

Supporting Information for

A Proton-Shuffle Mechanism of O-O Activation for the Formation of a High-Valent Oxo-Iron Species of Bleomycin

Devesh Kumar,¹ Hajime Hirao,¹ Sason Shaik,^{,1} and Pawel M. Kozłowski^{*,1,2,†}*

¹ Department of Organic Chemistry and the Lise Meitner-Minerva Center for Computational Quantum Chemistry, The Hebrew University, Jerusalem, 91904, Israel.

² Department of Chemistry, University of Louisville, Louisville, KY 40292, USA.

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a) Methods

We used the unrestricted hybrid density functional UB3LYP combined with an LACVP* basis set on iron and 6–31G* basis sets on the remaining atoms (hence UB3LYP/LACVP*, B1). Single point calculations were done with a triple zeta basis set, which includes polarization and diffuse functions on all atoms (hence UB3LYP/LACV3P++**, B2). The geometry optimizations were performed using the Jaguar 5.5 program package. Due to the extraordinary large size of the system, we limited frequency calculations to $\text{TS}_{\text{O-O}}$ (see Figs. 6 and 7 in the text), which were done with GAUSSIAN 03. Since bleomycin functions in aqueous solution, the relative energies of all the structures were corrected using the solvent model implemented in JAGUAR 5.5 (the program defines the solvent by its dielectric constant, ϵ , and probe radius, r ; for water $\epsilon = 80.4$ and $r = 1.40 \text{ \AA}$).

b) Reference 52 in Full

Frisch, M. J.; Trucks, G. W.; Schlegel, H. B.; Scuseria, G. E.; Robb, M. A.; Cheeseman, J. R.; Montgomery, Jr., J. A.; Vreven, T.; Kudin, K. N.; Burant, J. C.; Millam, J. M.; Iyengar, S. S.; Tomasi, J.; Barone, V.; Mennucci, B.; Cossi, M.; Scalmani, G.; Rega, N.; Petersson, G. A.; Nakatsuji, H.; Hada, M.; Ehara, M.; Toyota, K.; Fukuda, R.; Hasegawa, J.; Ishida, M.; Nakajima, T.; Honda, Y.; Kitao, O.; Nakai, H.; Klene, M.; Li, X.; Knox, J. E.; Hratchian, H. P.; Cross, J. B.; Bakken, V.; Adamo, C.; Jaramillo, J.; Gomperts, R.; Stratmann, R. E.; Yazyev, O.; Austin, A. J.; Cammi, R.; Pomelli, C.; Ochterski, J. W.; Ayala, P. Y.; Morokuma, K.; Voth, G. A.; Salvador, P.; Dannenberg, J. J.; Zakrzewski, V. G.; Dapprich, S.; Daniels, A. D.; Strain, M. C.; Farkas, O.; Malick, D. K.; Rabuck, A. D.; Raghavachari, K.; Foresman, J. B.; Ortiz, J. V.; Cui, Q.; Baboul, A. G.; Clifford, S.; Cioslowski, J.; Stefanov, B. B.; Liu, G.; Liashenko, A.; Piskorz, P.; Komaromi, I.; Martin, R. L.; Fox, D. J.; Keith, T.; Al-Laham, M. A.; Peng, C. Y.; Nanayakkara, A.; Challacombe, M.; Gill, P. M. W.; Johnson, B.; Chen, W.; Wong, M. W.; Gonzalez, C.; and Pople, J. A.; Gaussian, Inc., Wallingford CT, 2004. *Gaussian 03*, Revision C.02.

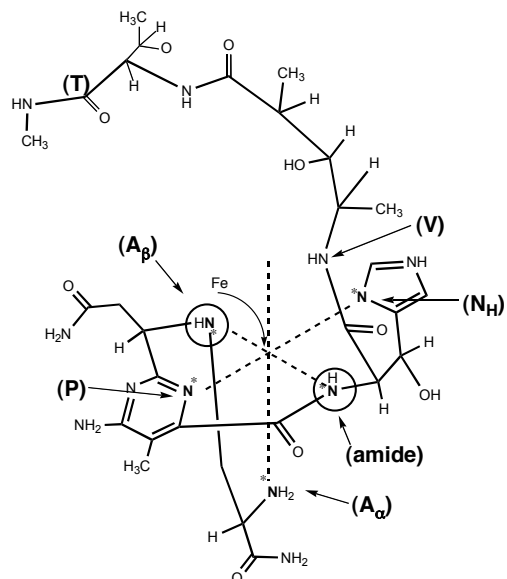
c) Definitions of “Unprotonated” and “Protonated”

In the following, we will often use “unprotonated” and “protonated” to differentiate states. These correspond to the protonation state of nitrogen $\text{N}(\text{A}_\text{p})$. See Figure S1.

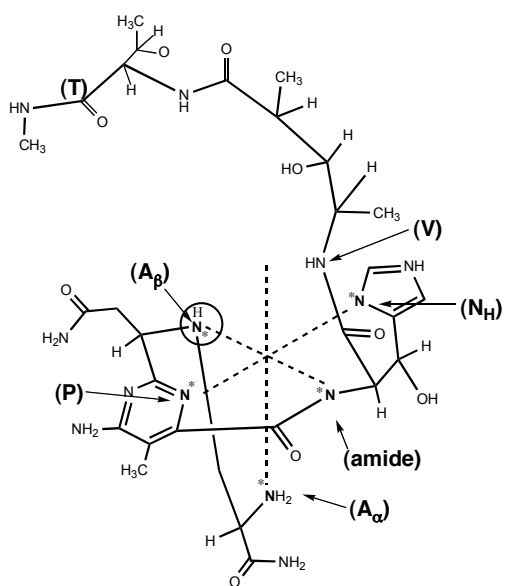
Part I: Species in Figures 1- 4 in the text

Figure S1: 3D structures of the (a) $\text{BLM}(\text{H}_2)$, (b) $\text{BLM}(\text{H})^{1-}$ and (c) BLM^{2-} ligands used in DFT calculations (see Figure 3, text).

(a) $\text{BLM}(\text{H}_2)$



(b) $\text{BLM}(\text{H})^{1-}$



(c) BLM^{2-}

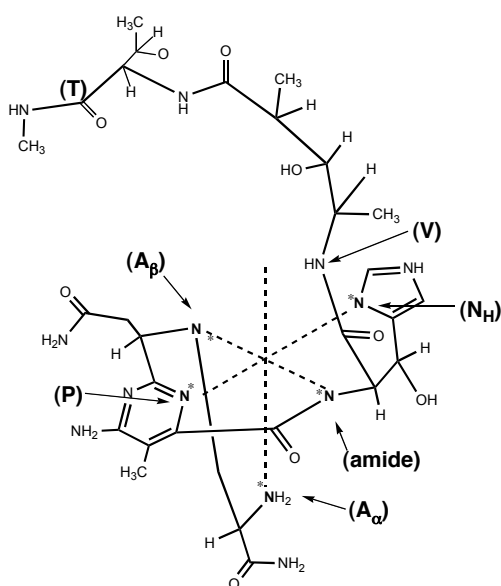
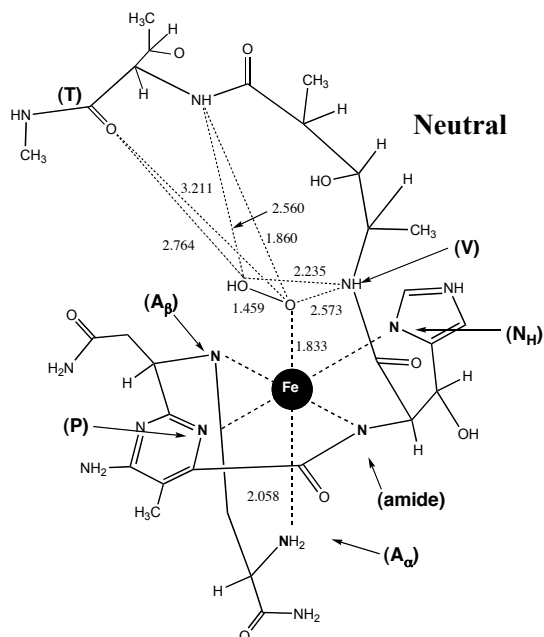


Figure S2: Structural models of (a) BLM-Fe^{III}-OOH (doublet) and (b) BLM(H)-Fe^{III}-OOH¹⁺ (doublet). The structures correspond to Figures 3b and 3c in the text.

(a) BLM-Fe^{III}-OOH



(b) BLM(H)-Fe^{III}-OOH¹⁺

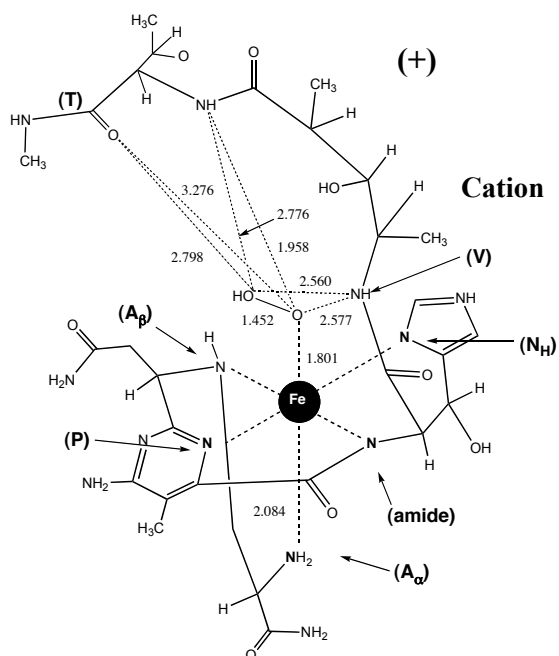
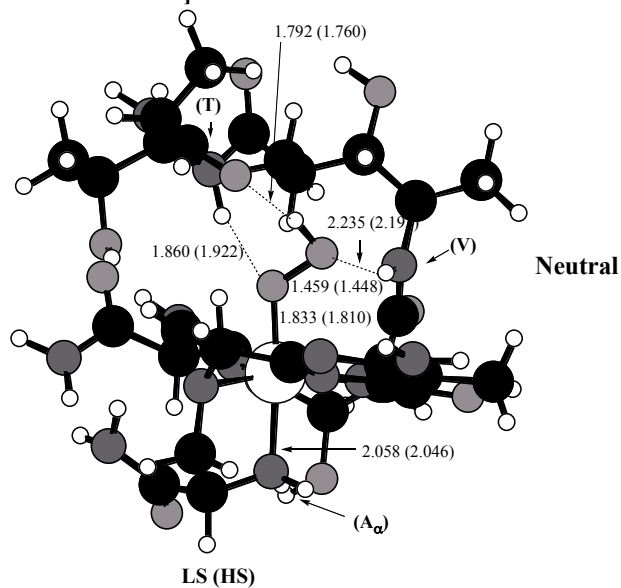


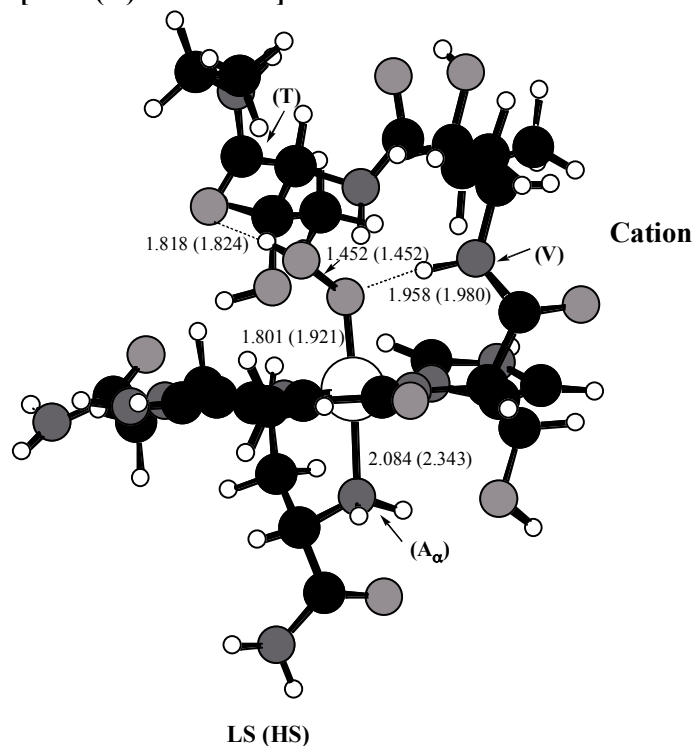
Figure S3: LACVP* Optimized Structures of Doulet (Quartet) States of (a) $^{2,4}[\text{BLM-Fe}^{\text{III}}\text{-OOH}]$ and (b) $^{2,4}[\text{BLM(H)-Fe}^{\text{III}}\text{-OOH}]^{1+}$ (see figure 3 in the text).

(a) $^{2,4}[\text{BLM-Fe}^{\text{III}}\text{-OOH}]$



	ρ_{Fe}	ρ_{O}	ρ_{OH}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	Q_{rest}
$^2[\text{BLM-Fe}^{\text{III}}\text{-OOH}]$	0.90	0.09	0.00	0.01	0.49	-0.44	-0.02	-0.03
$^4[\text{BLM-Fe}^{\text{III}}\text{-OOH}]$	2.72	0.02	-0.01	0.27	0.58	-0.43	0.01	-0.16

(b) $^{2,4}[\text{BLM(H)-Fe}^{\text{III}}\text{-OOH}]^{1+}$



	ρ_{Fe}	ρ_{O}	ρ_{OH}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	Q_{rest}
$^2[\text{BLM-Fe}^{\text{III}}\text{-OOH}]^{1+}$	0.87	0.12	0.00	0.01	0.56	-0.42	0.00	0.86
$^4[\text{BLM-Fe}^{\text{III}}\text{-OOH}]^{1+}$	2.65	0.24	0.03	0.08	0.73	-0.47	0.01	0.74

Figure S4: Geometry of active bleomycin taken from PDB file 1GJ2 (see Figure 3a in the text) and used as an initial structure to generate the ABLM complexes in Figure 3c,d.

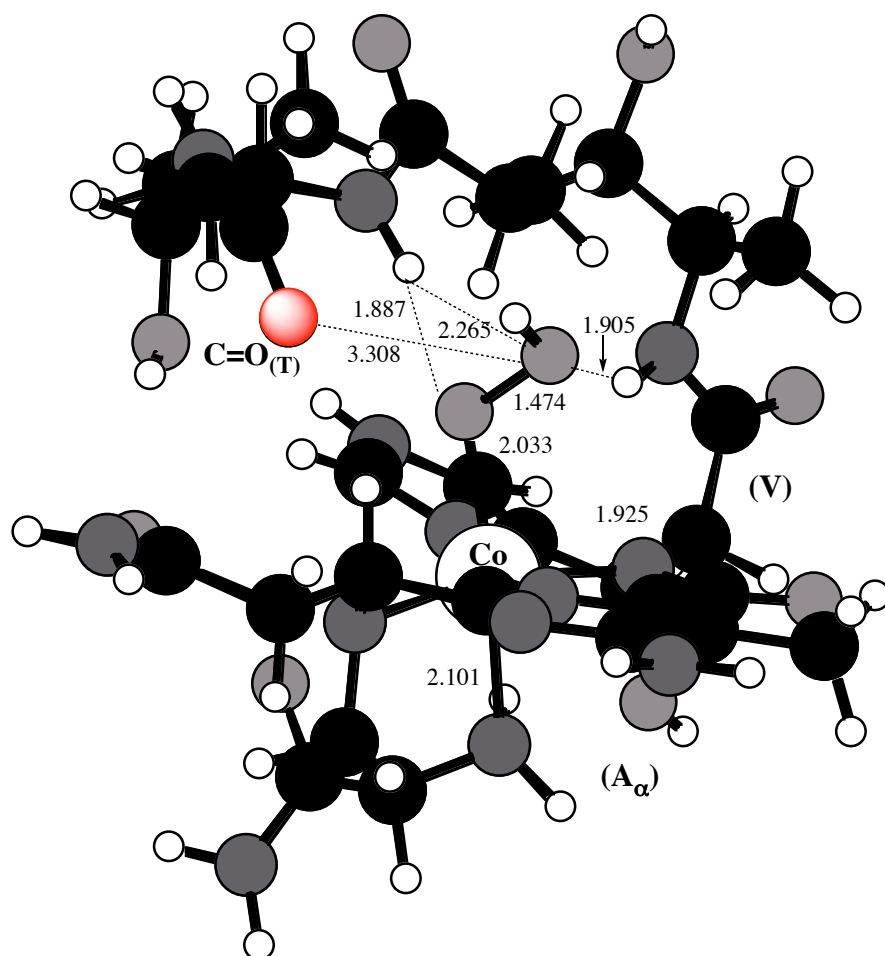
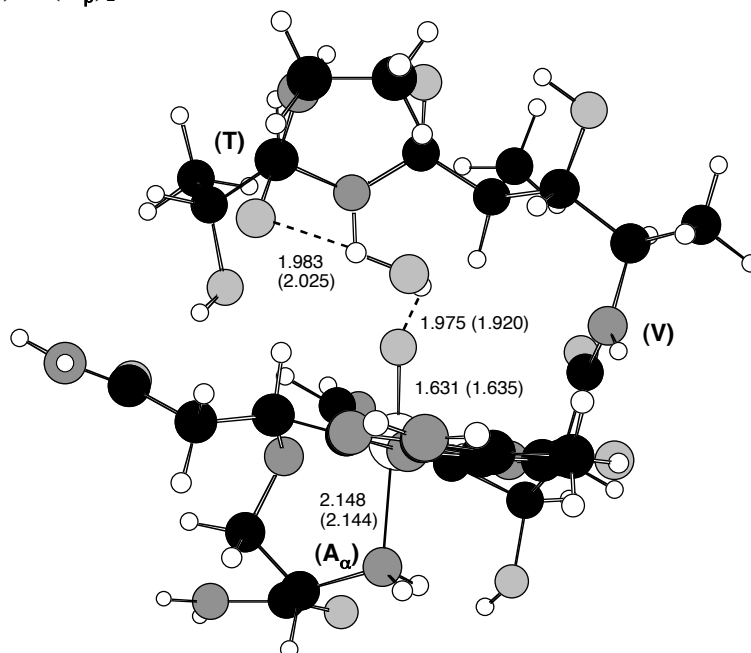


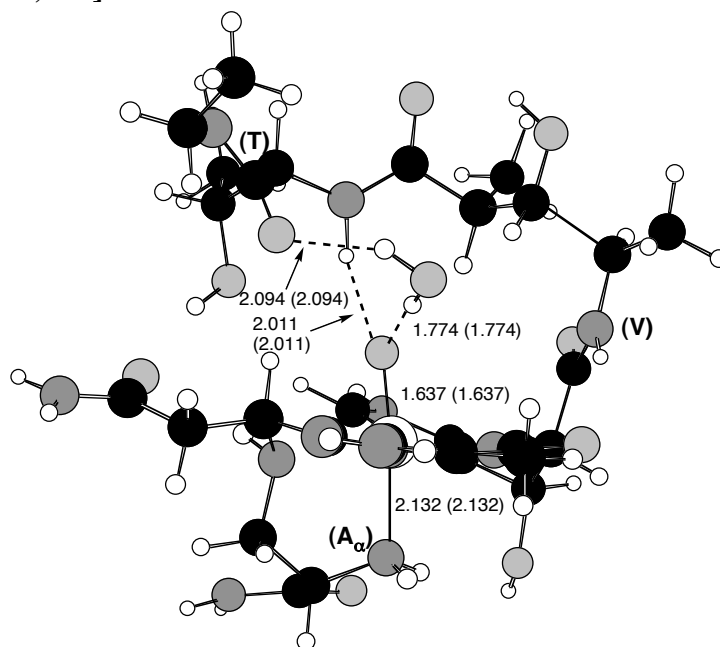
Figure S5: LACVP* Optimized Structures of (a) $^{2,4}[\text{BLM-Fe}^{\text{IV}}=\text{O}; \text{N}^*(\text{A}_\beta)]^{1+}$ and (b) $^{2,4}[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}=\text{O}; \text{V}^{*}]^{2+}$ (see figure 4 in the text).^a

(a) $^{2,4}[\text{BLM-Fe}^{\text{IV}}=\text{O}; \text{N}^*(\text{A}_\beta)]^{1+}$



	ρ_{Fe}	ρ_{O}	$\rho_{\text{N}(\text{A}\beta)}$	ρ_{rest}	Q_{Fe}	Q_{O}	$Q_{\text{N}(\text{A}\beta)}$	Q_{rest}
doublet	1.21	0.77	-0.85	-0.13	0.60	-0.52	-0.27	1.20
quarteeet	1.29	0.77	0.86	0.07	0.60	-0.52	-0.28	1.20

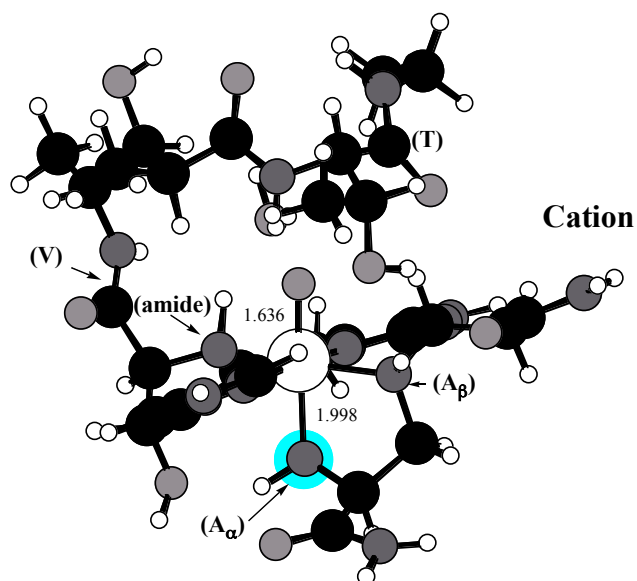
(b) $^{2,4}[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}=\text{O}; \text{V}^{*}]^{2+}$



	ρ_{Fe}	ρ_{O}	$\rho_{\text{V}(\text{V}) \text{ side}}$	ρ_{rest}	Q_{Fe}	Q_{O}	$Q_{\text{V}(\text{V}) \text{ side}}$	Q_{rest}
doublet	1.33	0.70	-0.84	-0.19	0.62	-0.56	0.01	1.93
quarteeet	1.34	0.70	0.86	0.11	0.61	-0.56	0.01	1.93

^a. Corresponding to Figure 4a and 4b in the text.

Figure S6: The LACVP* optimized structure of ${}^2[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}=\text{O}; \text{NH}^{*+}(\text{A}_\alpha)]^{2+}$.^{a,b}

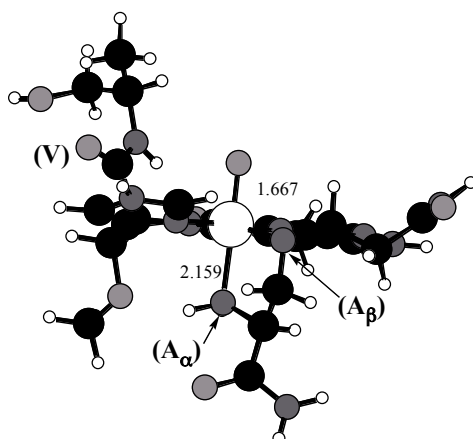


ρ_{Fe}	ρ_{O}	$\rho_{\text{N}(\text{A}\alpha)}$	ρ_{rest}	Q_{Fe}	Q_{O}	$Q_{\text{N}(\text{A}\alpha)}$	Q_{rest}
1.18	0.85	-0.92	-0.11	0.54	-0.48	-0.43	2.37

- ^a. One proton from the structure in Figure 4b (text) was shifted from $\text{NH}_2(\text{A}_\alpha)$ to $\text{N}(\text{amide})$. The so formed species ${}^2[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}=\text{O}; \text{NH}^{*+}(\text{A}_\alpha)]^{2+}$ is 22.5/ 24.1 kcal/mol less stable than the isomer structure $[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}=\text{O}; \text{V}^{*+}]^{2+}$ species (in Figure 4b) in the gas phase/ aqueous solution, respectively.
- ^b. Corresponds to Figure 4c in the text.

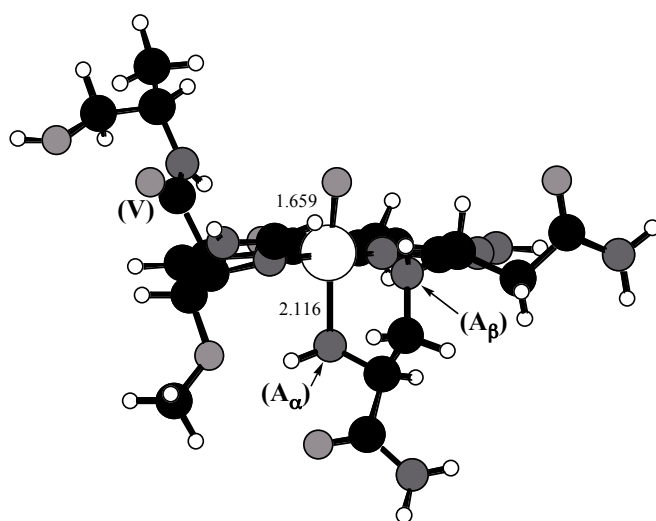
Figure S7: LACVP* Optimized Structures of (a) ${}^3\text{BLM-Fe}^{\text{IV}}=\text{O}$ and (b) ${}^3\text{BLM(H)-Fe}^{\text{IV}}=\text{O}^{1+}$. ^{a,b}

(a) ${}^3\text{BLM-Fe}^{\text{IV}}=\text{O}$



ρ_{Fe}	ρ_{O}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{rest}
1.11	0.91	-0.02	0.48	-0.35	-0.13

(b) ${}^3\text{BLM(H)-Fe}^{\text{IV}}=\text{O}^{1+}$

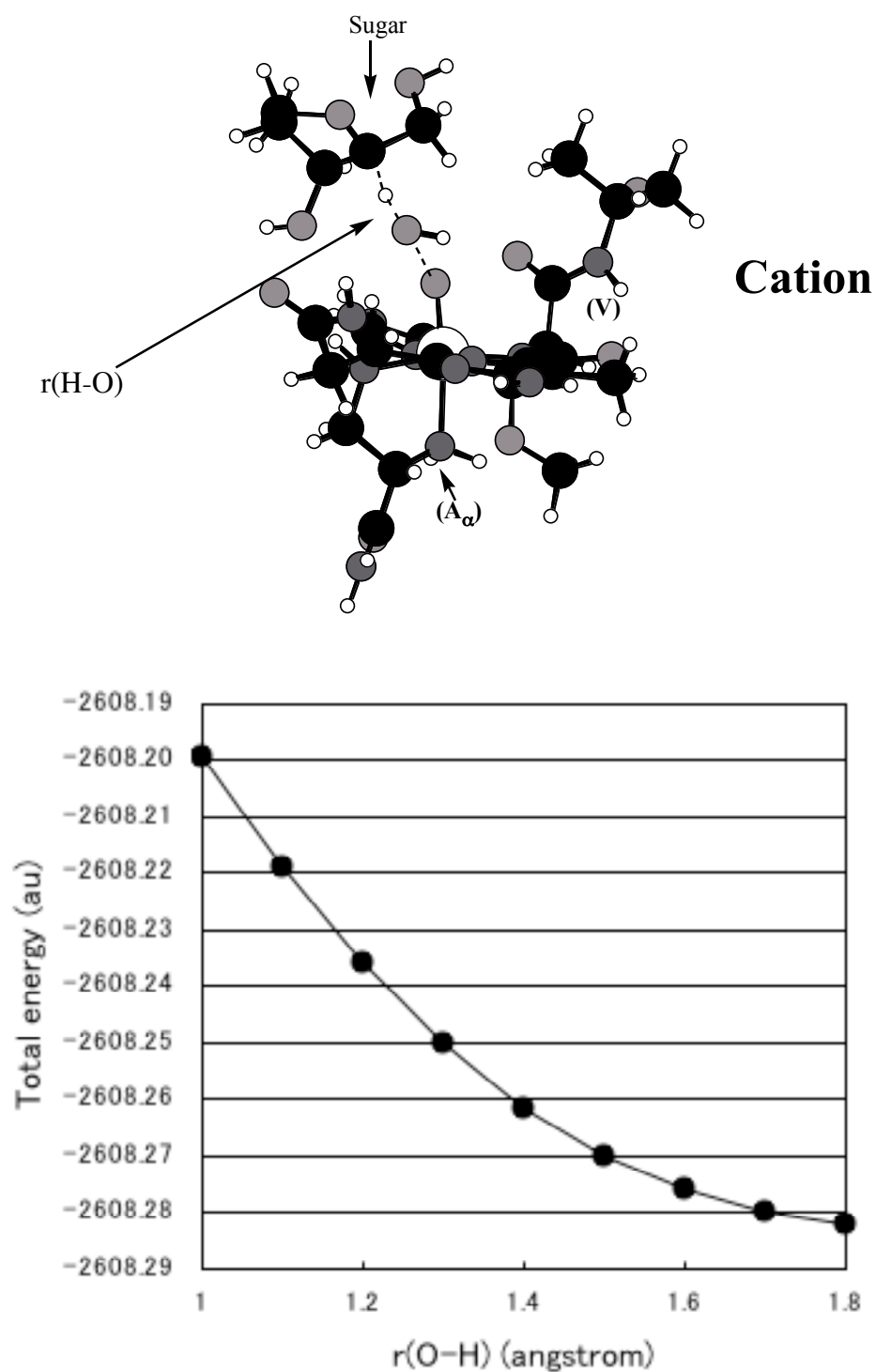


ρ_{Fe}	ρ_{O}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{rest}
1.08	0.95	-0.03	0.53	-0.32	0.79

^a This small model is more severely truncated than the one in Figure S5.

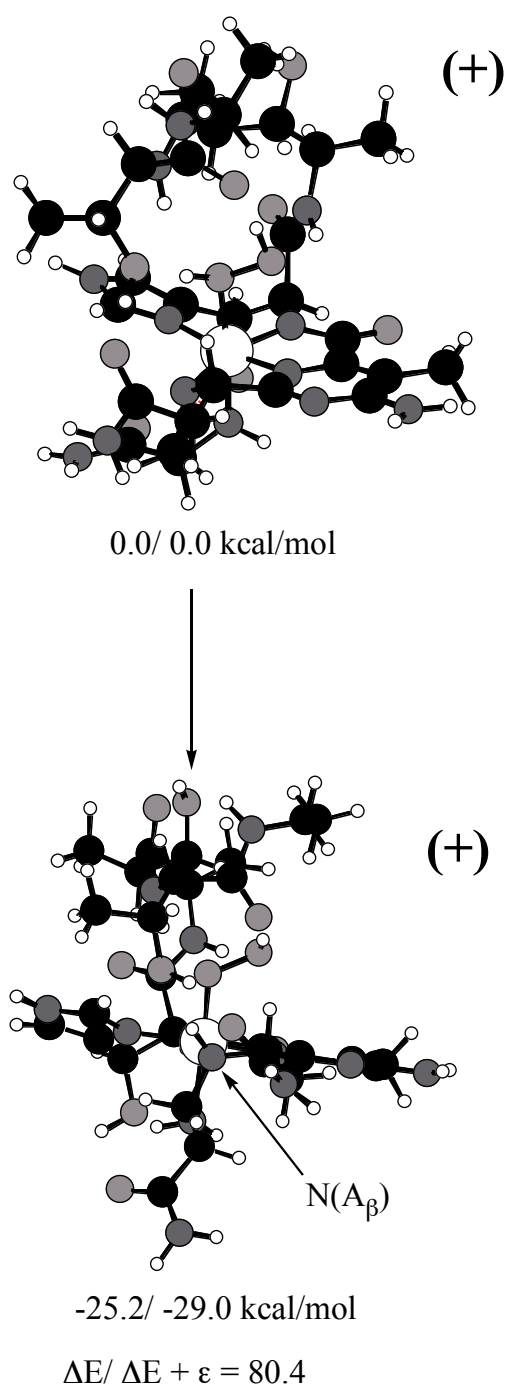
^b Corresponds to species due to hemolytic cleavage in Figure 2 in the text.

Figure S8: LACVP* One-Dimensional Energy Scan for the Direct H-Abstraction from ${}^2\text{BLM}(\text{H})\text{-Fe}^{\text{III}}\text{-OOH}^{1+}$.^a



^a Here we used the small model in Figure S7.

Figure S9: The behavior of ${}^2\text{BLM-Fe}^{\text{III}}\text{-(H}_2\text{O}_2\text{)}^{1+}$. The H_2O_2 ligand loses a proton to $\text{N}(\text{A}_\beta)$.

