247220 6.224041
H -0.131672 -0.230706 5.151928
H -0.733952 2.219072 4.347775
H -1.380106 -1.496061 -3.254069
H -2.734793 -3.491888 -3.819915
H -5.109351 -3.642194 -3.087241
H -6.123872 -1.765267 -1.800105
H -4.767325 0.235897 -1.248113
H -3.563585 2.311539 -2.779259
H 2.116153 -2.088767 -2.234713
H 3.110229 -4.356767 -2.276834
H 5.121551 -4.869593 -0.902167
H 6.144492 -3.082930 0.501175
H 5.151381 -0.812608 0.536850
H 4.891569 1.280699 -1.213734
O 0.066395 -1.606070 -1.349533
O 0.861096 -1.567787 1.096815
C -1.650572 4.423687 -1.836364
H -1.691685 4.887871 -0.844367
H -0.735556 4.776491 -2.324577
H -2.504061 4.788590 -2.413269
C 3.287866 3.801311 -1.010059
H 2.684859 4.292342 -1.780976
H 3.106580 4.328777 -0.066895
H 4.341488 3.928975 -1.270157
C 0.247790 4.331708 2.458343
H 0.082883 4.662279 3.486876
H 1.286709 4.559317 2.193978
H -0.394467 4.931787 1.803804

^{5}TS$_{23}$

Fe -0.079647 0.440178 -0.238064
N -0.961373 -2.360172 0.272674
N -1.319890 -1.241001 -0.423879
N -0.340686 -1.046471 2.302646
N -0.277473 0.202831 1.773364
N 1.485397 -1.956129 0.817464
N 1.696664 -0.853448 0.035838
B 0.085158 -2.244017 1.412428
C -2.259940 -1.608818 -1.328243
C -2.965416 -0.665095 -2.210061
C -3.350944 0.611061 -1.757278
C -4.050380 1.481472 -2.597971
C -4.385095 1.088271 -3.900111
C -4.017028 -0.183966 -4.355558
C -3.315262 -1.054763 -3.516994
C -2.482213 -2.997138 -1.213540
C -1.646576 -3.443586 -0.190767
C -0.736761 1.073752 2.704812
C -0.718351 2.502971 2.419982
C 0.359592 2.993882 1.588441
C 0.393665 4.403155 1.301264
C -0.627215 5.237433 1.722263
C -1.690792 4.728512 2.501631
C -1.726810 3.369724 2.846429
C -1.121379 0.349004 3.851615
C -0.851391 -0.992010 3.566414
C 2.978269 -0.906733 -0.393896
C 3.612368 0.112751 -1.247697

C 3.209899 1.462144 -1.226708
C 3.850828 2.407053 -2.034208
C 4.908212 2.026699 -2.869635
C 5.319436 0.688165 -2.894951
C 4.677960 -0.259058 -2.092723
C 3.590064 -2.072265 0.124655
C 2.621135 -2.714543 0.886857
H 0.147684 1.527668 -2.248835
H 0.107098 -3.251788 2.052898
H -3.114024 0.915661 -0.743313
H -4.339899 2.462309 -2.234322
H -4.929355 1.764706 -4.551375
H -4.270742 -0.495749 -5.363786
H -3.015109 -2.032384 -3.880319
H -3.191064 -3.588235 -1.770470
H 1.311112 2.475950 1.660555
H 1.228914 4.794360 0.730738
H -0.601869 6.294045 1.475812
H -2.482121 5.391130 2.835575
H -2.552889 2.981807 3.434370
H -1.498928 0.747301 4.779388
H 2.392516 1.772829 -0.586276
H 3.525132 3.442340 -2.007000
H 5.404354 2.762882 -3.494036
H 6.133972 0.380515 -3.543165
H 4.989947 -1.297497 -2.134872
H 4.612022 -2.387034 -0.010377
O 0.034191 2.189931 -0.052283
O 0.011888 0.588221 -2.036608
C -1.033961 -2.195627 4.436981
H -1.713423 -2.925497 3.983255
H -0.083752 -2.707386 4.626069
H -1.454247 -1.895245 5.399850
C 2.734817 -3.988446 1.666559
H 2.511268 -3.839899 2.728794
H 2.051089 -4.760307 1.295245
H 3.753517 -4.376589 1.586862
C -1.488627 -4.827460 0.358398
H -2.169893 -5.508245 -0.158095
H -0.468947 -5.205856 0.223091
H -1.713061 -4.870065 1.429889

^{3}TS$_{23}$

Fe -0.099299 0.421177 -0.280182
N -1.109108 -2.261962 0.513742
N -1.407146 -1.194137 -0.284752
N -0.315376 -0.817499 2.393838
N -0.220296 0.376860 1.751811
N 1.375650 -1.982481 0.931871
N 1.622390 -0.954752 0.065798
B -0.013180 -2.117038 1.601434
C -2.391452 -1.582332 -1.132493
C -3.054522 -0.686010 -2.094001
C -3.379270 0.641202 -1.755189
C -4.041494 1.465551 -2.669386
C -4.399847 0.974889 -3.931356
C -4.093259 -0.348400 -4.272756
C -3.428571 -1.173329 -3.360914
C -2.704332 -2.933379 -0.875971
C -1.876461 -3.334946 0.171540
C -0.533377 1.350586 2.640358
C -0.442968 2.752522 2.250283
C 0.595540 3.123060 1.327511
C 0.708312 4.496869 0.944317
C -0.216967 5.428909 1.384277
C -1.252759 5.042701 2.264856
C -1.357197 3.714324 2.694878
C -0.858535 0.752024 3.875074
C -0.700471 -0.622492 3.688424
C 2.874232 -1.127674 -0.414676
C 3.530007 -0.211958 -1.363888
C 3.238359 1.165431 -1.394683
C 3.893971 2.011763 -2.294196
C 4.858234 1.502042 -3.172551
C 5.160789 0.134930 -3.146399
C 4.503406 -0.713464 -2.251475
C 3.430866 -2.295928 0.157723
C 2.458761 -2.814134 1.005955
H 0.341367 1.265462 -2.366342
H -0.032321 -3.061696 2.331622
H -3.124338 1.022921 -0.772135
H -4.283479 2.487036 -2.393649
H -4.915220 1.615727 -4.639625
H -4.366151 -0.735973 -5.249190
H -3.176277 -2.192462 -3.635852
H -3.464946 -3.524629 -1.359562
H 1.487023 2.507097 1.293921
H 1.522164 4.790690 0.290633
H -0.137519 6.464926 1.071501
H -1.970406 5.779313 2.610343
H -2.161742 3.420787 3.361652
H -1.123100 1.252493 4.792329
H 2.496645 1.575268 -0.718972
H 3.654215 3.070507 -2.305084
H 5.366627 2.161233 -3.868904
H 5.902642 -0.271853 -3.826419
H 4.728917 -1.774897 -2.252676
H 4.421660 -2.690211 0.000295
O 0.006638 2.211307 -0.284069
O 0.013444 0.394350 -2.081998
C -0.878034 -1.733097 4.675876
H -1.641813 -2.447879 4.350333
H 0.050784 -2.294064 4.827726
H -1.187488 -1.323223 5.640396
C 2.521537 -4.035392 1.870912
H 2.362738 -3.796826 2.928467
H 1.767327 -4.778746 1.588410
H 3.504966 -4.502621 1.774291
C -1.799352 -4.666255 0.852149
H -2.539378 -5.344062 0.419437
H -0.812076 -5.127535 0.735040
H -1.997494 -4.587711 1.926755

^{5}3

Fe -0.081961 0.406907 -0.224801
N -0.991255 -2.352748 0.336707
N -1.313290 -1.248942 -0.401721
N -0.334883 -1.004257 2.332501
N -0.282744 0.225465 1.758443
N 1.461050 -1.977021 0.854180
N 1.677152 -0.880339 0.066663
B 0.063374 -2.230012 1.470553
C -2.255876 -1.620962 -1.302607
C -2.928702 -0.690231 -2.223431
C -3.313566 0.599263 -1.809710
C -3.983106 1.455999 -2.688014
C -4.288034 1.035579 -3.988870
C -3.921009 -0.250233 -4.405430
C -3.249282 -1.107599 -3.529314
C -2.516352 -2.997611 -1.142389
C -1.701931 -3.431536 -0.096857
C -0.730767 1.135781 2.660927
C -0.722370 2.543679 2.330803
C 0.196398 2.954885 1.194847
C 0.131684 4.424956 0.886766
C -0.625473 5.301129 1.614205
C -1.418002 4.850537 2.710855
C -1.456771 3.483008 3.039732
C -1.086404 0.446959 3.844950
C -0.819850 -0.900924 3.604716
C 2.949548 -0.954941 -0.385298
C 3.583158 0.061242 -1.242342
C 3.242444 1.424796 -1.156417
C 3.880447 2.369140 -1.966457
C 4.874292 1.971918 -2.869567
C 5.225301 0.619062 -2.958794
C 4.586420 -0.327008 -2.152892
C 3.550021 -2.130890 0.121502
C 2.583704 -2.755511 0.902820
H 0.222317 1.518465 -2.179053
H 0.072745 -3.223500 2.133018
H -3.100549 0.925369 -0.797097
H -4.272440 2.447507 -2.354542
H -4.808937 1.701598 -4.669300
H -4.152316 -0.583131 -5.412276
H -2.950230 -2.096567 -3.861567
H -3.236333 -3.587623 -1.685954
H 1.234487 2.702781 1.500123
H 0.721975 4.756215 0.038291
H -0.636663 6.355216 1.353172
H -2.012910 5.559484 3.276010
H -2.097071 3.154126 3.853615
H -1.450548 0.873144 4.765453
H 2.478374 1.746605 -0.458216
H 3.604416 3.416077 -1.888080
H 5.368893 2.707184 -3.496189
H 5.990901 0.299936 -3.658943
H 4.849778 -1.375983 -2.241847
H 4.564239 -2.461985 -0.032196
O -0.049978 2.235046 -0.044896
O 0.060641 0.573073 -2.009816
C -0.982464 -2.071970 4.522191
H -1.671412 -2.817506 4.110096
H -0.027859 -2.576696 4.708064
H -1.381226 -1.736998 5.482763
C 2.687535 -4.029527 1.683484
H 2.488393 -3.873563 2.749526
H 1.980841 -4.788080 1.328021
H 3.696225 -4.438701 1.584649
C -1.587109 -4.799763 0.500046
H -2.281896 -5.478895 -0.000250
H -0.576920 -5.209859 0.388426
H -1.822985 -4.799572 1.569892

^{3}3

Fe -0.078434 0.400523 -0.229607
N -1.108179 -2.297318 0.411893
N -1.390168 -1.195945 -0.345896
N -0.330887 -0.935685 2.355188
N -0.247601 0.274769 1.746090
N 1.372150 -2.032646 0.856259
N 1.623139 -0.961363 0.044511
B -0.019959 -2.200910 1.514747
C -2.371527 -1.538959 -1.216127
C -3.017923 -0.596254 -2.143884
C -3.333063 0.718327 -1.750662
C -3.978932 1.587753 -2.634211
C -4.329603 1.155622 -3.919621
C -4.032435 -0.154594 -4.315265
C -3.384465 -1.024818 -3.433902
C -2.698655 -2.896206 -1.016374
C -1.883220 -3.347649 0.020883
C -0.588946 1.232075 2.650162
C -0.515712 2.627794 2.293957
C 0.360582 2.971873 1.101208
C 0.341347 4.438467 0.760171
C -0.308054 5.365928 1.523212
C -1.045536 4.977026 2.683854
C -1.143753 3.621532 3.036024
C -0.915182 0.589038 3.869758
C -0.734961 -0.774907 3.651175
C 2.877529 -1.108267 -0.438778
C 3.539545 -0.138652 -1.327676
C 3.270736 1.241654 -1.255204
C 3.935036 2.140288 -2.095487
C 4.884252 1.679614 -3.016311
C 5.163813 0.309435 -3.092589
C 4.498413 -0.590884 -2.256300
C 3.430328 -2.305372 0.072678
C 2.454411 -2.866979 0.889250
H 0.232714 1.448459 -2.216461
H -0.041337 -3.176890 2.202393
H -3.084347 1.054609 -0.749535
H -4.214271 2.598597 -2.316687
H -4.832013 1.831577 -4.604150
H -4.299619 -0.496813 -5.310038
H -3.139472 -2.033655 -3.750320
H -3.460649 -3.460272 -1.529346
H 1.402904 2.693670 1.371206
H 0.882432 4.720456 -0.137523
H -0.282624 6.414703 1.242503
H -1.558136 5.728143 3.274624
H -1.748858 3.341404 3.893874

H -1.199402 1.056248 4.798371
H 2.542066 1.612352 -0.543577
H 3.714622 3.201000 -2.026903
H 5.399496 2.379420 -3.666451
H 5.894291 -0.058601 -3.806125
H 4.705991 -1.653114 -2.334978
H 4.421927 -2.690600 -0.101163
O 0.033247 2.231757 -0.100828
O 0.031309 0.515735 -2.021512
C -0.905834 -1.913744 4.606730
H -1.653750 -2.631642 4.252352
H 0.030565 -2.463384 4.753851
H -1.233036 -1.535638 5.578270
C 2.513469 -4.132173 1.688703
H 2.350763 -3.949328 2.756666
H 1.759771 -4.858778 1.364416
H 3.496920 -4.594404 1.571183
C -1.824236 -4.705593 0.648551
H -2.564908 -5.359381 0.181426
H -0.839434 -5.170070 0.523789
H -2.033681 -4.667972 1.723231

^{5}TS$_{34}$

Fe -0.134766 0.319861 -0.609540
N -1.110319 -1.739218 1.478400
N -1.472472 -1.166929 0.289089
N 0.273215 0.139474 2.480749
N 0.062430 1.013419 1.486653
N 1.427615 -1.736843 1.248626
N 1.660466 -1.008181 0.118073
B 0.234426 -1.391785 2.165782
C -2.657914 -1.711292 -0.068570
C -3.402680 -1.345741 -1.286827
C -3.372691 -0.042130 -1.819162
C -4.112321 0.272122 -2.963851
C -4.899980 -0.700955 -3.590689
C -4.942151 -1.998527 -3.064967
C -4.200107 -2.317706 -1.924937
C -3.051624 -2.654066 0.908906
C -2.054702 -2.645748 1.877526
C 0.106525 2.260376 2.020520
C -0.109646 3.442020 1.219000
C -0.573479 3.312288 -0.192634
C -0.850658 4.590238 -0.898440
C -0.625655 5.832437 -0.307065
C -0.174651 5.890557 1.015380
C 0.091817 4.722361 1.745423
C 0.368118 2.153914 3.414129
C 0.463372 0.794943 3.676158
C 2.774190 -1.520537 -0.450256
C 3.406821 -0.960843 -1.657767
C 3.416487 0.426262 -1.905211
C 4.058623 0.944058 -3.033969
C 4.709905 0.088303 -3.931563
C 4.712551 -1.291735 -3.692698
C 4.067486 -1.811644 -2.566647
C 3.244746 -2.608497 0.323033
C 2.371585 -2.717725 1.398742
H 0.966700 -0.447289 -2.704944
H 0.321805 -2.000311 3.189538
H -2.779536 0.727968 -1.339599
H -4.074002 1.280774 -3.363147
H -5.472724 -0.452290 -4.478606
H -5.545689 -2.762231 -3.545665
H -4.221451 -3.330192 -1.534500
H -3.958308 -3.236955 0.924328
H 0.465347 3.689557 -0.767803
H -1.195396 4.480184 -1.920044
H -0.807449 6.738536 -0.872504
H -0.007325 6.853895 1.484269
H 0.441087 4.818157 2.767265
H 0.450548 2.948373 4.137717
H 2.919605 1.090547 -1.207123
H 4.053915 2.015039 -3.210889
H 5.208411 0.492025 -4.807015
H 5.210358 -1.963060 -4.385368
H 4.059090 -2.883410 -2.395337
H 4.125226 -3.204512 0.143498
O -1.046726 2.189768 -0.687085
O 0.192966 0.076576 -2.454230
C 0.712130 0.098142 4.976758
H -0.113439 -0.570068 5.245047
H 1.624348 -0.507998 4.945200
H 0.824205 0.835624 5.775649
C 2.405506 -3.687230 2.540226
H 2.481451 -3.180494 3.508897
H 1.508098 -4.316015 2.572011
H 3.271357 -4.346546 2.435710
C -1.978842 -3.445253 3.142316
H -2.868783 -4.074020 3.230705
H -1.100753 -4.100539 3.163667
H -1.927967 -2.805382 4.030385

^{3}TS$_{34}$

Fe 0.161160 0.369863 -0.294343
N -1.443335 -1.984113 0.856222
N -1.609625 -1.024347 -0.098824
N -0.121520 -0.549661 2.444867
N -0.025490 0.538963 1.656235
N 1.091568 -2.142385 0.923938
N 1.479830 -1.174689 0.038678
B -0.191814 -1.950592 1.766461
C -2.729698 -1.339146 -0.784950
C -3.271111 -0.524055 -1.885348
C -3.052931 0.865984 -1.955705
C -3.596066 1.617376 -3.002609
C -4.371747 1.000651 -3.992328
C -4.598573 -0.379922 -3.928764
C -4.053364 -1.134389 -2.886446
C -3.283104 -2.530355 -0.254451
C -2.444330 -2.915054 0.784929
C -0.127116 1.640440 2.453110
C -0.055186 2.973751 1.920960
C -0.034703 3.186172 0.452967
C 0.029691 4.592094 -0.003490
C 0.074245 5.664893 0.891379
C 0.031813 5.409576 2.265841
C -0.016150 4.098029 2.758040
C -0.278395 1.207598 3.800350
C -0.279608 -0.176937 3.760074
C 2.630362 -1.595698 -0.535703
C 3.448109 -0.797922 -1.466858
C 3.665463 0.577337 -1.262250
C 4.496249 1.301969 -2.120591
C 5.129034 0.664832 -3.196403
C 4.926679 -0.704709 -3.403902
C 4.096754 -1.430781 -2.543724
C 2.960598 -2.870564 -0.022135
C 1.970225 -3.188352 0.901434
H 0.072989 1.097184 -2.503404
H -0.265742 -2.801334 2.601921
H -2.457630 1.356529 -1.194292
H -3.416730 2.687624 -3.041722
H -4.793049 1.587293 -4.802673
H -5.193399 -0.870039 -4.693352
H -4.216707 -2.206863 -2.857468
H -4.190106 -3.024505 -0.563680
H 1.167971 3.617362 0.287716
H 0.030062 4.725665 -1.078896
H 0.139491 6.677233 0.511940
H 0.052849 6.235610 2.967900
H -0.046296 3.948206 3.831434
H -0.390662 1.818298 4.681045
H 3.181312 1.073453 -0.428022
H 4.654893 2.362317 -1.948610
H 5.773457 1.229235 -3.863094
H 5.410293 -1.206879 -4.235984
H 3.931737 -2.489538 -2.716430
H 3.831646 -3.458387 -0.263062
O -0.365712 2.262885 -0.425548
O 0.485893 0.310373 -2.110264
C -0.430941 -1.157116 4.880038
H -1.333412 -1.768370 4.766192
H 0.421346 -1.842984 4.937316
H -0.502048 -0.623745 5.831340
C 1.836492 -4.413829 1.751899
H 1.816992 -4.171924 2.820426
H 0.919572 -4.971050 1.527642
H 2.684509 -5.079589 1.571291
C -2.556159 -4.099995 1.694555
H -3.461164 -4.663878 1.453343
H -1.701440 -4.778665 1.592325
H -2.612449 -3.805442 2.748631

^{5}4

Fe -0.122477 0.236107 -0.573351
N -0.319397 -1.980806 1.535429
N -0.848360 -1.643894 0.318972
N 0.098821 0.341112 2.477026
N -0.369872 1.050015 1.420158
N 1.996614 -0.934539 1.384716
N 1.956127 -0.266831 0.195640
B 0.718046 -1.070487 2.246595
C -1.683545 -2.644347 -0.041899
C -2.473530 -2.656598 -1.285986
C -2.940383 -1.471852 -1.886860
C -3.710915 -1.522929 -3.052517
C -4.036818 -2.753933 -3.634760
C -3.581961 -3.938924 -3.042697
C -2.807346 -3.890508 -1.880814
C -1.678596 -3.640173 0.962712
C -0.810824 -3.189303 1.949831
C -0.926551 2.183795 1.900992
C -1.575589 3.174759 1.039196
C -2.041286 2.801220 -0.304260
C -2.809908 3.823311 -1.124389
C -2.986539 5.179776 -0.523545
C -2.501372 5.463893 0.706213
C -1.806123 4.457941 1.476075
C -0.796780 2.196706 3.310530
C -0.145343 1.012691 3.643780
C 3.204648 -0.305855 -0.320161
C 3.588059 0.361004 -1.576844
C 3.037560 1.604175 -1.946977
C 3.438067 2.237657 -3.127777
C 4.402211 1.647209 -3.954392
C 4.963559 0.416228 -3.591590
C 4.560468 -0.221163 -2.414620
C 4.050829 -1.030466 0.551240
C 3.256459 -1.410946 1.627546
H 1.008790 0.024783 -2.748618
H 0.999370 -1.548654 3.303890
H -2.702699 -0.512054 -1.444949
H -4.056947 -0.598803 -3.504696
H -4.635252 -2.789652 -4.539634
H -3.823655 -4.898781 -3.488607
H -2.442126 -4.812154 -1.439179
H -2.257560 -4.549248 0.982514
H -2.310175 3.899456 -2.103181
H -3.792641 3.383767 -1.361033
H -3.514970 5.925436 -1.109391
H -2.624403 6.448789 1.142778
H -1.443391 4.744633 2.458623
H -1.153557 2.943914 4.000861
H 2.303546 2.073928 -1.301747
H 3.001287 3.193734 -3.398392
H 4.712849 2.140607 -4.869735
H 5.709301 -0.050290 -4.227562
H 4.986676 -1.182869 -2.147163
H 5.106564 -1.214281 0.431821
O -1.842894 1.674346 -0.810358
O 0.101615 0.156161 -2.436719
C 0.232333 0.500275 4.998861
H -0.264568 -0.448678 5.229163
H 1.311418 0.331560 5.084675
H -0.057678 1.227192 5.761906
C 3.644080 -2.180699 2.852690
H 3.457100 -1.612756 3.770909
H 3.092933 -3.124475 2.936372
H 4.710437 -2.418582 2.814144
C -0.450478 -3.848695 3.245912
H -0.992457 -4.793691 3.337906
H 0.621148 -4.068032 3.312740

H -0.708795 -3.226070 4.109844

^{3}4

Fe 0.006461 0.324681 -0.274653
N -1.285412 -2.121977 0.819433
N -1.535688 -1.110544 -0.063031
N -0.023063 -0.681162 2.438473
N -0.014832 0.447299 1.677516
N 1.250783 -2.136714 0.838715
N 1.539238 -1.118969 -0.026038
B -0.023488 -2.052314 1.722004
C -2.663945 -1.430370 -0.738097
C -3.301636 -0.551442 -1.731425
C -3.283066 0.849568 -1.592543
C -3.919783 1.665580 -2.531908
C -4.592921 1.097052 -3.620872
C -4.625553 -0.295814 -3.763050
C -3.987035 -1.113216 -2.826108
C -3.129207 -2.683582 -0.281429
C -2.235573 -3.095309 0.704438
C -0.022486 1.521826 2.507873
C -0.016362 2.891780 2.015543
C -0.009300 3.146601 0.621716
C -0.003474 4.567256 0.089610
C -0.009961 5.640117 1.139031
C -0.016675 5.331162 2.468915
C -0.019263 3.979605 2.917953
C -0.036713 1.045117 3.841481
C -0.037108 -0.344116 3.762080
C 2.666372 -1.460557 -0.691768
C 3.342944 -0.585699 -1.664154
C 3.450656 0.802173 -1.453314
C 4.125969 1.610336 -2.372741
C 4.712840 1.045326 -3.512227
C 4.622218 -0.335978 -3.724614
C 3.945091 -1.145147 -2.807677
C 3.091342 -2.732616 -0.249632
C 2.175389 -3.133754 0.720409
H 0.026088 1.188494 -2.396617
H -0.035714 -2.942882 2.517765
H -2.777038 1.297038 -0.743942
H -3.896842 2.743999 -2.409893
H -5.087835 1.731959 -4.348797
H -5.142167 -0.745081 -4.605317
H -3.999422 -2.191154 -2.951646
H -4.021206 -3.199659 -0.597810
H 0.871881 4.679579 -0.575370
H -0.867427 4.681379 -0.589475
H -0.008870 6.672185 0.802159
H -0.020694 6.123435 3.211506
H -0.023640 3.782203 3.983705
H -0.046060 1.627974 4.747321
H 3.018036 1.243344 -0.561817
H 4.202031 2.678519 -2.194931
H 5.238096 1.673805 -4.224321
H 5.073181 -0.781979 -4.605430
H 3.862328 -2.212653 -2.985102
H 3.972623 -3.267573 -0.564852
O -0.007670 2.226299 -0.303841
O 0.032953 0.268972 -2.078281
C -0.051880 -1.351067 4.869046
H -0.937804 -1.994203 4.820968
H 0.827144 -2.004328 4.835821
H -0.057193 -0.839293 5.834532
C 2.153902 -4.394242 1.528837
H 2.174478 -4.190069 2.604994
H 1.259293 -4.994862 1.328082
H 3.027460 -5.003391 1.282996
C -2.257305 -4.343663 1.531274
H -3.135895 -4.940211 1.272911
H -1.369212 -4.963067 1.361595
H -2.300444 -4.122907 2.603539