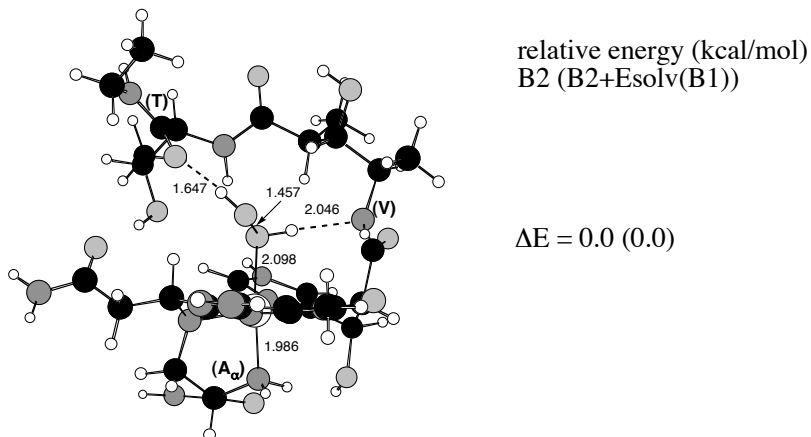


Explanation: One proton from the H_2O_2 ligand shifts spontaneously to the $\text{N}(\text{A}_\beta)$ ligand to generate ${}^2\text{BLM(H)-FeOOH}^+$.

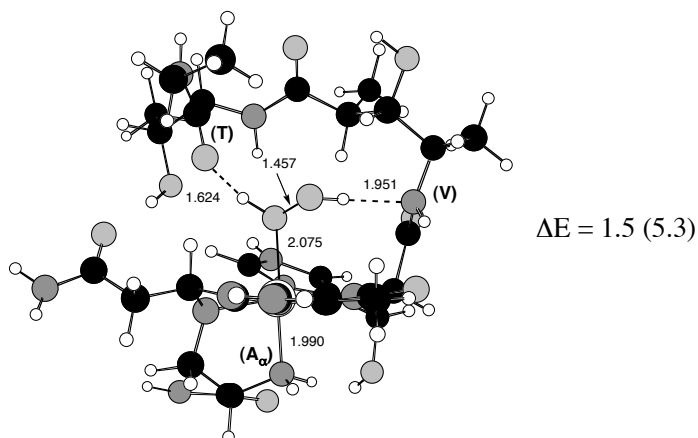
Part II: Species in the Heterolytic Reactions.

Figure S10: LACVP* Optimized Structures of **1**: (a) $^2[\text{BLM-Fe}^{\text{III}}(\text{H}_2\text{O}_2)]^{1+}$ (unprotonated) and (b) $^2[\text{BLM(H)-Fe}^{\text{III}}(\text{H}_2\text{O}_2)]^{2+}$ (protonated).

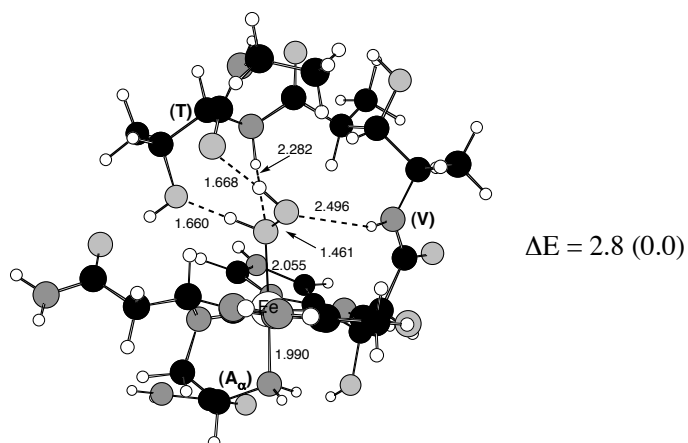
(a) Unprotonated **1a**



1b



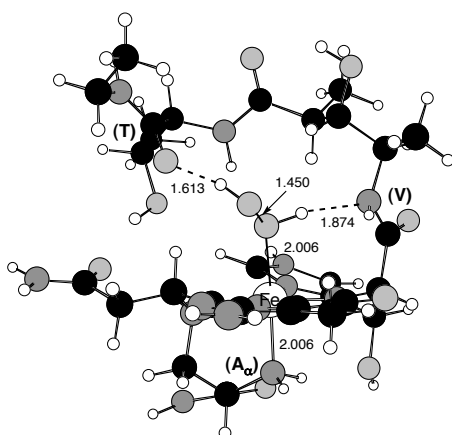
1c



	ρ_{Fe}	ρ_{HO}	ρ_{OH}	ρ_{rest}	Q_{Fe}	Q_{HO}	Q_{OH}	Q_{rest}
1a	0.74	0.00	0.00	0.26	0.42	0.05	0.05	0.47
1b	0.76	0.00	0.00	0.25	0.45	0.01	0.07	0.46
1c	0.80	0.00	0.00	0.21	0.46	0.02	0.04	0.48

(b) Protonated

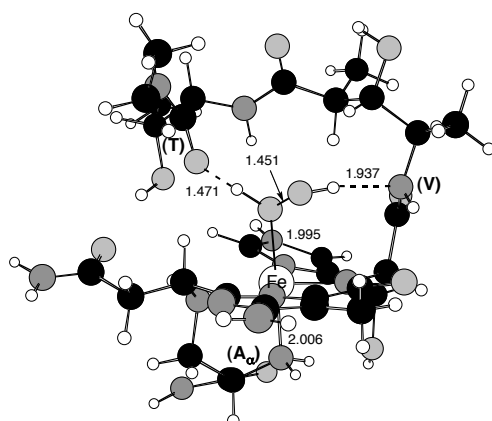
1a



relative energy (kcal/mol)
B2 (B2+Esolv(B1))

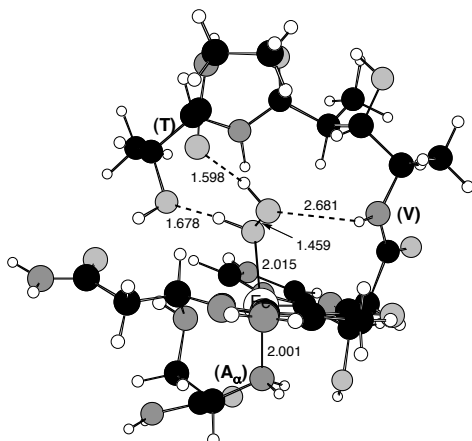
$\Delta E = 0.0$ (0.0)

1b



$\Delta E = 1.2$ (1.2)

1c

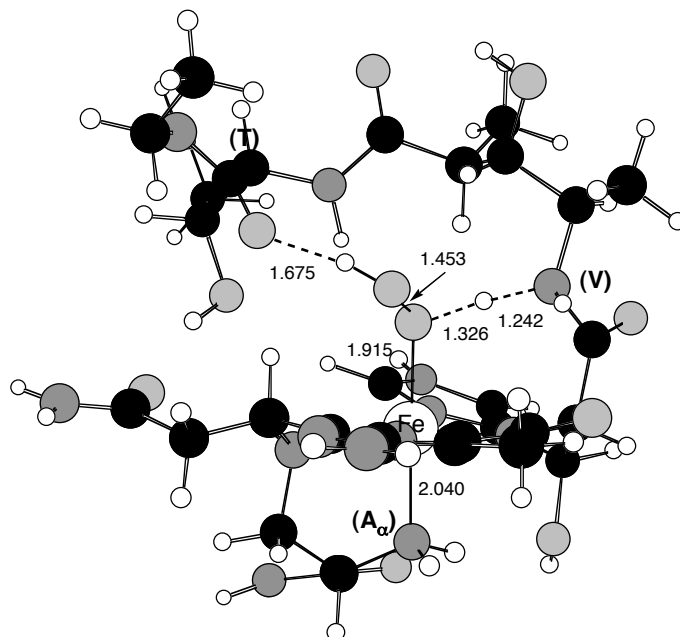


$\Delta E = 5.5$ (2.6)

	ρ_{Fe}	ρ_{HO}	ρ_{OH}	ρ_{rest}	Q_{Fe}	Q_{HO}	Q_{OH}	Q_{rest}
1a	0.95	0.00	0.00	0.05	0.52	0.06	0.07	1.35
1b	0.99	0.01	0.00	0.01	0.56	0.01	0.10	1.33
1c	0.90	0.01	0.00	0.09	0.62	0.18	0.10	1.10

Figure S11: LACVP* Optimized Structures for TSh-oh1 (Between **1a** and **2**, Protonated).

Protonated

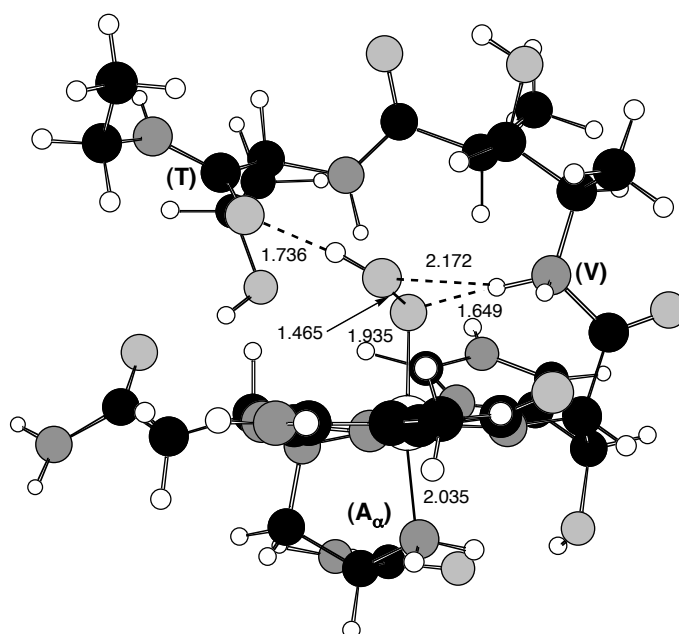


ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{NH2(V)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{N(V)}}$	Q_{rest}
0.99	0.02	0.00	0.00	-0.01	0.52	-0.47	0.04	0.15	1.75

Figure S12: LACVP* Optimized Structures for **2**: (a) $[\text{}^2\text{BLM-Fe}^{\text{III}}\text{-OOH; NH}_2^+(\text{V})]^{1+}$, (b) $[\text{}^2\text{BLM(H)-Fe}^{\text{III}}\text{-OOH; NH}_2^+(\text{V})]^{2+}$

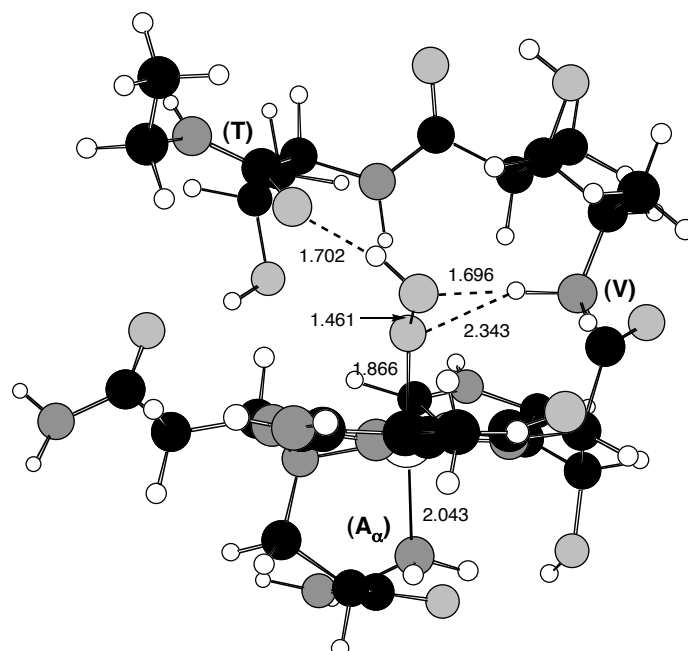
(a) Unprotonated

2'



barrier < 1 kcal/mol

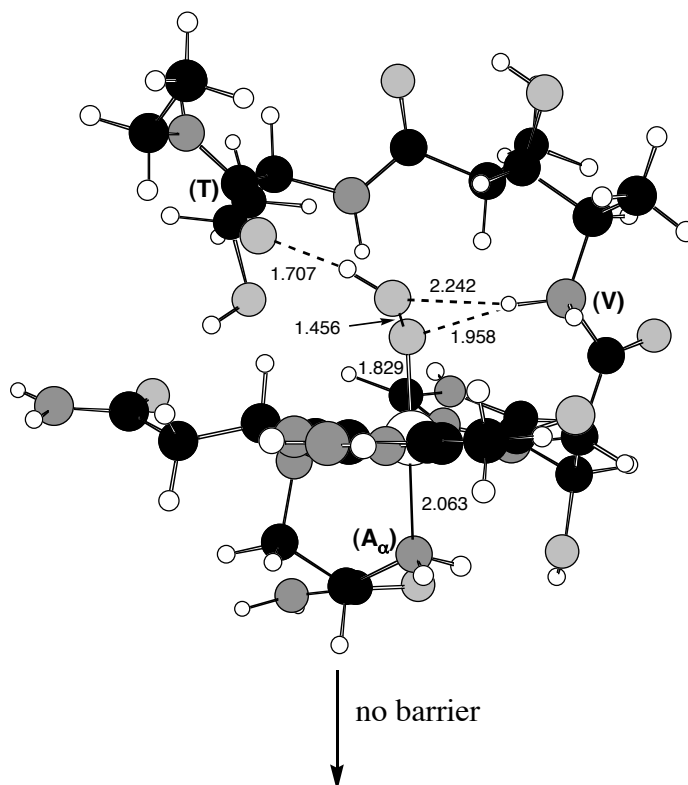
2



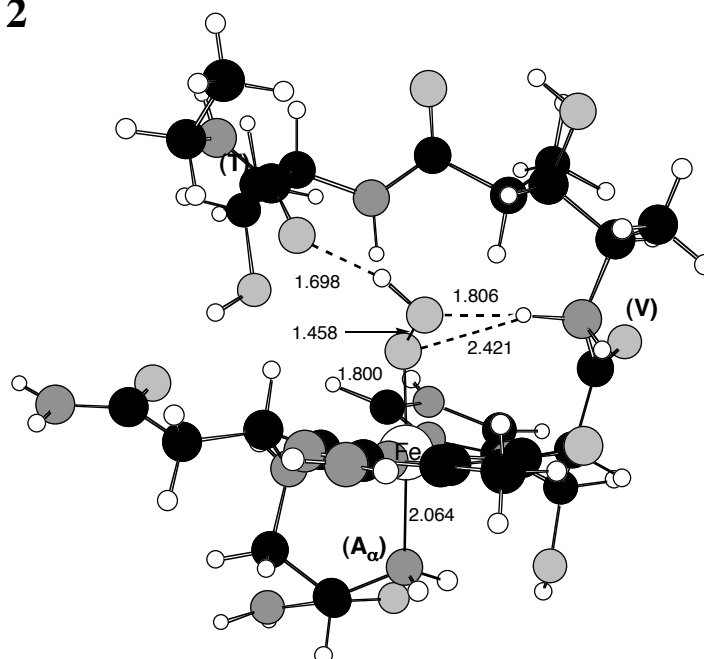
	ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{NH2(V)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{N(V)}}$	Q_{rest}
2'	0.84	0.01	0.00	0.00	0.15	0.43	-0.46	-0.01	0.14	0.90
2	0.86	0.05	0.00	0.00	0.09	0.48	-0.43	-0.03	0.12	0.87

- (b) **Protonated** (note that the proton transfer from **1a**, Figure 6 in the text, to NH(V) generates initially **2'**, which is converted to **2**, Figure 6 in the text. The **2'** $\rightarrow$ **2** surface is very flat).

2'



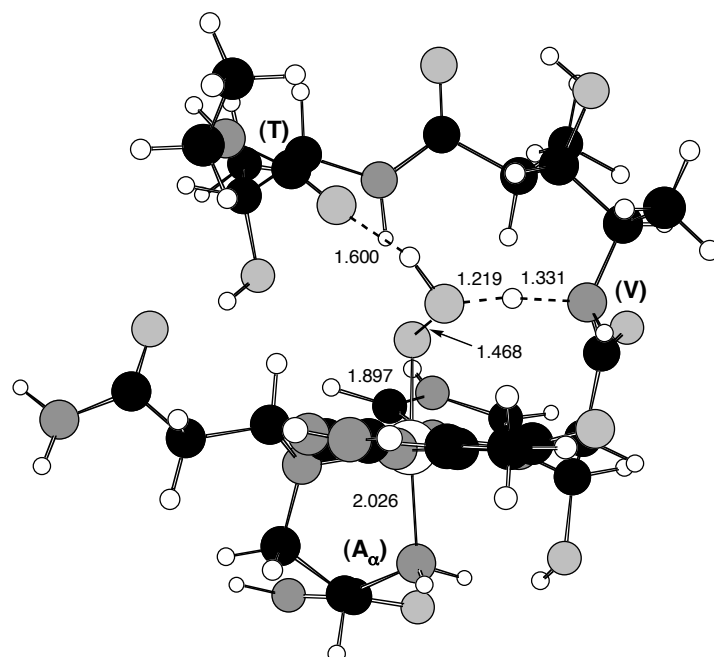
2



	ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{NH2(V)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{N(V)}}$	Q_{rest}
2'	0.93	0.09	0.00	0.00	-0.02	0.54	-0.44	0.01	0.13	1.75
2	0.91	0.12	0.00	0.00	-0.04	0.58	-0.41	0.00	0.12	1.71

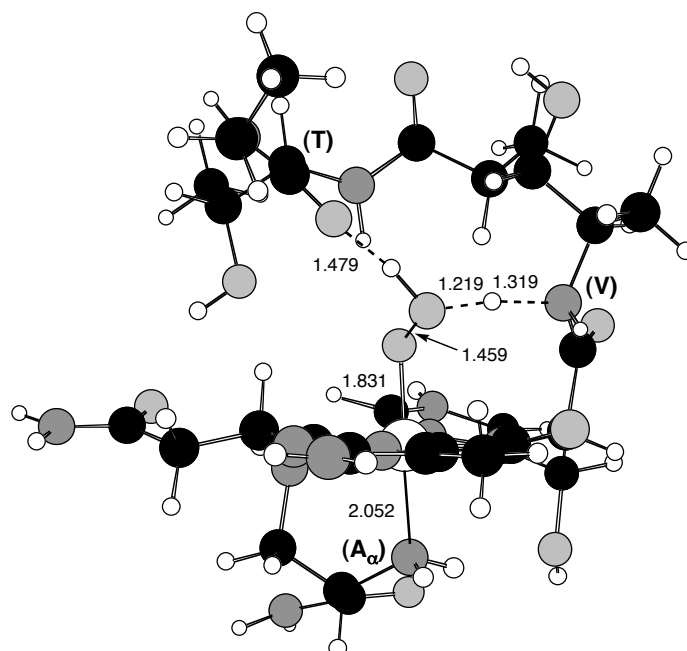
Figure S13: LACVP* Optimized Structures for $\text{TS}_{\text{h-oh2}}$: (a) Protonated, (b) Unprotonated (between **2** and **3**)

(a) Protonated



ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{NH2(V)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{N(V)}}$	Q_{rest}
0.85	0.03	0.00	0.00	0.13	0.47	-0.41	-0.03	0.14	0.83

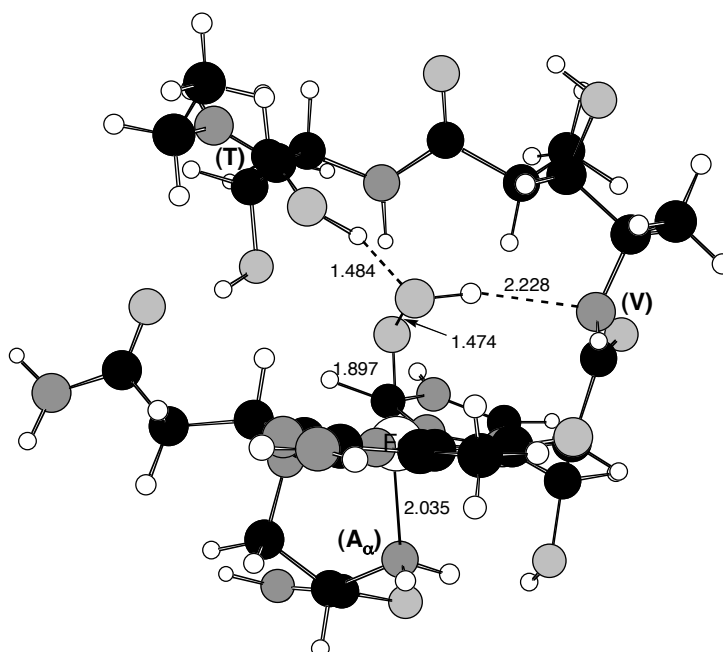
(b) Unprotonated



ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{NH2(V)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{N(V)}}$	Q_{rest}
0.97	0.08	0.00	0.00	-0.04	0.57	-0.39	-0.01	0.14	1.69

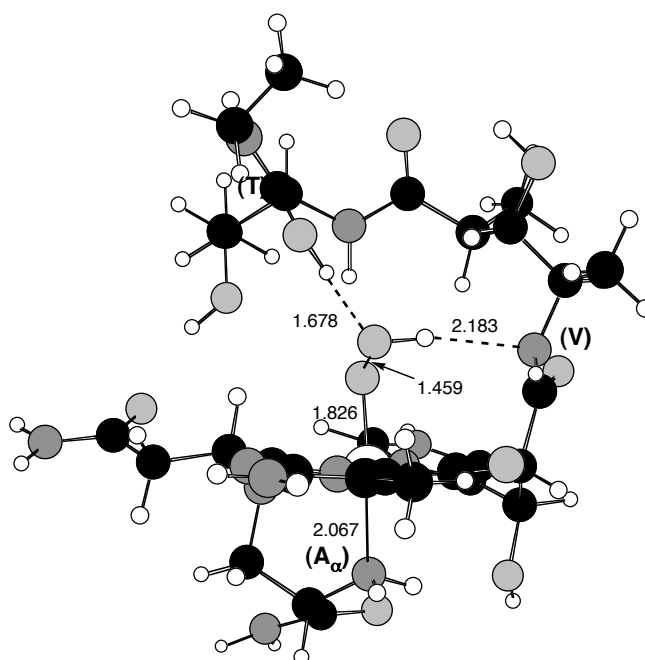
Figure S14: LACVP* Optimized Structures for **3**: (a) Protonated, (b) Unprotonated

(a) Unprotonated



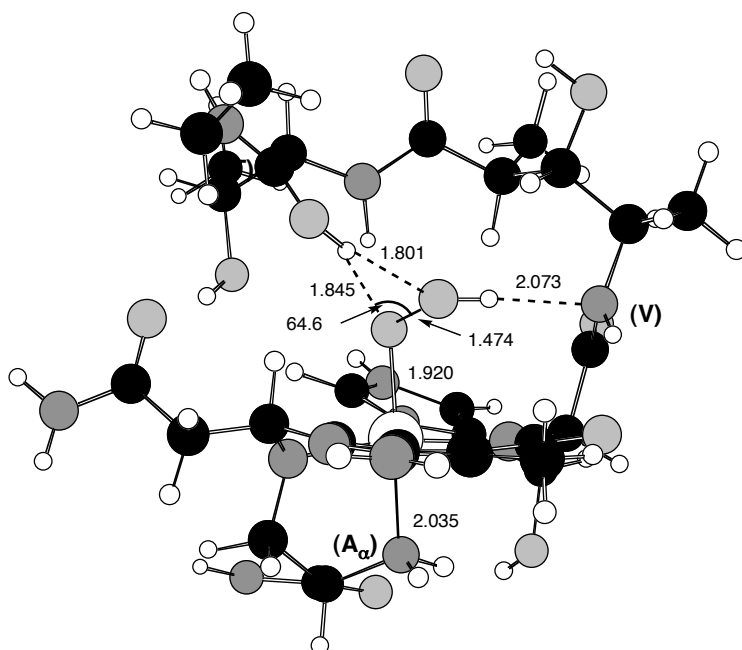
ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{COH(T)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{COH(T)}}$	Q_{rest}
0.87	0.02	0.00	0.00	0.11	0.47	-0.43	-0.04	0.54	0.46

(b) Protonated



ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{COH(T)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{COH(T)}}$	Q_{rest}
0.95	0.08	-0.01	0.00	-0.03	0.57	-0.39	-0.02	0.58	1.26

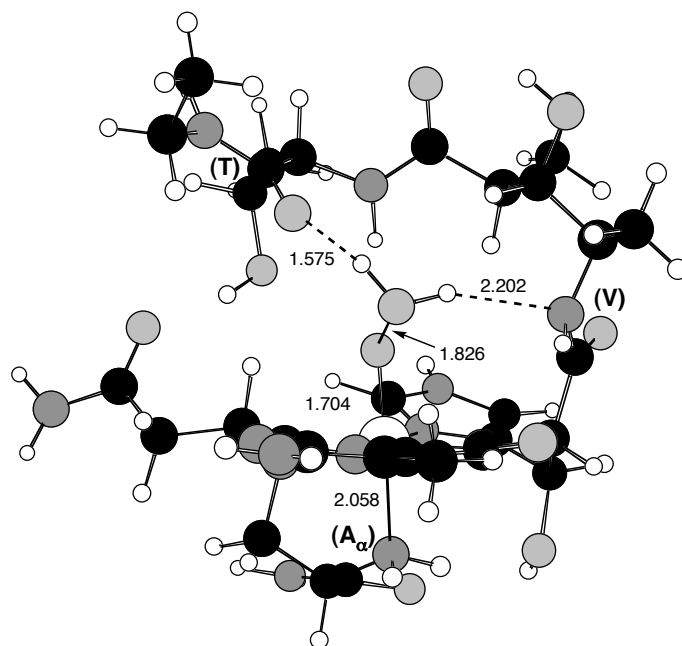
Figure S15: LACVP* Optimized Structures for TS_{coh} : (between **1b** and **3**, Unprotonated)



ρ_{Fe}	ρ_{O}	ρ_{OH}	$\rho_{\text{COH(T)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH}	$Q_{\text{COH(T)}}$	Q_{rest}
0.89	0.01	0.00	0.00	0.10	0.48	-0.47	-0.03	0.60	0.42

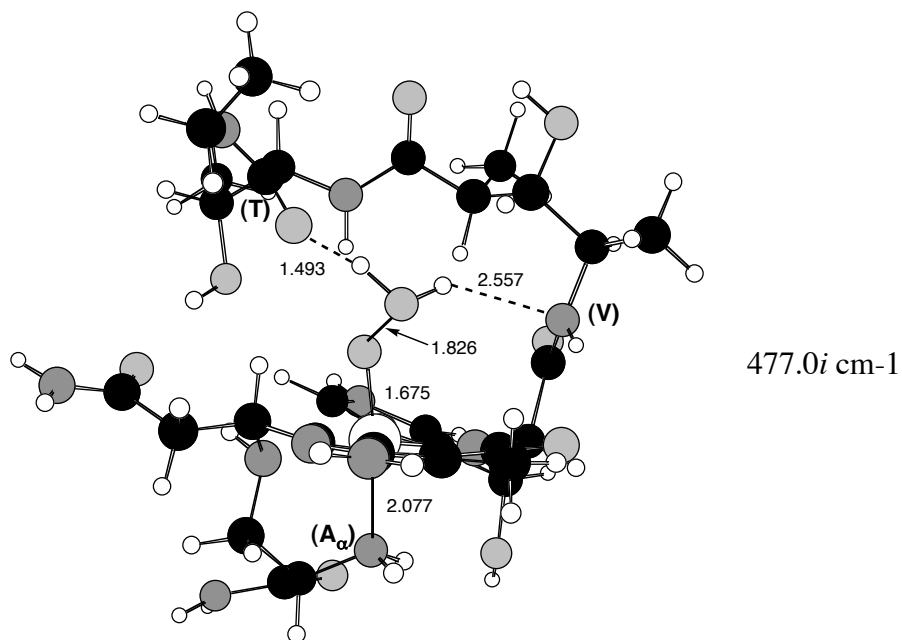
Figure S16: The LACVP* Optimized Structure of $^2\text{TS}_{\text{O}_2\text{O}}$ species in Figures 6 and 7 in the text.