^{5}TS$_{45}$

Fe 3.708023 2.025549 -0.054333
N 1.013975 0.652894 0.257795
N 1.653285 1.566232 -0.537432
N 2.360335 0.845821 2.412659
N 3.165348 1.841177 1.977791
N 2.945728 -0.921973 0.690466
N 4.008606 -0.268065 0.130281
B 1.784098 -0.136903 1.357745
C 0.755683 1.992687 -1.456492
C 1.058148 2.990731 -2.498619
C 1.886134 4.102078 -2.246651
C 2.137121 5.039525 -3.254603
C 1.561367 4.891156 -4.522330
C 0.728435 3.794582 -4.778874
C 0.479278 2.853039 -3.776618
C -0.474545 1.333060 -1.245409
C -0.280869 0.496122 -0.150088
C 3.523840 2.593929 3.036876
C 4.405064 3.751617 2.857209
C 4.445710 4.434653 1.570839
C 5.413542 5.517244 1.398545
C 6.131167 6.012684 2.551433
C 6.044467 5.366961 3.760734
C 5.183573 4.241871 3.895618
C 2.925718 2.048007 4.198971
C 2.192645 0.941953 3.768401
C 4.827398 -1.220358 -0.371467
C 6.137119 -0.940006 -0.990448
C 7.049304 -0.041905 -0.399754
C 8.309093 0.172794 -0.971369
C 8.682250 -0.512496 -2.134475
C 7.787906 -1.415924 -2.722973
C 6.527374 -1.628700 -2.156365
C 4.265012 -2.497322 -0.149149
C 3.074056 -2.274982 0.533936
H 5.759243 1.650873 -1.545065
H 1.036259 -0.901184 1.889847
H 2.321989 4.241728 -1.263913
H 2.776145 5.891484 -3.044130
H 1.757359 5.621840 -5.300681
H 0.278797 3.669358 -5.758961
H -0.152729 1.995647 -3.985512
H -1.391236 1.473916 -1.795004
H 6.229663 4.828391 0.633208
H 5.135846 6.250139 0.636369
H 6.764966 6.887154 2.435463
H 6.614466 5.704509 4.618835
H 5.140438 3.737875 4.857413
H 2.992072 2.416038 5.210305
H 6.771802 0.474293 0.512880
H 8.998589 0.867365 -0.502413
H 9.660255 -0.347428 -2.574862
H 8.069653 -1.950770 -3.624454
H 5.833352 -2.322310 -2.620382
H 4.693148 -3.451497 -0.411830
O 3.750497 4.060631 0.556201
O 5.253565 2.417783 -1.235327
C 1.348593 -0.000666 4.568774
H 0.305855 -0.000571 4.231865
H 1.712583 -1.032221 4.500165
H 1.362890 0.292091 5.621773
C 2.086770 -3.280599 1.042443
H 1.945649 -3.205742 2.126350
H 1.101447 -3.160832 0.577531
H 2.442639 -4.289442 0.817056
C -1.268256 -0.416829 0.510017
H -2.239249 -0.323738 0.016562
H -0.960334 -1.466938 0.452151
H -1.403113 -0.175876 1.570157
O 6.854846 4.029128 -0.287093
H 7.172133 4.600781 -1.006088
H 6.117860 3.298586 -0.739439

^{3}TS$_{45}$

Fe 3.829578 1.872408 0.157895
N 0.996089 0.633085 0.293091
N 1.656081 1.514720 -0.516995
N 2.349325 0.776533 2.440773
N 3.209066 1.723471 2.010176
N 2.962588 -0.894819 0.658935
N 4.002611 -0.183650 0.120062
B 1.774467 -0.181047 1.355838
C 0.749408 1.984416 -1.402447
C 1.057515 2.958470 -2.465382
C 2.068568 3.928970 -2.322781
C 2.317190 4.848708 -3.347169
C 1.562127 4.823920 -4.526191
C 0.552142 3.865264 -4.676319
C 0.304148 2.941529 -3.657548
C -0.510349 1.387665 -1.148262
C -0.322099 0.538168 -0.065786
C 3.519397 2.533747 3.044251
C 4.424751 3.666081 2.835711
C 4.514439 4.266733 1.515886
C 5.460690 5.363177 1.310346
C 6.139250 5.925726 2.457208
C 6.021901 5.344154 3.696125
C 5.161353 4.224257 3.870507
C 2.834118 2.067455 4.190102
C 2.094853 0.957651 3.771221
C 4.868799 -1.089624 -0.394835
C 6.190270 -0.776881 -0.976900
C 7.120803 0.032382 -0.294319
C 8.398741 0.245609 -0.821623
C 8.771042 -0.350105 -2.033732
C 7.856841 -1.161265 -2.717431
C 6.578062 -1.375408 -2.192529
C 4.350421 -2.390177 -0.211719
C 3.146360 -2.234661 0.464754
H 5.529024 1.486908 -1.656294
H 1.055176 -0.985945 1.868091
H 2.652100 3.970215 -1.411709
H 3.099592 5.590634 -3.219048
H 1.757596 5.541040 -5.317361
H -0.037100 3.832106 -5.587649
H -0.467254 2.189944 -3.791230
H -1.438110 1.573776 -1.665056
H 6.266540 4.666518 0.569333
H 5.173288 6.061904 0.519244
H 6.761927 6.804112 2.315713
H 6.560927 5.735289 4.551351
H 5.079605 3.784253 4.860608
H 2.846307 2.488926 5.182357
H 6.837834 0.489717 0.647509
H 9.102223 0.872862 -0.284005
H 9.763693 -0.184679 -2.440003
H 8.137075 -1.624896 -3.657899
H 5.869170 -2.001356 -2.725185
H 4.820413 -3.317462 -0.497240
O 3.886415 3.821882 0.481740
O 5.119443 2.254274 -1.231144
C 1.164604 0.089249 4.559165
H 0.138430 0.141221 4.177662
H 1.469740 -0.962699 4.531391
H 1.151915 0.410511 5.603706
C 2.192521 -3.289983 0.933467
H 2.057191 -3.267628 2.020518
H 1.201336 -3.177064 0.479926
H 2.576483 -4.276591 0.660985
C -1.322985 -0.334198 0.628548
H -2.304680 -0.206984 0.164382
H -1.057086 -1.395849 0.567672
H -1.418775 -0.084568 1.691473
O 6.836705 3.804454 -0.374248
H 7.158460 4.347737 -1.112778
H 6.059555 3.096414 -0.792846

^{5}5

Fe 3.823489 1.850022 -0.000682
N 1.107240 0.580667 0.207820
N 1.747900 1.557319 -0.502203
N 2.320906 0.888616 2.418990
N 3.208843 1.834311 2.009584
N 3.038677 -0.951302 0.823703
N 4.076317 -0.306637 0.209786
B 1.824287 -0.149870 1.387217
C 0.885446 2.007347 -1.441076
C 1.206311 3.115403 -2.358400
C 1.873906 4.269581 -1.902181
C 2.151715 5.323401 -2.779569

C 1.760197 5.246060 -4.122344
C 1.083648 4.108868 -4.581682
C 0.807120 3.053386 -3.707506
C -0.323641 1.286943 -1.341708
C -0.154241 0.395629 -0.283564
C 3.516187 2.615917 3.064028
C 4.467593 3.725978 2.963857
C 5.175032 4.030282 1.757405
C 6.096272 5.104814 1.773818
C 6.316308 5.867993 2.916669
C 5.615263 5.579325 4.097242
C 4.710687 4.520609 4.105207
C 2.787269 2.147985 4.190781
C 2.042323 1.059303 3.748068
C 4.937117 -1.258629 -0.220089
C 6.199731 -0.947671 -0.915528
C 7.017882 0.129775 -0.514974
C 8.217289 0.399407 -1.184493
C 8.626989 -0.408125 -2.252865
C 7.829639 -1.489634 -2.649476
C 6.626692 -1.756577 -1.989214
C 4.432275 -2.532092 0.116926
C 3.229161 -2.303330 0.781945
H 5.230813 1.122763 -2.166660
H 1.057669 -0.906698 1.903156
H 2.151062 4.350624 -0.855729
H 2.654836 6.212008 -2.410214
H 1.973136 6.065615 -4.801081
H 0.775211 4.042117 -5.620141
H 0.294595 2.168178 -4.070495
H -1.214496 1.425117 -1.932995
H 5.661896 4.024768 -0.810268
H 6.641288 5.318281 0.859696
H 7.031341 6.684881 2.889326
H 5.774789 6.168217 4.994214
H 4.171361 4.296215 5.019727
H 2.798299 2.537240 5.195596
H 6.726324 0.739933 0.333086
H 8.834156 1.232180 -0.862943
H 9.558760 -0.199246 -2.768107
H 8.140527 -2.120234 -3.476213
H 6.003916 -2.585215 -2.310761
H 4.897470 -3.487554 -0.064985
O 5.018092 3.350834 0.599437
O 4.604729 1.857071 -2.047243
C 1.096333 0.190057 4.517459
H 0.080706 0.229420 4.106985
H 1.409118 -0.860342 4.511163
H 1.051719 0.521906 5.557977
C 2.285791 -3.304683 1.374529
H 2.144001 -3.145909 2.449177
H 1.295843 -3.263165 0.906517
H 2.683307 -4.312791 1.231297
C -1.134084 -0.593216 0.269015
H -2.073950 -0.526864 -0.285028
H -0.767080 -1.622536 0.187491
H -1.350214 -0.407666 1.326795
O 5.921296 4.167455 -1.769302
H 5.428976 4.945310 -2.073832
H 5.131121 2.696974 -2.164546

^{3}5

Fe 3.814678 1.778128 0.115178
N 1.088501 0.563267 0.256836
N 1.754484 1.537404 -0.427844
N 2.367588 0.833739 2.408790
N 3.227480 1.786362 1.957770
N 3.007575 -0.998249 0.809013
N 4.058003 -0.326538 0.253923
B 1.811410 -0.199142 1.402197
C 0.912081 2.013184 -1.371043
C 1.254956 3.129730 -2.267120
C 2.057673 4.199945 -1.825896
C 2.354396 5.265345 -2.681929
C 1.848392 5.285455 -3.988372
C 1.041434 4.230582 -4.433199
C 0.746343 3.162692 -3.580325
C -0.312672 1.310092 -1.295491
C -0.169902 0.398867 -0.252568
C 3.554797 2.591676 2.989542
C 4.437187 3.750878 2.845344
C 5.004037 4.121317 1.589323
C 5.796282 5.293095 1.524883
C 6.068936 6.045500 2.664930
C 5.531582 5.674211 3.904084
C 4.721936 4.543282 3.978238
C 2.872689 2.124678 4.144879
C 2.134486 1.017685 3.744546
C 4.918151 -1.256981 -0.225024
C 6.201957 -0.915542 -0.864887
C 7.015616 0.126017 -0.370922
C 8.236400 0.425072 -0.984446
C 8.671552 -0.317079 -2.090180
C 7.878594 -1.362377 -2.580159
C 6.653861 -1.659517 -1.974435
C 4.394983 -2.543941 0.022310
C 3.184899 -2.345772 0.684908
H 4.893777 0.936344 -2.046197
H 1.050003 -0.943791 1.943199
H 2.438506 4.200111 -0.810034
H 2.967311 6.086862 -2.323330
H 2.076031 6.115275 -4.649871
H 0.645557 4.236864 -5.443938
H 0.132411 2.340921 -3.935455
H -1.195133 1.471595 -1.893742
H 5.744684 3.822942 -0.860373
H 6.216857 5.581074 0.567691
H 6.692894 6.931010 2.583460
H 5.736944 6.259800 4.793919
H 4.298305 4.260059 4.935897
H 2.904973 2.535149 5.140425
H 6.699787 0.684272 0.504002
H 8.850264 1.229966 -0.593795
H 9.620362 -0.084430 -2.562330
H 8.209233 -1.941341 -3.436483
H 6.035297 -2.460696 -2.366217
H 4.856438 -3.490031 -0.210618
O 4.830629 3.400475 0.455338
O 4.437812 1.769409 -1.840144
C 1.222272 0.148149 4.552656
H 0.184502 0.210343 4.204135
H 1.517342 -0.906154 4.509894
H 1.244121 0.462841 5.599301
C 2.217831 -3.368436 1.196789
H 2.034147 -3.256756 2.270805
H 1.247157 -3.301261 0.692032
H 2.616974 -4.371088 1.023613
C -1.164441 -0.588075 0.276585
H -2.094488 -0.514434 -0.293040
H -0.802150 -1.619333 0.196799
H -1.398632 -0.406751 1.331654
O 6.158086 3.790337 -1.777882
H 5.923565 4.620911 -2.218900
H 5.098142 2.497476 -2.017066