(a) Unprotonated



ρ_{Fe}	ρ_{O}	ρ_{OH2}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH2}	Q_{rest}
1.14	-0.08	-0.18	0.11	0.54	-0.40	0.32	0.54

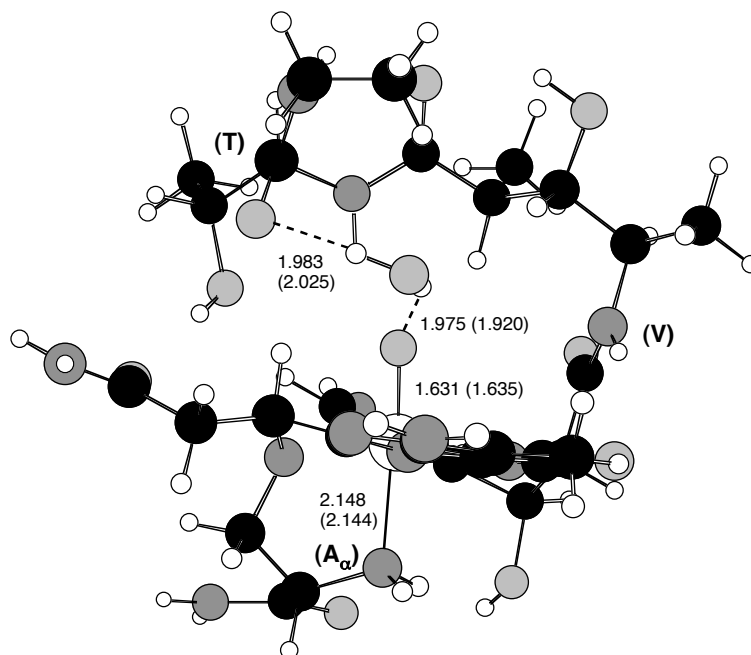
(b) Protonated



ρ_{Fe}	ρ_{O}	ρ_{OH2}	ρ_{rest}	Q_{Fe}	Q_{O}	Q_{OH2}	Q_{rest}
1.23	0.01	-0.23	-0.01	0.64	-0.38	0.36	1.38

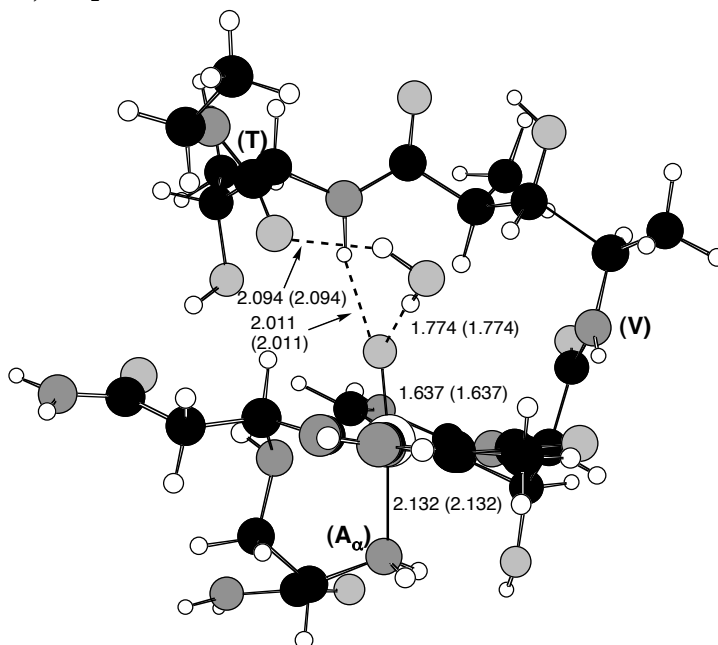
Figure S17: LACVP* Optimized Structures of Doulet (Quartet) CpdI species **(4)** (a) Unprotonated, (b) Protonated (same as Figure S5)

(a) Protonated



	ρ_{Fe}	ρ_{O}	$\rho_{\text{N(AB)}}$	ρ_{rest}	Q_{Fe}	Q_{O}	$Q_{\text{N(AB)}}$	Q_{rest}
doublet	1.21	0.77	-0.85	-0.13	0.60	-0.52	-0.27	1.20
quarteeet	1.29	0.77	0.86	0.07	0.60	-0.52	-0.28	1.20

(b) $^{2,4}[\text{BLM(H)}\text{-Fe}^{\text{IV}}\text{=O; V}^{\bullet+}]^{2+}$

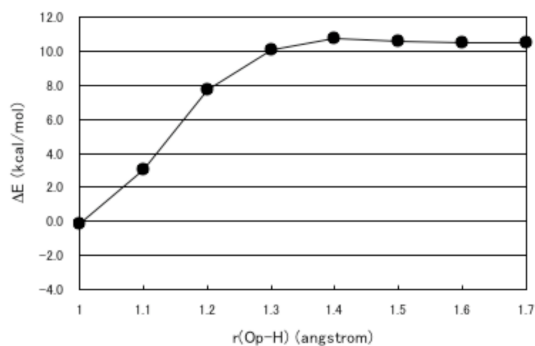


	ρ_{Fe}	ρ_{O}	$\rho_{\text{(V) side}}$	ρ_{rest}	Q_{Fe}	Q_{O}	$Q_{\text{(V) side}}$	Q_{rest}
doublet	1.33	0.70	-0.84	-0.19	0.62	-0.56	0.01	1.93
quarteeet	1.34	0.70	0.86	0.11	0.61	-0.56	0.01	1.93

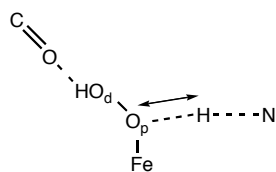
Figure S18: Energy scans for unprotonated state

$N(A_\beta)$ unprotonated state

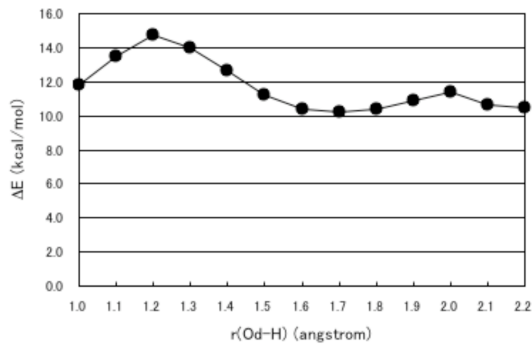
(a) **1a** $\rightarrow$ **2**



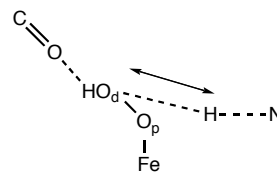
$\leftarrow$ **1a** **2** $\rightarrow$



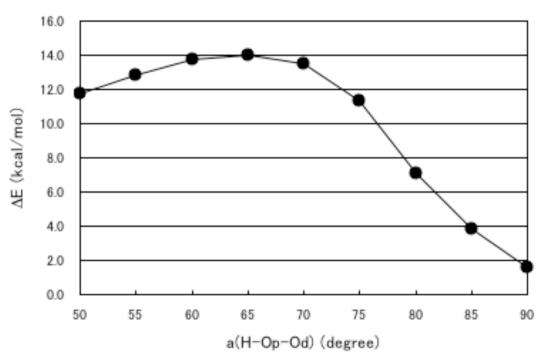
(b) **2** $\rightarrow$ **3**



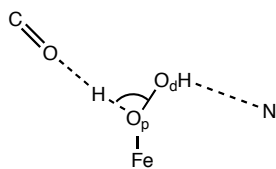
$\leftarrow$ **3** **2** $\rightarrow$



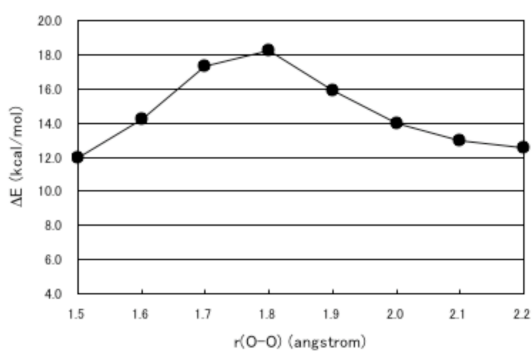
(c) **1b** $\rightarrow$ **3**



$\leftarrow$ **3** **1b** $\rightarrow$



(d) **3** $\rightarrow$ **4**



$\leftarrow$ **3** **4** $\rightarrow$

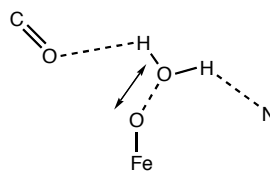
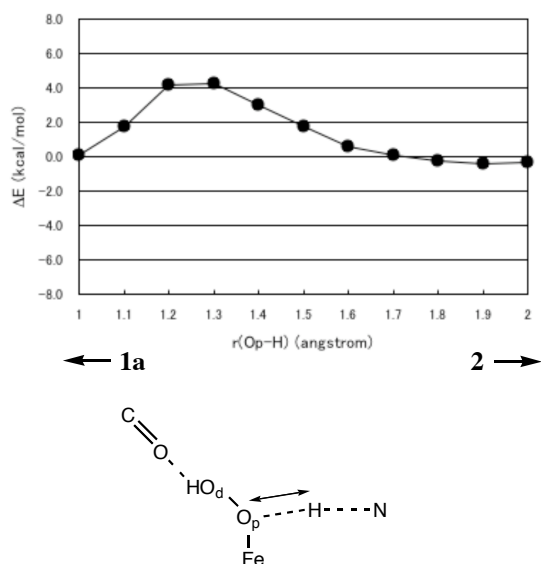


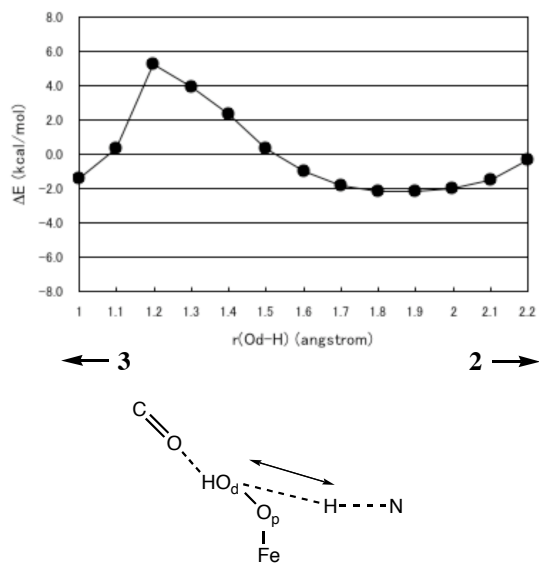
Figure S19: Energy scans for protonated state (used for Figure 6 and 7 in the text)

N(A_β) protonated state

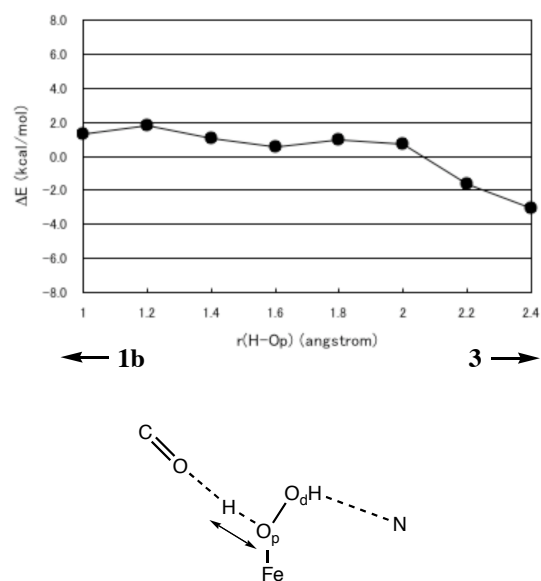
(a) **1a** --> **2**



(b) **2** --> **3**



(c) **1b** --> **3**



(d) **3** --> **4**

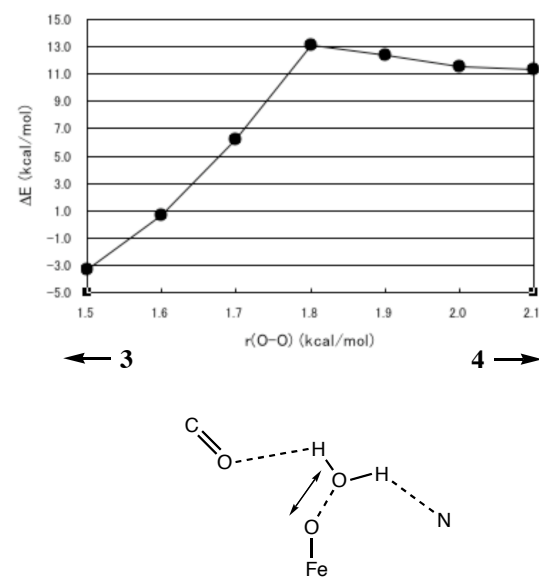
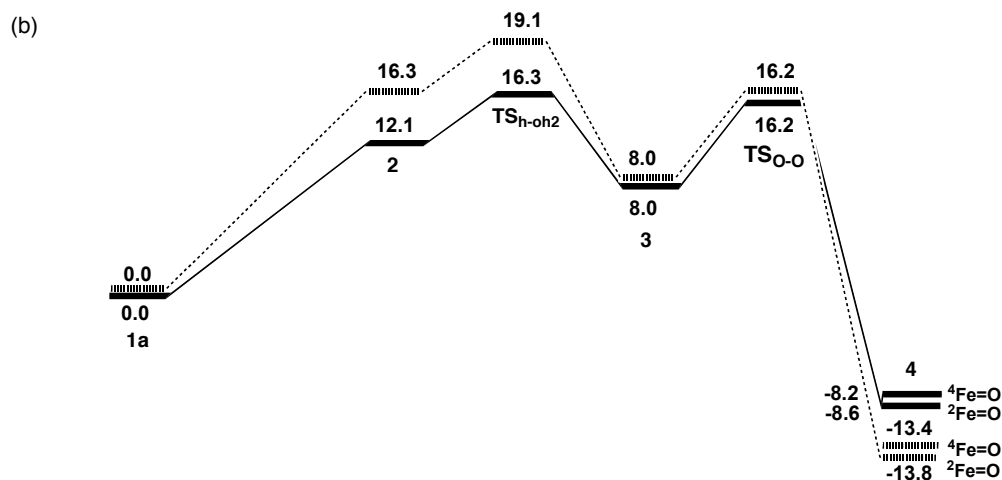
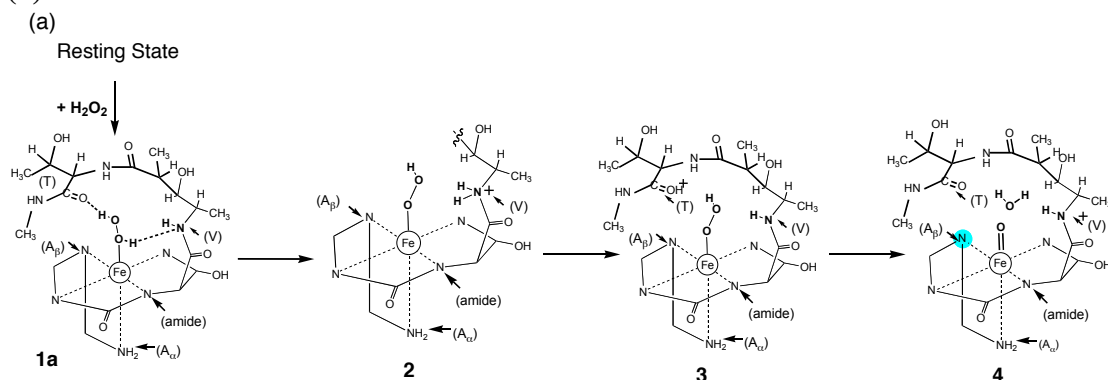


Figure S20: Energy profiles for **unprotonated state**: (a) path A, (b) path B

(a) Path A



(b) Path B (note that the barrier in solution drops to 10.9 kcal/mol)

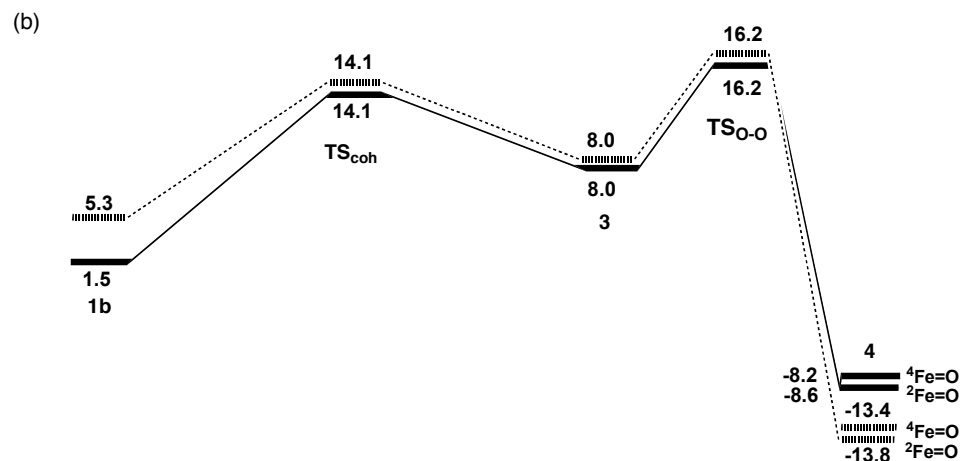
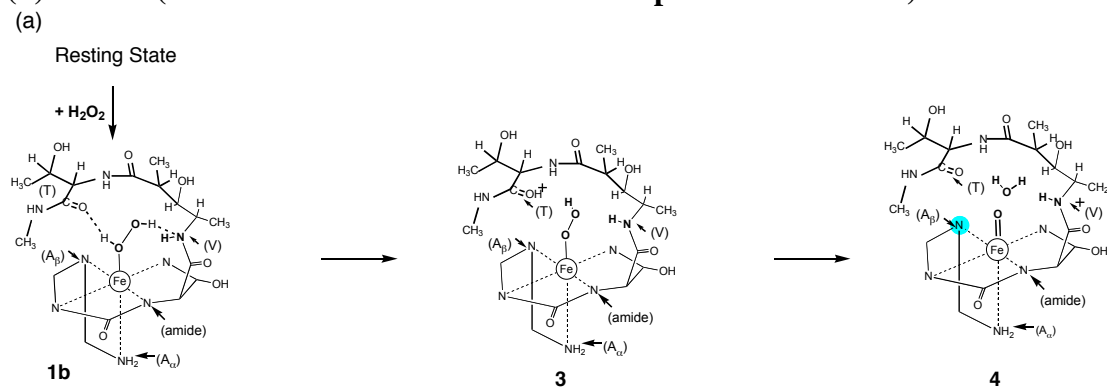
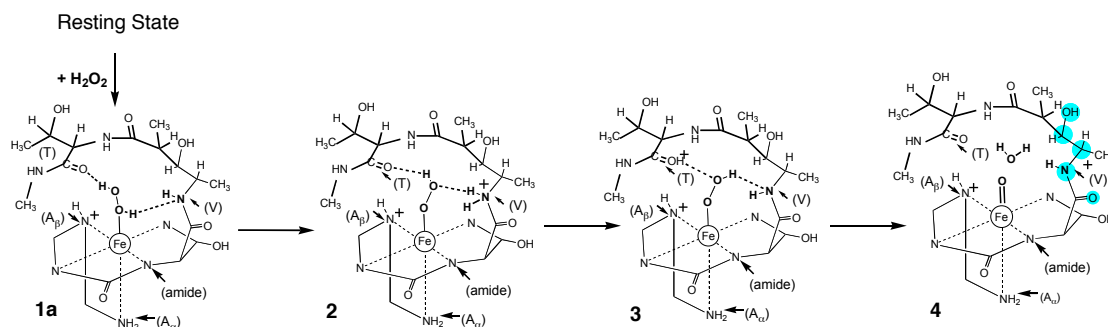


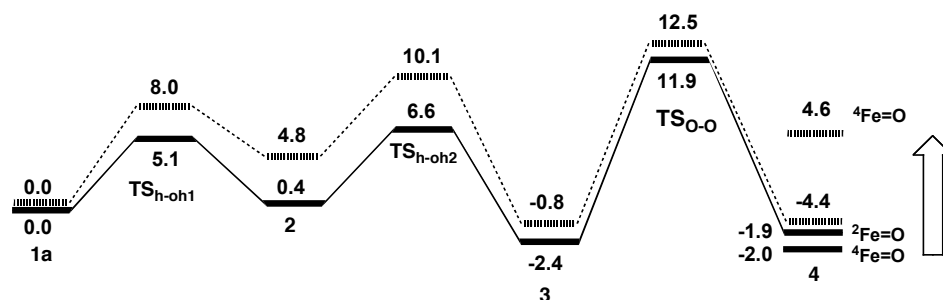
Figure S21: Energy profiles for protonated state: (a) path A, (b) path B (Figure 6 and 7 in the text)

(a) Path A

(a)

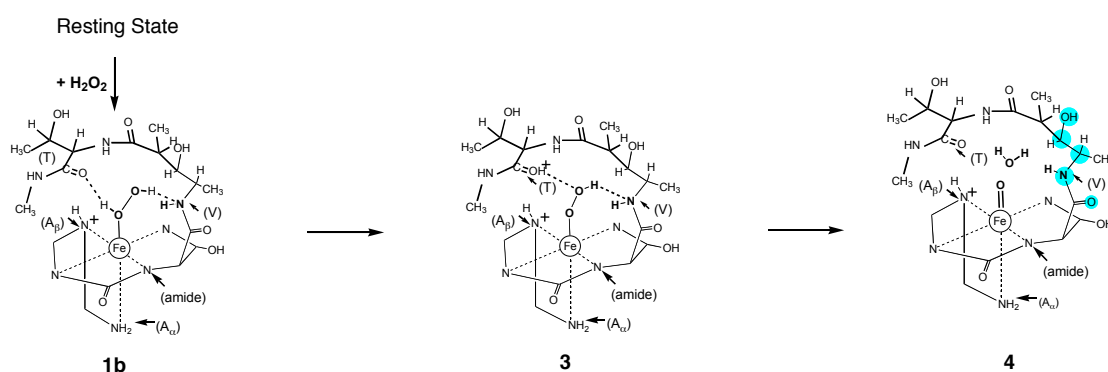


(b)



(b) Path B

(a)



(b)

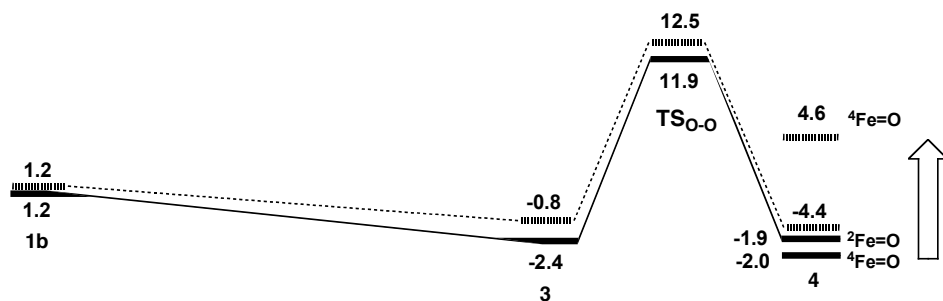


Table S1a: Relative intrinsic acidity of H_2O_2 in the presence of $[\text{BLM-Fe}^{\text{III}}]^+$ and $[\text{BLM(H)-Fe}^{\text{III}}]^{2+}$ in the gas phase, in chlorobenzene ($\epsilon = 5.7$) and in water ($\epsilon = 80.4$). All values are in kcal/mol.

A	$\text{H}_2\text{O}_2 \rightarrow \text{H}^+ + \text{HOO}^-$
B	$\text{BLM-Fe}^{\text{III}}(\text{H}_2\text{O}_2)^+ \rightarrow \text{H}^+ + \text{BLM-Fe}^{\text{III}}\text{-HOO}$
C	$\text{BLM(H)-Fe}^{\text{III}}(\text{H}_2\text{O}_2)^{2+} \rightarrow \text{H}^+ + \text{BLM(H)-Fe}^{\text{III}}\text{-HOO}^+$

	$\Delta E(\text{g})$	$\Delta E(\text{g})_{\text{rel}}$	$\Delta(E+\epsilon=5.7)_{\text{rel}}$	$\Delta(E+\epsilon=80.4)_{\text{rel}}$
A	406.0	0.00	0.00	0.00
B	259.8	-146.2	-54.3	-30.1
C	185.9	-220.1	-84.8	-49.9 ^a

^a using a solvation energy of -256.0 kcal/mol for H^+ , the absolute ΔE in water for the complex C would be -4.5 kcal/mol

Table S1b: Relative energies (in kcal/mol) of the $[\text{BLM(H)-Fe}^{\text{III}}\text{-OOH; NH}_2^+(\text{V})]^{2+}$ (**2a**) and $[\text{BLM(H)-Fe}^{\text{III}}\text{-OOH; C=OH}^+(\text{T})]^{2+}$ (**2b**) species with respect to $[\text{BLM(H)-Fe}^{\text{III}}\text{-(H}_2\text{O}_2)]^{2+}$ (**2**) in different solvents using the solvent model implemented in Jaguar 5.5.

	1	2a	2b
ΔE	0.00	-5.86	+6.22
Solvent Chlorobenzene $\epsilon = 5.7$			
$\Delta(E+E_{\text{sol}})$	0.00	-0.46	+7.15
Solvent Acetonitrile $\epsilon = 37.5$			
$\Delta(E+E_{\text{sol}})$	0.00	+2.88	+5.76
Solvent Water $\epsilon = 80.4$			
$\Delta(E+E_{\text{sol}})$	0.00	+2.20	-2.60

Table S2: Energies (in au) and relative energies (in kcal/mol) of different species in Figure in the gas phase and in water: (a) Unprotonated (b) Protonated.

(a) Unprotonated

B1 (LACVP*)

	Energy	ΔE	Esolv	ΔE
1a	-2835.256643	0.0	-74.5352	0.0
1b	-2835.256158	0.3	-70.7348	4.1
1c	-2835.252861	2.4	-77.2934	-0.4
2'	-2835.239946	10.5	-70.5153	14.5
2	-2835.240326	10.2	-70.2932	14.5
TSh-oh2	-2835.233104	14.8	-71.6260	17.7
3 (C=OH+)	-2835.238662	11.3	-74.4838	11.3
TScoh	-2835.234375	14.0	-74.6059	13.9
TSO-O	-2835.228006	18.0	-74.4736	18.0
² 4	-2835.270278	-8.6	-79.7375	-13.8
⁴ 4	-2835.269633	-8.2	-79.7582	-13.4

B2 (LACV3P+***)

	Energy	ΔE	Esolv (B1)	ΔE
1a	-2836.142404	0.0	-74.5352	0.0
1b	-2836.139987	1.5	-70.7348	5.3
1c	-2836.138000	2.8	-77.2934	0.0
2'	-2836.122862	12.3	-70.5153	16.3
2	-2836.123126	12.1	-70.2932	16.3
TSh-oh2	-2836.116533	16.2	-71.6260	19.1
3 (C=OH+)	-2836.129660	8.0	-74.4838	8.0
TScoh	-2836.119880	14.1	-74.6059	14.1
TSO-O	-2836.116645	16.2	-74.4736	16.2
² 4	-2836.160815	-11.6	-79.7375	-16.8
⁴ 4	-2836.160675	-11.5	-79.7582	-16.7

(b) Protonated

B1 (LACVP*)

	Energy	ΔE	Esolv	ΔE
1a	-2835.598253	0.0	-156.6909	0.0
1b	-2835.596962	0.8	-156.6190	0.9
1c	-2835.589359	5.6	-159.5738	2.7
TSh-oh1	-2835.591593	4.2	-153.8152	7.1
2'	-2835.598695	-0.3	-151.5166	4.9
2	-2835.601603	-2.1	-152.2916	2.3
TSh-oh2	-2835.589975	5.2	-153.2341	8.7
3 (C=OH+)	-2835.604220	-3.7	-155.0514	-2.1
TSO-O	-2835.577322	13.1	-156.0947	13.7
² 4	-2835.597168	0.7	-159.1360	-1.8
⁴ 4	-2835.596846	0.9	-150.0469	7.5
² 4(iso)	-2835.563104	22.1	-157.5106	21.2

B2 (LACV3P+***)

	Energy	ΔE	Esolv (B1)	ΔE
1a	-2836.479147	0.0	-156.6909	0.0
1b	-2836.477285	1.2	-156.6190	1.2
1c	-2836.470373	5.5	-159.5738	2.6
TSh-oh1	-2836.471034	5.1	-153.8152	8.0
2'	-2836.476638	1.6	-151.5166	6.7
2	-2836.478530	0.4	-152.2916	4.8
TSh-oh2	-2836.468631	6.6	-153.2341	10.1
3 (C=OH+)	-2836.482980	-2.4	-155.0514	-0.8
TSO-O	-2836.460156	11.9	-156.0947	12.5
² 4	-2836.482214	-1.9	-159.1360	-4.4
⁴ 4	-2836.482365	-2.0	-150.0469	4.6
² 4(iso)	-2836.446338	20.6	-157.5106	19.8

Part IV: Cartesian coordinates of LACVP* optimized geometry of various species.

²BLM-Fe^{III}-OOH (Figure S3(a))

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	X	Y	Z
Fe	0.0046910152	0.0282150447	0.0109970402
N	0.0110278609	0.0392460744	1.9031304939
C	1.1895280781	0.0283583400	2.5557259764
C	1.2063813050	0.1758470196	3.9353918778
C	-0.0769424721	0.3741710083	4.5347294548
N	-1.2348317076	0.4439040556	3.8393397140
C	-1.1419470157	0.2823421545	2.5262791156
C	2.3769848339	-0.0713422506	1.5976886162
O	3.5429291886	-0.1771386962	2.0036255755
C	2.4544599509	0.1653183031	4.7795331282
N	-0.1915955508	0.5163187018	5.8811482425
C	-2.2840050256	0.4397052194	1.5186925492
N	-1.9642785916	-0.3515119681	0.3168885093
C	-2.1531687447	-1.7854224975	0.5737355224
C	-1.2251593377	-2.5702654264	-0.3457183724
C	-1.5055031551	-2.4589908511	-1.8572304014
N	-2.6090735978	-1.7313451355	-2.1913651217
N	1.9630913107	0.0032835074	0.3056058647
C	2.9960695648	0.0099091816	-0.7170834366
C	3.5377214651	1.4225615717	-1.1074992720
O	4.3452979090	1.5226940071	-2.0339133492
C	2.5682110633	-0.6747417533	-2.0364498203
C	1.3565419197	-0.0546884239	-2.6714867395
N	0.1656097033	0.1614566829	-1.9953878001
C	-0.6535075557	0.7824518455	-2.8253023230
N	-0.0462005669	0.9544914622	-4.0266219739
C	1.2288723738	0.4321116528	-3.9462408641
O	2.3804211690	-2.0840944128	-1.7860846571
N	3.0803739466	2.4662608307	-0.3820985078
C	3.4839452619	3.8533395085	-0.6292586441
C	4.4119654400	4.3656600636	0.4809207854
C	2.2212596254	4.7342505041	-0.7593236632
C	1.2543847615	4.2506733451	-1.8741336327
C	-0.0680729454	4.9893150698	-1.6884351522
O	-0.1619560936	6.2182761585	-1.8174466873
O	2.6359250955	6.0744986929	-0.9828181631
C	-3.6693835330	0.2165276971	2.1382669989
C	-4.7865138344	0.7348643776	1.2416346679
N	-5.9427229623	0.0149809561	1.2714227003
O	-4.6971013047	1.7614235742	0.5620706569
N	0.1227026333	-2.0235937881	-0.0863944043
O	-0.7887279617	-3.0458644923	-2.6619034180
C	1.8112521334	4.4781619699	-3.2880632192
N	-1.1195328926	4.1864017759	-1.3665778637
C	-2.4477018738	4.6763627997	-1.1020233026
C	-2.7791699296	4.6228339060	0.4069450864

O	-2.0528743636	4.0853230532	1.2484322584
C	-3.4846959148	3.8614597457	-1.9448207722
O	-3.3010569164	2.4648239481	-1.7720409617
C	-3.3463258954	4.1595563199	-3.4342179826
N	-3.9585168635	5.1929631293	0.7547542098
C	-4.4905581110	5.1352265604	2.1137047536
C	-4.0146826645	6.2891587115	2.9977547196
H	-2.7309009509	-1.5635116132	-3.1833554294
H	-2.8417570207	-0.9644453363	-1.5544741073
H	-1.2670843176	-3.6460643964	-0.1209699246
H	-1.8909105254	-2.0785599043	1.6112189685
H	-3.1959077688	-2.1138134087	0.4230847339
H	0.8232756057	-2.2896042311	-0.7902781209
H	0.4716870911	-2.3531871695	0.8131853639
H	-6.0436439814	-0.8308563709	1.8155261565
H	-6.7282612125	0.3358413890	0.7220872641
H	-3.8361362065	-0.8349446572	2.3990585301
H	-3.7115879846	0.7787748092	3.0809471249
H	-2.2462799768	1.4934926675	1.2178487751
H	-1.1020831989	0.7182732204	6.2649667535
H	0.6147009233	0.5365009620	6.4829402705
H	2.5607942852	1.1063152946	5.3386310971
H	3.3312783821	0.0359741116	4.1445508168
H	2.4290968080	-0.6535914276	5.5136103092
H	3.8730017585	-0.5373179635	-0.3475564149
H	3.4102807349	-0.5375204311	-2.7221109733
H	1.9280235799	0.4757251451	-4.7669185104
H	-1.6377084486	1.1618577064	-2.5773008710
H	-0.4499780407	1.4217471644	-4.8252310586
H	2.3391615528	2.2954619188	0.2911038629
H	1.0813110599	3.1847437849	-1.7164100506
H	1.8249125678	6.5620504254	-1.2266633388
H	4.0310360827	3.8515375059	-1.5759393964
H	3.9102581224	4.3308462504	1.4572749315
H	5.3106838359	3.7428036034	0.5364681816
H	4.7037584804	5.4008686363	0.2812174493
H	1.6777447197	4.6600685820	0.1982686771
H	1.0761888424	4.1813944164	-4.0469665933
H	2.7141464843	3.8795847293	-3.4418696791
H	2.0592672450	5.5292450268	-3.4456066634
H	-0.9174549330	3.2208730594	-1.0900777504
H	-2.4719643839	5.7272948730	-1.4145122475
H	-4.4975393443	4.1440822881	-1.6191905570
H	-3.6460312105	2.1899982402	-0.8959652893
H	-3.5468495765	5.2149176207	-3.6488782937
H	-4.0535334244	3.5445914948	-4.0000352974
H	-2.3309693893	3.9303363108	-3.7734837048
H	-4.4884246667	5.6830493299	0.0489797963
H	-4.3220559717	7.2600466262	2.5882750484
H	-2.9229636071	6.2764688406	3.0781441359
H	-4.1773414749	4.1771397693	2.5345894816
H	-0.4773905851	3.2363197501	1.1680164581
H	-4.4371706517	6.1939923133	4.0054849490
H	2.0226409287	-2.4800683810	-2.5986168676

O	-0.1677594157	1.8507162060	-0.0804603453
O	0.2741417979	2.6027627147	1.0893148586
H	-5.5833387424	5.1262558103	2.0380694072

⁴BLM-Fe^{III}-OOH (Figure S3(a))

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	X	Y	Z
Fe	-0.0076127899	-0.0738378951	-0.0578073989
N	-0.0196314433	-0.0800944916	2.0542765249
C	1.1341591927	-0.0028417384	2.7335905993
C	1.1125736359	0.2705337377	4.0973105805
C	-0.1910905322	0.5079533579	4.6376259517
N	-1.3257011678	0.5211051395	3.9035846537
C	-1.1797992424	0.2298405839	2.6146208557
C	2.3621665026	-0.1369954793	1.8250762045
O	3.5017396215	-0.2516957688	2.3070216993
C	2.3299309174	0.3542030166	4.9804892762
N	-0.3504707494	0.7497059306	5.9690391432
C	-2.3019953456	0.3599514773	1.5673857282
N	-1.9738856953	-0.4454593581	0.3853593380
C	-2.1575862493	-1.8805521422	0.6379148032
C	-1.2672360257	-2.6610731537	-0.3230859109
C	-1.6031733750	-2.5446255728	-1.8266567400
N	-2.5830988146	-1.6547269980	-2.1448110752
N	2.0410785375	-0.0599866546	0.5066200287
C	3.1780818808	-0.0477473373	-0.4003603552
C	3.7009364728	1.3659565823	-0.8021686643
O	4.6227622618	1.4644362416	-1.6171042858
C	2.9415345564	-0.8151796399	-1.7224543999
C	1.8830961685	-0.2123264774	-2.6026747448
N	0.5831307726	0.0068581663	-2.1773917464
C	-0.0551185844	0.5948235923	-3.1704251067
N	0.7736576880	0.7546958744	-4.2338350336
C	2.0107274341	0.2488816735	-3.8880948546
O	2.6449187952	-2.1929310904	-1.4109228143
N	3.0878836768	2.4195612156	-0.2178500628
C	3.4851677241	3.8095753227	-0.4558631844
C	4.3998806994	4.3236091992	0.6632947392
C	2.2214052455	4.6839769702	-0.5974566176
C	1.2840468659	4.2325793171	-1.7506729444
C	-0.0535773867	4.9433341828	-1.5626704747
O	-0.1468413231	6.1783418445	-1.5263479384
O	2.6281989053	6.0334664873	-0.7710716483
C	-3.7066386910	0.1487742424	2.1514667295
C	-4.7900732483	0.5996470320	1.1814051182
N	-5.9189399363	-0.1588912428	1.1662902275
O	-4.6939017407	1.6045373900	0.4722643941
N	0.0953831806	-2.1163059122	-0.1123393385
O	-1.0192439530	-3.2563681811	-2.6368810948
C	1.8597113323	4.5362158835	-3.1434030416
N	-1.1263537143	4.1141587896	-1.4440139119

C	-2.4614600974	4.5780412497	-1.1702998976
C	-2.7628350557	4.5976918172	0.3437780293
O	-2.0913842165	3.9946186556	1.1887664196
C	-3.4835423436	3.6791574038	-1.9440678745
O	-3.1726311151	2.3047737473	-1.7822772003
C	-3.4616872853	3.9853608971	-3.4381454183
N	-3.8586645708	5.3116565332	0.6955793569
C	-4.3495564285	5.3790655724	2.0714090013
C	-3.6576297426	6.4598269276	2.9052802552
H	-2.7334894141	-1.4918813272	-3.1326943170
H	-2.7468997939	-0.8843641202	-1.4900295314
H	-1.2947711618	-3.7366452443	-0.1038259680
H	-1.8672984383	-2.1744973382	1.6652135967
H	-3.2071619450	-2.1951960983	0.5115457620
H	0.7896295206	-2.4098531470	-0.8096503475
H	0.4613452031	-2.3960810938	0.7975662134
H	-6.0232217267	-0.9870277873	1.7323821696
H	-6.6759274204	0.1116621126	0.5533049138
H	-3.8681885518	-0.8886534145	2.4651047212
H	-3.7872982604	0.7633084865	3.0570542608
H	-2.2658644698	1.4083797846	1.2506435593
H	-1.2600679362	1.0580972487	6.2791075794
H	0.4444094290	0.9300923572	6.5604683924
H	2.4155507274	1.3471382487	5.4460103940
H	3.2264540524	0.1665238417	4.3901483979
H	2.2795703469	-0.3866662836	5.7914627950
H	4.0308032056	-0.5333068454	0.0910131269
H	3.8916432451	-0.7572355477	-2.2625170043
H	2.8598811723	0.2910189644	-4.5519753252
H	-1.0791574195	0.9416047044	-3.1413334451
H	0.5327162008	1.1924561549	-5.1114248778
H	2.2998494949	2.2341123239	0.3961187639
H	1.1280361338	3.1566114316	-1.6489926710
H	1.8038665393	6.5224646385	-0.9658228995
H	4.0448948734	3.8142565212	-1.3949384393
H	3.8839431030	4.2930947318	1.6309995617
H	5.2928288800	3.6944769990	0.7308660753
H	4.6990057869	5.3559966056	0.4645855354
H	1.6536403752	4.5811233120	0.3423292299
H	1.1525451284	4.2374500353	-3.9270719065
H	2.7913085691	3.9837484248	-3.3015611498
H	2.0682842431	5.6026772510	-3.2545856078
H	-0.9554186533	3.1203627283	-1.2819579518
H	-2.5334893791	5.6088152093	-1.5351162829
H	-4.4888508665	3.8838017079	-1.5469384859
H	-3.5139331681	2.0009742074	-0.9152012461
H	-3.7668764420	5.0189841256	-3.6353271690
H	-4.1460044255	3.3107902700	-3.9616497748
H	-2.4531297455	3.8427533652	-3.8396699327
H	-4.3379399383	5.8462625000	-0.0151277239
H	-3.8077806181	7.4546983981	2.4712084347
H	-2.5829397462	6.2645932631	2.9591181384
H	-4.1906376934	4.3937308216	2.5168519723
H	-0.5868309702	3.0907380906	1.0565282048

H	-4.0597201393	6.4679523336	3.9250346890
H	2.6716510584	-2.6857247076	-2.2476092029
O	-0.2220689822	1.7185241987	-0.1903793420
O	0.1960308222	2.4931436262	0.9598057557
H	-5.4298229473	5.5538431587	2.0244051672

²BLM(H)-Fe^{III}-OOH¹⁺ (Figure S3(b))

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	X	Y	Z
Fe	-0.0077734995	-0.0200310638	0.0266753088
N	0.0066262999	-0.0220541515	1.9197271400
C	1.2118214384	-0.0051756362	2.5362248280
C	1.2828535434	0.0623887706	3.9163537527
C	0.0115653907	0.1235305690	4.5821099601
N	-1.1737069696	0.1126446057	3.9310965661
C	-1.1239067951	0.0501801371	2.6089069415
C	2.3555959281	-0.0324674098	1.5300689263
O	3.5382875288	-0.0613247728	1.8698913942
C	2.5610623096	0.0844718554	4.7116172759
N	-0.0521488404	0.1834585223	5.9304304440
C	-2.3812240718	0.1636945577	1.7537977053
N	-2.0773465087	-0.2891377682	0.3464536062
C	-2.4359473613	-1.6645272821	-0.0611392150
C	-1.3683388918	-2.6660195786	0.4170608613
C	-1.5566216934	-4.0089560247	-0.3259685492
N	-2.3299875824	-4.9363428467	0.2992986674
N	1.8838736560	-0.0150958761	0.2438124308
C	2.8666795869	-0.0245418333	-0.8314980000
C	3.2379462283	1.3660515935	-1.4307792772
O	3.8812375681	1.4062109288	-2.4789476741
C	2.4446462839	-0.9315887861	-2.0042623761
C	1.1899014228	-0.4623375284	-2.6883318550
N	0.0503736447	-0.0975964046	-1.9849509857
C	-0.8644487342	0.2583446946	-2.8753314519
N	-0.3607261875	0.1314225674	-4.1247506500
C	0.9374916747	-0.3201854642	-4.0270847906
O	2.2865150221	-2.2696576832	-1.4970711601
N	2.8376575949	2.4528787850	-0.7354072350
C	3.1311168855	3.8334236974	-1.1366745093
C	4.0731132806	4.5059211352	-0.1311892722
C	1.7988309704	4.6041209886	-1.2764932351
C	0.8772591049	4.0336504651	-2.3951489041
C	-0.5075512510	4.6256582601	-2.1677381484
O	-0.7163405045	5.8466063015	-2.2089929757
O	2.0910271092	5.9708740058	-1.5002870862
C	-3.6094841617	-0.4471191534	2.4350950331
C	-4.9263809187	-0.0172544148	1.7892106716
N	-6.0462323749	-0.4829542415	2.3924425473
O	-4.9800810333	0.6840096275	0.7819579141
N	-0.0428177035	-2.1023523879	0.0936452029
O	-1.0767589660	-4.1589919801	-1.4403068538
C	1.3841795450	4.3412125642	-3.8141699419

N	-1.4948002753	3.7207968144	-1.8853894354
C	-2.8058484001	4.1679323466	-1.4200679374
C	-2.6847487967	4.4744914279	0.0840849972
O	-2.7487421966	3.5845861360	0.9542588569
C	-3.9042289241	3.1418185995	-1.7709361131
O	-3.5688472929	1.8179961823	-1.3260737412
C	-4.1542109486	3.0895201447	-3.2764649067
N	-2.4323270968	5.7674232624	0.3648199255
C	-2.0935627649	6.2510505693	1.7045085120
C	-0.5862915500	6.2318326400	1.9796664774
H	-2.4210173651	-5.8461680684	-0.1394677070
H	-2.5298473648	-4.8808723848	1.2875778917
H	-1.4374182284	-2.8026077997	1.5031061471
H	-3.4354195755	-1.9630391508	0.2724296635
H	-2.4436361341	-1.6709819356	-1.1562915673
H	0.2799449772	-2.4523557820	-0.8152345493
H	0.6649872283	-2.4192737326	0.7541857202
H	-6.0226233434	-0.9574834103	3.2819966342
H	-6.9441916290	-0.1696192801	2.0450184912
H	-3.5589210717	-1.5419249284	2.4745065171
H	-3.5892362632	-0.1148733943	3.4792671734
H	-2.5756006744	1.2370647303	1.6464346537
H	-0.9531924832	0.3228567282	6.3645846080
H	0.7765483663	0.3050879666	6.4909436439
H	2.6419681704	1.0111617359	5.2971336146
H	3.4233662396	0.0209808565	4.0487120833
H	2.5975297781	-0.7569909969	5.4172750212
H	3.8012004925	-0.4348663969	-0.4307767303
H	3.2627665726	-0.8880376944	-2.7279331527
H	1.5640076980	-0.4734148389	-4.8924926935
H	-1.8571389338	0.6289671852	-2.6544645858
H	-0.8518447198	0.3501068054	-4.9803520106
H	2.2411954581	2.3070709094	0.0697458313
H	0.8223563499	2.9507355017	-2.2563765297
H	1.2437985787	6.3935192444	-1.7368914525
H	3.6284811817	3.7675704388	-2.1069694824
H	3.6183629307	4.5499699735	0.8666309977
H	5.0076855454	3.9408317286	-0.0581494840
H	4.2954667868	5.5279354827	-0.4485552028
H	1.2641394425	4.4840607246	-0.3168631338
H	0.6806682002	3.9650019618	-4.5657896180
H	2.3495021423	3.8562088242	-3.9864922433
H	1.5049632832	5.4162041124	-3.9636526007
H	-1.1818065932	2.8265626941	-1.5056927571
H	-3.0300708078	5.0951834689	-1.9530238327
H	-4.8247484293	3.4614699812	-1.2646149141
H	-4.0757262084	1.6277054268	-0.5125911534
H	-4.4865428197	4.0614150938	-3.6573145770
H	-4.9248431098	2.3465677222	-3.4980632203
H	-3.2370385356	2.8138551775	-3.8086524717
H	-2.1858704992	6.3558300496	-0.4262370090
H	-0.0368077407	6.8304896216	1.2440834667
H	-0.1954957676	5.2099219256	1.9432522175
H	-2.6279015063	5.6165452242	2.4156091049

H	-2.4910192938	7.2674946145	1.7963659373
H	-0.3793855127	6.6437394869	2.9733184058
H	2.4064824514	-2.8847123716	-2.2366972859
O	-0.2658817660	1.7534639613	-0.1487674031
O	-0.1495367171	2.5531500969	1.0566521997
H	-1.0573443100	2.9357856011	1.1119240341
H	-2.5379177534	0.3728905746	-0.2817397918

⁴BLM(H)-Fe^{III}-OOH¹⁺ (Figure S3(b))

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	X	Y	Z
Fe	-0.0091755932	0.0735290323	0.0204190618
N	0.0862578646	-0.1216326535	1.9244705756
C	1.3217366646	-0.2187096957	2.4839747469
C	1.4577007809	-0.3413543070	3.8542997238
C	0.2203656125	-0.3591619232	4.5837889497
N	-0.9957715389	-0.2842103230	3.9932969580
C	-1.0181683740	-0.1577241924	2.6789465872
C	2.4338450046	-0.1691728460	1.4427053029
O	3.6225510282	-0.2748771959	1.7423944636
C	2.7684625897	-0.4461098560	4.5874825114
N	0.2175025824	-0.4714968284	5.9256639644
C	-2.3091870842	0.0617815670	1.9131965943
N	-2.1615397372	-0.4522396709	0.5157319099
C	-2.4949232736	-1.8644434920	0.2383745355
C	-1.3197165991	-2.8180378395	0.5433881631
C	-1.6473033632	-4.2002360170	-0.0629053507
N	-2.1254637379	-5.1430453363	0.7892084343
N	1.9290455557	0.0076767390	0.1844391192
C	2.8790752609	0.0437532191	-0.9192342720
C	3.2256976502	1.4641544071	-1.4504289108
O	3.7752805565	1.5797122100	-2.5456259534
C	2.4206171923	-0.8169078746	-2.1126307632
C	1.1306246083	-0.3352843759	-2.7231676895
N	0.0280525549	0.0313061595	-1.9622867723
C	-0.9385758693	0.4029270020	-2.7945447931
N	-0.5004235560	0.2810804435	-4.0646735286
C	0.8016933087	-0.1795689456	-4.0426114181
O	2.3058508898	-2.1720626098	-1.6538562471
N	2.9146043299	2.4953117770	-0.6344262371
C	3.2083909561	3.9012603437	-0.9264481466
C	4.0237956194	4.5255346075	0.2107650941
C	1.8830566292	4.6629246146	-1.1597522770
C	1.0677093590	4.1190267268	-2.3672896482
C	-0.3052217906	4.7732583206	-2.3085380802
O	-0.4541672765	6.0012551257	-2.4143787829
O	2.1865732351	6.0367743286	-1.3166816282
C	-3.5827207009	-0.3432874708	2.6576867713
C	-4.8149861015	0.2188562853	1.9387888887
N	-6.0060297135	-0.0395484272	2.5344158789
O	-4.7272321283	0.8454891206	0.8847740565

N	-0.1193586172	-2.2638530285	-0.0873341658
O	-1.5098335519	-4.3775760528	-1.2659076383
C	1.7408005984	4.3766904804	-3.7267416565
N	-1.3521624634	3.9198927471	-2.1144055832
C	-2.7022914100	4.4253376987	-1.8680219086
C	-2.7750146725	4.8136778110	-0.3820174035
O	-3.0783996477	3.9725325426	0.4911866117
C	-3.7591057849	3.3642406639	-2.2479909736
O	-3.4955747312	2.1198363261	-1.5974818926
C	-3.8005003386	3.1062299567	-3.7492786563
N	-2.4135554055	6.0779952079	-0.1063025100
C	-2.2023760333	6.5756155473	1.2552831530
C	-0.7518739697	6.4109526998	1.7213313065
H	-2.3176917427	-6.0663989116	0.4206782106
H	-2.1010230514	-5.0314062749	1.7920358969
H	-1.1536016562	-2.8850791695	1.6249041971
H	-3.3998756941	-2.1999598113	0.7596387762
H	-2.7001990826	-1.9305674344	-0.8348804826
H	-0.1064568504	-2.5491981167	-1.0685797081
H	0.7436502769	-2.6395854720	0.3028727944
H	-6.0755275432	-0.4625160393	3.4484357034
H	-6.8415638486	0.3601067428	2.1273288553
H	-3.6774015485	-1.4301075427	2.7739994129
H	-3.5269071771	0.0600573051	3.6752851078
H	-2.3474836287	1.1483507692	1.7820655607
H	-0.6646128130	-0.4172056380	6.4153385198
H	1.0719150239	-0.4618998493	6.4608648958
H	2.8895686002	0.3900371989	5.2904585491
H	3.6004260862	-0.4285012478	3.8852148904
H	2.8187710105	-1.3784781924	5.1667545734
H	3.8243990981	-0.3872299577	-0.5683189880
H	3.2045878086	-0.7273940423	-2.8694550408
H	1.3763306172	-0.3292161902	-4.9437755147
H	-1.9071891095	0.7973864526	-2.5071084072
H	-1.0354640917	0.5139939367	-4.8907291501
H	2.3977833311	2.2835230175	0.2095583250
H	0.9444163668	3.0421206229	-2.2224184563
H	1.3842816568	6.4568085071	-1.6839643659
H	3.8005644751	3.9057655388	-1.8438153610
H	3.4701440630	4.4910110618	1.1586244747
H	4.9664116476	3.9850402709	0.3430287723
H	4.2392913179	5.5724201005	-0.0150295619
H	1.2655292797	4.5101790580	-0.2544907645
H	1.0802311812	4.0768690274	-4.5487040985
H	2.6620907581	3.7924847890	-3.8063499407
H	1.9804652536	5.4353765242	-3.8501869962
H	-1.1351068077	3.0332066007	-1.6508496058
H	-2.8391402239	5.3138371761	-2.4907096983
H	-4.7387225064	3.7439439325	-1.9220088169
H	-3.6035656782	2.2858344011	-0.6402336724
H	-4.1118640153	4.0036690560	-4.2938202794
H	-4.5136416479	2.3047955066	-3.9651656052
H	-2.8113391229	2.8133242689	-4.1193978137
H	-1.9950099169	6.5968437639	-0.8749481979

H	-0.0542790786	6.9219122085	1.0475951261
H	-0.4729015719	5.3522491957	1.7577349518
H	-2.8861694747	6.0244677735	1.9048409713
H	-2.4993751027	7.6294061556	1.2709202951
H	-0.6266138900	6.8351927801	2.7240021984
H	2.4189018471	-2.7569045167	-2.4194546192
O	-0.5950808791	1.8979183948	-0.1207282951
O	-0.6975127680	2.6309167030	1.1279490683
H	-1.5381938215	3.1249507306	0.9772608026
H	-2.7855600504	0.1288339088	-0.0432310495

²[BLM-Fe^{IV}Fe=O;N[•](A_p)]¹⁺ (Figures S5(a), S17(a))

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	X	Y	Z
Fe	0.0238493155	0.0625113521	0.0903618732
N	-0.0199635974	-0.0234451229	2.0007418969
C	1.1605042247	0.0322071594	2.6591198433
C	1.1721239333	0.1611656923	4.0349701291
C	-0.1297107041	0.2387232431	4.6467055393
N	-1.2895441305	0.2346361093	3.9455253729
C	-1.1767876813	0.1505273644	2.6376019675
C	2.3280029694	0.0503950916	1.6875086739
O	3.5018517958	0.1917365556	2.0590298385
C	2.4170280655	0.2458722719	4.8743883721
N	-0.2518885149	0.3194128635	5.9871171784
C	-2.3462782430	0.3472639867	1.6628016229
N	-1.9439791271	-0.3775265780	0.4478654840
C	-2.4323267141	-1.7301501891	0.2623180863
C	-1.3267735447	-2.6316647365	-0.3575768401
C	-1.3535973603	-2.8675782046	-1.8861311628
N	-2.5772399275	-3.0217470478	-2.4533336891
N	1.9147822162	-0.0365110070	0.3940793058
C	2.9335997508	0.0674556313	-0.6509144158
C	3.2409482637	1.5410432373	-1.0767614784
O	3.2943926874	1.8502270260	-2.2671443717
C	2.5637725379	-0.7532751888	-1.9026038623
C	1.3234395883	-0.2587405869	-2.5855283733
N	0.1705509258	0.0504027761	-1.8884137887
C	-0.7238642993	0.5009536728	-2.7589647337
N	-0.1894791217	0.4653898028	-4.0002374941
C	1.1023709391	-0.0089184977	-3.9123802676
O	2.4295121831	-2.1277814198	-1.4938672927
N	3.4261733708	2.4098450208	-0.0557820770
C	3.6850653808	3.8466360439	-0.2305699234
C	4.7132718494	4.3003393685	0.8065765506
C	2.3661419870	4.6499841405	-0.1125534626
C	1.3608523710	4.3638447038	-1.2622966109
C	0.0178097602	5.0071075897	-0.9261099839
O	-0.0906812407	6.2019812740	-0.5987010795
O	2.7001310841	6.0269053769	-0.0646210838
C	-3.7268175945	0.0990751845	2.2665455886
C	-4.8249602974	0.5811404031	1.3195922510

N	-6.0147634050	0.8717990614	1.8861088734
O	-4.6406180848	0.6507803938	0.0990896498
N	-0.0116720348	-2.0842121024	0.0211498550
O	-0.3113990362	-2.9842913033	-2.5197115644
C	1.8431787761	4.8854735083	-2.6304741609
N	-1.0632255038	4.1900047899	-1.0571493826
C	-2.4216502084	4.6299723969	-0.7782292056
C	-2.6548959145	4.6595631325	0.7470747847
O	-2.9721106345	3.6437004297	1.3945097120
C	-3.4243957135	3.7208870052	-1.5414019776
O	-3.0172763280	2.3494427584	-1.4862804674
C	-3.5208222050	4.1259386881	-3.0132492525
N	-2.4682535183	5.8783116942	1.2941021088
C	-2.4889199748	6.1598518008	2.7298036521
C	-1.0854793089	6.3286870575	3.3154745952
H	-2.6076868986	-3.3245950755	-3.4195481584
H	-3.4385379651	-3.0592487588	-1.9274514116
H	-1.4582973047	-3.6376697007	0.0677773869
H	-2.7476535339	-2.1625989328	1.2224583553
H	-3.3366654295	-1.6662592271	-0.3602246274
H	0.7276926498	-2.3461595772	-0.6494830658
H	0.2816174319	-2.4290536658	0.9340965301
H	-6.1522517274	0.8855256256	2.8870359041
H	-6.7657959559	1.2084199431	1.2954261015
H	-3.9046932585	-0.9568382055	2.5057360789
H	-3.7585408571	0.6320756918	3.2219951137
H	-2.2916301687	1.4101528395	1.3830957833
H	-1.1688058134	0.5018717720	6.3719932934
H	0.5515251621	0.4742570409	6.5776125429
H	2.4461131771	1.1940905691	5.4290292371
H	3.3052482915	0.1918331520	4.2458578849
H	2.4530168858	-0.5727231792	5.6060069115
H	3.8571406598	-0.3621686400	-0.2422620591
H	3.3964425053	-0.6554325828	-2.6058536237
H	1.7510152412	-0.0866251519	-4.7702741600
H	-1.6958380818	0.9144673595	-2.5164854537
H	-0.6524655278	0.7786539336	-4.8428635474
H	3.5258040056	2.0239666443	0.8770518463
H	1.2178055605	3.2822930590	-1.3290412708
H	1.8505326776	6.5093081144	-0.1289723620
H	4.0977092155	3.9775883985	-1.2337460881
H	4.3368276782	4.1513421407	1.8270990671
H	5.6421412561	3.7335838154	0.6942953009
H	4.9238626803	5.3628340319	0.6816951566
H	1.8869503084	4.3405936652	0.8370081346
H	1.0531403962	4.7791825019	-3.3818591874
H	2.7031398003	4.3025353284	-2.9676183190
H	2.1227532957	5.9397576088	-2.5674134967
H	-0.9197391657	3.1832254269	-1.0517896983
H	-2.5188843721	5.6502967942	-1.1608401605
H	-4.4116589714	3.8270669616	-1.0673584718
H	-3.4916047292	1.8952947682	-0.7663918987
H	-3.8889451651	5.1484736024	-3.1191753120
H	-4.2055307769	3.4589632931	-3.5372643560

H	-2.5373988972	4.0654241720	-3.4936691055
H	-1.9852678906	6.5493293874	0.7005946706
H	-0.5536188307	7.1496437423	2.8212156976
H	-0.5019517189	5.4089681571	3.1942945192
H	-3.0266592869	5.3356526602	3.2077783871
H	-3.0771906859	7.0714264198	2.8810173493
H	-1.1535135991	6.5675705949	4.3835821547
H	2.1150772015	-2.6310719275	-2.2661026337
O	-0.1413226253	1.6853522837	0.0841209662
O	-0.3942790091	3.0112094245	2.6026921116
H	-1.3194069016	3.2691326256	2.4244698783
H	-0.0593309865	2.8020411735	1.7115021910

⁴[BLM-Fe^{IV}Fe=O;N⁺(A_p)]¹⁺ (Figure S5(a), S17(a))

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	X	Y	Z
Fe	-0.0296906647	0.0467840033	0.0551695182
N	-0.0701600644	0.0192727987	1.9691288554
C	1.1114485766	0.0997622049	2.6227616338
C	1.1266426100	0.2579870016	3.9956032584
C	-0.1726588515	0.3345741314	4.6105802474
N	-1.3341003857	0.3083529486	3.9127702704
C	-1.2269908126	0.1995551919	2.6072156722
C	2.2773796635	0.1061582989	1.6485311656
O	3.4491180589	0.2671699467	2.0152012976
C	2.3726942506	0.3701881917	4.8293863774
N	-0.2914106430	0.4447017176	5.9478915086
C	-2.4020006145	0.3730772578	1.6311809413
N	-1.9866844844	-0.3844636414	0.4423075147
C	-2.4850047143	-1.7330758455	0.2639582724
C	-1.3783339907	-2.6497028956	-0.3286738195
C	-1.3880303313	-2.9233602347	-1.8508830573
N	-2.6046939149	-3.0646458086	-2.4365458761
N	1.8656309822	-0.0159768126	0.3570568040
C	2.8885368993	0.0486631487	-0.6869829397
C	3.1949110111	1.5036104110	-1.1697871640
O	3.2563607296	1.7650710128	-2.3710463888
C	2.5215123179	-0.8191060459	-1.9072641342
C	1.2818148461	-0.3490865523	-2.6076454014
N	0.1284140575	-0.0198935285	-1.9209719342
C	-0.7654133062	0.4046395077	-2.8045524049
N	-0.2298602355	0.3323836269	-4.0432777576
C	1.0613265685	-0.1394405105	-3.9411160862
O	2.3876103972	-2.1773592216	-1.4477231854
N	3.3682269884	2.4129603822	-0.1825778344
C	3.6153667798	3.8438718649	-0.4128258805
C	4.6337210057	4.3522945657	0.6098203596
C	2.2852739409	4.6400623421	-0.3319479855
C	1.2843838473	4.3005865943	-1.4708951284
C	-0.0623082660	4.9475608480	-1.1606343624
O	-0.1731909910	6.1534650630	-0.8782269700
O	2.6069343013	6.0188454888	-0.3367858450

C	-3.7846319826	0.1376782956	2.2390290323
C	-4.8794969325	0.6093752020	1.2827141024
N	-6.0448581072	0.9845844153	1.8497487826
O	-4.7112934921	0.6045035127	0.0585542370
N	-0.0644364617	-2.0964771644	0.0487404957
O	-0.3386767357	-3.0802011438	-2.4625814880
C	1.7633512604	4.7691446152	-2.8588337895
N	-1.1390189414	4.1227475677	-1.2627860349
C	-2.5001183531	4.5585888276	-0.9815273274
C	-2.7163750615	4.6305000861	0.5452264062
O	-3.1014937389	3.6528940001	1.2154343277
C	-3.5022875845	3.6248062688	-1.7103742771
O	-3.0998857006	2.2563262351	-1.6096980296
C	-3.5996680256	3.9750973581	-3.1926954902
N	-2.4255598734	5.8404775736	1.0642540464
C	-2.4364136326	6.1619856923	2.4917145890
C	-1.0290466455	6.4059326356	3.0409498597
H	-2.6239210416	-3.4004347614	-3.3910917804
H	-3.4729459767	-3.0747290475	-1.9231937726
H	-1.5116699689	-3.6468855136	0.1165015667
H	-2.8069892599	-2.1477941891	1.2287171994
H	-3.3872207434	-1.6753749259	-0.3593398969
H	0.6798214801	-2.3782421818	-0.6079458484
H	0.2179505723	-2.4177039400	0.9736187539
H	-6.1713108798	1.0423021739	2.8496994977
H	-6.7977963527	1.2986655923	1.2510788935
H	-3.9663796459	-0.9143500222	2.4924923131
H	-3.8175945085	0.6854337946	3.1862510927
H	-2.3537357228	1.4288699863	1.3303912366
H	-1.2101569956	0.5987863883	6.3388987802
H	0.5126608684	0.5745330685	6.5421147614
H	2.3880079343	1.3227024382	5.3762348486
H	3.2586553117	0.3243598742	4.1977115488
H	2.4258614786	-0.4420327409	5.5672358353
H	3.8112060100	-0.3636190621	-0.2597365301
H	3.3544190386	-0.7464056316	-2.6131499697
H	1.7106086047	-0.2415330279	-4.7958139889
H	-1.7376681612	0.8236493196	-2.5748235674
H	-0.6924534584	0.6192311921	-4.8948093796
H	3.4596534768	2.0650832324	0.7662618738
H	1.1468789908	3.2166660604	-1.4933559602
H	1.7540157471	6.4891410403	-0.4261976864
H	4.0301856125	3.9398624385	-1.4190611689
H	4.2559312130	4.2354758568	1.6341396139
H	5.5730086592	3.7968557546	0.5217217032
H	4.8276482478	5.4133613853	0.4459197307
H	1.8077599730	4.3623382299	0.6266877779
H	0.9740815872	4.6265435421	-3.6055874699
H	2.6281286920	4.1790257391	-3.1711330757
H	2.0350875601	5.8269992619	-2.8385655884
H	-0.9872474834	3.1184768428	-1.2105112330
H	-2.6057782964	5.5684587879	-1.3884365099
H	-4.4851834419	3.7504377593	-1.2397679298
H	-3.5831268028	1.8265324581	-0.8800508694

H	-3.9752018093	4.9940516833	-3.3348169303
H	-4.2802297916	3.2804364228	-3.6938020540
H	-2.6148555938	3.9040988475	-3.6675575993
H	-1.9027068988	6.4624554422	0.4507096318
H	-0.5279346697	7.2128467404	2.4941622385
H	-0.4230435237	5.4991403594	2.9590468594
H	-2.9243787896	5.3272271460	3.0000662967
H	-3.0667171225	7.0478838001	2.6366012672
H	-1.0835243862	6.7010602695	4.0947197542
H	2.0781015809	-2.7088715034	-2.2019348397
O	-0.2486326519	1.6660957308	0.0024019366
O	-0.5067815240	3.0574619075	2.4577960155
H	-1.4344033298	3.3231525804	2.3167723956
H	-0.2255739709	2.7829818869	1.5638354366

$^2[\text{BLM}(\text{H})\text{-Fe}^{\text{IV}}\text{Fe}=\text{O};\text{N}^+(\text{A}_\text{p})]^{2+}$ (Figure S5(b), Figure 17(b))

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	X	Y	Z
Fe	0.0814672165	0.0704647903	-0.0205020358
N	0.0495214455	0.0147537596	1.8894840366
C	1.2374828046	-0.0330649933	2.5445072525
C	1.2767954711	0.0304581817	3.9224091856
C	-0.0111476437	0.1849719131	4.5543536814
N	-1.1679066193	0.3265789416	3.8593467632
C	-1.0861204070	0.2598228257	2.5455220579
C	2.3929194587	-0.0354135506	1.5670425898
O	3.5774406591	0.0767371224	1.9202130655
C	2.5280862901	-0.0251996509	4.7531705123
N	-0.1189053253	0.2185936352	5.8916895124
C	-2.2469835357	0.5634033346	1.6136615899
N	-2.0088951671	-0.2225607176	0.3515772975
C	-2.3454058068	-1.6673182634	0.4969041451
C	-1.3793937993	-2.5675526163	-0.2895718521
C	-1.6008830522	-2.7236962668	-1.8124908455
N	-2.8900686784	-2.8319569232	-2.2326726078
N	1.9771022845	-0.0854785804	0.2713616256
C	3.0120107140	-0.0872802529	-0.7638418527
C	3.4343640590	1.3529534317	-1.1413347304
O	3.4225789363	1.7895358806	-2.2789929954
C	2.5949036350	-0.8750436166	-2.0235041165
C	1.3795028656	-0.3213697993	-2.7064008417
N	0.2426777902	0.0540384649	-2.0142502569
C	-0.6163403586	0.5466131979	-2.8953758079
N	-0.0818886762	0.4743985485	-4.1340867131
C	1.1785174849	-0.0704994616	-4.0375664892
O	2.4055983615	-2.2330569990	-1.6014425611
N	3.8286153385	2.1339374391	-0.0544284914
C	4.1403178508	3.4966926897	-0.1267838977
C	5.1438230958	3.9480367234	0.9180040264
C	2.6682458374	4.4548585358	0.1066746114
C	1.6986802327	4.3042832672	-1.0546649265

C	0.4461102466	5.1364997463	-0.6874446920
O	0.5711771408	6.3393367157	-0.4194995216
O	3.0460314759	5.7364872289	0.3487541370
C	-3.6358748765	0.4235743920	2.2419860948
C	-4.7258035969	0.9481578307	1.3065692394
N	-5.9684216817	1.0156650333	1.8206041922
O	-4.4826232621	1.2744674177	0.1352747171
N	-0.0143890009	-2.0585477858	-0.0638751806
O	-0.6440541772	-2.7774989237	-2.5727361265
C	2.2213658869	4.8307248732	-2.4101012161
N	-0.7208727136	4.4761535449	-0.7521398189
C	-2.0135805345	5.0720361950	-0.4774558144
C	-2.3773988867	4.9153622283	1.0143488855
O	-2.0021530930	3.9400642094	1.6825208015
C	-3.0715846830	4.3860975357	-1.4053950243
O	-2.8706371676	2.9725267046	-1.4036675397
C	-2.9643157462	4.8841647760	-2.8423967454
N	-3.1710090793	5.8889383652	1.5055756106
C	-3.6166045167	5.9505236905	2.9015819361
C	-2.7747046512	6.9089019725	3.7454277794
H	-3.0267549513	-3.1236453067	-3.1940833943
H	-3.6489012650	-3.0345502989	-1.5967946874
H	-1.4827912188	-3.5863190445	0.1145264143
H	-2.2393486129	-1.9270781812	1.5544810070
H	-3.3923816552	-1.8475799779	0.2315173722
H	0.6292670548	-2.3610133965	-0.8093793207
H	0.3662162863	-2.4172469754	0.8111619071
H	-6.1848237956	0.7423736429	2.7692326333
H	-6.7279960383	1.3268404680	1.2273676444
H	-3.8639095629	-0.6111112188	2.5268825994
H	-3.6348931129	0.9951058235	3.1769303068
H	-2.1177506808	1.6136254805	1.3205056149
H	-1.0273498283	0.3780993078	6.3062260715
H	0.6841265660	0.1574800164	6.4995428828
H	2.6220808125	0.8782717108	5.3701813756
H	3.4116989232	-0.0999586623	4.1219244010
H	2.5100464277	-0.8920076095	5.4276989324
H	3.8930565048	-0.5936402731	-0.3477960280
H	3.4323098834	-0.8171592261	-2.7281565629
H	1.8178434878	-0.2044691752	-4.8962052336
H	-1.5664068640	1.0113895604	-2.6709783788
H	-0.5340187433	0.7778462665	-4.9868996370
H	3.9176387705	1.6470906226	0.8449072889
H	1.4170942196	3.2546108400	-1.1469176200
H	2.4023214553	6.3444428767	-0.1089145886
H	4.3930373371	3.7758783183	-1.1514469707
H	4.8103418745	3.7064949885	1.9330964318
H	6.0956802140	3.4360617703	0.7365977688
H	5.3035523288	5.0247343992	0.8536509044
H	2.3175837161	3.9683033157	1.0375035307
H	1.4108454399	4.8366115088	-3.1449979279
H	3.0090594401	4.1791323288	-2.7942234099
H	2.5986120182	5.8541550733	-2.3281903404
H	-0.7142351931	3.4590684218	-0.8154574676