2. Substrate oxidation

2.1 Sulfide oxidation

^{5}RC

Fe 3.129464 1.846532 0.171894
N 0.845213 -0.083898 0.319051
N 1.159866 1.068315 -0.345544
N 1.989381 0.439697 2.525640
N 2.590540 1.630014 2.221180
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C 0.163578 2.439712 -2.168385
C 0.589308 3.714435 -1.741879
C 0.544497 4.808762 -2.614352
C 0.060514 4.652575 -3.919925
C -0.379295 3.393481 -4.347576
C -0.326712 2.297111 -3.481676
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C -0.313092 -0.617068 -0.178491
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C 3.134535 3.752316 3.407826
C 4.198375 4.164782 2.581950
C 4.704372 5.465978 2.663885
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C 2.601123 4.676654 4.328881
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C 6.638460 1.180154 -0.466426
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C 8.359758 1.159355 -2.176485
C 7.916098 -0.099682 -2.600816
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H 5.144342 5.055395 -1.444260
H 5.276563 6.783010 -1.871666
H 6.194935 5.548483 -2.791165
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C 10.195386 8.648240 -0.883899
H 9.536841 7.115333 0.478287
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H 7.122932 7.689543 -3.056585
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C 3.261476 3.684859 3.438803
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C 5.253427 5.059673 3.156398
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C 2.627830 4.770002 4.075287
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C 6.392709 1.512323 -0.547713
C 7.400063 2.215972 -1.215993
C 8.108924 1.606916 -2.258770
C 7.803006 0.290864 -2.629333
C 6.790807 -0.409138 -1.967662
C 4.976172 -1.955859 0.029359
C 3.794243 -2.190731 0.726533
H 2.769987 3.265440 -1.814830
H 1.287153 -1.627930 1.946250
H 0.759371 3.757894 -0.852314
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H -0.301199 1.025694 -4.009885
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H 5.090857 3.007062 2.516203
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H 5.132754 7.077909 3.916160
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H 1.606117 4.659198 4.424692
H 1.598142 2.110519 5.314006
H 5.873282 1.985392 0.280068
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H 8.893023 2.151233 -2.775150
H 8.347380 -0.187429 -3.437469
H 6.544541 -1.421054 -2.272941
H 5.728145 -2.684363 -0.226958
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H 1.138920 -1.509050 4.450775
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C 3.255175 -3.484106 1.254422
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H 2.305107 -3.756277 0.780604
H 3.969734 -4.287506 1.057975
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H -0.110596 -2.894117 0.134580
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C 5.538730 6.210291 -1.077883
H 4.881523 5.526967 -0.533508
H 5.081094 7.202453 -1.104584
H 5.671463 5.829470 -2.093663
C 8.176145 7.286838 -1.157332
C 9.510273 7.436408 -0.724856
C 7.752556 7.963850 -2.313936
C 10.396993 8.246946 -1.436575
H 9.849776 6.916356 0.166334
C 8.650861 8.773665 -3.022055
H 6.733546 7.868865 -2.668732
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C -0.525232 3.449603 -4.257147
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C -0.284846 -0.657545 -0.185898
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C 3.115367 3.818933 3.292255
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C 4.803295 5.472935 2.694286
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C 2.465423 4.797976 4.071103
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C 7.696842 1.833136 -1.262623
C 8.365105 1.149934 -2.285940
C 7.949329 -0.137971 -2.647136
C 6.870412 -0.736237 -1.991706
C 4.965878 -2.101802 0.029727
C 3.763308 -2.260276 0.713755
H 2.916854 2.935954 -2.424467
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H 9.201418 1.616592 -2.796533
H 8.459470 -0.672600 -3.442156
H 6.539345 -1.726367 -2.288200
H 5.687100 -2.872185 -0.188949
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O 3.622139 2.352754 -2.088307
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H 1.496137 -1.536134 4.470582
H 0.696223 -0.355298 5.520062
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H 3.850265 -4.351345 1.103878
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H 7.045034 7.752978 -2.825481
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C -0.326176 -0.681730 -0.144843
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C 8.287051 0.986984 -2.241710
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C 3.616798 -2.266356 0.839193
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H -4.619676 2.567299 3.031574
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H 2.561693 -1.898729 -1.998442
H 3.754626 -0.638190 -2.365811
H 4.287118 -2.334935 -2.143672
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C 5.524166 0.089048 1.475366
C 6.250058 -0.378114 -0.794651
C 6.741262 0.723840 1.732716
H 4.767292 0.032974 2.252025
C 7.465507 0.266359 -0.527776
H 6.080555 -0.802923 -1.776701
C 7.718623 0.817717 0.732188
H 6.922531 1.151513 2.713805
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C -2.665956 -2.783675 -3.807028
C -1.952932 -3.942497 -3.475113
C -0.703666 -3.845153 -2.856667
C 2.264397 -3.413749 -2.145877
C 3.330860 -2.923675 -1.399103
H -1.588827 -0.392010 0.262528
H 4.770317 -1.217372 0.341077
H 0.129374 1.821053 2.573558
H -1.947836 2.700744 3.591717
H -3.213443 1.327802 5.239353
H -2.384836 -0.941026 5.849677
H -0.320224 -1.831772 4.808018
H 2.316183 -1.592132 4.756460
H 0.866986 2.138108 -2.992653
H -0.779619 3.789887 -3.838796
H -1.006451 6.006354 -2.728542
H 0.427755 6.561381 -0.770763
H 2.071498 4.904876 0.075480
H 4.489686 3.598069 -1.124305
H -0.457432 -0.450598 -2.667095
H -2.660721 -0.625251 -3.774407
H -3.635478 -2.857930 -4.289102
H -2.370583 -4.920335 -3.693171
H -0.163563 -4.747374 -2.588341
H 2.271787 -4.282910 -2.783405
O -0.367109 1.272748 -0.815046
O -0.766366 -0.825775 0.562383
C 6.014227 1.179565 -0.231441
H 6.225824 0.892624 0.804567
H 6.350288 0.357720 -0.873014
H 6.615479 2.061110 -0.467242
C 4.715062 -3.479496 -1.264128
H 5.477964 -2.757859 -1.576373
H 4.943404 -3.768800 -0.232045
H 4.814975 -4.369361 -1.890888
C 4.646424 -2.203254 2.977599
H 4.747324 -2.525398 4.017007
H 4.739438 -3.090627 2.341089
H 5.488746 -1.543332 2.742898
S -3.638049 1.170034 0.186670
C -3.676587 1.909255 -1.482269
H -2.706668 2.397002 -1.602762
H -3.781830 1.140632 -2.252041
H -4.474041 2.650069 -1.579110
C -5.131232 0.186342 0.258334
C -5.269844 -0.670300 1.370258
C -6.152954 0.229979 -0.705747
C -6.411022 -1.462816 1.510326
H -4.481553 -0.718089 2.115601
C -7.291592 -0.573705 -0.558036
H -6.073355 0.881279 -1.567731
C -7.428082 -1.420508 0.546285
H -6.502107 -2.119042 2.370203
H -8.072004 -0.531276 -1.311727
H -8.311902 -2.040298 0.655562

^{5}TS$_{SO,\mathrm{a}}$

Fe 0.185441 0.106738 -0.195733
N 2.988483 -0.432542 -1.334065
N 1.705776 -0.884584 -1.452009
N 3.036702 -0.139501 1.175844
N 1.799046 -0.677599 1.379297
N 2.637600 1.874928 -0.291302
N 1.301471 1.961001 -0.014386
B 3.391019 0.518258 -0.174905
C 1.657630 -1.679049 -2.543456
C 0.452400 -2.414271 -2.962907
C -0.397247 -3.027502 -2.022622
C -1.518650 -3.752088 -2.439778
C -1.806577 -3.882201 -3.804823
C -0.962310 -3.284234 -4.748956
C 0.158099 -2.559241 -4.332324
C 2.936076 -1.721737 -3.142341
C 3.758770 -0.924875 -2.351110
C 1.794517 -1.173800 2.636463
C 0.691130 -1.963862 3.209556
C 0.370374 -1.845205 4.575815
C -0.617874 -2.651096 5.151760
C -1.299465 -3.595658 4.372901
C -0.986800 -3.723511 3.011795
C -0.001308 -2.915343 2.436205
C 3.042520 -0.917782 3.251646
C 3.811497 -0.261500 2.296702
C 0.941638 3.256692 -0.173698
C -0.410351 3.779285 0.085860
C -1.201266 3.283494 1.140030
C -2.453575 3.845364 1.408834
C -2.936802 4.907075 0.633502
C -2.158184 5.404169 -0.419287
C -0.905168 4.846901 -0.689291
C 2.072019 4.004683 -0.565092
C 3.130467 3.102222 -0.628704
H -1.691075 0.878394 -1.557610
H 4.565920 0.725962 -0.231778
H -0.165623 -2.953707 -0.965315

H -2.156880 -4.228032 -1.701345
H -2.674217 -4.448237 -4.128609
H -1.177924 -3.379066 -5.808553
H 0.799999 -2.084338 -5.067255
H 3.229827 -2.290485 -4.009886
H 0.893430 -1.112915 5.182737
H -0.852058 -2.544507 6.206419
H -2.058182 -4.229299 4.821182
H -1.500749 -4.461310 2.403382
H 0.254345 -3.029729 1.388905
H 3.356229 -1.219252 4.238395
H -0.834807 2.459108 1.740395
H -3.047321 3.461232 2.232704
H -3.907144 5.343691 0.848184
H -2.525885 6.222987 -1.029696
H -0.309596 5.227814 -1.512638
H 2.120236 5.067846 -0.736959
O -1.085698 -0.060508 1.060938
O -0.791672 0.571742 -1.751202
C 5.223888 0.226527 2.399735
H 5.875564 -0.243657 1.654693
H 5.294786 1.310761 2.255378
H 5.621331 -0.006462 3.391199
C 4.562613 3.367190 -0.977613
H 5.241654 3.089129 -0.164227
H 4.876016 2.810790 -1.868142
H 4.698234 4.432177 -1.183233
C 5.219878 -0.638770 -2.515789
H 5.600457 -1.171840 -3.391019
H 5.416720 0.429310 -2.661220
H 5.800482 -0.960442 -1.644152
S -2.787089 -1.116354 0.997433
C -3.210431 -0.606852 2.685047
H -2.549842 -1.172254 3.343371
H -3.011465 0.458358 2.812231
H -4.252967 -0.845911 2.907274
C -3.977050 -0.268662 -0.010596
C -4.076582 -0.704446 -1.351131
C -4.767357 0.808876 0.433640
C -4.964520 -0.073429 -2.224282
H -3.457385 -1.523341 -1.703065
C -5.657718 1.426585 -0.450901
H -4.692726 1.169308 1.451618
C -5.760252 0.991521 -1.777870
H -5.034029 -0.413293 -3.252057
H -6.267102 2.253395 -0.100982
H -6.450149 1.478385 -2.458730

^{3}TS$_{SO,a}$

Fe -0.328246 -0.113629 0.035300
N -3.039251 0.551490 1.136413
N -1.854298 -0.032040 1.480390
N -2.981462 -0.044597 -1.305838
N -1.871208 -0.829895 -1.183988
N -2.269020 2.266564 -0.556801
N -0.930224 2.019204 -0.642604
B -3.247823 1.101058 -0.300531
C -1.929200 -0.353727 2.793184
C -0.881985 -1.071603 3.541277
C -0.202421 -2.172835 2.989380
C 0.756772 -2.865817 3.733678
C 1.047992 -2.474762 5.046939
C 0.369477 -1.387090 5.610713
C -0.589252 -0.693597 4.865838
C -3.185380 0.052907 3.293732
C -3.866340 0.620465 2.220557
C -1.978377 -1.815951 -2.104972
C -1.068917 -2.970381 -2.217511
C -0.719570 -3.472552 -3.485439
C 0.060979 -4.627603 -3.606356
C 0.500408 -5.304359 -2.461401
C 0.155295 -4.814581 -1.193401
C -0.623436 -3.659572 -1.073328
C -3.163502 -1.625886 -2.850128
C -3.781272 -0.500391 -2.314991
C -0.325721 3.219861 -0.795069
C 1.120214 3.404763 -1.005225
C 1.882429 2.478891 -1.743899
C 3.233208 2.728607 -2.008612
C 3.847712 3.894830 -1.535968
C 3.100176 4.816049 -0.791514
C 1.748682 4.574653 -0.530924
C -1.300970 4.244795 -0.794116
C -2.526242 3.606662 -0.642205
H 1.324476 1.205848 1.034174
H -4.372720 1.486865 -0.417573
H -0.434702 -2.492985 1.979766
H 1.269910 -3.714574 3.292325
H 1.791573 -3.014067 5.625083
H 0.588581 -1.076697 6.627574
H -1.102674 0.157497 5.301805
H -3.559878 -0.089342 4.294608
H -1.054532 -2.949227 -4.375368
H 0.323167 -4.998880 -4.592103
H 1.099223 -6.204728 -2.554477
H 0.482378 -5.338659 -0.300754
H -0.908687 -3.294752 -0.093070
H -3.540731 -2.258691 -3.637291
H 1.412617 1.570873 -2.104537
H 3.806120 2.011502 -2.586500
H 4.896110 4.083127 -1.744375
H 3.568184 5.720252 -0.414770
H 1.174145 5.289565 0.049476
H -1.135881 5.301331 -0.932280
O 0.867339 -0.698681 -1.113722
O 0.963307 0.336820 1.277139
C -5.080444 0.133423 -2.705939
H -5.811607 0.107018 -1.890081
H -4.952955 1.182749 -2.994577
H -5.506680 -0.401174 -3.558910
C -3.897720 4.207073 -0.592216
H -4.554096 3.795818 -1.367038
H -4.387434 4.035068 0.373287
H -3.830829 5.287669 -0.744323
C -5.247506 1.198978 2.188376
H -5.715101 1.084313 3.169792
H -5.241179 2.266943 1.942573
H -5.882802 0.699024 1.449192
S 2.447916 -1.425926 -0.310367
C 2.885201 -2.209117 -1.891961
H 2.076440 -2.902144 -2.118873
H 2.945254 -1.463561 -2.687833
H 3.827511 -2.753048 -1.795821
C 3.943848 -0.492398 0.039640
C 4.085477 -0.023833 1.363849
C 4.955705 -0.230108 -0.903179
C 5.234672 0.674560 1.737117
H 3.286093 -0.197833 2.075661
C 6.103610 0.471526 -0.515343
H 4.864630 -0.567228 -1.927947
C 6.248880 0.924630 0.800597
H 5.338305 1.024990 2.758789
H 6.882427 0.663056 -1.246704
H 7.140373 1.468716 1.094406