H	-1.9524524735	6.1358328226	-0.7250807218
H	-4.0685716545	4.6234713092	-1.0116157248
H	-3.4754642236	2.5469818800	-0.7675140392
H	-3.1517078558	5.9611407738	-2.9044660864
H	-3.7003495306	4.3681819872	-3.4651636223
H	-1.9664844457	4.6834180504	-3.2465691245
H	-3.3416150283	6.7042970573	0.9297616788
H	-2.8135509250	7.9295057589	3.3495132948
H	-1.7280105826	6.5895911235	3.7698958189
H	-3.5569881313	4.9321886952	3.2906984163
H	-4.6693347392	6.2527430879	2.9036409632
H	-3.1520235839	6.9351684294	4.7729756329
H	2.2275989701	-2.7690533559	-2.3935510045
O	-0.0664518726	1.6995898114	-0.0892920339
O	0.7714120461	3.1294382726	2.1110758183
H	-0.0122327389	3.6857104282	2.2822136275
H	0.4839587581	2.6218733721	1.3228301443
H	-2.6094784653	0.2062633031	-0.3549134373

⁴[BLM(H)-Fe^{IV}Fe=O;N⁺(A_g)]²⁺ (Figure S5(b), Figure 17(b))

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	X	Y	Z
Fe	0.0000000000	0.0000000000	0.0000000000
N	0.0000000000	0.0000000000	1.9110654223
C	1.1991070513	0.0000000000	2.5472544799
C	1.2589075779	0.1051315737	3.9218692134
C	-0.0221434548	0.2473833073	4.5704819651
N	-1.1929909839	0.3406690675	3.8910761033
C	-1.1306396674	0.2370983087	2.5785723392
C	2.3384628683	-0.0035769452	1.5510958219
O	3.5253944452	0.1472754848	1.8809967294
C	2.5243214150	0.1040063590	4.7328670216
N	-0.1092699632	0.3179167872	5.9078836485
C	-2.3133348979	0.4851437755	1.6577934845
N	-2.0763625001	-0.3318454550	0.4153543497
C	-2.3751340369	-1.7793174429	0.6083416092
C	-1.4001458340	-2.6790208924	-0.1675947865
C	-1.6421054627	-2.8853506394	-1.6813993190
N	-2.9348244383	-3.0368006739	-2.0766374744
N	1.9033058147	-0.1018410639	0.2645570186
C	2.9212472274	-0.1094619969	-0.7873090123
C	3.3022191641	1.3286838411	-1.2136342629
O	3.2615712894	1.7310536127	-2.3631801596
C	2.5033860946	-0.9438575907	-2.0163226485
C	1.2640562010	-0.4398485981	-2.6946573844
N	0.1296299999	-0.0714666276	-1.9948381455
C	-0.7551505409	0.3741591334	-2.8754659669
N	-0.2389911052	0.2781862497	-4.1203060794
C	1.0357249465	-0.2333021709	-4.0290248158
O	2.3540691309	-2.2929484639	-1.5517464439
N	3.6946345219	2.1506535001	-0.1566993877

C	3.9717783647	3.5177449146	-0.2739512057
C	4.9805610715	4.0236489512	0.7403143297
C	2.4806797374	4.4468868373	-0.0439493625
C	1.4966142387	4.2389024915	-1.1840359828
C	0.2301398317	5.0513914971	-0.8203455505
O	0.3300785421	6.2642687959	-0.5897072411
O	2.8308920044	5.7437825974	0.1543164891
C	-3.6881635649	0.3307428684	2.3130563855
C	-4.8054066813	0.8012239429	1.3810947605
N	-6.0409153062	0.8541328411	1.9136432990
O	-4.5890441658	1.0985084780	0.1968842020
N	-0.0445360128	-2.1310485455	0.0203182910
O	-0.6965397678	-2.9386792065	-2.4556413286
C	1.9845298606	4.7374224241	-2.5627907890
N	-0.9212609194	4.3616834028	-0.8462463139
C	-2.2235678361	4.9343147076	-0.5674793349
C	-2.5595278768	4.8131263174	0.9341318040
O	-2.1499378837	3.8672566326	1.6240853660
C	-3.2792289447	4.1961340271	-1.4572122762
O	-3.0438312254	2.7884454716	-1.4176366891
C	-3.2071659002	4.6539484470	-2.9097150891
N	-3.3687040605	5.7815205069	1.4099657301
C	-3.7932678907	5.8736459130	2.8108369486
C	-2.9616158214	6.8764127197	3.6121943526
H	-3.0797205355	-3.3599565106	-3.0267171431
H	-3.6782097493	-3.2386190867	-1.4225279212
H	-1.4721608043	-3.6875849898	0.2677025555
H	-2.2458526913	-2.0051026680	1.6711207621
H	-3.4215110404	-1.9923461842	0.3658611488
H	0.5942966585	-2.4399194293	-0.7267068637
H	0.3586699171	-2.4545246903	0.8989556223
H	-6.2353693947	0.6038897902	2.8733203286
H	-6.8172580156	1.1293767303	1.3243676800
H	-3.8862820647	-0.7002337876	2.6317668255
H	-3.6861693285	0.9295097293	3.2307949594
H	-2.2144876071	1.5290371925	1.3320269129
H	-1.0145859119	0.4678150309	6.3327219505
H	0.7046411978	0.2940257828	6.5037516330
H	2.6060964395	1.0273049313	5.3216203391
H	3.3992784800	0.0317960047	4.0893861382
H	2.5382466364	-0.7426758820	5.4325850608
H	3.8209382653	-0.5820778480	-0.3714645974
H	3.3277433902	-0.8867952316	-2.7362628085
H	1.6643051911	-0.3772454723	-4.8939602572
H	-1.7125664998	0.8224930962	-2.6488628396
H	-0.7119868002	0.5453958387	-4.9739254949
H	3.8099001449	1.6928623241	0.7548327923
H	1.2392962659	3.1805244792	-1.2409296629
H	2.1652891963	6.3223705958	-0.3100563703
H	4.2011734117	3.7725004453	-1.3103988402
H	4.6693665496	3.8042945401	1.7674493442
H	5.9416072324	3.5294636622	0.5580240854
H	5.1129077472	5.1014891272	0.6419397920
H	2.1569441629	3.9797951821	0.9063995450

H	1.1624480248	4.7021933595	-3.2838952149
H	2.7816460058	4.0938020576	-2.9408681785
H	2.3379422753	5.7715609175	-2.5170671518
H	-0.8908105662	3.3436217556	-0.8799892756
H	-2.1923989047	5.9914882568	-0.8469978212
H	-4.2752827998	4.4211117682	-1.0539094125
H	-3.6278295208	2.3675305888	-0.7593266601
H	-3.4217628739	5.7238270322	-3.0000126960
H	-3.9402581013	4.1023230911	-3.5047847023
H	-2.2113285743	4.4652843840	-3.3244870216
H	-3.5683586448	6.5751928421	0.8135597090
H	-3.0316977849	7.8836505283	3.1874003834
H	-1.9071811354	6.5831048807	3.6284603065
H	-3.7025888651	4.8689714543	3.2284234159
H	-4.8528943156	6.1505140125	2.8216822276
H	-3.3229677570	6.9239917525	4.6447034854
H	2.1765515178	-2.8562218382	-2.3248067695
O	-0.1887274500	1.6223743983	-0.1137704551
O	0.6490939586	3.1362556487	2.0296660615
H	-0.1450573040	3.6784283011	2.1975904402
H	0.3615368534	2.5988878917	1.2614671494
H	-2.6984667533	0.0614204886	-0.2931988896

[²BLM(H)-Fe^{IV}=O; NH⁺(A_α)]²⁺ (Figure S6)

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	X	Y	Z
Fe	-0.0040276900	0.0324800676	0.0138127904
N	-0.0149722677	0.0195919137	1.9265729813
C	1.1529109314	0.0035944802	2.6120879008
C	1.1612819478	-0.0193128428	3.9912524882
C	-0.1542699470	0.0159767213	4.5952110963
N	-1.3036631435	0.0427281263	3.8730371166
C	-1.1897225754	0.0428427762	2.5596381674
C	2.3429096687	0.0148057523	1.6805587499
O	3.4453735706	-0.3913505541	1.9285467448
C	2.3940771135	-0.0522036606	4.8484740750
N	-0.2935182944	0.0181454939	5.9273496385
C	-2.3510914498	0.1127556834	1.5821586281
N	-1.8974119772	-0.6520199060	0.3522711107
C	-1.9483711477	-2.1401141167	0.5352120199
C	-0.7141530416	-2.8329481453	-0.0785513030
C	-0.7875134404	-3.4168570413	-1.5506761977
N	-1.9849562526	-3.9192338740	-1.9292928759
N	1.9762282865	0.5827771731	0.3651192838
C	3.0298532888	0.5528925581	-0.7052180546
C	3.1777091706	1.9486047293	-1.3897944733
O	3.2322439313	2.0232535634	-2.6109974803
C	2.7757449387	-0.5132350866	-1.7934701266
C	1.4882399466	-0.3377006686	-2.5516492459
N	0.2526327500	-0.1228407318	-1.9543424662

C	-0.6426266438	0.0473082020	-2.9218160306
N	-0.0271279881	-0.0699004316	-4.1170217891
C	1.3114073938	-0.3087772395	-3.9087610890
O	2.8857971569	-1.8013602224	-1.1622174687
N	3.2141943970	3.0219859998	-0.5611310388
C	3.2658726910	4.4243518877	-1.0283242375
C	4.2756098639	5.2084454894	-0.1912839805
C	1.8422461368	5.0378198599	-0.9545711730
C	0.8453262715	4.4052286091	-1.9622201857
C	-0.5759260659	4.8328218984	-1.5986492392
O	-0.8500216872	5.9883237630	-1.2358551500
O	1.9525146920	6.4264143213	-1.1434506446
C	-3.7309748996	-0.2769272619	2.1234378476
C	-4.8061829143	-0.0862205374	1.0470545999
N	-6.0561578961	0.1389891225	1.4834295461
O	-4.5327790292	-0.1828143357	-0.1590950700
N	0.3831122453	-1.9272131533	-0.0108502549
O	0.2126756135	-3.4180764654	-2.2452724502
C	1.1455305627	4.7912453172	-3.4246733731
N	-1.5177601009	3.8636163099	-1.7338041965
C	-2.9405690167	4.0590799089	-1.4829364777
C	-3.2245941627	3.9355819742	0.0327241303
O	-3.6207656359	2.8756895775	0.5495006983
C	-3.7523459792	3.0371185852	-2.3100896724
O	-3.2949708571	1.7025173738	-2.0411675256
C	-3.6468023873	3.2809216478	-3.8087929328
N	-2.9901358500	5.0726734071	0.7193846419
C	-3.1393168988	5.2039313078	2.1660433503
C	-1.7988610030	5.2322887276	2.9048732710
H	-2.0133398672	-4.4199532241	-2.8110574659
H	-2.7391907882	-4.0980260805	-1.2827708273
H	-0.4778281331	-3.7315733361	0.5205231019
H	-1.9445362235	-2.3506978454	1.6072251305
H	-2.8969648600	-2.5057897720	0.1349698120
H	1.2727173769	-2.2793298265	-0.4043802835
H	1.7117588423	1.5622146903	0.5679204780
H	-6.2856287612	0.2544221925	2.4603900025
H	-6.7982904671	0.2456896214	0.8022133175
H	-3.7625183465	-1.3157512805	2.4750766701
H	-3.9323687972	0.3470484473	2.9999504685
H	-2.4261459859	1.1553548645	1.2437364240
H	-1.2243343730	0.0546669295	6.3231241288
H	0.4947166924	0.0034481210	6.5579382977
H	2.4402618701	0.8327224884	5.4967908299
H	3.3026884841	-0.0871013635	4.2495239696
H	2.3932947373	-0.9400802467	5.4944081161
H	3.9719344316	0.2834763667	-0.2144732005
H	3.5907389998	-0.3900923998	-2.5119625893
H	2.0161396093	-0.4002617316	-4.7204573495
H	-1.6830460561	0.3230063314	-2.7908967318
H	-0.4795631012	0.0252550471	-5.0179350193
H	3.3233113555	2.8851212968	0.4360335674
H	0.9017872103	3.3148410028	-1.8715756372
H	1.0356743663	6.7682199847	-1.1549582662

H	3.5987527092	4.3914080596	-2.0673487942
H	3.9915331091	5.2215531048	0.8698252818
H	5.2731872044	4.7678384265	-0.2802870467
H	4.3124932040	6.2435326902	-0.5335423404
H	1.4661014763	4.8237504341	0.0649615995
H	0.3642300950	4.4114156770	-4.0907766232
H	2.0968199088	4.3574628616	-3.7442871197
H	1.1991270475	5.8761201493	-3.5355158757
H	-1.2226111778	2.8963843142	-1.7872007890
H	-3.1929895863	5.0727651216	-1.8088773924
H	-4.8021784659	3.1223765550	-2.0019277003
H	-3.6763239167	1.4605524856	-1.1761509673
H	-4.0350373780	4.2703128547	-4.0706132461
H	-4.2307790614	2.5285975666	-4.3462210951
H	-2.6059233000	3.2240806940	-4.1447376880
H	-2.5480769916	5.8330162447	0.2055644076
H	-1.1718360627	6.0602737935	2.5514287362
H	-1.2493017393	4.2936287182	2.7633715590
H	-3.7555803932	4.3644724563	2.4972741977
H	-3.6968904586	6.1252786009	2.3663708852
H	-1.9613721960	5.3739627829	3.9779697657
H	2.9489183743	-2.4747051443	-1.8622596860
O	-0.4894164003	1.5869411093	-0.1416335130
O	0.9543223222	2.9025420578	1.8614380011
H	1.1290111678	3.8399220339	2.0425402488
H	0.1847737492	2.9003417011	1.2587992966
H	-2.5823837321	-0.3937781792	-0.3674540025

³BLM-Fe^{IV}=O (Figure S7(a))

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	X	Y	Z
Fe	-0.0276621926	-0.0343290086	0.0928583404
N	-0.0301879362	0.0321680997	2.0488882693
N	0.1376374127	-0.0162196630	-1.7956355902
N	1.8862389633	-0.6188029396	-0.0573048059
N	-1.7310801003	0.9040866976	-0.2417103679
N	0.7846062780	1.9657559940	0.0567242462
H	1.6035175294	1.9300283568	-0.5471779334
H	1.1288540710	2.1805895493	0.9998353601
H	-2.1215637760	0.0112106848	2.4701468382
C	2.7830941157	-0.9398778458	1.0609710862
O	3.4625415293	-1.3294320573	-1.6401237969
H	-2.6229995787	-0.4595280443	-1.5128494799
C	-1.6065565462	2.3234200170	0.0849604546
C	0.2599505664	-0.0478593877	-4.4670345381
C	1.3107581922	-0.4173886693	-2.3549125449
C	-0.9472558655	0.2998808880	-2.5138439689
N	-0.9148308690	0.2921105824	-3.8580793814
C	1.4318325774	-0.4423530809	-3.7430571272
C	2.3283006447	-0.8183335630	-1.3114843685
C	-2.1771446362	0.5417014413	-1.6292686967

C	2.4921381622	-0.0757106239	2.3091867287
H	3.8127945071	-0.7194117709	0.7368103113
H	3.1727189436	-0.4088513076	3.1007607049
H	1.2359791833	-0.4902622957	5.0467130774
C	1.1005704046	-0.1363100059	2.8468095843
C	-1.1069870553	-0.0405489139	2.8246042649
N	-0.7076658829	-0.2422615080	4.1155270173
C	0.6812702963	-0.3043585731	4.1444629316
H	-1.3191832214	-0.3584169044	4.9067341382
H	-2.4408237043	2.9285348572	-0.2933366909
C	-0.2443375900	2.9215986785	-0.4021834876
H	-1.6147652010	2.4207744942	1.1785657226
H	-0.2374914070	2.9467451813	-1.4985777613
C	-0.0123311141	4.3214307186	0.1515093301
O	0.6643468557	4.5208698347	1.1852445362
N	-0.6484823713	5.3358936088	-0.5099103841
H	-1.1958061381	5.1830346017	-1.3416559122
H	-0.5779874302	6.2728520553	-0.1421032174
C	2.6792596932	-0.8562110008	-4.4808050213
H	3.0737589258	-0.0300846986	-5.0904846830
H	3.4453764381	-1.1605271044	-3.7665494301
H	2.4767256804	-1.7004442295	-5.1554206724
N	0.2606110646	-0.0025379176	-5.8268226855
H	1.0720862355	-0.2498736479	-6.3655316907
H	-0.5807745898	0.2769686117	-6.3043009650
C	-3.2532955111	1.4806092545	-2.2315529508
H	-3.8414102454	1.8904999260	-1.4091465336
H	-2.7814524101	2.3155796745	-2.7685142796
C	-4.2849475071	0.8191555539	-3.1473855768
O	-5.5091105409	0.8803161923	-2.8909700258
N	-3.7951167209	0.1901347550	-4.2528714273
H	-4.4495325010	-0.2751070749	-4.8633636414
H	-2.7937821006	0.1567266646	-4.4295054239
O	2.7549387993	1.3475522525	2.0213884355
C	2.7747934492	-2.4461072153	1.4627127407
O	2.5049576151	-2.7862169650	2.6385140913
N	3.1115978873	-3.2744189971	0.4397838190
H	3.3870783304	-2.8120111165	-0.4296687930
C	3.1672580284	-4.7479012122	0.4458099880
H	2.8970470387	-5.0455611974	-0.5790654728
C	2.1680229986	-5.4083991720	1.4067082358
H	1.1576003365	-5.0311427218	1.2231862918
H	2.1715459336	-6.4922697763	1.2371273870
H	2.4325869811	-5.2016057736	2.4421758020
C	4.6026408464	-5.2531643329	0.6498367685
H	4.6230763346	-6.3374953253	0.4557483849
H	5.2657821265	-4.7611508871	-0.0777943905
O	5.0164625424	-4.9586789902	2.0092501065
H	5.9431294041	-5.2359108186	2.1497364640
C	4.1508333788	1.7463963334	2.0781816438
H	4.5870248491	1.5074597812	3.0575672745
H	4.7486324499	1.2678482991	1.2919340121
H	4.1550645655	2.8272242163	1.9313789139
O	-0.6830100592	-1.5670200008	0.1138796138

³BLM(H)-Fe^{IV}=O¹⁺ (Figure S7(b))

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	X	Y	Z
Fe	-0.0264993882	-0.0231131422	0.0807763335
N	-0.0315984705	-0.0145737137	2.0763617181
N	0.1328652296	-0.0259489292	-1.8152912712
N	1.4045895048	-1.3216076770	-0.0629693190
N	-1.2265511423	1.6828347793	-0.3345894869
N	1.4896969361	1.4520397293	0.0550963017
H	2.1934373128	1.1010042066	-0.5930362353
H	1.9374849293	1.4237297274	0.9835249589
H	-2.0307241985	0.6132925689	2.5899412617
C	2.1370078526	-1.9579401619	1.0477632629
O	2.5863655035	-2.6003128908	-1.6174397749
H	-2.5612240262	0.9322335943	-1.7658923904
C	-0.4771769979	2.8975018502	0.1073187849
C	0.3154025989	-0.0401623552	-4.4973914483
C	1.0150641998	-0.9015273441	-2.3777756736
C	-0.6285581904	0.7818919154	-2.5590386658
N	-0.5500789929	0.8259218250	-3.8893746861
C	1.1453184059	-0.9591204995	-3.7607791994
C	1.7426672858	-1.6940798189	-1.3252339321
C	-1.6644569908	1.5703311355	-1.7875707395
C	2.2749862239	-1.0418938354	2.2752783497
H	3.1557573081	-2.1536227936	0.6871237443
H	2.8130522641	-1.6121719109	3.0395209143
H	1.0101625905	-1.0307544178	5.0412744327
C	0.9835614444	-0.5751299312	2.8584572644
C	-1.0640171744	0.2468970211	2.8846394616
N	-0.7372754205	-0.1035665770	4.1591267313
C	0.5479622906	-0.6233158470	4.1599026652
H	-1.3467983699	-0.0396978329	4.9596098015
H	-0.9279217361	3.8245958703	-0.2644791552
C	1.0016363247	2.7974412709	-0.3146413623
H	-0.5241043104	2.9133477454	1.2008578390
H	1.0880123859	2.9190191218	-1.4005691682
C	1.8224256235	3.8810910286	0.4117152090
O	2.3279622842	3.6365178330	1.5272007307
N	1.9144428298	5.0898712847	-0.2020811659
H	1.5587368484	5.2664673294	-1.1283428373
H	2.4160976775	5.8334107127	0.2637895077
C	2.0718648098	-1.8937077219	-4.4920505717
H	2.7966012684	-1.3351422926	-5.1010242239
H	2.6224804068	-2.5127174523	-3.7841490384
H	1.5085869690	-2.5543635191	-5.1656897202
N	0.3549712861	0.0129703028	-5.8470376076
H	0.9453572867	-0.5931548408	-6.3914309062
H	-0.2712562896	0.6435553301	-6.3236442266
C	-2.0995382118	2.8751262673	-2.4746136900
H	-2.5191118223	3.5655037123	-1.7304114634
H	-1.2609469620	3.3776547260	-2.9680148246

C	-3.2254351622	2.5847629889	-3.4798738016
O	-3.9925209015	1.6131211547	-3.3224241943
N	-3.3584983058	3.4754946802	-4.4987548360
H	-4.1199186207	3.3520298006	-5.1504076005
H	-2.7264783525	4.2467728670	-4.6404281629
O	3.0957074786	0.1149756123	1.8713824746
C	1.5235748606	-3.3238323322	1.4881706605
O	1.0525506953	-3.4576875394	2.6411234051
N	1.5867455678	-4.2734739414	0.5229180967
H	2.0609433339	-4.0019178564	-0.3368527844
C	1.1545888727	-5.6851593033	0.6125153486
H	0.8861729264	-5.9645513796	-0.4169823139
C	-0.0749602298	-5.9048468837	1.5050250181
H	-0.8890127096	-5.2354227892	1.2112502797
H	-0.4201685589	-6.9388850105	1.3871520002
H	0.1666653814	-5.7211292377	2.5505995363
C	2.3340181022	-6.5888600236	0.9981412815
H	2.0031013530	-7.6363174678	0.9401990916
H	3.1546573747	-6.4475839296	0.2783103918
O	2.7619654146	-6.2389417791	2.3390244161
H	3.3966922555	-6.8980183398	2.6814063019
C	3.8684519474	0.7141799017	2.9608723060
H	3.2174707813	1.0185341743	3.7885714985
H	4.6258659190	0.0086749006	3.3205907296
H	4.3446385593	1.5974561963	2.5372813369
O	-1.3596359729	-1.0108861262	0.0846349855
H	-2.0565766425	1.5613969524	0.2441450702

[²BLM-Fe^{III}(H₂O₂)]¹⁺ (Figure S10(a))

===1a===

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	X	Y	Z
Fe	-0.0342223369	-0.0347562659	-0.0056611785
N	-0.0148530364	-0.0003498982	1.8980340029
C	1.1661340435	0.0429289967	2.5576168521
C	1.1773034424	0.2204804383	3.9309927423
C	-0.1192673842	0.3866141798	4.5300649968
N	-1.2710424200	0.4509346464	3.8191790697
C	-1.1675750056	0.2721731901	2.5155840318
C	2.3462894469	0.0403597513	1.5895555433
O	3.5141679984	0.2250995166	1.9705809501
C	2.4202249916	0.2707411117	4.7799705753
N	-0.2428027661	0.5227571033	5.8671517463
C	-2.2808950171	0.5061774910	1.4892958722
N	-1.8957223374	-0.2344515027	0.2656490763
C	-2.3539451712	-1.6232746713	0.2691256978
C	-1.3579721517	-2.5156289367	-0.4909135539
C	-1.4197038278	-2.6143453543	-2.0284139690
N	-2.6470226665	-2.5284950915	-2.5981460517
N	1.9333219090	-0.0605524379	0.3042802567
C	2.9577746016	0.0077438051	-0.7337764782
C	3.3158091674	1.4664477942	-1.1593560840

O	3.6712451497	1.7311016045	-2.2990957124
C	2.5517198681	-0.7629085428	-2.0112842232
C	1.3349301053	-0.1827617605	-2.6751033168
N	0.1795520401	0.1361889855	-1.9770740098
C	-0.6813992097	0.6531765211	-2.8429414312
N	-0.1231740693	0.6703393798	-4.0752007758
C	1.1499381878	0.1480766911	-3.9896558559
O	2.3628037607	-2.1415789422	-1.6535637606
N	3.1334782234	2.4263302314	-0.1785713290
C	3.6449680346	3.8099106054	-0.3615390892
C	4.5879030705	4.1678883845	0.7893011410
C	2.4477843679	4.7839330220	-0.4465280747
C	1.5959849001	4.6041306174	-1.7391174623
C	0.2792133942	5.3410982149	-1.5119746522
O	0.2410439997	6.5460913888	-1.2425692064
O	2.9378592236	6.1055802624	-0.3561391084
C	-3.6971967443	0.3359631227	2.0409426730
C	-4.7415679724	1.1015340231	1.2279029341
N	-6.0302771555	0.8063501128	1.5389868124
O	-4.4638916669	1.9477261583	0.3758673659
N	-0.0220575540	-2.0184167650	-0.1079066570
O	-0.4035092232	-2.8433698846	-2.6764719645
C	2.2989550760	5.1321060836	-3.0033947381
N	-0.8496500946	4.5847007846	-1.6201273218
C	-2.1745439544	5.1041829877	-1.3743165397
C	-2.4572269056	5.2826947701	0.1269045841
O	-2.0272104607	4.4990390356	0.9872041913
C	-3.2063506953	4.1137757139	-2.0137630908
O	-2.8416073953	2.7692971406	-1.7213302983
C	-3.2527353503	4.2720602357	-3.5316670175
N	-3.2791975584	6.3033302683	0.4399699368
C	-3.6683462533	6.6328948216	1.8135481597
C	-2.7406805130	7.6641264842	2.4583897615
H	-2.7296050707	-2.7674299227	-3.5776924319
H	-3.4943875120	-2.4255057492	-2.0614979295
H	-1.4905722144	-3.5555692538	-0.1545300706
H	-2.3995468686	-2.0263167533	1.2971418069
H	-3.3787881704	-1.7249667726	-0.1247043794
H	0.7233901507	-2.3035497638	-0.7611421352
H	0.2395770151	-2.3637650831	0.8155086694
H	-6.2796260091	0.1279877507	2.2443240481
H	-6.7716706080	1.2997070105	1.0605420685
H	-3.9946049635	-0.7145902088	2.1326893672
H	-3.7000589009	0.7385986232	3.0628956754
H	-2.1911094996	1.5707972463	1.2444283096
H	-1.1585901515	0.6973327739	6.2549587951
H	0.5564759997	0.5194420903	6.4806531094
H	2.4692268931	1.2102446835	5.3478807652
H	3.3105346860	0.2003327660	4.1556607687
H	2.4347367344	-0.5559187321	5.5047218207
H	3.8824050896	-0.4448488558	-0.3495059656
H	3.3858667090	-0.6748533198	-2.7139723126
H	1.8106845877	0.0856718399	-4.8403719245
H	-1.6575208917	1.0544963044	-2.6010048771

H	-0.5657895504	1.0226820045	-4.9125568064
H	3.2467560333	2.0621274417	0.7671714333
H	1.3880659670	3.5387181371	-1.8836376458
H	2.1688323836	6.6856208328	-0.5283253494
H	4.1973526488	3.8232014224	-1.3039759018
H	4.0682544951	4.1308196353	1.7557394104
H	5.4337241904	3.4729553287	0.8231835237
H	4.9670289224	5.1826866822	0.6545837785
H	1.7994576824	4.5597194840	0.4201220783
H	1.6336085824	5.0626825519	-3.8721892258
H	3.1906466642	4.5355955132	-3.2172064003
H	2.5949791215	6.1759376729	-2.8767981561
H	-0.7806015186	3.5738129682	-1.6257478253
H	-2.2559561226	6.0805369970	-1.8636350287
H	-4.1961998539	4.3297195482	-1.5909009630
H	-3.2840717416	2.4767671787	-0.8954926379
H	-3.5848320750	5.2760455482	-3.8169236295
H	-3.9480390601	3.5419164987	-3.9567337047
H	-2.2606518985	4.1053823491	-3.9659111341
H	-3.4869840449	6.9811149533	-0.2816288101
H	-2.7320591367	8.6029352324	1.8936976109
H	-1.7161291131	7.2835953216	2.5054570859
H	-3.6572249353	5.6971494874	2.3755714675
H	-4.7005002737	6.9977198146	1.7864470988
H	-3.0753456365	7.8862101142	3.4777619459
H	1.9742856153	-2.5931329429	-2.4241096227
O	0.1231451112	2.0568588350	-0.0014580438
O	-0.0824174764	2.7542308137	1.2608154805
H	-0.7778430634	3.4265334150	0.9913351845
H	1.1020849336	2.1912760946	-0.1068121771

===1b===

104

	X	Y	Z
Fe	-0.1096057090	-0.1220427958	0.0057524279
N	-0.0445024679	-0.0181927108	1.9073116050
C	1.1487420418	0.1092115161	2.5320412106
C	1.1831505299	0.2926416572	3.9047072675
C	-0.1044320578	0.3763605785	4.5377247858
N	-1.2785937756	0.3509574022	3.8612386931
C	-1.1981381511	0.1629481346	2.5562432269
C	2.3021498099	0.1502069102	1.5335629785
O	3.4723277130	0.3926729629	1.8859144670
C	2.4413108839	0.4278437366	4.7205218840
N	-0.1999040191	0.5148070904	5.8776354222
C	-2.3509645899	0.2840210375	1.5562862854
N	-1.9434790330	-0.4550903649	0.3389904610
C	-2.2912896722	-1.8752222822	0.4018718660
C	-1.2466431979	-2.7161457235	-0.3493090096
C	-1.3328261975	-2.8779844349	-1.8803096125
N	-2.5741279432	-2.8984200582	-2.4222983938
N	1.8697354857	-0.0050102725	0.2635103712
C	2.8819436034	0.0321475528	-0.7931979534

C	3.2246346937	1.4775902607	-1.2712916821
O	3.3205093937	1.7575223067	-2.4593444159
C	2.4694341759	-0.7928350474	-2.0318268505
C	1.2062384756	-0.3040844648	-2.6809730077
N	0.0401233409	-0.0434397390	-1.9776134949
C	-0.8577839103	0.3967101786	-2.8464324872
N	-0.3164917685	0.4150874156	-4.0865606391
C	0.9871346626	-0.0236773162	-4.0020704842
O	2.3691297170	-2.1698988878	-1.6288517242
N	3.3584741607	2.4156293670	-0.2659688012
C	3.8359737255	3.7923110336	-0.5654776254
C	4.8817598957	4.2064107020	0.4717297414
C	2.6274649516	4.7619629350	-0.5776945630
C	1.6188487804	4.4822705725	-1.7326289906
C	0.2929444073	5.1527685352	-1.3796235950
O	0.2251373613	6.2906803551	-0.9072290074
O	3.1131766428	6.0889655790	-0.6435152002
C	-3.7486638770	0.0242863447	2.1178862042
C	-4.8316716737	0.6252364793	1.2167696901
N	-6.0858106034	0.1492547571	1.4371914199
O	-4.6100125707	1.4760099618	0.3557925485
N	0.0541161610	-2.1053191049	-0.0118878859
O	-0.3185467863	-3.0829392472	-2.5406413888
C	2.1278808972	4.9766662644	-3.1006748780
N	-0.8275163845	4.4070938022	-1.6377567964
C	-2.1458473988	4.8055576012	-1.1792288765
C	-2.2706400439	4.6576419329	0.3446786001
O	-2.0326188377	3.5712156688	0.9076952875
C	-3.2287880104	3.9167750243	-1.8654679242
O	-2.9227246939	2.5346675541	-1.6871946317
C	-3.3250713291	4.1989390953	-3.3624497311
N	-2.7230154176	5.7297734254	1.0152461981
C	-2.8844222030	5.7676054301	2.4711816433
C	-1.6851488594	6.4027756036	3.1777863236
H	-2.6612854553	-3.1113236148	-3.4071143703
H	-3.4117395121	-2.7019959349	-1.8970691018
H	-1.2923888147	-3.7500721664	0.0257004689
H	-2.2814478130	-2.2402916907	1.4449618976
H	-3.3140817804	-2.0728960341	0.0412524514
H	0.8118347477	-2.3679539792	-0.6609818997
H	0.3502807721	-2.3892079675	0.9221198318
H	-6.3005877580	-0.4337031644	2.2337367457
H	-6.8572244918	0.6027985035	0.9645759900
H	-3.9519302909	-1.0372784993	2.2965076608
H	-3.8075298955	0.5139087636	3.0993824905
H	-2.3629794174	1.3464032035	1.2932948941
H	-1.1144309171	0.6310329731	6.2894850126
H	0.6146752280	0.5854487986	6.4662066812
H	2.4462113260	1.3732320866	5.2809153540
H	3.3161988084	0.4088733629	4.0717306712
H	2.5281184522	-0.3902008608	5.4497357932
H	3.8117469007	-0.4051157603	-0.4017082658
H	3.2747032512	-0.6876598823	-2.7657737399
H	1.6423239058	-0.0675983809	-4.8580381875

H	-1.8507164788	0.7494478033	-2.6059468482
H	-0.7888377236	0.7178613660	-4.9269494746
H	3.6428579400	2.0173666094	0.6337640289
H	1.4519206861	3.4034371368	-1.8076189556
H	2.3145432712	6.6509656329	-0.6294002432
H	4.2932981901	3.7679320485	-1.5582765437
H	4.4592556302	4.2055577971	1.4849878251
H	5.7363452179	3.5213890231	0.4522665222
H	5.2338681375	5.2174339469	0.2584925250
H	2.0975175270	4.6169920786	0.3775147666
H	1.3642954141	4.8268759786	-3.8721679503
H	3.0168270526	4.4118267675	-3.3951587194
H	2.3829732341	6.0379814465	-3.0623586815
H	-0.7075550427	3.4150534347	-1.7993950813
H	-2.3060702743	5.8504702463	-1.4632088337
H	-4.1923400162	4.1470328626	-1.3908986769
H	-3.3863235142	2.1943690737	-0.8936088821
H	-3.5899162815	5.2447400746	-3.5519465873
H	-4.0936383811	3.5593358467	-3.8066931721
H	-2.3702675683	3.9947629938	-3.8580603193
H	-2.7380750660	6.6122545490	0.5193935209
H	-1.5245768585	7.4343245828	2.8445700249
H	-0.7728955268	5.8322287129	2.9774187281
H	-3.0250254728	4.7348922147	2.7960981639
H	-3.8055559390	6.3189759233	2.6902945182
H	-1.8535930661	6.4216135800	4.2602619678
H	1.9343599962	-2.6582547049	-2.3517816942
O	-0.2197274372	1.9498308760	-0.0166789894
O	0.6835506012	2.6091639492	0.9165810989
H	-1.0525827612	2.4793362057	0.2122539484
H	1.5368486573	2.5181196000	0.4244168130

===1c===

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	X	Y	Z
Fe	-0.0128418190	-0.0073867223	0.0214389223
N	-0.0267257865	-0.0796268523	1.9269989104
C	1.1418050070	-0.0704593150	2.6078399178
C	1.1271029824	0.0064126531	3.9904281603
C	-0.1783445981	0.1129296668	4.5795762672
N	-1.3244607659	0.1806187862	3.8576624413
C	-1.1960309419	0.0884467683	2.5467985651
C	2.3439672907	-0.0689400337	1.6686788749
O	3.5041827624	-0.1450566136	2.0846589430
C	2.3586010183	0.0110663547	4.8574046207
N	-0.3206977394	0.1715718340	5.9205848924
C	-2.3107291537	0.3123812234	1.5223556093
N	-1.8806048328	-0.3305158790	0.2595051297
C	-2.2328505168	-1.7498733186	0.2177665870
C	-1.1857238902	-2.5345311631	-0.5875024521
C	-1.2514685398	-2.5405376532	-2.1277554907
N	-2.4872605097	-2.4895199641	-2.6827440228
N	1.9491383881	0.0581439459	0.3699723515

C	3.0222616397	0.0605016185	-0.6200887093
C	3.6271914211	1.4572444370	-0.9626062077
O	4.4485271132	1.5511396306	-1.8728646419
C	2.6276258249	-0.5917978393	-1.9599051994
C	1.4292954084	0.0439800391	-2.6049036102
N	0.2263922392	0.2503806612	-1.9441743814
C	-0.6093751258	0.8054992650	-2.8082739416
N	0.0062599335	0.9659361874	-4.0027064646
C	1.2959051510	0.4896300955	-3.8929614640
O	2.4237363760	-1.9999944873	-1.7397727341
N	3.1956478660	2.5063396468	-0.2203233096
C	3.8022199827	3.8400402819	-0.2899888032
C	4.7445916590	4.0820499420	0.8956694651
C	2.6656075488	4.8833539530	-0.3475140211
C	1.8614922540	4.8373667827	-1.6858261881
C	0.5487749092	5.5426382102	-1.3807058183
O	0.4984662907	6.7472149942	-1.0985394671
O	3.2035920795	6.1724904180	-0.1236957311
C	-3.7216215683	0.0207474788	2.0352155132
C	-4.7996567886	0.6707172189	1.1681793674
N	-6.0561352528	0.2101285242	1.3756473290
O	-4.5785479814	1.5611249495	0.3409891698
N	0.1176430114	-1.9840837286	-0.1652685587
O	-0.2335125082	-2.6814366108	-2.7982498108
C	2.6030113508	5.4898656047	-2.8617758484
N	-0.5562174381	4.7401844779	-1.3369320930
C	-1.8106225780	5.1614025684	-0.7090225716
C	-1.6171346283	5.2777725927	0.8224286717
O	-1.8481253954	4.3134694777	1.5831146969
C	-2.9537187039	4.1868432443	-1.0643538013
O	-2.5017213494	2.8227327458	-0.8952984477
C	-3.4520986956	4.3765884857	-2.4942777345
N	-1.1711930953	6.4643775794	1.2528981936
C	-0.8219599791	6.7298841345	2.6506735097
C	0.6516756648	6.4518518778	2.9594651054
H	-2.5647628984	-2.6318305031	-3.6808685193
H	-3.3312162739	-2.3954591882	-2.1426269846
H	-1.2566274191	-3.5988860819	-0.3156650408
H	-2.2273318418	-2.1937447191	1.2304356568
H	-3.2537968252	-1.9205238837	-0.1624383393
H	0.8911585951	-2.2008815731	-0.8166060154
H	0.3824513871	-2.3585181232	0.7459631112
H	-6.2728265114	-0.4383012074	2.1189560285
H	-6.8245975823	0.6769939935	0.9111074845
H	-3.9201267843	-1.0514032755	2.1415001497
H	-3.7962086047	0.4423675384	3.0471726675
H	-2.3009867940	1.3959380715	1.3550897506
H	-1.2444857662	0.2994326789	6.3071345587
H	0.4733549140	0.1654151763	6.5406762569
H	2.4111788623	0.9278314701	5.4612888449
H	3.2538481324	-0.0509722828	4.2393294148
H	2.3554596377	-0.8423841821	5.5499389800
H	3.8682043170	-0.5175749143	-0.2262905390
H	3.4840302761	-0.4476862853	-2.6249841208

H	1.9960733882	0.5145193348	-4.7135806259
H	-1.6168971681	1.1272949600	-2.5882191739
H	-0.4129519124	1.3609103988	-4.8330946496
H	2.5461371211	2.3126344801	0.5327203091
H	1.6672840618	3.7833673375	-1.9145640245
H	2.4847301895	6.8059679303	-0.3083623123
H	4.3815107254	3.8591584401	-1.2163275740
H	4.2027925182	4.0319888162	1.8486895632
H	5.5279513206	3.3181221297	0.9065413818
H	5.2074864787	5.0688040618	0.8195252114
H	1.9659807505	4.6243024917	0.4677373437
H	2.0074117180	5.4224327851	-3.7787967489
H	3.5560386421	4.9844146438	-3.0414343192
H	2.8081383092	6.5436769682	-2.6630267844
H	-0.3920224231	3.7441592706	-1.4007265483
H	-2.0599238642	6.1494415805	-1.1087429962
H	-3.7690861802	4.3634547962	-0.3551780994
H	-3.2250585311	2.3015583338	-0.4615791012
H	-3.8680635426	5.3795452977	-2.6356745020
H	-4.2369686866	3.6471001319	-2.7161546306
H	-2.6354695427	4.2410748658	-3.2105904405
H	-0.8229653628	7.1009932101	0.5367129954
H	1.3164145427	7.0389816378	2.3189574258
H	0.8900979418	5.3926493598	2.8161681087
H	-1.4739756158	6.1024064496	3.2662623925
H	-1.0698536913	7.7784076946	2.8547284716
H	0.8680265575	6.7101324711	3.9999038543
H	1.9908488037	-2.3706601387	-2.5299407448
O	-0.1881468848	2.0386538851	0.1012025366
O	0.2172661636	2.6582046985	1.3606032039
H	-0.5506893027	3.2656654142	1.5576537055
H	-1.1264374338	2.3570313042	-0.0916613223

[²BLM(H)-Fe^{III}(H₂O₂)]²⁺ (Figure S10(b))

===1a===

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	X	Y	Z
Fe	-0.0004557779	-0.0009450162	-0.0001702630
N	-0.0009672830	-0.0070153096	1.9075826732
C	1.2079614782	0.0008268912	2.5256180588
C	1.2902167543	0.0935100104	3.9007378014
C	0.0144517816	0.2020763058	4.5729605317
N	-1.1678119484	0.2912723384	3.9123388294
C	-1.1216448194	0.2007875274	2.5985318456
C	2.3357140387	0.0304832074	1.5070189335
O	3.5179431671	0.1521210131	1.8096466956
C	2.5680358316	0.0982148559	4.6941086992
N	-0.0500977209	0.2472211544	5.9114449736
C	-2.3222212571	0.4532129874	1.7010344066
N	-2.0644207392	-0.2811749688	0.4090775751
C	-2.3511236473	-1.7439628028	0.5284533809
C	-1.3770457524	-2.5824662050	-0.3066202229

C	-1.6453189436	-2.7412362810	-1.8227044874
N	-2.9351618096	-2.9603762012	-2.1877522948
N	1.8635973784	-0.0059783019	0.2072472072
C	2.8491925666	0.0877753326	-0.8691625085
C	3.0813987599	1.5488951412	-1.3607790525
O	3.4439371081	1.7683988819	-2.5009280440
C	2.4532651570	-0.7581460182	-2.0975615395
C	1.1965238234	-0.2458718636	-2.7410735310
N	0.0893919962	0.1304757232	-1.9937979594
C	-0.8325629099	0.5676989780	-2.8482487797
N	-0.3550891719	0.4801743966	-4.1074978417
C	0.9222396293	-0.0290197870	-4.0631691084
O	2.3232284066	-2.1181172306	-1.6546237180
N	2.7654210869	2.5560302899	-0.4479869569
C	3.2145017001	3.9600057657	-0.7160946463
C	4.2714761923	4.3722215235	0.3085466054
C	1.9738685957	4.8787352581	-0.6923988386
C	1.0450213806	4.6623668025	-1.9264423903
C	-0.3099130799	5.2678933842	-1.5756325179
O	-0.4296962475	6.4329429774	-1.1946929395
O	2.4073164539	6.2150199934	-0.6163724100
C	-3.6976379046	0.2263986172	2.3378229010
C	-4.8085183647	0.7418760529	1.4203337292
N	-6.0157571676	0.9169565264	1.9851151581
O	-4.6041124258	0.9590432089	0.2159871397
N	-0.0279394230	-2.0031462730	-0.1239494618
O	-0.7148200755	-2.7064523143	-2.6153150304
C	1.6002335548	5.2945301626	-3.2165219323
N	-1.3842930860	4.4309693320	-1.6933424448
C	-2.7331817263	4.8308428992	-1.3640071572
C	-2.9733993727	4.8382652211	0.1555922068
O	-2.5312904666	3.9331295155	0.8967850725
C	-3.7222708970	3.8472567162	-2.0659562313
O	-3.3333702351	2.4919613477	-1.8013715462
C	-3.7494855554	4.0521057120	-3.5770514405
N	-3.7596929184	5.8179562336	0.6191819055
C	-4.1065833030	5.9965799857	2.0358057834
C	-3.1815787323	6.9864387870	2.7463046191
H	-3.0933144300	-3.2456372248	-3.1478195489
H	-3.6536331855	-3.2133873428	-1.5231253855
H	-1.3920693048	-3.6076895810	0.0919545069
H	-2.2102024591	-2.0260091435	1.5758914246
H	-3.3971734582	-1.9482959921	0.2798826907
H	0.6099311175	-2.2618124584	-0.8984260268
H	0.3991685233	-2.3591116078	0.7317426306
H	-6.1938380933	0.7377663937	2.9638222293
H	-6.7926069801	1.2098524618	1.4048072406
H	-3.8837430674	-0.8293116139	2.5714915944
H	-3.7120584100	0.7514896478	3.2992452922
H	-2.2693720842	1.5136032977	1.4347433889
H	-0.9504752672	0.3607752555	6.3579821327
H	0.7740305563	0.2043117213	6.4923736687
H	2.6388090896	1.0033191188	5.3120849832
H	3.4375550079	0.0631840644	4.0393964185

H	2.6094622458	-0.7688589223	5.3678703223
H	3.8075169905	-0.2890738557	-0.4919899470
H	3.2694223846	-0.6732139327	-2.8198216045
H	1.5224642441	-0.1657011808	-4.9496879101
H	-1.8023257466	0.9833455018	-2.5992077900
H	-0.8558976522	0.7522157702	-4.9437447200
H	2.9261188428	2.2774933166	0.5191047190
H	0.9242581283	3.5846902369	-2.0990224170
H	1.6022413072	6.7663472497	-0.6671315256
H	3.6554505300	3.9558978708	-1.7146586211
H	3.8694961842	4.3511363113	1.3296539826
H	5.1387173267	3.7059070889	0.2571819565
H	4.6004881311	5.3926133629	0.1060181316
H	1.4032330375	4.6154947722	0.2165816915
H	0.9066905214	5.1380327455	-4.0498714521
H	2.5583654298	4.8413933999	-3.4887396411
H	1.7517092571	6.3680435755	-3.0903726420
H	-1.2396549518	3.4413431161	-1.8375790687
H	-2.8937201519	5.8410463796	-1.7549710615
H	-4.7258856743	4.0247746873	-1.6583448636
H	-3.8072092526	2.1684608968	-1.0127002276
H	-4.0877245047	5.0619001629	-3.8300904109
H	-4.4357623043	3.3332110280	-4.0332569493
H	-2.7535716107	3.9108368603	-4.0097663577
H	-3.9921147824	6.5749164191	-0.0125075329
H	-3.2192099721	7.9758867395	2.2784785083
H	-2.1450505312	6.6358427340	2.7242567637
H	-4.0527411778	5.0093392320	2.4985968463
H	-5.1473049728	6.3338462662	2.0777256614
H	-3.4875156456	7.0980861500	3.7920206444
H	2.2809489261	-2.6888506476	-2.4408000122
O	-0.0297952312	2.0037699722	-0.0789158543
O	-0.2373985394	2.7352337301	1.1554493213
H	-1.0607625149	3.2703237156	0.9150201036
H	0.9174657160	2.2774261674	-0.3073611874
H	-2.7227978313	0.1283819167	-0.2589178957

===1b===

105

	X	Y	Z
Fe	-0.0068504506	0.0070964156	-0.0006719464
N	-0.0047552508	-0.0041930706	1.9004362816
C	1.1988262537	0.0029098880	2.5292601625
C	1.2635363211	0.0513263366	3.9081272675
C	-0.0176643395	0.1248998487	4.5688445363
N	-1.1976696255	0.2195407338	3.9001641640
C	-1.1384069824	0.1648567702	2.5850778674
C	2.3309771581	0.0677453007	1.5204844894
O	3.5098113738	0.2367371000	1.8377977947
C	2.5345533700	0.0436095007	4.7129691625
N	-0.0968871583	0.1290294987	5.9079864684
C	-2.3347261640	0.4203491991	1.6797435218
N	-2.0710078282	-0.3089941222	0.3836008789

C	-2.3351228140	-1.7782434252	0.5002939604
C	-1.3022607536	-2.6147505141	-0.2693397841
C	-1.5107993012	-2.8410515081	-1.7862040512
N	-2.7812487356	-3.1110156260	-2.1863116374
N	1.8730688226	-0.0012236873	0.2293624763
C	2.8756021381	0.0528676359	-0.8410571235
C	3.2036246303	1.5072047953	-1.3003342274
O	3.2308326495	1.8001140841	-2.4857557383
C	2.4520220210	-0.7697208364	-2.0716346514
C	1.1929873164	-0.2647936551	-2.7158204049
N	0.0673960701	0.1019223638	-1.9906615297
C	-0.8423654507	0.5226733553	-2.8648767532
N	-0.3447259669	0.4259923616	-4.1156031946
C	0.9368911098	-0.0692054019	-4.0445386409
O	2.3241741473	-2.1358341210	-1.6361959380
N	3.4027767365	2.4258965753	-0.2868744846
C	3.9077703258	3.7990408272	-0.5958310578
C	4.9841952395	4.1776781922	0.4211994308
C	2.7165781776	4.7892498237	-0.5754096828
C	1.6984285741	4.5497677338	-1.7320736799
C	0.3646654407	5.1693223172	-1.3318065750
O	0.2679858381	6.2427074452	-0.7384874563
O	3.2303159968	6.1019924149	-0.6104594859
C	-3.7228508468	0.1954910904	2.2843329383
C	-4.8027506139	0.7216952181	1.3300736658
N	-6.0655349774	0.7045597013	1.7959501743
O	-4.5244095983	1.1189413948	0.1889906525
N	0.0242020825	-1.9981807489	-0.0555539653
O	-0.5558878848	-2.8145699719	-2.5486507335
C	2.1827903539	5.1221971473	-3.0798083845
N	-0.7504836244	4.4417086575	-1.6776508301
C	-2.0768899767	4.8272045165	-1.2453173491
C	-2.2443631083	4.5987604301	0.2616839301
O	-1.9150037566	3.5028598976	0.7857342188
C	-3.1624220796	4.0123407894	-2.0107044452
O	-2.9842422491	2.6050361734	-1.7913018327
C	-3.1282147673	4.2768192861	-3.5121614746
N	-2.8168340253	5.5700187317	0.9690757559
C	-3.0444988724	5.5319987971	2.4201136595
C	-2.6225493767	6.8433338058	3.0783586444
H	-2.8924730628	-3.4481202027	-3.1365193791
H	-3.5079630257	-3.3760902819	-1.5361577663
H	-1.3078179786	-3.6251592382	0.1661151659
H	-2.2483841653	-2.0463989783	1.5571985605
H	-3.3616169954	-2.0060403727	0.1969389841
H	0.6939085725	-2.2542186184	-0.8068916798
H	0.4389882414	-2.3251455607	0.8173499891
H	-6.3012133266	0.4048999894	2.7322884240
H	-6.8144240910	1.0324574314	1.1992116353
H	-3.9196136300	-0.8565777225	2.5232586582
H	-3.7671973144	0.7307862890	3.2398035392
H	-2.2876845599	1.4826694830	1.4217563266
H	-1.0030217081	0.2151791529	6.3482939450
H	0.7218593868	0.0759132232	6.4956355412

H	2.5899211166	0.9270523470	5.3628346511
H	3.4080149754	0.0438473162	4.0624353633
H	2.5833003456	-0.8459991223	5.3560795234
H	3.8002856139	-0.3913066927	-0.4505821381
H	3.2594276500	-0.6908725175	-2.8053604306
H	1.5550123678	-0.2059140902	-4.9186278175
H	-1.8088135085	0.9521321397	-2.6344492042
H	-0.8337703361	0.6860295982	-4.9623176937
H	3.7572728720	2.0139240234	0.5783491783
H	1.5510120705	3.4729220554	-1.8617780474
H	2.4600748336	6.6930171999	-0.5260983754
H	4.3417105905	3.7668252803	-1.5987592860
H	4.5831170761	4.1881904784	1.4430325255
H	5.8204028190	3.4714943200	0.3800285207
H	5.3603754449	5.1786358464	0.2030616077
H	2.1913095780	4.6317653110	0.3812408952
H	1.4267868026	4.9703859621	-3.8577554015
H	3.0967147632	4.6129590215	-3.3981230884
H	2.3921477143	6.1907736442	-3.0000873850
H	-0.6284557107	3.4954522186	-2.0120656248
H	-2.2148414891	5.8907358969	-1.4665525949
H	-4.1392471455	4.3196552201	-1.6146852836
H	-3.5393683626	2.3182213769	-1.0431354058
H	-3.2717087108	5.3404405267	-3.7259904536
H	-3.9286030471	3.7143369931	-4.0010293962
H	-2.1705798312	3.9725563743	-3.9465433089
H	-2.9915771221	6.4505864344	0.4988606315
H	-3.1977528399	7.6913718737	2.6910544778
H	-1.5595645693	7.0426212730	2.9158778044
H	-2.4665518930	4.6892008689	2.8041094912
H	-4.1062463759	5.3262173655	2.6046372207
H	-2.8018922549	6.7916538689	4.1556985826
H	2.1555029365	-2.6856494155	-2.4208334341
O	-0.0638749042	2.0013290397	0.0355522576
O	0.8046798907	2.5863533302	1.0402841065
H	-0.9085645070	2.6057383803	0.1966846278
H	1.6557536301	2.6127856204	0.5281600504
H	-2.7265963113	0.0989454035	-0.2872632302

===1c===
105

	X	Y	Z
Fe	0.0448740010	0.0423952665	0.0012959796
N	0.0158513686	-0.0156147305	1.8904781106
C	1.1991587335	-0.0537307270	2.5576592503
C	1.2162862527	0.0160535267	3.9371326805
C	-0.0821082908	0.1688226630	4.5512078013
N	-1.2312758369	0.3092619284	3.8399261056
C	-1.1282679934	0.2223473432	2.5290760520
C	2.3661452150	-0.0250281990	1.5840526247
O	3.5396873753	0.1465165964	1.9445782552
C	2.4565991631	-0.0385512473	4.7865354922

N	-0.2072281094	0.2006135706	5.8868523984
C	-2.2850741420	0.5170828735	1.5839567089
N	-1.9997815757	-0.1794227650	0.2675750357
C	-2.3677569988	-1.6331875737	0.2742823747
C	-1.3369590805	-2.4854906616	-0.4897937506
C	-1.3983968144	-2.5818066001	-2.0334832701
N	-2.6252527169	-2.5793985253	-2.6038531179
N	1.9491773091	-0.0756539595	0.2912244625
C	2.9608356438	-0.0191828340	-0.7486066906
C	3.3859241522	1.4252157500	-1.0890496870
O	3.7320681121	1.7811313714	-2.1844381048
C	2.5256031908	-0.7267438018	-2.0597703955
C	1.3252240885	-0.0794013802	-2.6916060134
N	0.1604305855	0.2034978907	-1.9911389599
C	-0.6610978278	0.8171260143	-2.8336660142
N	-0.0803074233	0.9137919672	-4.0496800573
C	1.1752415450	0.3543462092	-3.9814579251
O	2.3082400632	-2.1052733444	-1.7461150756
N	3.3270755115	2.3734572749	0.0343524125
C	3.9989319540	3.7236025858	-0.1893373117
C	4.9340808062	4.0160299783	0.9890238597
C	2.8999023335	4.7916335897	-0.3398333609
C	1.9659148193	4.5664983400	-1.5735878718
C	0.7167675330	5.3811588983	-1.2657125505
O	0.7776190841	6.5896231604	-1.0363494271
O	3.5365688051	6.0411165624	-0.3985663438
C	-3.6755747033	0.3316112993	2.1950318888
C	-4.7240890664	1.1759635177	1.4640479404
N	-5.9991162926	0.7426965001	1.5553039152
O	-4.4162198377	2.1896950682	0.8315782191
N	-0.0052588827	-1.9884892260	-0.0922762434
O	-0.3676865164	-2.7554096101	-2.6734199171
C	2.6132635055	4.9876714737	-2.9022317465
N	-0.4452148090	4.6668477226	-1.1811949917
C	-1.6335736296	5.2405169287	-0.5997831823
C	-1.5919289927	5.0641907018	0.9412081956
O	-0.7023804566	4.4144138421	1.5259214398
C	-2.8903294561	4.5748298751	-1.2373922420
O	-2.7444059555	3.1457516797	-1.1897977817
C	-3.0863703449	5.0030387331	-2.6872172788
N	-2.5850984807	5.6566680210	1.6220073066
C	-2.6922822227	5.6591731647	3.0871828353
C	-1.9900501486	6.8552588974	3.7331260475
H	-2.6851987055	-2.7337354250	-3.6033552325
H	-3.4883332849	-2.4559530437	-2.0973243640
H	-1.4678767412	-3.5264377569	-0.1576309430
H	-2.3448922358	-1.9705078019	1.3143325156
H	-3.3923183484	-1.7845800594	-0.0803369116
H	0.7403751373	-2.2728519160	-0.7496285766
H	0.2584603913	-2.3570264366	0.8218172994
H	-6.2708259848	-0.0143400627	2.1680010831
H	-6.7360171965	1.3311359366	1.1839942891
H	-3.9880328066	-0.7180026601	2.2250817898
H	-3.6180273232	0.6712618608	3.2367375519

H	-2.1839641434	1.5821512390	1.3418449349
H	-1.1144891940	0.3950354855	6.2898238728
H	0.5930642282	0.1720097437	6.5012919100
H	2.5272916356	0.8462098610	5.4336715264
H	3.3496200311	-0.0773680973	4.1644831278
H	2.4461654819	-0.9252019829	5.4352444978
H	3.8677890072	-0.5282299500	-0.3883686157
H	3.3589918328	-0.6331413055	-2.7638486309
H	1.8475012273	0.3316067872	-4.8258035870
H	-1.6144567382	1.2665480498	-2.5886453653
H	-0.4933369972	1.3463064719	-4.8664586315
H	3.7293708323	1.8886478054	0.8555853319
H	1.6836979579	3.5095145867	-1.6378742499
H	2.8265520665	6.6978315007	-0.5496024422
H	4.5727287726	3.6457764209	-1.1141068243
H	4.3813263755	4.0590069210	1.9354392330
H	5.7161137820	3.2531652026	1.0687688600
H	5.4083256752	4.9863185363	0.8316345276
H	2.2776379931	4.7387273403	0.5735116608
H	1.9155959864	4.8295225946	-3.7317242013
H	3.5117336900	4.3966664497	-3.1008032616
H	2.8899548764	6.0431901963	-2.8844974932
H	-0.4134397964	3.6524922874	-1.1842808368
H	-1.6262489669	6.3148325417	-0.8099146219
H	-3.7733641184	4.8502289358	-0.6473743181
H	-3.2894449215	2.8228673764	-0.4465057437
H	-3.2407571713	6.0844474044	-2.7656727349
H	-3.9599090468	4.4962602921	-3.1080693412
H	-2.2076755670	4.7412692025	-3.2856585672
H	-3.2229202142	6.2520797613	1.1087651792
H	-2.4143166234	7.8032760720	3.3852306452
H	-0.9211807409	6.8488772146	3.4980307573
H	-2.2581800251	4.7198847391	3.4373647216
H	-3.7590953775	5.6509363274	3.3335073084
H	-2.1045599097	6.8144935187	4.8216882236
H	1.7716671787	-2.4995104079	-2.4602795214
O	-0.0445513830	1.8762010394	0.0197849024
O	0.9271865410	2.5193867345	0.8977478771
H	0.4244944901	3.4005094017	1.0540307077
H	2.1372187818	2.5064857079	0.3894084584
H	-2.5304229683	0.3170550249	-0.4491640980

TSh-oh1 (protonated) (Figure S11)

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	X	Y	Z
Fe	-0.0052806656	-0.0069102547	0.0016661221
N	-0.0046039846	-0.0090058194	1.9119994031
C	1.2016277910	-0.0034397079	2.5344680238
C	1.2848319082	0.1034985100	3.9083130548
C	0.0116457077	0.2245045524	4.5781445433
N	-1.1678360984	0.3163663811	3.9151005164
C	-1.1227636145	0.2159359651	2.6004842298

C	2.3281427433	0.0172719621	1.5180299794
O	3.5000319854	0.2652619103	1.8032138173
C	2.5648047516	0.1048307624	4.6983053100
N	-0.0527149226	0.2799948387	5.9174135007
C	-2.3298954900	0.4681177341	1.7109229920
N	-2.0822484909	-0.2622840800	0.4149838199
C	-2.4122216375	-1.7170081878	0.5165107393
C	-1.4521019610	-2.5812215220	-0.3090337111
C	-1.6911683182	-2.7217968827	-1.8306752775
N	-2.9798488910	-2.8680956743	-2.2288061115
N	1.8679443153	-0.1611609686	0.2349286398
C	2.8516259964	-0.0843563692	-0.8325618557
C	3.1569145989	1.3604268469	-1.2818648515
O	3.7544131330	1.6241277798	-2.2897200072
C	2.4299117814	-0.8788281135	-2.0940305135
C	1.1998860331	-0.3035311972	-2.7380285347
N	0.0897276547	0.0822877698	-2.0010858243
C	-0.8107197219	0.5430219834	-2.8614900114
N	-0.3197020548	0.4619569966	-4.1180778633
C	0.9485018985	-0.0674382107	-4.0633460783
O	2.2502813413	-2.2382859953	-1.6853970058
N	2.5977671484	2.4216508491	-0.4188700451
C	3.0619010975	3.8398232327	-0.7543694495
C	4.1283956451	4.2691347192	0.2500641100
C	1.8315427942	4.7666139833	-0.7768399946
C	0.9217532720	4.5103069082	-2.0175245890
C	-0.4317698668	5.1278110397	-1.6873163538
O	-0.5514192454	6.3234360761	-1.4205930339
O	2.3011577314	6.0943870660	-0.7560570141
C	-3.6882750256	0.2263285908	2.3812720600
C	-4.8421718747	0.6912048363	1.4944418494
N	-6.0190239308	0.8999457489	2.1109187700
O	-4.7056504787	0.8370026771	0.2705697319
N	-0.0957218130	-2.0428053582	-0.0925239419
O	-0.7425814482	-2.7395358252	-2.6027759001
C	1.4885679966	5.1085157854	-3.3182581477
N	-1.4863320746	4.2600503869	-1.6852129005
C	-2.8262407898	4.6520927765	-1.3129147107
C	-3.0138834010	4.6340086721	0.2149651632
O	-2.4764677765	3.7670308741	0.9337864551
C	-3.8337752761	3.6818994085	-2.0032713233
O	-3.4337764068	2.3241231302	-1.7627589649
C	-3.9022746630	3.9102954130	-3.5091249899
N	-3.8502886299	5.5582410819	0.7111979298
C	-4.1510950264	5.7098649557	2.1410575897
C	-3.2486164556	6.7371455725	2.8271365336
H	-3.1306114167	-3.1465964823	-3.1917477341
H	-3.7281435588	-3.0689711393	-1.5816623765
H	-1.5139709713	-3.6087645989	0.0799028845
H	-2.2884922064	-2.0124848570	1.5623711370
H	-3.4625359776	-1.8846914230	0.2583842598
H	0.5517186332	-2.3277209976	-0.8447205034
H	0.2974226118	-2.3987632387	0.7786725947
H	-6.1474606792	0.7639213275	3.1040544045