^{5}TS$_{SO,b}$

Fe 4.420343 2.139831 -0.624189
N 1.604106 1.709532 0.371174
N 2.210121 2.067079 -0.801607
N 3.378387 1.973335 2.211458
N 4.404039 2.569796 1.534022
N 3.214856 -0.177251 0.871090
N 4.225121 0.046482 -0.025802
B 2.413077 1.002144 1.498438
C 1.226734 2.369218 -1.684829
C 1.441667 2.688994 -3.109933
C 2.674883 3.148462 -3.613826
C 2.832239 3.412313 -4.979494
C 1.766584 3.230685 -5.868761
C 0.535341 2.777611 -5.378879
C 0.375915 2.507165 -4.017733
C -0.026396 2.238385 -1.037726
C 0.244948 1.812104 0.256243
C 5.108172 3.293758 2.436118
C 6.321934 4.072198 2.130211
C 7.191850 3.726854 1.078853
C 8.351483 4.471504 0.839459
C 8.671920 5.567810 1.649602
C 7.816595 5.918631 2.702259
C 6.654040 5.179828 2.938692
C 4.505615 3.156857 3.709041
C 3.417953 2.310755 3.536691
C 4.655616 -1.164048 -0.453267
C 5.756534 -1.349809 -1.414121
C 6.890469 -0.515395 -1.408337
C 7.932620 -0.727106 -2.317306
C 7.864860 -1.779631 -3.238500
C 6.745162 -2.621610 -3.246085
C 5.700349 -2.409115 -2.342350
C 3.900028 -2.174479 0.178694
C 2.997610 -1.518684 1.011498
H 5.978421 2.415437 -2.713704
H 1.644943 0.562809 2.298752
H 3.502361 3.332815 -2.937535
H 3.789833 3.770929 -5.344994
H 1.892297 3.438957 -6.926451
H -0.298996 2.626927 -6.056815
H -0.576943 2.132189 -3.660335
H -1.001756 2.433503 -1.452351
H 6.961841 2.889341 0.433926
H 9.004463 4.190269 0.019391
H 9.574853 6.140919 1.464005
H 8.051939 6.768310 3.335833
H 5.987612 5.472284 3.743281
H 4.839968 3.588635 4.638228
H 6.954643 0.296899 -0.694989
H 8.798740 -0.073296 -2.299422
H 8.676006 -1.943865 -3.940637
H 6.683226 -3.438963 -3.957642
H 4.827802 -3.054398 -2.363332
H 4.020834 -3.240304 0.071497
O 4.987962 3.859592 -1.438623
O 6.148650 2.522386 -1.762302
C 2.446719 1.816442 4.564346
H 1.416426 2.106635 4.329541
H 2.464133 0.724627 4.654903
H 2.700687 2.239243 5.540009
C 1.969303 -2.114364 1.923153
H 2.124225 -1.815325 2.965579
H 0.952707 -1.814131 1.645536
H 2.023143 -3.204968 1.872845
C -0.720241 1.504629 1.359734
H -1.735380 1.752453 1.038303
H -0.704720 0.444400 1.636738
H -0.502099 2.079926 2.266138
S 3.727393 5.690793 -1.222758
C 5.220722 6.726872 -1.312102
H 5.643806 6.545545 -2.301733
H 4.969622 7.785353 -1.208752
H 5.951709 6.422088 -0.561427
C 3.020383 6.116227 0.363313
C 1.718131 5.636075 0.615038
C 3.678000 6.878263 1.344417
C 1.087126 5.922900 1.827810
H 1.205832 5.041079 -0.134673
C 3.032327 7.165110 2.553963
H 4.684403 7.242654 1.182292
C 1.739557 6.691584 2.801753
H 0.083372 5.551478 2.007961
H 3.547478 7.758981 3.302457
H 1.245176 6.918190 3.740608

^{3}TS$_{SO,b}$

Fe 4.355211 2.039098 -0.556967
N 1.598335 1.687717 0.325386
N 2.234917 2.031904 -0.836957
N 3.337459 2.013053 2.188570
N 4.384562 2.557433 1.501430
N 3.217486 -0.151858 0.893842
N 4.198926 0.107608 -0.023420
B 2.385157 1.014799 1.490799
C 1.275976 2.351629 -1.740092
C 1.522665 2.664962 -3.161265

C 2.756733 3.156888 -3.631305
C 2.943759 3.422334 -4.992909
C 1.908046 3.208993 -5.910497
C 0.676700 2.723241 -5.453595
C 0.487160 2.451579 -4.096252
C 0.007757 2.241090 -1.118453
C 0.244353 1.817166 0.183132
C 5.076678 3.328748 2.370399
C 6.320119 4.045966 2.040410
C 7.205638 3.585691 1.047443
C 8.395274 4.270094 0.780328
C 8.730436 5.420045 1.506280
C 7.860989 5.883973 2.501877
C 6.668192 5.204373 2.765773
C 4.440765 3.281487 3.634200
C 3.344792 2.440181 3.488091
C 4.676311 -1.086272 -0.448622
C 5.762842 -1.253815 -1.431103
C 6.932558 -0.471846 -1.388650
C 7.962283 -0.683406 -2.311934
C 7.845013 -1.682659 -3.285939
C 6.689389 -2.473126 -3.330928
C 5.658266 -2.261907 -2.410934
C 3.974301 -2.121968 0.208785
C 3.059803 -1.499945 1.051958
H 5.656346 2.240597 -2.712534
H 1.606866 0.585998 2.287949
H 3.554709 3.362662 -2.925659
H 3.900243 3.807235 -5.334088
H 2.057056 3.418140 -6.965031
H -0.134012 2.548068 -6.153964
H -0.464385 2.051786 -3.762628
H -0.954551 2.449834 -1.556367
H 6.961188 2.700377 0.474658
H 9.061343 3.900918 0.006969
H 9.656921 5.946654 1.300299
H 8.109484 6.774967 3.070323
H 5.991476 5.581820 3.525090
H 4.760387 3.766136 4.542356
H 7.033878 0.298154 -0.634339
H 8.856887 -0.070647 -2.265291
H 8.646138 -1.845913 -3.999780
H 6.589482 -3.249853 -4.082598
H 4.759254 -2.868611 -2.455858
H 4.142193 -3.181829 0.105616
O 4.876440 3.720451 -1.319221
O 5.923630 2.350503 -1.783382
C 2.335007 2.026537 4.513896
H 1.318917 2.326715 4.233602
H 2.323707 0.941305 4.664563
H 2.571552 2.497643 5.471590
C 2.071644 -2.121138 1.990040
H 2.235705 -1.803794 3.025912
H 1.039685 -1.860232 1.729011
H 2.163245 -3.209737 1.951878
C -0.746407 1.534338 1.270396
H -1.753585 1.774999 0.919941
H -0.736807 0.480512 1.570940
H -0.549973 2.129753 2.168981
S 3.630028 5.545882 -1.017669
C 5.106568 6.592637 -1.203246
H 5.517578 6.344990 -2.183428
H 4.844025 7.652957 -1.173497
H 5.852375 6.353250 -0.443298
C 2.971308 6.034876 0.571598
C 1.712274 5.498941 0.914925
C 3.617907 6.906226 1.465313
C 1.113881 5.836871 2.130974
H 1.206374 4.824208 0.231048
C 3.004417 7.243549 2.678741
H 4.590651 7.319679 1.231720
C 1.755349 6.712874 3.017764
H 0.142817 5.421803 2.381632
H 3.509751 7.923117 3.357932
H 1.285599 6.978886 3.958912
^{5}PC
Fe 0.332073 0.069975 0.233594
N 3.234526 -0.889708 -0.433104
N 2.550318 -0.523258 0.689787
N 2.261541 0.887870 -1.959324
N 1.342813 1.450160 -1.120546
N 1.426917 -1.537194 -2.076646
N 0.424609 -1.617805 -1.151166
B 2.652845 -0.610558 -1.841741
C 3.273414 -0.957019 1.744426
C 2.898825 -0.699458 3.146275
C 2.387660 0.550575 3.550086
C 2.064820 0.789242 4.890968
C 2.256850 -0.211220 5.852303
C 2.777378 -1.452269 5.463881
C 3.095485 -1.694535 4.124013
C 4.430499 -1.628821 1.284315
C 4.379432 -1.566137 -0.103513
C 1.294690 2.771231 -1.407255
C 0.467240 3.742356 -0.673086
C 0.069728 4.939911 -1.305307
C -0.676966 5.900147 -0.617038
C -1.045910 5.683431 0.717604
C -0.660241 4.497242 1.354784
C 0.092818 3.536682 0.669880
C 2.191925 3.049024 -2.463469
C 2.792440 1.837769 -2.788125
C -0.392846 -2.626058 -1.533655
C -1.540200 -3.101389 -0.743127
C -1.629376 -2.874571 0.644662
C -2.697390 -3.393384 1.383294
C -3.689453 -4.157403 0.756386
C -3.611529 -4.389053 -0.622912
C -2.550598 -3.863593 -1.365283
C 0.090619 -3.179747 -2.742104
C 1.244257 -2.471665 -3.058466
H 0.169394 0.077977 2.697259
H 3.478569 -0.854297 -2.668645
H 2.265903 1.336920 2.812928
H 1.674145 1.758430 5.184764
H 2.008150 -0.024286 6.891989
H 2.929556 -2.233151 6.202397
H 3.485238 -2.662663 3.825633
H 5.215932 -2.060562 1.884128
H 0.338783 5.111066 -2.342450
H -0.972235 6.814601 -1.121893
H -1.622379 6.430361 1.253846
H -0.938000 4.318110 2.388588
H 0.388051 2.628762 1.185026
H 2.404841 4.008656 -2.905752
H -0.868551 -2.290650 1.150351
H -2.748077 -3.204527 2.450945
H -4.512408 -4.566101 1.334121
H -4.375959 -4.978043 -1.120689
H -2.507306 -4.039976 -2.435227
H -0.318412 -4.012368 -3.290961
O -1.678897 0.605261 -0.686576
O -0.435749 0.204292 1.951412
C 3.837004 1.564023 -3.826209
H 4.765407 1.185935 -3.383906
H 3.501554 0.823056 -4.560128
H 4.070679 2.487744 -4.362203
C 2.163661 -2.658877 -4.226228
H 2.265722 -1.742668 -4.818337
H 3.170731 -2.957275 -3.913781
H 1.768969 -3.440312 -4.881055
C 5.359937 -2.098086 -1.103484
H 6.201533 -2.561519 -0.581573
H 4.911601 -2.856220 -1.756135
H 5.756959 -1.307052 -1.749545
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C -3.208938 2.720951 -1.211604
H -2.354771 3.370687 -1.411091
H -3.500830 2.181159 -2.115564
H -4.045932 3.307636 -0.824248
C -4.243112 0.583884 0.160332
C -5.182498 0.978143 1.123124
C -4.488726 -0.493407 -0.696669
C -6.403507 0.298210 1.203823
H -4.963681 1.795835 1.803838
C -5.710330 -1.170360 -0.602934
H -3.726585 -0.808244 -1.400523
C -6.667683 -0.771973 0.339162
H -7.138199 0.596244 1.944408
H -5.906789 -2.012877 -1.256709
H -7.612321 -1.301513 0.407916
^{3}PC
Fe -0.338456 -0.162906 0.110559
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N -1.951521 -0.868598 1.116772
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N -1.606602 -0.120401 -1.544892
N -2.249528 2.175785 0.539358
N -0.925301 2.131345 0.218784
B -3.191960 1.049469 0.046639
C -2.156727 -1.851862 2.022299
C -1.160965 -2.873619 2.391611
C -0.342304 -3.490055 1.427482
C 0.555684 -4.497688 1.791156
C 0.649123 -4.911371 3.126547
C -0.166018 -4.310489 4.093538
C -1.065323 -3.303622 3.728968
C -3.488189 -1.773342 2.490087
C -4.075540 -0.707501 1.815620
C -1.521781 -0.412480 -2.862773
C -0.511701 -1.307589 -3.453941
C 0.024180 -1.029296 -4.726602
C 0.913024 -1.919758 -5.338883
C 1.280518 -3.107219 -4.691719
C 0.752583 -3.395185 -3.424975
C -0.136305 -2.504868 -2.813093
C -2.613883 0.173870 -3.542491
C -3.377476 0.807371 -2.567537
C -0.366848 3.242955 0.744619
C 1.024885 3.649162 0.484304
C 1.610917 3.440582 -0.780503
C 2.893110 3.925251 -1.059844
C 3.616025 4.621853 -0.080860
C 3.046297 4.825216 1.183129
C 1.762037 4.346280 1.461873
C -1.347707 3.990945 1.438299
C -2.537638 3.286404 1.285532
H 1.406992 0.355216 1.634286
H -4.319117 1.450773 0.012658
H -0.418968 -3.182716 0.390605
H 1.174035 -4.967321 1.031953
H 1.344701 -5.695508 3.408706
H -0.100391 -4.622960 5.131102
H -1.685544 -2.831990 4.484462
H -3.966983 -2.435271 3.193694
H -0.254475 -0.109418 -5.230681
H 1.314918 -1.688675 -6.320433
H 1.961772 -3.803008 -5.170963
H 1.019237 -4.319647 -2.922067
H -0.567460 -2.744079 -1.847136
H -2.840436 0.097350 -4.593906
H 1.048222 2.909426 -1.539371
H 3.322387 3.772218 -2.045679
H 4.606388 5.007179 -0.302762
H 3.598706 5.360925 1.949026
H 1.325491 4.506545 2.442681
H -1.218667 4.940830 1.932805
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O 0.698627 -0.307079 1.659228
C -4.658639 1.567021 -2.722867
H -5.480102 1.103044 -2.165368
H -4.567201 2.599369 -2.366919
H -4.941282 1.598066 -3.778509
C -3.904041 3.623985 1.797311
H -4.648979 3.647159 0.994243
H -4.251790 2.899925 2.544078
H -3.887627 4.608178 2.273406
C -5.482230 -0.200979 1.908313
H -6.046185 -0.816116 2.614610
H -5.526590 0.836782 2.256623