H	-6.8285234155	1.1479156482	1.5548857902
H	-3.8440662256	-0.8283473752	2.6403869462
H	-3.6855426756	0.7668351034	3.3337850545
H	-2.2914331869	1.5297573689	1.4456303369
H	-0.9522025988	0.4016757576	6.3628823398
H	0.7706577195	0.2328018243	6.4986576219
H	2.6377921533	1.0061174905	5.3213958296
H	3.4309191272	0.0782517303	4.0389526396
H	2.6112700033	-0.7662603600	5.3664927597
H	3.8030108843	-0.5012695092	-0.4765160500
H	3.2585269028	-0.8063160223	-2.8061125567
H	1.5527994837	-0.2161804080	-4.9455997969
H	-1.7826275563	0.9584226293	-2.6194380413
H	-0.8089782404	0.7438470064	-4.9581452600
H	2.8910652454	2.2036984145	0.5434136089
H	0.7951758753	3.4290563068	-2.1540778327
H	1.5133811054	6.6649337739	-0.8497621970
H	3.5013755457	3.7784137162	-1.7506611608
H	3.7275705435	4.3077028349	1.2707031817
H	4.9850770186	3.5862520025	0.2277524345
H	4.4778380973	5.2711777126	-0.0048712441
H	1.2475523995	4.5560190773	0.1341614983
H	0.8216984397	4.8920496507	-4.1599818599
H	2.4711958211	4.6867725526	-3.5529309621
H	1.5954223136	6.1917226460	-3.2367502344
H	-1.3036678989	3.2652852686	-1.6817603815
H	-2.9894453085	5.6689775352	-1.6829376658
H	-4.8260903733	3.8495963524	-1.5650667920
H	-3.9509418377	1.9677438142	-1.0159918381
H	-4.2526039589	4.9219229170	-3.7383745626
H	-4.5958182841	3.1940672962	-3.9588975085
H	-2.9162105457	3.7809719870	-3.9673209549
H	-4.1619780101	6.2964015306	0.0914369212
H	-3.3519704452	7.7278838544	2.3719083906
H	-2.1983078495	6.4364126618	2.7616163516
H	-4.0315669308	4.7233492902	2.5932195741
H	-5.2044753795	5.9956959032	2.2256311483
H	-3.5179437032	6.8245556077	3.8852687430
H	2.0524113879	-2.7674317422	-2.4775830295
O	0.1104955499	1.9019968046	-0.1058130418
O	-0.0791396706	2.6416873055	1.1304446076
H	-0.9278677199	3.1277731513	0.9288504900
H	1.3737066043	2.2259115121	-0.3456240394
H	-2.7190146624	0.1675712405	-0.2586358887

[²BLM-Fe^{III}-OOH; NH₂⁺(V)]¹⁺ (Figure S12(a))

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	X	Y	Z
Fe	-0.0069831096	0.0257386280	0.0066176145
N	-0.0183339801	0.0476662673	1.9068744881
C	1.1540709030	0.0535134136	2.5794858076

C	1.1653938472	0.2291427335	3.9517740150
C	-0.1291465926	0.4332588880	4.5404514389
N	-1.2696615615	0.5365257022	3.8206500841
C	-1.1645954423	0.3575483274	2.5134502663
C	2.3337847574	0.0113670103	1.6205997559
O	3.4927000784	0.3208780673	1.9655154327
C	2.4045205478	0.2297439388	4.8070207496
N	-0.2601384891	0.5656671068	5.8788602535
C	-2.2724190245	0.6161333049	1.4905779034
N	-1.9223602909	-0.1012372186	0.2420051679
C	-2.4239021771	-1.4750566494	0.2332908649
C	-1.4712440476	-2.3989926455	-0.5402737593
C	-1.4917495548	-2.4197517068	-2.0793580049
N	-2.6907510868	-2.2183587286	-2.6716813305
N	1.9434203404	-0.2475975664	0.3550128548
C	2.9816442729	-0.2719861450	-0.6509941605
C	3.5798381100	1.1058060723	-0.9723565888
O	4.4378544048	1.3155029993	-1.7806015726
C	2.5201441024	-0.8968083544	-2.0054481078
C	1.3886610467	-0.1478247469	-2.6506743578
N	0.2223148660	0.1761110997	-1.9767361178
C	-0.5659906894	0.8110069191	-2.8274710953
N	0.0457196647	0.8953538112	-4.0349721997
C	1.2833385139	0.2959112738	-3.9435227177
O	2.1978574972	-2.2658878709	-1.7637846282
N	2.9789958611	2.2507621055	-0.1950986918
C	3.5442817662	3.6299783265	-0.5222108414
C	4.6588342885	3.9615016284	0.4655609022
C	2.3811183921	4.6428146334	-0.5083668181
C	1.4372607361	4.4707849617	-1.7346048391
C	0.1369945129	5.1969111472	-1.3943607046
O	0.1151959075	6.4172371233	-1.2092572278
O	2.9433568541	5.9391913623	-0.4788514302
C	-3.6752923741	0.4194239857	2.0791866879
C	-4.7870501473	1.0121613066	1.2203391057
N	-6.0306502315	0.5270823077	1.4762016390
O	-4.6083515133	1.8884122584	0.3729594759
N	-0.1278852135	-2.0031715435	-0.0879285420
O	-0.4836125707	-2.7186523659	-2.7198359627
C	2.0334356915	5.0279282397	-3.0389755244
N	-0.9588033319	4.3967042454	-1.3160527478
C	-2.2822578469	4.8759571169	-1.0002740894
C	-2.5709359503	4.8122253650	0.5129142124
O	-1.9660837179	4.0560598481	1.2849251993
C	-3.3170413938	4.0218254219	-1.8100924799
O	-2.9908723347	2.6412013491	-1.7150476309
C	-3.3187803753	4.4063444895	-3.2868688621
N	-3.5775774410	5.6057426779	0.9376295096
C	-4.0214431052	5.6614021175	2.3331610196
C	-3.2703328009	6.7097785454	3.1601046675
H	-2.7495731394	-2.3081545255	-3.6773144938
H	-3.4997113731	-1.8874903047	-2.1680171301
H	-1.6884252392	-3.4425570311	-0.2623995490
H	-2.4723547915	-1.9033093443	1.2528564224

H	-3.4574098722	-1.5481171238	-0.1495699063
H	0.6274576406	-2.3530033486	-0.6873997418
H	0.0467236929	-2.3508679409	0.8543606620
H	-6.2109147747	-0.1442503991	2.2078364756
H	-6.8197176961	0.9351710222	0.9930066584
H	-3.8922181036	-0.6316295521	2.3008551740
H	-3.6913515553	0.9365068475	3.0484348960
H	-2.1890700240	1.6866866003	1.2653495717
H	-1.1743929784	0.7647103340	6.2581067642
H	0.5318386236	0.5341613421	6.5002579150
H	2.4799989364	1.1594780992	5.3876605627
H	3.2982870363	0.1439241219	4.1895121920
H	2.3905871230	-0.6057927614	5.5213869748
H	3.8365443136	-0.8709882110	-0.3055738709
H	3.3851585235	-0.8393634849	-2.6776927189
H	1.9630944397	0.2358345378	-4.7798660863
H	-1.5281853649	1.2507574769	-2.5887543014
H	-0.3425721449	1.3351311791	-4.8578940386
H	3.1706338895	2.0203749197	0.7974896998
H	1.2158744220	3.4070199852	-1.8690954394
H	2.1908758560	6.5534902579	-0.5871078301
H	3.9629987165	3.5447189078	-1.5263902584
H	4.2783770031	4.0175155197	1.4925355265
H	5.4556036977	3.2116308155	0.4210324523
H	5.0795009634	4.9362045091	0.2125025467
H	1.7969941980	4.4562281535	0.4060206925
H	1.3468217982	4.8525651193	-3.8754626516
H	2.9866120229	4.5455773890	-3.2821755079
H	2.2077836992	6.1027049956	-2.9609325031
H	-0.8206963000	3.3911449812	-1.2378762592
H	-2.3391728893	5.9225437813	-1.3183132916
H	-4.3148458341	4.1948510737	-1.3845048646
H	-3.4001268639	2.2710422545	-0.9034002584
H	-3.6205462255	5.4503202400	-3.4270478927
H	-4.0183362786	3.7656473851	-3.8329389996
H	-2.3189954851	4.2795478212	-3.7168854323
H	-3.9637434933	6.2793033838	0.2896138684
H	-3.4059805288	7.7172931315	2.7493517319
H	-2.1988090481	6.4872953278	3.1783538312
H	-3.8715410590	4.6627917245	2.7502397217
H	-5.0978320766	5.8646902688	2.3279316551
H	-3.6406509734	6.7130841789	4.1926523867
H	1.5324618727	-2.5476011178	-2.4239624558
O	0.2732668746	1.9380657964	-0.0922982777
O	0.3581439503	2.6500040347	1.1855657437
H	-0.4591005639	3.2069100562	1.1413863307
H	1.8961013422	2.1685209354	-0.2701947757

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	X	Y	Z
Fe	0.0021057842	-0.0022750825	-0.0013491845
N	0.0047454749	0.0002622898	1.8984535163
C	1.1718255258	-0.0039439248	2.5785290762

C	1.1642092098	0.0746885584	3.9610072342
C	-0.1415713220	0.2018894764	4.5454593506
N	-1.2803115220	0.3122861090	3.8233632455
C	-1.1599493505	0.2127225021	2.5086539189
C	2.3562259326	0.0536165188	1.6260669169
O	3.5163738581	0.3369773509	2.0122662510
C	2.3929144774	0.0429358726	4.8316070550
N	-0.2905082305	0.2268333384	5.8899497491
C	-2.2609066054	0.4622283771	1.4746524523
N	-1.9052335133	-0.2586032982	0.2318538582
C	-2.2937974878	-1.6670567445	0.2723990213
C	-1.2771925213	-2.5418662079	-0.4826057760
C	-1.3027195486	-2.6071641837	-2.0212528850
N	-2.5188736445	-2.5426428538	-2.6092244633
N	1.9688484079	-0.0861678909	0.3463662551
C	2.9734502329	0.0242566962	-0.6875080713
C	3.3876300521	1.4726770141	-0.9890879791
O	3.8360199379	1.8784001161	-2.0227479768
C	2.5599629010	-0.6600074814	-2.0275094592
C	1.3458315845	-0.0458849992	-2.6645158164
N	0.1539371761	0.1372196489	-1.9855167354
C	-0.6898273486	0.7256696732	-2.8131698605
N	-0.0924516010	0.9071322172	-4.0172377148
C	1.1968064266	0.4255287980	-3.9424659890
O	2.3913704165	-2.0522918205	-1.7565838868
N	3.2610343196	2.4145613567	0.1904292965
C	3.8419343423	3.8144442293	0.0100111725
C	4.7599346878	4.1338968712	1.1870527058
C	2.6634919507	4.8039610234	-0.1124888691
C	1.7452617219	4.5426983479	-1.3424988216
C	0.4450824902	5.2933980251	-1.0621399797
O	0.4485564992	6.5065726074	-0.8235596342
O	3.2067618647	6.1027377446	-0.1444015339
C	-3.6775366110	0.2863998977	2.0323764290
C	-4.7209786534	1.0685804431	1.2411195226
N	-5.9829122207	0.5766301591	1.2962077511
O	-4.4681455120	2.0937740016	0.6136884702
N	0.0424681989	-2.0441580795	-0.0612696467
O	-0.2723830135	-2.8188336424	-2.6603271566
C	2.3707183039	5.0068635823	-2.6682375306
N	-0.6777591334	4.5288455520	-1.0800799025
C	-1.9716055317	5.0282467237	-0.6819343235
C	-2.1920091580	4.8252125136	0.8359999831
O	-1.4423218347	4.1385171432	1.5452685373
C	-3.0723646815	4.3193761609	-1.5368264578
O	-2.8799819562	2.9126747791	-1.5208861771
C	-3.0313649386	4.7820663352	-2.9904269622
N	-3.2801594321	5.4373648177	1.3451793976
C	-3.6870133298	5.3240533683	2.7477620074
C	-3.1540698750	6.4629210318	3.6197208560
H	-2.5765969812	-2.6749078735	-3.6100176565
H	-3.3587901095	-2.3116245307	-2.1020394242
H	-1.4197050542	-3.5894635911	-0.1733079512
H	-2.3056496570	-2.0644238618	1.3064840928

H	-3.3183584154	-1.8384341242	-0.1030023470
H	0.8027567127	-2.3385144221	-0.6823945852
H	0.2671384419	-2.3766807690	0.8757035222
H	-6.2316273493	-0.1736522572	1.9204790524
H	-6.7315751431	1.1297175467	0.9012854243
H	-3.9675441652	-0.7664206562	2.1144015444
H	-3.6799380054	0.6828071968	3.0567756670
H	-2.1595015467	1.5308787895	1.2404250314
H	-1.2046842881	0.4450228707	6.2605761080
H	0.5032377492	0.2891858467	6.5076050051
H	2.4447430447	0.9330031874	5.4737362593
H	3.2957425150	0.0137289322	4.2226247566
H	2.3853719073	-0.8368473450	5.4898246207
H	3.9048694126	-0.4630148559	-0.3512347003
H	3.3993461394	-0.5216244842	-2.7193318890
H	1.8803607375	0.4647344645	-4.7766026832
H	-1.6759053959	1.0865110523	-2.5536518146
H	-0.5208773886	1.3373061421	-4.8248880038
H	3.6805758837	1.8952132386	0.9992849129
H	1.5135556507	3.4758430120	-1.4120031522
H	2.4397326628	6.6952732054	-0.2889149131
H	4.4115799065	3.7919611277	-0.9206537385
H	4.2141147090	4.1157700351	2.1382143352
H	5.5930319858	3.4244152694	1.2443322476
H	5.1661016269	5.1384115929	1.0517515605
H	2.0520907539	4.6782197486	0.7965908580
H	1.6791382096	4.8220519621	-3.4972490955
H	3.2959790744	4.4610807028	-2.8769572519
H	2.5970719616	6.0743454417	-2.6417909141
H	-0.5806955497	3.5118792726	-1.0657776895
H	-1.9889916352	6.1056618147	-0.8804245510
H	-4.0538903446	4.5650403478	-1.1068939983
H	-3.3047482250	2.5401512538	-0.7201080368
H	-3.2011196061	5.8610059021	-3.0709947160
H	-3.8058459796	4.2629343959	-3.5629522076
H	-2.0570509750	4.5555431749	-3.4352369668
H	-3.8198783860	6.0407599293	0.7396264116
H	-3.5123836525	7.4370310793	3.2690624214
H	-2.0601152728	6.4753099936	3.6087617272
H	-3.3159968459	4.3600241983	3.1039934807
H	-4.7820302403	5.2924154119	2.7729094212
H	-3.4877695832	6.3340143081	4.6559325991
H	1.7646375282	-2.4165067345	-2.4130173034
O	0.0624729816	1.8582530211	-0.1290610508
O	0.6380783500	2.5177750034	1.0403466683
H	-0.0510413507	3.2183318633	1.2093437014
H	2.2362027057	2.4920341377	0.4717304951

[²BLM-Fe^{III}-OOH; NH₂⁺(V)]¹⁺ (Figure S12(b))

===2'===

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X

Y

Z

Fe	0.0685321921	0.0454762450	-0.0289081479
N	0.0055102159	-0.0252930721	1.8779407061
C	1.1838459846	-0.0398084792	2.5492191472
C	1.2095627797	0.0233921885	3.9286856296
C	-0.0902940046	0.1263085722	4.5471702987
N	-1.2397382173	0.2519856117	3.8388627794
C	-1.1381545925	0.1916090060	2.5241402249
C	2.3473834324	0.0196570880	1.5807922777
O	3.5051723044	0.3070413685	1.9206335752
C	2.4549974972	-0.0031320689	4.7717573010
N	-0.2122796942	0.1329551567	5.8847517249
C	-2.2956919697	0.5008636346	1.5866452684
N	-2.0164728153	-0.2071698743	0.2859828485
C	-2.3706657183	-1.6572936441	0.3315857332
C	-1.3841311094	-2.5102874232	-0.4764735450
C	-1.5363822191	-2.5793381477	-2.0138830959
N	-2.8028713084	-2.6413778597	-2.4970149223
N	1.9518570086	-0.1437219844	0.2849210498
C	2.9924522370	-0.1153507922	-0.7268892479
C	3.5143065910	1.2913742762	-1.0585643713
O	4.2228727220	1.5774931317	-1.9734509319
C	2.5762278927	-0.7969285275	-2.0586405603
C	1.3999511551	-0.1321787847	-2.7143698894
N	0.2503546855	0.2151926281	-2.0214407969
C	-0.5778874679	0.7733827557	-2.8929161606
N	-0.0082497894	0.7843714694	-4.1202818598
C	1.2419367371	0.2183108763	-4.0298868428
O	2.3352592660	-2.1709749343	-1.7498586114
N	3.0611128312	2.3750939174	-0.0870365169
C	3.5828506805	3.7946415616	-0.3551365159
C	4.6398145181	4.1408745029	0.6879777921
C	2.3663981128	4.7456588748	-0.3530041375
C	1.4378425956	4.5339576705	-1.5870286323
C	0.1144538204	5.2230836764	-1.2619030331
O	0.0719698583	6.4143928089	-0.9496470191
O	2.8699170088	6.0568621669	-0.3089510052
C	-3.6939583166	0.2960529624	2.1793609189
C	-4.7744960209	0.8625937848	1.2576798140
N	-5.9891350554	1.0414562150	1.8082118284
O	-4.5492198513	1.1137755928	0.0640084530
N	-0.0332437092	-2.0110878872	-0.1635144911
O	-0.5428390370	-2.6188884638	-2.7289026046
C	2.0266249831	5.1044444101	-2.8908283975
N	-0.9927986593	4.4325259894	-1.3481990003
C	-2.3241032395	4.9068100840	-1.0407799494
C	-2.6280037841	4.8017500481	0.4647041311
O	-2.2063510052	3.8551017300	1.1585437130
C	-3.3498927317	4.0727419328	-1.8717461596
O	-3.0636608707	2.6754416959	-1.7334409711
C	-3.2992568402	4.4308400553	-3.3530509614
N	-3.4364468763	5.7514259965	0.9630173015
C	-3.8361357702	5.8273025215	2.3743868788
C	-2.9132742154	6.7246554901	3.2015745066
H	-2.9080740729	-2.8758613514	-3.4776903453

H	-3.6024949204	-2.8185119763	-1.9053863030
H	-1.4951026761	-3.5525240532	-0.1391909112
H	-2.2949123327	-1.9847302644	1.3730222315
H	-3.4117496910	-1.8081351118	0.0274794056
H	0.6495681570	-2.2884693709	-0.8834810729
H	0.2978785926	-2.3973277953	0.7203448562
H	-6.1838634386	0.8433364344	2.7800111345
H	-6.7485275488	1.3756518597	1.2273348125
H	-3.9128246075	-0.7604080618	2.3798036512
H	-3.7174872932	0.7934623079	3.1551796142
H	-2.2035956757	1.5661679759	1.3476551462
H	-1.1295708463	0.2463297821	6.2945995547
H	0.5846919491	0.0588425629	6.4988724284
H	2.5004500631	0.8755112643	5.4290400593
H	3.3484545171	-0.0065757845	4.1492143363
H	2.4750744525	-0.8969979596	5.4106900892
H	3.8736982734	-0.6565402871	-0.3516679068
H	3.4346074695	-0.7138524720	-2.7352921147
H	1.8975132747	0.1214609923	-4.8824602566
H	-1.5422013225	1.2155454299	-2.6707626551
H	-0.4358377327	1.1476138377	-4.9626335781
H	3.3697011270	2.0437888149	0.8474894291
H	1.2462722776	3.4628396982	-1.7229112557
H	2.0946502912	6.6472562677	-0.4005675326
H	4.0368219072	3.7557574139	-1.3466415399
H	4.2184428043	4.1532428199	1.7003365854
H	5.4755090926	3.4329209371	0.6547266442
H	5.0250256180	5.1401928776	0.4768814745
H	1.7827526541	4.5250583901	0.5575104306
H	1.3366725410	4.9366370647	-3.7248837592
H	2.9782692253	4.6248519298	-3.1435378508
H	2.2017644950	6.1782064533	-2.8026626993
H	-0.8753073025	3.4248711847	-1.3547269764
H	-2.3804704996	5.9562959721	-1.3456863836
H	-4.3551282736	4.2811630693	-1.4823712620
H	-3.6293238333	2.2932628425	-1.0366610008
H	-3.5586208927	5.4822995740	-3.5145109296
H	-4.0102113183	3.8102748447	-3.9060798292
H	-2.2956829419	4.2620835135	-3.7574914509
H	-3.6510534787	6.5485600289	0.3762357300
H	-2.9011863860	7.7501449255	2.8167403236
H	-1.8881682550	6.3407333847	3.1914785015
H	-3.8299638725	4.8048282674	2.7577560534
H	-4.8675319696	6.1938529905	2.4031690052
H	-3.2588229032	6.7602324657	4.2403626002
H	2.0210817110	-2.6109176386	-2.5601054304
O	0.1124112854	1.8725102234	-0.0921367953
O	0.1658969967	2.5858301258	1.1759583644
H	-0.6528352628	3.1492590508	1.1035763579
H	2.0163581425	2.3300646981	-0.0642838500
H	-2.6097633179	0.2577731177	-0.4037426060

	X	Y	Z
Fe	-0.0037459097	-0.0116218801	-0.0058964542
N	-0.0011610641	-0.0055076849	1.8990818916
C	1.1916482414	-0.0035862796	2.5469285247
C	1.2424043185	0.0777084307	3.9247993111
C	-0.0459392832	0.1893711461	4.5652662022
N	-1.2100795543	0.2950755667	3.8778543848
C	-1.1348127266	0.2083889603	2.5630503038
C	2.3324483094	0.0596241757	1.5537763381
O	3.5046818505	0.3213155298	1.8759888464
C	2.5032210247	0.0638572333	4.7467949381
N	-0.1426762942	0.2249354477	5.9041167691
C	-2.3160868542	0.4704615244	1.6405531691
N	-2.0709979602	-0.3055920698	0.3707961927
C	-2.3734646021	-1.7609435988	0.5106153411
C	-1.3689409754	-2.6359287977	-0.2590206485
C	-1.5660346493	-2.8192399711	-1.7828772476
N	-2.8413666458	-3.0116702810	-2.2095214254
N	1.8959443690	-0.0669952287	0.2729512709
C	2.8852286656	0.0249223292	-0.7823843896
C	3.2363568835	1.4739243616	-1.1531945630
O	3.5889216061	1.8687371897	-2.2304001027
C	2.4815537402	-0.7513596345	-2.0633330828
C	1.2411065828	-0.2123163225	-2.7161103604
N	0.0838735667	0.0718309267	-2.0079872450
C	-0.7909867941	0.5684766057	-2.8700119552
N	-0.2469880126	0.5909966125	-4.1088255842
C	1.0375209276	0.1030731785	-4.0334711967
O	2.3477865129	-2.1186550261	-1.6637629888
N	3.1657105090	2.4479453332	0.0241126913
C	3.7134912024	3.8622715684	-0.2237658982
C	4.6774844119	4.2267634517	0.9028407798
C	2.5035795937	4.8170618934	-0.3209372760
C	1.5685084384	4.5228167636	-1.5320402459
C	0.2516062654	5.2339840639	-1.2326152001
O	0.2202861000	6.4340774317	-0.9504850655
O	3.0132017633	6.1229803904	-0.3666728357
C	-3.6959945584	0.2916407867	2.2801503348
C	-4.8001400363	0.8194913702	1.3628673477
N	-6.0354274031	0.8786801437	1.8947020577
O	-4.5706780237	1.1555968836	0.1917992131
N	-0.0238018826	-2.0755115670	-0.0288802613
O	-0.5998519467	-2.8234812668	-2.5335173524
C	2.1525227714	5.0018302774	-2.8734173127
N	-0.8614400341	4.4494824975	-1.2856820124
C	-2.1666083507	4.9354916645	-0.9058887328
C	-2.3752036436	4.8116580744	0.6182946895
O	-1.7860341931	3.9549100953	1.3085994461
C	-3.2538138753	4.1442660788	-1.6988750068
O	-3.0235538437	2.7374080418	-1.5632777287
C	-3.2345981243	4.4969595530	-3.1824241577
N	-3.2803861269	5.6586805258	1.1443412917
C	-3.6007820351	5.7390382140	2.5754402876

C	-2.8240633792	6.8517846521	3.2877879875
H	-2.9586152107	-3.3142059097	-3.1700248294
H	-3.5940585232	-3.2407104327	-1.5753031254
H	-1.4359125599	-3.6527036128	0.1575701231
H	-2.2783337360	-2.0192071022	1.5698561523
H	-3.4104554975	-1.9685275383	0.2259907068
H	0.6267505858	-2.3489362367	-0.7799532139
H	0.3716650604	-2.4224594640	0.8445930953
H	-6.2363768139	0.6050742625	2.8471382508
H	-6.8042048324	1.1947555844	1.3161204373
H	-3.9052828652	-0.7536644783	2.5397518885
H	-3.6980443071	0.8378114750	3.2304200054
H	-2.2257687662	1.5221458021	1.3399396715
H	-1.0529362044	0.3407739077	6.3286093519
H	0.6648935562	0.1620096151	6.5052271047
H	2.5619141286	0.9544712703	5.3866992156
H	3.3879837966	0.0430551350	4.1110518108
H	2.5302991572	-0.8169578459	5.4031130907
H	3.8297423366	-0.4146315883	-0.4202059204
H	3.3092641732	-0.6477869105	-2.7746549869
H	1.6841807976	0.0364814730	-4.8957473361
H	-1.7629318010	0.9824563058	-2.6319990480
H	-0.7093122167	0.9189881596	-4.9469751569
H	3.6588958608	1.9706012570	0.8117508460
H	1.3705490400	3.4473843673	-1.5966804527
H	2.2351733035	6.7071547700	-0.4777406322
H	4.2397178143	3.8175026808	-1.1795286659
H	4.1752724909	4.2344519853	1.8786473991
H	5.5258910694	3.5337032498	0.9425989022
H	5.0628815758	5.2317295161	0.7180984192
H	1.9165752173	4.6739722000	0.6034765312
H	1.4507649737	4.7958119465	-3.6886013772
H	3.0906864769	4.4858178022	-3.1010289103
H	2.3478584669	6.0753501446	-2.8525743242
H	-0.7546636500	3.4389333884	-1.2920654170
H	-2.2182867687	5.9944210623	-1.1784677732
H	-4.2354547554	4.3987608526	-1.2774893346
H	-3.6095758865	2.3706976971	-0.8763983159
H	-3.4378766909	5.5613460850	-3.3396138686
H	-3.9986515394	3.9171740846	-3.7081571106
H	-2.2572469404	4.2688086062	-3.6201432595
H	-3.6382111990	6.3984301906	0.5503872842
H	-3.0414802711	7.8364337262	2.8530198981
H	-1.7422504746	6.6767875002	3.2213266747
H	-3.3631428634	4.7608727701	3.0039407787
H	-4.6839692572	5.8972801637	2.6651895907
H	-3.1059773971	6.8846392956	4.3463533904
H	2.1009108153	-2.6368254232	-2.4502342794
O	-0.0819931830	1.7808435561	-0.1549898658
O	0.4658928832	2.5386534881	0.9638067249
H	-0.2830960457	3.1959409698	1.0914748776
H	2.1675341483	2.5143729630	0.3580393522
H	-2.6953199731	0.1104602619	-0.3230873305

²TS_{h-oh2} (unprotonated, Figure S13a)

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	X	Y	Z
Fe	0.0005301169	-0.0018042199	-0.0034767711
N	-0.0020531895	-0.0037957976	1.9001477249
C	1.1635846864	-0.0008635152	2.5835775109
C	1.1489833078	0.0709501922	3.9666121204
C	-0.1591640296	0.1776339860	4.5504974233
N	-1.2994020273	0.2693640753	3.8261012383
C	-1.1719761784	0.1782723212	2.5118106355
C	2.3506073502	0.0832871638	1.6339946049
O	3.5032686438	0.3627141933	2.0319461511
C	2.3774364732	0.0604596038	4.8368213870
N	-0.3094419575	0.2078116877	5.8940769033
C	-2.2756003541	0.4071042240	1.4768635623
N	-1.8895496637	-0.2963697056	0.2331580989
C	-2.2541772010	-1.7119938091	0.2519559016
C	-1.2179069354	-2.5553690106	-0.5124552577
C	-1.2534260361	-2.6218801965	-2.0521047576
N	-2.4762997461	-2.5897313518	-2.6323602702
N	1.9609687370	-0.0282436351	0.3511012009
C	2.9584376445	0.1650939841	-0.6835838387
C	3.2479634903	1.6554732636	-0.9647789515
O	3.5573433680	2.0849313945	-2.0507979570
C	2.5827859828	-0.5329939900	-2.0213927699
C	1.3413922622	0.0200384780	-2.6637331780
N	0.1448073715	0.1589683020	-1.9827750913
C	-0.7249705965	0.7098413450	-2.8102680458
N	-0.1389090247	0.9110007742	-4.0155250257
C	1.1690538036	0.4812267757	-3.9418963668
O	2.4707096227	-1.9346877737	-1.7480633013
N	3.1386580200	2.5335491549	0.1936210798
C	3.7492569132	3.9118708499	0.0490059143
C	4.6354085827	4.2029244589	1.2592393156
C	2.6103510782	4.9410166653	-0.0933785295
C	1.7344472474	4.7396812852	-1.3692654678
C	0.4264467293	5.4597474422	-1.0703222919
O	0.4027559338	6.6627344645	-0.7912512351
O	3.1781958218	6.2302173036	-0.0618778855
C	-3.6898725213	0.1897294565	2.0249354895
C	-4.7377291933	1.0078677477	1.2758791678
N	-5.9986165820	0.5103039654	1.3089734345
O	-4.4835273196	2.0725648848	0.7084401682
N	0.0932424137	-2.0228844052	-0.1036197184
O	-0.2215256698	-2.8029809805	-2.6946584220
C	2.3991180848	5.2752840764	-2.6465691055
N	-0.6847475828	4.6712218617	-1.0707383843
C	-1.9401152881	5.1217254234	-0.5242925721
C	-1.9699286915	4.8896076730	1.0046464914
O	-1.0943695366	4.2538797966	1.6187152957
C	-3.1092506571	4.4008438413	-1.2695792610
O	-2.8530770835	3.0047441301	-1.3361249298

C	-3.2640221057	4.9286358880	-2.6935417456
N	-3.0216574474	5.4273880437	1.6490126898
C	-3.2324202445	5.3238668247	3.0953064832
C	-2.6338213471	6.4989607234	3.8709280948
H	-2.5369486716	-2.7346444828	-3.6312174262
H	-3.3232533870	-2.4009716175	-2.1189516642
H	-1.3261750864	-3.6063938978	-0.2021474046
H	-2.2615383543	-2.1193574849	1.2818372497
H	-3.2747992676	-1.8954879140	-0.1288122631
H	0.8487656829	-2.2730371018	-0.7527656229
H	0.3545669887	-2.3733109028	0.8171977127
H	-6.2406349460	-0.3103754310	1.8440197321
H	-6.7479683115	1.0635013802	0.9144396318
H	-3.9709323199	-0.8684304248	2.0528219517
H	-3.6946262026	0.5331544335	3.0687063025
H	-2.2000638223	1.4789631681	1.2482418737
H	-1.2299774939	0.3829502968	6.2700734352
H	0.4823577413	0.2381114454	6.5162330317
H	2.4093408090	0.9473102164	5.4850930518
H	3.2774336088	0.0580177562	4.2229692678
H	2.3919727340	-0.8247288725	5.4878034648
H	3.9166931135	-0.2637345337	-0.3499236001
H	3.4151234265	-0.3580552842	-2.7128710721
H	1.8512582744	0.5552723864	-4.7746037331
H	-1.7259521732	1.0238251109	-2.5505155836
H	-0.5850229578	1.3226101033	-4.8231748701
H	3.5337084613	2.0183834157	1.0021339958
H	1.5245994896	3.6747474152	-1.5042308107
H	2.4308642912	6.8446734740	-0.2077487597
H	4.3500791981	3.9046282642	-0.8629179939
H	4.0588649174	4.1837693355	2.1925557950
H	5.4486032159	3.4727657581	1.3362014137
H	5.0684820337	5.1996941969	1.1545906748
H	1.9587629414	4.8132735244	0.7903263373
H	1.7385763339	5.1234906392	-3.5072212096
H	3.3348889046	4.7455151879	-2.8449471357
H	2.6121392532	6.3422920306	-2.5612997739
H	-0.5812362940	3.6590691689	-1.1246425826
H	-2.0078582863	6.2024102987	-0.6899010647
H	-4.0405249790	4.5792571399	-0.7142638230
H	-3.2918032280	2.5700677077	-0.5763289705
H	-3.4987056722	5.9989202659	-2.7005152316
H	-4.0732544506	4.3905935187	-3.1965928155
H	-2.3394222189	4.7766928354	-3.2600064171
H	-3.6669629285	5.9954803148	1.1160081164
H	-3.0679946450	7.4525238202	3.5508290214
H	-1.5509294824	6.5470364279	3.7215349370
H	-2.7819499128	4.3814911827	3.4140643674
H	-4.3123330825	5.2537009198	3.2635280160
H	-2.8293117228	6.3817011956	4.9425380173
H	1.9592366591	-2.3406213257	-2.4727333306
O	0.0198359514	1.8912598429	-0.1241623442
O	0.7263563626	2.5225277116	0.9974725637
H	0.1344177990	3.3359881394	1.1623220635

H	1.8680998043	2.6192399790	0.5819171880
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²TS_{h-oh2} (protonated, Figure S13b)

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	X	Y	Z
Fe	0.0011005302	-0.0007298235	0.0016055000
N	0.0002723705	-0.0011439326	1.9049298527
C	1.1971126522	-0.0027350096	2.5463867517
C	1.2500209961	0.0415303816	3.9261193601
C	-0.0363754164	0.1137960345	4.5752086979
N	-1.2078399920	0.2123583031	3.8964373849
C	-1.1379665133	0.1630508786	2.5793567853
C	2.3365701547	0.0907973882	1.5476707698
O	3.5028144725	0.3501817457	1.8727661073
C	2.5153354245	0.0256413428	4.7400194430
N	-0.1275130065	0.1122473594	5.9151487167
C	-2.3388014078	0.3861200769	1.6707122789
N	-2.0688452275	-0.3678976549	0.3921740686
C	-2.3010375419	-1.8376029014	0.5364803824
C	-1.2733599788	-2.6687905967	-0.2483561874
C	-1.4920223631	-2.8692548946	-1.7668725524
N	-2.7666696191	-3.1232648277	-2.1654208331
N	1.8910827577	-0.0179362989	0.2656683432
C	2.8554756665	0.1639682160	-0.8082448231
C	3.0385793073	1.6488316036	-1.1906907410
O	3.1776279525	2.0329661644	-2.3251702657
C	2.4880141615	-0.6500729937	-2.0700031087
C	1.2124575449	-0.1926844015	-2.7192678380
N	0.0556591436	0.0592598251	-1.9990619210
C	-0.8600037004	0.4661490845	-2.8647815023
N	-0.3439168977	0.4703180897	-4.1132749271
C	0.9664821808	0.0572764098	-4.0424612281
O	2.4224827392	-2.0210102027	-1.6566231134
N	3.0209273559	2.5769169291	-0.0703726494
C	3.5957310384	3.9608244314	-0.3387216542
C	4.6731421201	4.2656860885	0.7000348172
C	2.4442573414	4.9844510993	-0.3090549840
C	1.4029929832	4.7956768221	-1.4631463135
C	0.1457882238	5.4952112508	-0.9660192655
O	0.1657468437	6.6691665317	-0.5938691216
O	3.0146989096	6.2680672360	-0.3390452439
C	-3.6996850457	0.1188377050	2.3260091377
C	-4.8600255698	0.5029490026	1.4047978174
N	-6.0813670704	0.5185895997	1.9710805682
O	-4.6872920843	0.7642366588	0.2040784062
N	0.0509625196	-2.0521036614	-0.0405377995
O	-0.5426150612	-2.8320165159	-2.5368820644
C	1.8856682755	5.3692411039	-2.8058031687
N	-0.9853739305	4.7246851707	-0.8726888057
C	-2.0836457745	5.1807053792	-0.0489552751
C	-1.7142307011	5.0428919342	1.4479955081
O	-0.8250335068	4.2651643571	1.8589755197

C	-3.3787592892	4.4069973539	-0.3815471871
O	-3.0603397234	3.0222221435	-0.2186090578
C	-3.8992798221	4.7086973983	-1.7857692596
N	-2.4260390425	5.7938617596	2.2968077379
C	-2.2014687487	5.8455293919	3.7495513490
C	-1.3120315995	7.0185498557	4.1647571314
H	-2.8863951048	-3.4444469161	-3.1196467341
H	-3.4921473805	-3.3887064258	-1.5139045977
H	-1.2866582441	-3.6853904103	0.1731430175
H	-2.1771667844	-2.0919855967	1.5934073202
H	-3.3322570387	-2.0895694285	0.2686070715
H	0.7033960413	-2.2937352584	-0.8036240773
H	0.4789568353	-2.3865527450	0.8224917301
H	-6.2368165454	0.3081612626	2.9474064289
H	-6.8870590575	0.7292742061	1.3945659325
H	-3.8134801325	-0.9294672054	2.6290518561
H	-3.7440203085	0.6966194769	3.2560676550
H	-2.3103057964	1.4416553466	1.3701298402
H	-1.0384815105	0.1879785204	6.3470862301
H	0.6842564290	0.0405734006	6.5099076869
H	2.5603068473	0.8950932321	5.4095428264
H	3.3927479518	0.0474074157	4.0947641176
H	2.5671109119	-0.8770868746	5.3644338503
H	3.8336211156	-0.1953384833	-0.4561425083
H	3.3004213268	-0.5136335945	-2.7917651435
H	1.6022060750	0.0002748708	-4.9128123288
H	-1.8641171337	0.7854529979	-2.6283674402
H	-0.8372699608	0.7368218707	-4.9555478138
H	3.5011399052	2.1236745399	0.7230012443
H	1.1901957468	3.7292531844	-1.5971324110
H	2.2648068720	6.8954233648	-0.3406525387
H	4.0339130737	3.9320876828	-1.3381524345
H	4.2618964664	4.2688444657	1.7171459560
H	5.4856564763	3.5323182070	0.6500274020
H	5.0884258372	5.2563007653	0.5064373456
H	1.9184871126	4.8414433802	0.6537885667
H	1.1214066347	5.2257828909	-3.5771720177
H	2.7960200153	4.8608508503	-3.1368473291
H	2.0971299962	6.4369269164	-2.7249506874
H	-0.9049065660	3.7189127430	-0.9879287295
H	-2.2395747563	6.2432545302	-0.2594587131
H	-4.1382384672	4.7028716620	0.3583895082
H	-3.8672526266	2.4795151587	-0.2909102786
H	-4.1718702490	5.7648368350	-1.8890303253
H	-4.7962211402	4.1131560099	-1.9902280427
H	-3.1440195351	4.4719773624	-2.5406808866
H	-3.0483280882	6.4888587313	1.9015360838
H	-1.7530279895	7.9786237149	3.8750531833
H	-0.3226924859	6.9400359541	3.7034804937
H	-1.7494479954	4.8925136419	4.0307268553
H	-3.1841445723	5.9101474833	4.2290027273
H	-1.1870368881	7.0232866394	5.2527313252
H	2.2774903264	-2.5657901127	-2.4493473962
O	-0.0741988421	1.8242632328	-0.1192475360

O	0.6952839990	2.4983086084	0.9213791329
H	0.0834248935	3.3105229623	1.1876780154
H	1.7959106120	2.6355431530	0.4155582374
H	-2.7412253820	0.0117920863	-0.2780014889

²³ (unprotonated, Figure S14a)

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	X	Y	Z
Fe	0.0495246123	0.0697665018	-0.0176304806
N	0.1167698601	0.0861933405	1.8843192007
C	1.3033278840	-0.0005722982	2.5230913116
C	1.3405848279	0.0606797128	3.9078884681
C	0.0643219954	0.2446264597	4.5368022835
N	-1.0935775699	0.4283692940	3.8555016496
C	-1.0138563263	0.3507629706	2.5357007385
C	2.4612021702	-0.0334199736	1.5320568938
O	3.6510755081	0.0865136684	1.8994489728
C	2.5966295560	-0.0347464727	4.7351757844
N	-0.0335867122	0.2825044039	5.8849868837
C	-2.1161462933	0.6836250742	1.5322848313
N	-1.8646525462	-0.0872613090	0.2976544779
C	-2.3128513777	-1.4732789314	0.4080356939
C	-1.3768905958	-2.4115138142	-0.3724381060
C	-1.5097310136	-2.5239439261	-1.9019364223
N	-2.7619664703	-2.4049680664	-2.4092600146
N	2.0177836402	-0.0927894088	0.2599737672
C	3.0114590250	-0.0964008315	-0.8081227507
C	3.5051809751	1.3268112615	-1.1928092858
O	3.6549151608	1.6630329105	-2.3621893377
C	2.5111971360	-0.8104297043	-2.0864513247
C	1.3021830312	-0.1768937588	-2.7102223883
N	0.1630023509	0.1474816854	-1.9971930672
C	-0.6890374605	0.7095381755	-2.8370922475
N	-0.1476615072	0.7452897977	-4.0793294130
C	1.1114747052	0.1876041778	-4.0175174830
O	2.2729248667	-2.1869790908	-1.7514153860
N	3.7380357629	2.1793267892	-0.1345929490
C	4.3938665267	3.4872310715	-0.3538419951
C	5.4569032424	3.7137844919	0.7183205135
C	3.3182005086	4.5970274798	-0.3300807427
C	2.2584114884	4.4537763984	-1.4609013703
C	1.0418265327	5.2718313434	-1.0606462844
O	1.1140742214	6.4560009461	-0.7304514168
O	3.9573589754	5.8544065863	-0.3854201624
C	-3.5322229789	0.6772566136	2.1193790571
C	-4.4437550701	1.6686518683	1.4014800305
N	-5.7536158178	1.3344754925	1.3586483756
O	-4.0364246015	2.7313497936	0.9140648767
N	-0.0125101333	-1.9638511547	-0.0511806754
O	-0.5368534328	-2.8156792132	-2.5959615843
C	2.7888909593	4.9035202738	-2.8300974624
N	-0.1519641404	4.5959626522	-1.0747191329
C	-1.3711619555	5.2293300817	-0.6528491559
C	-1.5823488829	5.1156538960	0.8587498557
O	-0.9046532841	4.3426977415	1.6341681452
C	-2.5984729312	4.6433773633	-1.4470434190

O	-2.5740171126	3.2331997759	-1.4261736410
C	-2.5594822441	5.1000615608	-2.9037169492
N	-2.5335193049	5.8382011933	1.4139508052
C	-2.9429978075	5.7656586615	2.8268546107
C	-2.1243188586	6.6842160781	3.7265884938
H	-2.8936144996	-2.5703073252	-3.3965055374
H	-3.5534528878	-2.1078183395	-1.8547853728
H	-1.5453718602	-3.4406665780	-0.0198861703
H	-2.2897907205	-1.8327964273	1.4570350407
H	-3.3634733462	-1.6126241184	0.0892091824
H	0.6956859989	-2.2960212690	-0.7173041475
H	0.2635728931	-2.2921679615	0.8730010481
H	-6.1163378317	0.5214053637	1.8345785335
H	-6.4106476363	1.9959204888	0.9694618722
H	-3.9762577657	-0.3260678668	2.1334289358
H	-3.4611043164	0.9980327118	3.1706081755
H	-1.9130641957	1.7284159007	1.2674680850
H	-0.9512166111	0.3575602916	6.2970051049
H	0.7536975934	0.0630313152	6.4765776152
H	2.6967752198	0.8372364144	5.3962413458
H	3.4724855834	-0.0831923985	4.0896920581
H	2.5866922024	-0.9307404835	5.3715779753
H	3.8979840838	-0.6493206771	-0.4607886868
H	3.3230145287	-0.7510735823	-2.8186695451
H	1.7605680388	0.1296289102	-4.8757644613
H	-1.6440723508	1.1375653078	-2.5681027186
H	-0.5921213081	1.1230894226	-4.9054900667
H	3.9403520128	1.6997485063	0.7475440843
H	1.9601686308	3.4087039647	-1.5393309049
H	3.2428771639	6.5148489245	-0.4168152080
H	4.8637911057	3.4676364033	-1.3406799824
H	5.0135263288	3.7025585972	1.7218127376
H	6.2212463681	2.9318327512	0.6711979892
H	5.9334586703	4.6844110840	0.5738228249
H	2.7941489470	4.4935868381	0.6409976406
H	2.0055943239	4.8281497908	-3.5855099239
H	3.6075800067	4.2548033303	-3.1333338670
H	3.1434711262	5.9326001371	-2.7985012385
H	-0.1627561438	3.5738522908	-1.1323537931
H	-1.2838385918	6.2997934181	-0.8676700669
H	-3.5171189332	5.0192274951	-0.9703497413
H	-3.0003246180	2.9132336405	-0.6023708337
H	-2.6170714808	6.1911327206	-2.9864255742
H	-3.4047614461	4.6643447190	-3.4408519048
H	-1.6354971316	4.7620843730	-3.3799033836
H	-3.0330116844	6.4844417284	0.8112551992
H	-2.1940111436	7.7262654277	3.4024356232
H	-1.0751963643	6.3846024669	3.7332236758
H	-2.8491690797	4.7234041284	3.1325825177
H	-4.0020985686	6.0302866446	2.8475374731
H	-2.5059249671	6.6237432383	4.7478256433
H	1.7185438426	-2.5751350863	-2.4525206257
O	0.0754443468	1.9638024636	-0.1287802820
O	0.7796444292	2.6232319591	0.9857431163

H	-0.1351900230	3.7733986417	1.1909235259
H	1.7051249920	2.6466498227	0.6477536670

²³ (protonated, Figure S14b)

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	X	Y	Z
Fe	-0.0043804123	-0.0009278293	-0.0044834527
N	-0.0044140020	-0.0053594417	1.9023868222
C	1.1936066806	0.0039224015	2.5373478706
C	1.2502662496	0.0331110131	3.9189899967
C	-0.0324923288	0.0815388338	4.5731638845
N	-1.2090957877	0.1686568451	3.9011225903
C	-1.1403318166	0.1310695891	2.5830801170
C	2.3314099903	0.0950203935	1.5374415783
O	3.5048210102	0.3022804500	1.8725518978
C	2.5190058128	0.0225256219	4.7288027926
N	-0.1174038807	0.0676155910	5.9149697369
C	-2.3432277750	0.3480467838	1.6763271509
N	-2.0844039036	-0.4213314557	0.4085203138
C	-2.2847420538	-1.8914863534	0.5806878193
C	-1.2375264656	-2.7190088103	-0.1864839585
C	-1.4820896190	-2.9713399075	-1.6924611380
N	-2.7500779748	-3.3268757863	-2.0407090511
N	1.8833202240	0.0140972983	0.2545747609
C	2.8728228395	0.1347153276	-0.8152358984
C	3.1279949150	1.6090104230	-1.2321559336
O	3.1218487866	1.9524968172	-2.4072229368
C	2.4911017122	-0.6889281058	-2.0585555215
C	1.2162847289	-0.2440960677	-2.7151294782
N	0.0588903033	0.0246548730	-2.0033192214
C	-0.8671079158	0.3727274765	-2.8839129018
N	-0.3560375104	0.3272475351	-4.1335969442
C	0.9619610053	-0.0609304909	-4.0473639778
O	2.4140105518	-2.0621610282	-1.6367384656
N	3.3358565364	2.4852549230	-0.1876789248
C	3.8730832403	3.8442996961	-0.4523450081
C	5.0096958364	4.1458739641	0.5259631220
C	2.7264570892	4.8702660722	-0.3323353047
C	1.6116609429	4.6950885152	-1.4159070903
C	0.3952390388	5.4390197713	-0.8984945621
O	0.4481144246	6.5938204795	-0.4634820639
O	3.2817514298	6.1624940524	-0.3746222943
C	-3.7090660662	0.1109860914	2.3285746794
C	-4.8503058513	0.5660173842	1.4138701128
N	-6.0945697750	0.4019048881	1.8997871113
O	-4.6415605634	1.0456067483	0.2876640321
N	0.0730812151	-2.0666441720	-0.0147686212
O	-0.5673176546	-2.8811815634	-2.4978447116
C	2.0330085530	5.2169607587	-2.8030635835
N	-0.7972259066	4.7520113804	-0.8649758394
C	-1.9159148711	5.3759937756	-0.1962359744
C	-1.5926682991	5.5408321018	1.2904266429

O	-0.8762910591	4.6771910545	1.9352186118
C	-3.2244920283	4.5683478854	-0.3746247447
O	-2.9606718201	3.2923000383	0.1861420283
C	-3.6668042657	4.4935613017	-1.8357998234
N	-2.0796159969	6.5555575964	1.9594459781
C	-1.8207050140	6.8666188877	3.3829964629
C	-0.7566047560	7.9538632246	3.5340693541
H	-2.8709818662	-3.6825127960	-2.9825946922
H	-3.4149487013	-3.6606016554	-1.3571517108
H	-1.2241209338	-3.7213066715	0.2680545449
H	-2.1588404439	-2.1193079342	1.6434104158
H	-3.3073888487	-2.1780682919	0.3144862220
H	0.7225015293	-2.3069495676	-0.7816968417
H	0.5224924066	-2.3750286686	0.8466167337
H	-6.2784241980	0.0128304039	2.8141823285
H	-6.8853574012	0.6796069112	1.3310743094
H	-3.8589358888	-0.9375996112	2.6137783175
H	-3.7384674049	0.6759200467	3.2683696075
H	-2.2951677941	1.3986033562	1.3692459695
H	-1.0280543948	0.1102193836	6.3513735525
H	0.6976992971	-0.0148158112	6.5034028326
H	2.5604334976	0.8890725169	5.4022110744
H	3.3931492002	0.0516179577	4.0793293811
H	2.5791312427	-0.8822845002	5.3495365757
H	3.8212084248	-0.2698807587	-0.4369644439
H	3.3017414626	-0.5673707330	-2.7842689415
H	1.5990087414	-0.1420487738	-4.9148499088
H	-1.8829632528	0.6640268941	-2.6622255628
H	-0.8569085334	0.5418514596	-4.9860195329
H	3.6637153186	2.0394860510	0.6704698332
H	1.3607763557	3.6341371909	-1.5111022920
H	2.5325135965	6.7857964423	-0.3302302557
H	4.2568441818	3.8509850138	-1.4759334803
H	4.6585255683	4.1219551495	1.5656535356
H	5.8161813843	3.4137041887	0.4152301588
H	5.4119248108	5.1415041915	0.3321567200
H	2.2632337495	4.6954941229	0.6599905806
H	1.1952228505	5.1562690140	-3.5090812653
H	2.8478951740	4.6014203235	-3.1967605263
H	2.3688605019	6.2552119189	-2.7469161532
H	-0.8113433749	3.7415314792	-0.9844421417
H	-2.0581738604	6.3797370560	-0.6086519667
H	-4.0046499683	5.0886810795	0.2060736934
H	-3.7121378432	2.6820945713	0.0452110741
H	-3.8677054202	5.4893253221	-2.2430923389
H	-4.5930020433	3.9137375406	-1.9088565927
H	-2.9051357651	4.0136593121	-2.4558995231
H	-2.5683250855	7.2616657550	1.4200802771
H	-1.0663945094	8.8902972105	3.0574574640
H	0.1934561286	7.6376090869	3.0940192820
H	-1.5172194457	5.9360074327	3.8647864748
H	-2.7761954434	7.1788847872	3.8150518777
H	-0.5969270862	8.1560910487	4.5974364019
H	2.2760928788	-2.6093614938	-2.4286617578

O	-0.1994699760	1.8115183874	-0.1168983473
O	0.4026624287	2.5641979513	0.9780465133
H	-0.4976086275	3.9217305660	1.3790856041
H	1.3280292034	2.6741533061	0.6492844952
H	-2.7503113951	-0.0563443877	-0.2738688099

²TS_{coh} (Figure S15)

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	X	Y	Z
Geometry:	9	Total energy:	-2835.60421963344
Fe	-0.0043804123	-0.0009278293	-0.0044834527
N	-0.0044140020	-0.0053594417	1.9023868222
C	1.1936066806	0.0039224015	2.5373478706
C	1.2502662496	0.0331110131	3.9189899967
C	-0.0324923288	0.0815388338	4.5731638845
N	-1.2090957877	0.1686568451	3.9011225903
C	-1.1403318166	0.1310695891	2.5830801170
C	2.3314099903	0.0950203935	1.5374415783
O	3.5048210102	0.3022804500	1.8725518978
C	2.5190058128	0.0225256219	4.7288027926
N	-0.1174038807	0.0676155910	5.9149697369
C	-2.3432277750	0.3480467838	1.6763271509
N	-2.0844039036	-0.4213314557	0.4085203138
C	-2.2847420538	-1.8914863534	0.5806878193
C	-1.2375264656	-2.7190088103	-0.1864839585
C	-1.4820896190	-2.9713399075	-1.6924611380
N	-2.7500779748	-3.3268757863	-2.0407090511
N	1.8833202240	0.0140972983	0.2545747609
C	2.8728228395	0.1347153276	-0.8152358984
C	3.1279949150	1.6090104230	-1.2321559336
O	3.1218487866	1.9524968172	-2.4072229368
C	2.4911017122	-0.6889281058	-2.0585555215
C	1.2162847289	-0.2440960677	-2.7151294782
N	0.0588903033	0.0246548730	-2.0033192214
C	-0.8671079158	0.3727274765	-2.8839129018
N	-0.3560375104	0.3272475351	-4.1335969442
C	0.9619610053	-0.0609304909	-4.0473639778
O	2.4140105518	-2.0621610282	-1.6367384656
N	3.3358565364	2.4852549230	-0.1876789248
C	3.8730832403	3.8442996961	-0.4523450081
C	5.0096958364	4.1458739641	0.5259631220
C	2.7264570892	4.8702660722	-0.3323353047
C	1.6116609429	4.6950885152	-1.4159070903
C	0.3952390388	5.4390197713	-0.8984945621
O	0.4481144246	6.5938204795	-0.4634820639
O	3.2817514298	6.1624940524	-0.3746222943
C	-3.7090660662	0.1109860914	2.3285746794
C	-4.8503058513	0.5660173842	1.4138701128
N	-6.0945697750	0.4019048881	1.8997871113
O	-4.6415605634	1.0456067483	0.2876640321
N	0.0730812151	-2.0666441720	-0.0147686212
O	-0.5673176546	-2.8811815634	-2.4978447116

C	2.0330085530	5.2169607587	-2.8030635835
N	-0.7972259066	4.7520113804	-0.8649758394
C	-1.9159148711	5.3759937756	-0.1962359744
C	-1.5926682991	5.5408321018	1.2904266429
O	-0.8762910591	4.6771910545	1.9352186118
C	-3.2244920283	4.5683478854	-0.3746247447
O	-2.9606718201	3.2923000383	0.1861420283
C	-3.6668042657	4.4935613017	-1.8357998234
N	-2.0796159969	6.5555575964	1.9594459781
C	-1.8207050140	6.8666188877	3.3829964629
C	-0.7566047560	7.9538632246	3.5340693541
H	-2.8709818662	-3.6825127960	-2.9825946922
H	-3.4149487013	-3.6606016554	-1.3571517108
H	-1.2241209338	-3.7213066715	0.2680545449
H	-2.1588404439	-2.1193079342	1.6434104158
H	-3.3073888487	-2.1780682919	0.3144862220
H	0.7225015293	-2.3069495676	-0.7816968417
H	0.5224924066	-2.3750286686	0.8466167337
H	-6.2784241980	0.0128304039	2.8141823285
H	-6.8853574012	0.6796069112	1.3310743094
H	-3.8589358888	-0.9375996112	2.6137783175
H	-3.7384674049	0.6759200467	3.2683696075
H	-2.2951677941	1.3986033562	1.3692459695
H	-1.0280543948	0.1102193836	6.3513735525
H	0.6976992971	-0.0148158112	6.5034028326
H	2.5604334976	0.8890725169	5.4022110744
H	3.3931492002	0.0516179577	4.0793293811
H	2.5791312427	-0.8822845002	5.3495365757
H	3.8212084248	-0.2698807587	-0.4369644439
H	3.3017414626	-0.5673707330	-2.7842689415
H	1.5990087414	-0.1420487738	-4.9148499088
H	-1.8829632528	0.6640268941	-2.6622255628
H	-0.8569085334	0.5418514596	-4.9860195329
H	3.6637153186	2.0394860510	0.6704698332
H	1.3607763557	3.6341371909	-1.5111022920
H	2.5325135965	6.7857964423	-0.3302302557
H	4.2568441818	3.8509850138	-1.4759334803
H	4.6585255683	4.1219551495	1.5656535356
H	5.8161813843	3.4137041887	0.4152301588
H	5.4119248108	5.1415041915	0.3321567200
H	2.2632337495	4.6954941229	0.6599905806
H	1.1952228505	5.1562690140	-3.5090812653
H	2.8478951740	4.6014203235	-3.1967605263
H	2.3688605019	6.2552119189	-2.7469161532
H	-0.8113433749	3.7415314792	-0.9844421417
H	-2.0581738604	6.3797370560	-0.6086519667
H	-4.0046499683	5.0886810795	0.2060736934
H	-3.7121378432	2.6820945713	0.0452110741
H	-3.8677054202	5.4893253221	-2.2430923389
H	-4.5930020433	3.9137375406	-1.9088565927
H	-2.9051357651	4.0136593121	-2.4558995231
H	-2.5683250855	7.2616657550	1.4200802771
H	-1.0663945094	8.8902972105	3.0574574640
H	0.1934561286	7.6376090869	3.0940192820

H	-1.5172194457	5.9360074327	3.8647864748
H	-2.7761954434	7.1788847872	3.8150518777
H	-0.5969270862	8.1560910487	4.5974364019
H	2.2760928788	-2.6093614938	-2.4286617578
O	-0.1994699760	1.8115183874	-0.1168983473
O	0.4026624287	2.5641979513	0.9780465133
H	-0.4976086275	3.9217305660	1.3790856041
H	1.3280292034	2.6741533061	0.6492844952
H	-2.7503113951	-0.0563443877	-0.2738688099

²TS_{o-o} (unprotonated, Figure S16a)

104			
	X	Y	Z
Fe	-0.0006274264	-0.0034419927	-0.0030445603
N	-0.0019474428	-0.0016662782	1.8876484951
C	1.1764782331	0.0001519276	2.5517779143
C	1.1806816648	0.1418443495	3.9279523365
C	-0.1169588783	0.3248081635	4.5204783488
N	-1.2639211537	0.4265079726	3.8051646013
C	-1.1589973335	0.2688310702	2.4976029804
C	2.3563933884	-0.0149554305	1.5882015542
O	3.5291725604	0.1421300252	1.9733930828
C	2.4181148687	0.1400361033	4.7848573270
N	-0.2473818063	0.4327729528	5.8585268789
C	-2.2520081890	0.5184063687	1.4596417225
N	-1.9217483724	-0.2590584116	0.2478762766
C	-2.3109863152	-1.6629373213	0.3745542901
C	-1.3315170731	-2.5708856509	-0.3836652138
C	-1.4339051407	-2.7114778390	-1.9157192060
N	-2.6772345136	-2.6514370833	-2.4502199097
N	1.9458453000	-0.1135643527	0.3054021834
C	2.9642862349	-0.0742569647	-0.7394049766
C	3.3835915544	1.3697947151	-1.1501998884
O	3.5363713764	1.6729214061	-2.3283568699
C	2.5349044020	-0.8388998727	-2.0143755335
C	1.3120600076	-0.2763257880	-2.6805644883
N	0.1409607611	-0.0008462912	-1.9981358622
C	-0.7229155544	0.5061384319	-2.8621349396
N	-0.1571050823	0.5440651971	-4.0905069428
C	1.1281515195	0.0538813390	-3.9962526699
O	2.3527865207	-2.2178811248	-1.6504873236
N	3.5526869336	2.2680634093	-0.1168562568
C	4.1713337862	3.5935814518	-0.3715548497
C	5.1982100899	3.9026867306	0.7186253278
C	3.0609370593	4.6685213065	-0.4246701601
C	2.0438848698	4.4619628138	-1.5876677627
C	0.8068256992	5.2874623571	-1.2560361844
O	0.8757105878	6.4854058877	-0.9629929359
O	3.6609634827	5.9422083665	-0.4938190269
C	-3.6798073808	0.4258919651	2.0014194784
C	-4.6501548139	1.2851100859	1.1921768719
N	-5.9507481606	0.9013016961	1.2474728431

O	-4.3005241967	2.2796217284	0.5546053800
N	0.0094981731	-2.0603805209	-0.0508436160
O	-0.4357914973	-2.9643698072	-2.5850197602
C	2.6140654307	4.8644543070	-2.9597113344
N	-0.3758297085	4.6072862257	-1.2867684191
C	-1.6255357208	5.1961264258	-0.8767295448
C	-1.7890452639	5.1385073025	0.6558824141
O	-1.1086763146	4.4012414521	1.3895652729
C	-2.7966702154	4.4685255893	-1.6174963253
O	-2.6251346108	3.0604211991	-1.5434477189
C	-2.8475013420	4.8617347188	-3.0911838494
N	-2.7513786111	5.9311335710	1.1615121976
C	-3.0533844505	6.0273978090	2.5923032104
C	-2.2602451346	7.1332461813	3.2928916311
H	-2.7850009606	-2.8625514633	-3.4331635290
H	-3.4996986070	-2.4343604295	-1.9093295204
H	-1.4544663254	-3.6011828973	-0.0160223680
H	-2.2847630577	-2.0056282934	1.4283176396
H	-3.3514294852	-1.8361578372	0.0467794162
H	0.7380294079	-2.3625196990	-0.7130626245
H	0.2966974811	-2.3781031937	0.8740584717
H	-6.2668621325	0.1647160647	1.8613940328
H	-6.6471971615	1.5045661048	0.8300630552
H	-4.0398690239	-0.6061701312	2.0705289250
H	-3.6715666621	0.8173410452	3.0281268530
H	-2.1058692563	1.5724233132	1.1845312367
H	-1.1605874592	0.6304182739	6.2416902697
H	0.5491731848	0.4195951328	6.4755393586
H	2.4837712801	1.0600838415	5.3819231866
H	3.3092460497	0.0723232680	4.1618364690
H	2.4131156304	-0.7091411159	5.4825983405
H	3.8682115220	-0.5686917302	-0.3559226210
H	3.3625636556	-0.7546484261	-2.7255621290
H	1.7958848713	0.0107230293	-4.8423070799
H	-1.7009632182	0.8945224266	-2.6182694572
H	-0.6004656234	0.8919607863	-4.9292886156
H	3.7641767100	1.8313644107	0.7827929326
H	1.7619297393	3.4055340285	-1.6338181696
H	2.9196794532	6.5747125460	-0.5837549789
H	4.6688656388	3.5433854547	-1.3437885511
H	4.7305519591	3.9238876606	1.7117519394
H	5.9924515712	3.1485893259	0.7266263345
H	5.6432381935	4.8832543221	0.5386578347
H	2.5073244826	4.5805422266	0.5323912821
H	1.8440142870	4.7684018030	-3.7344761675
H	3.4440819146	4.2046017515	-3.2285123037
H	2.9680135575	5.8978887377	-2.9481931023
H	-0.3837105431	3.5963846499	-1.3779510684
H	-1.6115018031	6.2527338441	-1.1656785570
H	-3.7383909871	4.7557572722	-1.1306973082
H	-3.0682165477	2.7233238664	-0.7381055137
H	-3.0159413257	5.9374878778	-3.2112909542
H	-3.6621421040	4.3240250868	-3.5854171726
H	-1.9077110320	4.6049010766	-3.5901206021

H	-3.2084626664	6.5827730794	0.5369599222
H	-2.4754006506	8.1161092879	2.8595218247
H	-1.1854750732	6.9481697135	3.2083625800
H	-2.8263620210	5.0529451116	3.0285439048
H	-4.1308302335	6.1961441943	2.6885543708
H	-2.5216884489	7.1687484730	4.3559227650
H	1.9112018103	-2.6640952075	-2.3962393325
O	-0.0790428705	1.6901293672	-0.1775037383
O	0.7316389989	2.6305310012	1.1618761533
H	0.0928145325	3.4236024378	1.1071855952
H	1.5548328415	2.7894263186	0.6477687388

²TS_{O-O} (protonated, Figure S16b)

105			
	X	Y	Z
Fe	-0.0013624640	-0.0044634893	-0.0030228904
N	-0.0033340299	-0.0027248318	1.8959644313
C	1.1990805246	-0.0001453352	2.5265520892
C	1.2653154975	0.1194518572	3.9007433368
C	-0.0135758310	0.2679074313	4.5546358492
N	-1.1862648606	0.3777458887	3.8765219440
C	-1.1297362671	0.2550966081	2.5667690821
C	2.3309049883	-0.0125003779	1.5198919169
O	3.5160853961	0.1157986755	1.8330497363
C	2.5356928988	0.1186475553	4.7058754221
N	-0.0948899924	0.3382423255	5.8908083787
C	-2.3062408102	0.5299590017	1.6462831663
N	-2.0927876009	-0.2928591261	0.4068909070
C	-2.4066495824	-1.7365234367	0.6091210980
C	-1.4304595409	-2.6449480563	-0.1567480901
C	-1.7060175697	-2.8915878125	-1.6590370608
N	-2.9945128226	-3.1775658971	-1.9878302913
N	1.8710288239	-0.1053633906	0.2327828274
C	2.8687262761	-0.1018744023	-0.8426228944
C	3.2301325298	1.3302210451	-1.3424099592
O	3.2281438559	1.5917871191	-2.5394421613
C	2.4359802675	-0.9651275320	-2.0431995687
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