H -5.994958 -0.240064 0.940695
S 2.427472 -1.113110 -0.813784
C 3.440684 -0.923337 -2.317201
H 2.817654 -1.205602 -3.167112
H 3.757754 0.118211 -2.404378
H 4.308040 -1.584557 -2.245782
C 3.643532 -0.549547 0.404768
C 4.165695 -1.514604 1.276572
C 4.043104 0.790299 0.479134
C 5.123714 -1.131831 2.222965
H 3.814548 -2.540571 1.233276
C 4.991422 1.163514 1.437903
H 3.604865 1.534018 -0.176362
C 5.535333 0.204408 2.303301
H 5.532219 -1.871046 2.903495
H 5.295349 2.202128 1.509507
H 6.269641 0.499950 3.045299

2.2. Cyclohexane oxidation

^{5}RC

Fe 3.257530 1.552865 0.147592
N 0.877177 -0.227897 0.345328
N 1.256751 0.922711 -0.285957
N 2.122231 0.119405 2.533824
N 2.805801 1.276501 2.278557
N 3.127178 -1.352489 0.715052
N 3.948219 -0.450813 0.092290
B 1.808694 -0.891918 1.401966
C 0.284112 1.237092 -1.171903
C 0.330246 2.440628 -2.018363
C 0.873519 3.651345 -1.541549
C 0.906106 4.787420 -2.359351
C 0.385664 4.736502 -3.659506
C -0.170338 3.542635 -4.135505
C -0.197517 2.404616 -3.323546
C -0.732311 0.259658 -1.107527
C -0.328542 -0.654165 -0.136888
C 2.870735 1.966698 3.438684
C 3.542883 3.269733 3.581248
C 4.666272 3.616290 2.806595
C 5.296079 4.853194 2.977956
C 4.822997 5.761854 3.932830
C 3.709792 5.425136 4.714010
C 3.075206 4.192660 4.539232
C 2.209628 1.233958 4.452068
C 1.749137 0.069125 3.850363
C 4.985995 -1.143486 -0.435072
C 6.099469 -0.517026 -1.166748
C 6.558915 0.776599 -0.854151
C 7.629385 1.339987 -1.555509
C 8.266829 0.617832 -2.571487
C 7.823821 -0.673656 -2.884911
C 6.749858 -1.235744 -2.190401
C 4.814392 -2.513978 -0.146293
C 3.632360 -2.614097 0.583297
H 3.286512 3.469714 -2.055834
H 1.257683 -1.843964 1.862798
H 1.251615 3.708485 -0.526132
H 1.322571 5.713046 -1.974472
H 0.408295 5.618561 -4.290935
H -0.575909 3.494880 -5.141000
H -0.611996 1.477383 -3.705863
H -1.654449 0.240568 -1.665573
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H 6.158743 5.102519 2.368656
H 5.316194 6.719078 4.067674
H 3.332659 6.123827 5.454162
H 2.202344 3.947252 5.135510
H 2.112411 1.501953 5.491623
H 6.085701 1.345004 -0.060986
H 7.965616 2.340586 -1.304320
H 9.098757 1.056084 -3.113200
H 8.309249 -1.239367 -3.673836
H 6.398652 -2.228785 -2.451641
H 5.479826 -3.321643 -0.404202
O 4.016092 3.240910 -0.288765
O 4.050319 2.948796 -1.740462
C 0.993508 -1.067087 4.467904
H 0.005596 -1.198925 4.012075
H 1.527902 -2.018353 4.367760
H 0.848015 -0.872983 5.533763
C 2.989898 -3.840653 1.153792
H 2.864011 -3.768453 2.239497
H 1.999288 -4.023097 0.722261
H 3.614025 -4.712700 0.942813
C -1.038410 -1.881403 0.345848
H -1.991140 -1.984910 -0.179700
H -0.453917 -2.790619 0.165940
H -1.247954 -1.836319 1.420250
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C 3.556068 9.279245 0.082336
C 4.970831 9.843103 0.329300
C 6.008865 9.191809 -0.607979
C 5.986386 7.653705 -0.491733
C 4.572861 7.086424 -0.737642
H 2.528259 7.360085 -0.028495
H 3.752832 7.450278 1.235670
H 3.223944 9.570909 -0.926332
H 2.842545 9.723625 0.789446
H 4.972988 10.933762 0.199010
H 5.257995 9.649476 1.374534
H 5.785008 9.478127 -1.647447
H 7.013766 9.575466 -0.385348
H 6.700620 7.209312 -1.197735
H 6.319124 7.364048 0.517377
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^{3}RC

Fe 3.621059 1.505837 0.167392
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C 0.578396 1.320152 -1.383724
C 0.757962 2.387831 -2.383373
C 1.363333 3.618185 -2.052058
C 1.511870 4.621442 -3.019075
C 1.047188 4.420350 -4.324667
C 0.431011 3.207387 -4.658506
C 0.289387 2.200259 -3.699322
C -0.527171 0.447088 -1.267484
C -0.255224 -0.370353 -0.175120
C 3.354131 2.195095 3.176731
C 4.318411 3.308181 3.215584
C 5.591766 3.197780 2.625606
C 6.511172 4.246703 2.714683
C 6.178322 5.420202 3.403391
C 4.917775 5.537113 4.003579
C 3.995729 4.490029 3.911290
C 2.539135 1.743649 4.238682
C 1.854934 0.630714 3.760046
C 4.894862 -1.312843 -0.390689
C 6.047262 -0.822053 -1.163501
C 6.708129 0.375707 -0.829911
C 7.803059 0.819144 -1.578460
C 8.265573 0.066663 -2.664780
C 7.624684 -1.133743 -2.997880
C 6.525564 -1.573661 -2.255863
C 4.558746 -2.653255 -0.098402
C 3.397843 -2.604408 0.668639
H 3.493061 2.866348 -2.017323
H 1.157846 -1.475475 2.003668
H 1.698755 3.794532 -1.034967
H 1.980153 5.561442 -2.744646
H 1.159591 5.199831 -5.071117
H 0.068001 3.042163 -5.668009
H -0.171976 1.256235 -3.970858
H -1.418778 0.438590 -1.873741
H 5.862544 2.282323 2.111313
H 7.489311 4.144877 2.255517
H 6.895010 6.231897 3.476295
H 4.652418 6.441992 4.541006
H 3.015837 4.589009 4.367435
H 2.490339 2.152603 5.234858
H 6.380454 0.951060 0.029783
H 8.297968 1.746099 -1.307535
H 9.116829 0.410192 -3.243417
H 7.976134 -1.722903 -3.838938
H 6.020584 -2.493916 -2.531363
H 5.108655 -3.536912 -0.378872
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O 4.258570 2.637518 -1.445645
C 0.869457 -0.244538 4.470340
H -0.112566 -0.232405 3.983838
H 1.201214 -1.288036 4.508356
H 0.740058 0.106961 5.497197
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H 2.519425 -3.646703 2.343647
H 1.596453 -3.785490 0.845857
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C -1.095060 -1.465810 0.407283
H -2.039506 -1.533883 -0.138987
H -0.600335 -2.441827 0.344610
H -1.327109 -1.286955 1.462996
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C 2.446941 9.029442 0.890808
C 3.759542 9.756226 1.249777
C 4.853198 9.499307 0.192278
C 5.085929 7.989590 -0.023580
C 3.774549 7.259659 -0.380903
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H 2.985206 7.060283 1.627360
H 2.034313 9.466630 -0.031905
H 1.697357 9.189896 1.677574
H 3.579946 10.834663 1.356087
H 4.113953 9.396954 2.228464
H 4.546572 9.957354 -0.761158
H 5.790170 9.989589 0.489627
H 5.834853 7.830502 -0.811095
H 5.499067 7.551013 0.897683
H 3.421099 7.616047 -1.362021
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^{5}TS$_{OO}$

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C -0.029313 2.497333 -1.635279
C 0.413539 3.709446 -1.068123
C 0.261972 4.914686 -1.762801
C -0.344207 4.931697 -3.025172
C -0.799582 3.733857 -3.590888
C -0.642752 2.527248 -2.903658
C -0.788846 0.128575 -0.927155
C -0.240115 -0.832701 -0.080289
C 2.883278 1.854663 3.484481
C 3.452445 3.202037 3.658286
C 4.577125 3.633040 2.928739
C 5.110269 4.909620 3.134323
C 4.536245 5.772592 4.076005
C 3.422150 5.350658 4.813061
C 2.885062 4.077134 4.606664
C 2.334120 1.027801 4.487640
C 1.948951 -0.151773 3.854556
C 5.087785 -0.810970 -0.602878
C 6.140635 -0.040063 -1.285746
C 6.610306 1.187222 -0.781529
C 7.628881 1.882242 -1.440365
C 8.202211 1.359306 -2.605566
C 7.749104 0.133820 -3.110457
C 6.727806 -0.559976 -2.456810
C 5.006438 -2.213679 -0.478510
C 3.865193 -2.474807 0.275526

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H 1.534608 -2.011735 1.771040
H 0.862929 3.713209 -0.081080
H 0.609527 5.838656 -1.312248
H -0.462417 5.867898 -3.560788
H -1.268049 3.738016 -4.569788
H -0.977476 1.599621 -3.356430
H -1.731084 0.065046 -1.446720
H 5.036079 2.969623 2.205745
H 5.976773 5.225916 2.562818
H 4.953450 6.761639 4.235264
H 2.969205 6.013787 5.543194
H 2.011858 3.761266 5.168562
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H 8.993414 1.900276 -3.114513
H 8.185327 -0.277353 -4.015240
H 6.367033 -1.499502 -2.863003
H 5.707673 -2.939712 -0.856279
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O 3.509657 2.497035 -1.866383
C 1.320224 -1.373078 4.450385
H 0.317187 -1.553757 4.047305
H 1.915518 -2.272567 4.259968
H 1.230115 -1.249342 5.532468
C 3.321979 -3.799000 0.715754
H 3.262922 -3.873983 1.807082
H 2.316169 -3.980943 0.321283
H 3.973622 -4.599430 0.356634
C -0.788779 -2.176418 0.287781
H -1.753652 -2.326053 -0.203100
H -0.123172 -2.989009 -0.024374
H -0.939123 -2.274406 1.368316
C 3.692009 7.562018 -0.224090
C 3.819175 9.095962 -0.326417
C 5.199977 9.580006 0.163366
C 6.345208 8.866558 -0.584765
C 6.215897 7.332565 -0.481421
C 4.836060 6.845299 -0.970615
H 2.721000 7.235288 -0.620840
H 3.714006 7.266111 0.836172
H 3.682877 9.400072 -1.375963
H 3.021024 9.584063 0.249340
H 5.286469 10.668262 0.041435
H 5.291412 9.374559 1.241315
H 6.319089 9.158808 -1.646119
H 7.317018 9.194755 -0.191534
H 7.015189 6.845141 -1.055702
H 6.352799 7.030088 0.568859
H 4.746294 7.048819 -2.049289
H 4.745483 5.759483 -0.841692

^{3}**TS**$_{OO}$

Fe 3.574252 1.554092 0.189557
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N 2.354112 0.277968 2.481632
N 3.168462 1.318679 2.132255
N 3.149976 -1.301811 0.680873
N 4.010173 -0.430273 0.075162
B 1.896276 -0.754816 1.422527
C 0.444930 1.309361 -1.212178
C 0.533260 2.431696 -2.163228
C 1.131677 3.658741 -1.810120
C 1.191083 4.711914 -2.731645
C 0.642273 4.564811 -4.011449
C 0.032711 3.354409 -4.366211
C -0.019654 2.297558 -3.453001
C -0.626510 0.394523 -1.082019
C -0.268701 -0.471312 -0.055030
C 3.380163 2.062077 3.244512
C 4.251919 3.248163 3.303647
C 5.497515 3.284703 2.648663
C 6.328942 4.402721 2.761942
C 5.934248 5.500050 3.537688
C 4.699875 5.472161 4.199848
C 3.866453 4.355674 4.085201
C 2.665739 1.485925 4.317981
C 2.030441 0.358890 3.806279
C 4.939272 -1.164577 -0.584836
C 6.070205 -0.577709 -1.324264
C 6.802907 0.508019 -0.808412
C 7.883751 1.038650 -1.519146
C 8.257167 0.485680 -2.750174
C 7.544127 -0.604284 -3.265560
C 6.460431 -1.132989 -2.558755
C 4.648343 -2.532092 -0.404722
C 3.511147 -2.586462 0.400346
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H 1.325003 -1.656131 1.957852
H 1.537983 3.789576 -0.813313
H 1.658079 5.648087 -2.442499
H 0.686119 5.383406 -4.722461
H -0.394310 3.230431 -5.356426
H -0.476126 1.356210 -3.741667
H -1.550783 0.390170 -1.637169
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H 7.286412 4.414255 2.251239
H 6.582977 6.365263 3.628709
H 4.386245 6.318198 4.803028
H 2.905906 4.342505 4.590231
H 2.651711 1.826595 5.340524
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H 8.436957 1.877153 -1.108752
H 9.096683 0.897729 -3.300591
H 7.827738 -1.038190 -4.219077
H 5.899513 -1.966854 -2.968658
H 5.215047 -3.369256 -0.778732
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O 4.164002 2.535030 -1.556877
C 1.156770 -0.629389 4.514576
H 0.148058 -0.663166 4.087612
H 1.565311 -1.644788 4.466206
H 1.067255 -0.350483 5.567567
C 2.779527 -3.790084 0.908016
H 2.704779 -3.790990 2.000654
H 1.759485 -3.845627 0.511069
H 3.307723 -4.696881 0.602896
C -1.038101 -1.624040 0.513849
H -2.011218 -1.694705 0.020855
H -0.518853 -2.578394 0.368904
H -1.212046 -1.509337 1.589536
C 2.826223 7.468956 0.577652
C 2.575772 8.986900 0.693649
C 3.866736 9.744210 1.067858
C 5.009036 9.433933 0.078238
C 5.258903 7.915949 -0.037718
C 3.969224 7.156111 -0.410520
H 1.905819 6.956259 0.266576
H 3.089741 7.068237 1.568411
H 2.202735 9.366136 -0.270621
H 1.790546 9.187021 1.435265
H 3.676621 10.825561 1.101320
H 4.177660 9.446554 2.081308
H 4.744166 9.832829 -0.913447
H 5.928965 9.947963 0.388451
H 6.043788 7.716883 -0.779790
H 5.631915 7.535479 0.925640
H 3.659386 7.451296 -1.425882
H 4.159798 6.074447 -0.435814

^{5}**IM**$_{OO}$

Fe -0.388385 0.038869 0.009306
N -3.098734 -0.553482 1.121167
N -1.774872 -0.738570 1.394032
N -2.811215 -1.086188 -1.298998
N -1.444882 -1.137617 -1.358380
N -3.083028 1.330823 -0.574214
N -1.763995 1.681285 -0.496492
B -3.521804 -0.127689 -0.310681
C -1.675452 -1.164531 2.676734
C -0.412949 -1.570784 3.315290
C 0.564178 -2.296768 2.607654
C 1.742139 -2.705127 3.239516
C 1.958428 -2.404493 4.590479
C 0.986209 -1.694976 5.306604
C -0.191366 -1.283651 4.675390
C -2.970326 -1.226186 3.232653
C -3.849576 -0.836375 2.223299
C -1.112790 -2.128619 -2.225448
C 0.259788 -2.538616 -2.597980
C 1.168097 -1.647890 -3.198682
C 2.429347 -2.092985 -3.607525
C 2.800816 -3.431563 -3.426397
C 1.900455 -4.327649 -2.837638
C 0.636561 -3.885606 -2.431909
C -2.296909 -2.715051 -2.714517
C -3.353600 -2.032036 -2.116090
C -1.695848 3.027121 -0.625815
C -0.453868 3.822284 -0.598244
C 0.744682 3.365202 -1.178129
C 1.890832 4.167406 -1.160691
C 1.859868 5.437687 -0.572253
C 0.670585 5.903394 0.002707
C -0.475715 5.104122 -0.011014
C -3.004248 3.536509 -0.790559
C -3.859460 2.440952 -0.754056
H 1.305536 1.114479 1.153067
H -4.705095 -0.222134 -0.428182
H 0.393640 -2.556792 1.567793
H 2.485704 -3.264171 2.680392
H 2.872744 -2.723360 5.080512
H 1.146560 -1.457593 6.353467
H -0.934226 -0.718215 5.228817
H -3.233586 -1.557390 4.224060
H 0.885865 -0.611848 -3.335954
H 3.119650 -1.395153 -4.070297
H 3.780370 -3.773314 -3.745341
H 2.178900 -5.367110 -2.696126
H -0.062559 -4.581419 -1.978330
H -2.365966 -3.514055 -3.434628
H 0.779370 2.381819 -1.630661
H 2.806394 3.800146 -1.613817
H 2.750763 6.057579 -0.561772
H 0.636558 6.884686 0.465493
H -1.389469 5.464340 0.450711
H -3.282180 4.565768 -0.949128
O 0.891039 0.226034 -0.986182
O 0.435523 0.787633 1.436441
C -4.825449 -2.233695 -2.302127
H -5.320799 -2.516609 -1.366736
H -5.317487 -1.327059 -2.670848
H -4.996566 -3.031063 -3.029545
C -5.350424 2.409709 -0.892349
H -5.670201 1.776947 -1.727565
H -5.839431 2.028288 0.011136
H -5.722319 3.421390 -1.073440
C -5.342987 -0.739464 2.262194
H -5.706067 -1.049635 3.245176
H -5.689998 0.284693 2.083850
H -5.813962 -1.380129 1.508677
C 4.982629 1.541007 0.499422
C 6.503311 1.652422 0.735181
C 7.147366 0.263352 0.926292
C 6.825060 -0.677106 -0.253773
C 5.304093 -0.786418 -0.487072
C 4.661447 0.602261 -0.681920
H 4.551241 2.535378 0.321893
H 4.505231 1.149291 1.411638
H 6.966801 2.148372 -0.132030
H 6.707663 2.287635 1.607598
H 8.234651 0.362721 1.046629
H 6.766288 -0.184481 1.857214
H 7.302586 -0.287422 -1.166439
H 7.255359 -1.671590 -0.073514
H 5.095313 -1.424898 -1.355743
H 4.840611 -1.278218 0.382638
H 5.048619 1.049685 -1.611338
H 3.575577 0.502165 -0.805115

^{3}**IM**$_{OO}$

Fe -0.452792 0.201881 -0.247898

N -2.863006 -0.373733 1.427037
N -1.501769 -0.440285 1.487791
N -2.961144 -1.251844 -0.903635
N -1.614906 -1.302099 -1.128660
N -3.107937 1.230639 -0.485464
N -1.784570 1.548221 -0.600915
B -3.522209 -0.168656 0.040298
C -1.165890 -0.710373 2.770146
C 0.208611 -0.968289 3.232431
C 1.101868 -1.743530 2.468919
C 2.385625 -2.023118 2.945697
C 2.796298 -1.537858 4.194315
C 1.911597 -0.773955 4.965316
C 0.626449 -0.494653 4.490197
C -2.346676 -0.790508 3.542447
C -3.405005 -0.577051 2.662611
C -1.355265 -2.469661 -1.765242
C -0.024315 -2.968919 -2.177867
C 0.845889 -2.230550 -3.001082
C 2.065777 -2.778272 -3.412768
C 2.434235 -4.069734 -3.015368
C 1.571196 -4.816720 -2.204204
C 0.350340 -4.272568 -1.792969
C -2.571363 -3.167214 -1.945923
C -3.568627 -2.373363 -1.390272
C -1.686590 2.878873 -0.857099
C -0.442109 3.654948 -1.038159
C 0.548231 3.292295 -1.969582
C 1.681039 4.095451 -2.143266
C 1.838120 5.270845 -1.398179
C 0.851538 5.644589 -0.477131
C -0.282205 4.845912 -0.301623
C -2.991336 3.406682 -0.906980
C -3.864739 2.347028 -0.667427
H 1.287378 1.586002 0.380253
H -4.710580 -0.240865 0.116482
H 0.785281 -2.136471 1.508196
H 3.061570 -2.625173 2.346850
H 3.793354 -1.756231 4.563299
H 2.221995 -0.393206 5.933228
H -0.051954 0.109216 5.084517
H -2.416618 -1.019828 4.593429
H 0.569012 -1.229820 -3.304960
H 2.725779 -2.196380 -4.048162
H 3.381423 -4.490696 -3.337473
H 1.846658 -5.819126 -1.891942
H -0.316688 -4.852416 -1.162605
H -2.697923 -4.114501 -2.444549
H 0.435537 2.380962 -2.542700
H 2.436819 3.804323 -2.865637
H 2.718344 5.890628 -1.535916
H 0.964815 6.553605 0.104811
H -1.041492 5.132076 0.419014
H -3.257245 4.428979 -1.120068
O 0.503077 0.305936 -1.539153
O 0.593458 1.142923 0.895518
C -5.042710 -2.624673 -1.310772
H -5.385507 -2.732739 -0.275243
H -5.619870 -1.810466 -1.762358
H -5.286651 -3.547770 -1.842643
C -5.360464 2.356687 -0.613243
H -5.797265 1.651716 -1.328489
H -5.735038 2.088881 0.380871
H -5.728650 3.356834 -0.854389
C -4.876861 -0.572134 2.937040
H -5.054654 -0.778555 3.995415
H -5.332385 0.396797 2.702410
H -5.405671 -1.332072 2.350884
C 4.565358 1.546980 0.009085
C 6.055483 1.638885 0.398122
C 6.585793 0.285384 0.915628
C 6.337831 -0.845890 -0.104111
C 4.847609 -0.935941 -0.492256
C 4.315872 0.416110 -1.010710
H 4.218039 2.506681 -0.397046
H 3.969692 1.352137 0.914687
H 6.640887 1.942287 -0.483933
H 6.202851 2.418415 1.157738
H 7.657110 0.360573 1.146444
H 6.075335 0.037178 1.859002
H 6.935670 -0.653188 -1.008652
H 6.683967 -1.805468 0.303521
H 4.695916 -1.717454 -1.248783
H 4.262699 -1.234766 0.391318
H 4.824615 0.664835 -1.955627
H 3.244506 0.338073 -1.235684
^{5}TS$_{H,\mathrm{a}}$
Fe -0.211911 0.041175 0.042163
N -2.693712 -0.998399 1.271258
N -1.343659 -0.953436 1.461109
N -2.468264 -1.446184 -1.177002
N -1.119959 -1.255768 -1.334008
N -3.127801 0.871397 -0.386589
N -1.889820 1.446241 -0.412924
B -3.272569 -0.643970 -0.125420
C -1.097923 -1.327535 2.740507
C 0.252004 -1.506471 3.298822
C 1.279447 -2.102042 2.542596
C 2.544444 -2.308007 3.101409
C 2.801173 -1.928607 4.425261
C 1.782175 -1.344786 5.188470
C 0.516702 -1.138380 4.631469
C -2.326676 -1.593051 3.378321
C -3.318356 -1.376531 2.421520
C -0.697725 -2.152533 -2.262213
C 0.683151 -2.320988 -2.773195
C 1.327295 -1.316490 -3.517656
C 2.588913 -1.547328 -4.074333
C 3.225973 -2.783273 -3.897383
C 2.590436 -3.791522 -3.163312
C 1.323956 -3.563790 -2.611934
C -1.798490 -2.922851 -2.688253
C -2.905312 -2.449035 -1.989791
C -2.072365 2.780092 -0.546911
C -0.985969 3.772162 -0.635748
C 0.239089 3.481680 -1.266408
C 1.232662 4.461880 -1.367997
C 1.021681 5.745335 -0.848375
C -0.194408 6.043534 -0.220857
C -1.188903 5.067006 -0.116333
C -3.459170 3.052236 -0.606718
C -4.101612 1.823833 -0.503290
H 1.208470 1.606279 1.001228
H -4.424705 -0.952491 -0.171377
H 1.079325 -2.421835 1.524826
H 3.324430 -2.775024 2.508417
H 3.782669 -2.091483 4.858880
H 1.973187 -1.047589 6.214733
H -0.266291 -0.672187 5.220877
H -2.470223 -1.943318 4.387622
H 0.840814 -0.358183 -3.648081
H 3.073365 -0.764066 -4.648810
H 4.204759 -2.959513 -4.332515
H 3.074072 -4.753286 -3.024033
H 0.827108 -4.349195 -2.050564
H -1.784255 -3.703673 -3.431267
H 0.413812 2.488582 -1.664535
H 2.169312 4.223677 -1.862901
H 1.793906 6.503562 -0.931693
H -0.367153 7.033176 0.190428
H -2.122470 5.301269 0.385097
H -3.926967 4.013645 -0.744167
O 1.056879 0.348830 -1.143268
O 0.517193 1.030441 1.364842
C -4.330789 -2.899442 -2.077911
H -4.699436 -3.281768 -1.119643
H -4.998020 -2.085629 -2.382422
H -4.415961 -3.700554 -2.816504
C -5.569728 1.527406 -0.524031
H -5.836821 0.839175 -1.333613
H -5.911758 1.074738 0.413609
H -6.128626 2.455169 -0.671503
C -4.801934 -1.526398 2.555935
H -5.045620 -1.890935 3.557015
H -5.322846 -0.573147 2.410095
H -5.208713 -2.235924 1.827316
C 3.711316 1.868454 0.607094
C 5.238948 2.085744 0.805342
C 5.969069 0.742450 1.002378
C 5.689789 -0.231272 -0.159928
C 4.163228 -0.438545 -0.370135
C 3.470870 0.905200 -0.546732
H 3.218525 2.832852 0.430081
H 3.304496 1.449397 1.538986
H 5.647402 2.599935 -0.077062
H 5.406705 2.745260 1.666872
H 7.049751 0.912695 1.099568
H 5.634477 0.285555 1.945940
H 6.128127 0.170590 -1.085462
H 6.171165 -1.200594 0.026265
H 3.986505 -1.086076 -1.236233
H 3.752431 -0.949937 0.512870
H 3.670105 1.361541 -1.526224
H 2.159645 0.638657 -0.734836
^{3}TS$_{H,\mathrm{a}}$
Fe -0.208578 0.071077 0.042125
N -2.641182 -1.085157 1.275023
N -1.292917 -0.983299 1.454458
N -2.410227 -1.519043 -1.176153
N -1.070697 -1.276881 -1.337343
N -3.171368 0.764494 -0.372739
N -1.960179 1.392149 -0.389941
B -3.243891 -0.755430 -0.116928
C -1.020765 -1.370518 2.724793
C 0.338530 -1.501964 3.274095
C 1.383078 -2.054122 2.508503
C 2.655074 -2.226276 3.063063
C 2.902923 -1.853397 4.390469
C 1.868004 -1.309839 5.161835
C 0.595003 -1.139085 4.609868
C -2.231083 -1.701294 3.367336
C -3.239038 -1.513617 2.421504
C -0.617670 -2.156668 -2.266945
C 0.767522 -2.266538 -2.782690
C 1.360709 -1.238834 -3.537996
C 2.630213 -1.413631 -4.097090
C 3.325790 -2.616473 -3.912497
C 2.740993 -3.647921 -3.168454
C 1.466828 -3.476180 -2.614169
C -1.688385 -2.969243 -2.690035
C -2.810262 -2.538835 -1.987083
C -2.201101 2.717323 -0.518827
C -1.158973 3.757239 -0.593659
C 0.079766 3.528414 -1.223467
C 1.029546 4.552682 -1.310145
C 0.760971 5.819395 -0.776340
C -0.469022 6.056407 -0.149840
C -1.419917 5.035911 -0.060086
C -3.598353 2.928918 -0.584229
C -4.186359 1.672729 -0.490148
H 1.078406 1.736987 0.984437
H -4.380682 -1.117665 -0.157648
H 1.190879 -2.365582 1.486721
H 3.448129 -2.662384 2.463914
H 3.890036 -1.990273 4.820343
H 2.051991 -1.017345 6.190736
H -0.201652 -0.706169 5.206308
H -2.350355 -2.074434 4.371604
H 0.827988 -0.306324 -3.676033
H 3.074942 -0.613023 -4.679737
H 4.310392 -2.749663 -4.349822
H 3.269965 -4.584723 -3.023877
H 1.009555 -4.279787 -2.045007
H -1.646551 -3.749099 -3.433066
H 0.299934 2.549557 -1.634609
H 1.976737 4.361989 -1.805628
H 1.499272 6.611805 -0.848287
H -0.686448 7.032628 0.272211
H -2.364530 5.222881 0.440511
H -4.107408 3.869638 -0.718516

O 1.032860 0.429913 -1.182900
O 0.478361 1.076872 1.368741
C -4.216864 -3.046256 -2.070012
H -4.565325 -3.445916 -1.111266
H -4.917960 -2.259320 -2.368946
H -4.272963 -3.848097 -2.810628
C -5.639583 1.310817 -0.518889
H -5.872082 0.615016 -1.332698
H -5.964825 0.838761 0.415216
H -6.239161 2.213120 -0.664711
C -4.712836 -1.736197 2.562769
H -4.933045 -2.118486 3.562682
H -5.280189 -0.808585 2.425425
H -5.088731 -2.460218 1.831707
C 3.668966 1.961980 0.520623
C 5.190459 2.195355 0.736710
C 5.921702 0.865994 1.009922
C 5.669664 -0.159906 -0.113009
C 4.149412 -0.385656 -0.343265
C 3.454817 0.946717 -0.595993
H 3.173681 2.913772 0.291325
H 3.242922 1.580138 1.459060
H 5.614664 2.669865 -0.160362
H 5.338982 2.894910 1.569568
H 6.999500 1.045381 1.121072
H 5.569039 0.450685 1.965871
H 6.124792 0.202342 -1.046674
H 6.151128 -1.117485 0.125634
H 3.992689 -1.072015 -1.182908
H 3.721772 -0.856791 0.553040
H 3.690917 1.360334 -1.586507
H 2.203752 0.698031 -0.770660

^{5}TS$_{H,\mathrm{b}}$

Fe 3.736190 2.079427 -0.137139
N 1.022752 0.819398 0.165226
N 1.684887 1.624292 -0.722042
N 2.321892 1.112409 2.361391
N 3.292586 2.017249 2.035752
N 2.980837 -0.695525 0.706648
N 4.021032 -0.060671 0.080261
B 1.789259 0.106376 1.314311
C 0.830591 1.877468 -1.744100
C 1.162066 2.655488 -2.952989
C 2.066019 3.735271 -2.938861
C 2.341511 4.446841 -4.112754
C 1.716759 4.101765 -5.317162
C 0.811310 3.033485 -5.340514
C 0.537766 2.317318 -4.172239
C -0.402583 1.237289 -1.483256
C -0.248909 0.572380 -0.272879
C 3.655038 2.639407 3.181481
C 4.725904 3.646419 3.285222
C 5.853367 3.629348 2.442629
C 6.873959 4.572654 2.594420
C 6.795429 5.543904 3.600118
C 5.684105 5.565865 4.452478
C 4.659419 4.628304 4.295448
C 2.878400 2.133255 4.250338
C 2.050071 1.162096 3.701853
C 4.855726 -1.020061 -0.384428
C 6.118917 -0.739311 -1.088484
C 6.940014 0.346758 -0.731354
C 8.148848 0.574048 -1.396442
C 8.562460 -0.283874 -2.422687
C 7.757756 -1.373256 -2.780586
C 6.547341 -1.599382 -2.119683
C 4.330365 -2.288066 -0.056106
C 3.145767 -2.049818 0.635203
H 4.759952 3.192446 -2.297036
H 1.045931 -0.655209 1.852284
H 3.037802 5.279467 -4.080450
H 1.930909 4.657291 -6.224582
H 0.323509 2.753070 -6.268820
H -0.148406 1.477553 -4.206748
H -1.294962 1.274826 -2.086580
H 5.937941 2.871347 1.673768
H 7.732692 4.543358 1.931527
H 7.590581 6.272746 3.719364
H 5.612394 6.314684 5.235060
H 3.794505 4.662864 4.949964
H 2.942825 2.409323 5.290319
H 6.639285 1.006503 0.073830
H 8.767753 1.417859 -1.109225
H 9.501842 -0.106969 -2.936522
H 8.069680 -2.042523 -3.576141
H 5.920080 -2.435842 -2.411118
H 4.774256 -3.248623 -0.261762
O 4.088991 4.022373 -0.492664
O 5.135940 2.916659 -1.443601
C 1.044534 0.292529 4.391968
H 0.042342 0.405245 3.963826
H 1.307379 -0.769519 4.328992
H 0.991260 0.563644 5.449639
C 2.196215 -3.045813 1.226448
H 2.071560 -2.901795 2.305187
H 1.201089 -2.983206 0.771906
H 2.577376 -4.056966 1.062088
C -1.248252 -0.264177 0.465370
H -2.204587 -0.243274 -0.063720
H -0.930702 -1.309873 0.545902
H -1.417076 0.103467 1.483461
C 1.579116 5.311904 1.381178
C 0.734895 6.530259 1.837343
C 1.623066 7.627081 2.459854
C 2.745524 8.060325 1.495108
C 3.590356 6.845728 1.034160
C 2.686826 5.768422 0.432680
H 0.937151 4.566621 0.895548
H 2.021102 4.832813 2.264087
H 0.200031 6.945189 0.969844
H -0.029115 6.202765 2.554794
H 1.010343 8.494187 2.740837
H 2.073700 7.242968 3.387502
H 2.300376 8.548030 0.614765
H 3.396317 8.803426 1.974545
H 4.345070 7.163075 0.304308
H 4.127052 6.432976 1.898598
H 2.268819 6.096479 -0.529686
H 3.387776 4.854334 0.102095

^{3}TS$_{H,\mathrm{b}}$

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N -1.073918 1.655776 0.613196
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N -2.172816 -0.847080 1.830339
N -1.900509 -1.216182 0.541237
B -1.211381 0.113321 2.596554
C -1.451939 2.915575 0.292148
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C -0.486340 3.111345 -2.036558
C -0.519732 3.665476 -3.322186
C -1.504005 4.599369 -3.667272
C -2.458798 4.975185 -2.713860
C -2.433232 4.417402 -1.432555
C -1.895540 3.587619 1.457479
C -1.782505 2.672782 2.495468
C 1.906308 -1.492050 1.565533
C 2.766293 -2.129768 0.552279
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C 3.099151 -3.279285 -1.574915
C 4.457527 -3.455800 -1.285582
C 4.972584 -2.971024 -0.076638
C 4.137364 -2.313568 0.830485
C 2.118879 -1.521642 2.963606
C 1.032079 -0.876395 3.539771
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C -3.014434 -2.579041 -1.232446
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C -3.204837 -3.826548 -3.753360
C -4.309896 -3.154206 -3.216050
C -4.216831 -2.537402 -1.965109
C -3.914823 -2.032586 1.123865
C -3.393522 -1.324125 2.205763
H -1.008613 0.724002 -2.488778
H -1.549585 0.178685 3.740019
H 0.290835 2.404106 -1.773320
H 0.231409 3.372075 -4.049178
H -1.526483 5.029568 -4.663372
H -3.228890 5.696206 -2.970040
H -3.191762 4.698462 -0.709363
H -2.227928 4.610468 1.533435
H 1.210794 -2.512569 -0.897914
H 2.687616 -3.652820 -2.507019
H 5.105564 -3.964518 -1.991830
H 6.024516 -3.099650 0.157896
H 4.551115 -1.927314 1.755997
H 2.936141 -1.990831 3.486257
H -0.993585 -3.339108 -1.206943
H -1.151048 -4.411039 -3.433560
H -3.276651 -4.304542 -4.724988
H -5.241067 -3.106674 -3.771642
H -5.070447 -2.005736 -1.556722
H -4.848410 -2.570716 1.093330
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O -0.706844 -0.182265 -2.288575
C 0.740156 -0.644903 4.989937
H 0.612692 0.419580 5.215716
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H -4.198584 -0.038982 3.744387
H -4.951964 -1.635306 3.624043
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H -1.241159 2.653203 4.588029
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C 5.452804 1.544759 -1.598771
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C 2.970463 1.417207 -1.144722
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H 4.640113 2.834892 1.555169
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H 6.314678 0.996202 -2.001305
H 3.982057 0.501357 -2.834149
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N -3.188947 0.990320 -0.237140
N -1.935416 1.492254 -0.434612
B -3.368843 -0.486536 0.175496
C -0.910701 -1.023828 2.841202
C 0.486946 -1.213630 3.262719
C 1.399824 -1.922643 2.458691
C 2.712313 -2.133873 2.891806
C 3.131510 -1.646657 4.136634
O 0.865167 0.283616 -1.662909
C 2.227126 -0.949963 4.948120
C 0.914307 -0.738101 4.516843
C -2.069178 -1.189701 3.626478
C -3.153670 -1.008299 2.767434
C -1.091565 -2.364826 -2.003523
C 0.238996 -2.704670 -2.563726
C 0.905526 -1.865380 -3.474146
C 2.115001 -2.265959 -4.050383

C 2.677094 -3.508616 -3.727593
C 2.017413 -4.354651 -2.828732
C 0.802564 -3.957876 -2.257202
C -2.269405 -3.097407 -2.254836
C -3.283500 -2.475230 -1.532119
C -2.067769 2.819400 -0.663415
C -0.947913 3.739547 -0.931978
C 0.195255 3.334894 -1.648458
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C 1.132387 5.571271 -1.468063
C -0.003107 5.983445 -0.759207
C -1.033349 5.076925 -0.493972
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C -4.124281 1.981790 -0.339700
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H 3.402571 -2.688366 2.264002
H 4.149669 -1.814031 4.473160
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H 0.220163 -0.185174 5.141566
H -2.110907 -1.454697 4.670490
H 0.481189 -0.899158 -3.713034
H 2.617671 -1.608777 -4.753049
H 3.616256 -3.815738 -4.177176
H 2.441959 -5.321200 -2.575965
H 0.286603 -4.618184 -1.566745
H -2.363753 -3.955999 -2.899723
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H 2.098433 3.918465 -2.466640
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C 5.685493 2.047463 0.618455
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C 4.569070 -0.462137 -0.579456
C 4.025427 0.904398 -0.888440
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H 7.283875 0.734926 1.297475
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H 6.412046 -1.356766 0.192288
H 4.472715 -1.135706 -1.438365
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H 1.763520 0.412348 -1.109333

^{3}IM$_{H}$

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H 3.566454 -3.861091 -4.173264
H 2.374658 -5.346949 -2.566775
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^{5}PC

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H -2.172768 -4.795980 -1.618270
H 0.210279 -4.871530 -2.133551
H 1.584662 -1.463338 3.048898
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H 4.305818 1.859730 3.300867
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H 2.356754 -4.480437 -3.699510
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H -3.064461 -0.357442 1.064548
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^{3}PC

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H -3.477471 2.380461 0.391481
H -4.031113 1.098332 1.485879
H -2.669049 0.663531 -1.231378
H -1.424143 1.308853 0.756636