

Supplementary Information for

**Effect of Porphyrin Ligand on Catalytic CH₄ Oxidation
Activity of Monocationic μ -Nitrido-Bridged Iron
Porphyrinoid Dimer by Using H₂O₂ as An Oxidant**

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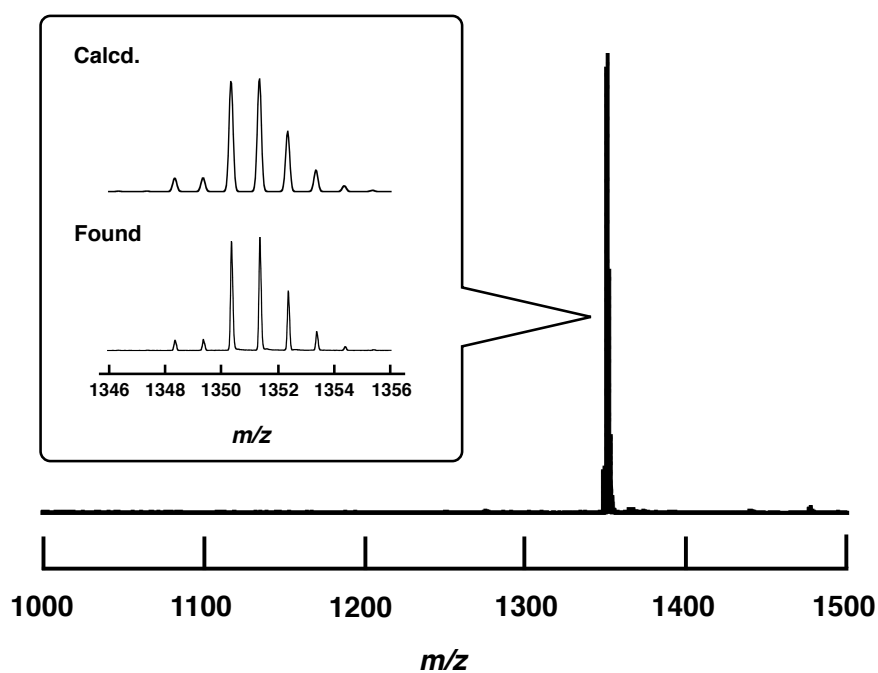


Figure S1. MALDI-TOF MS spectrum of $4^+ \cdot \text{I}_3^-$. Inset: Comparison of the calculated (top) and observed (bottom) spectrum of 4^+ .

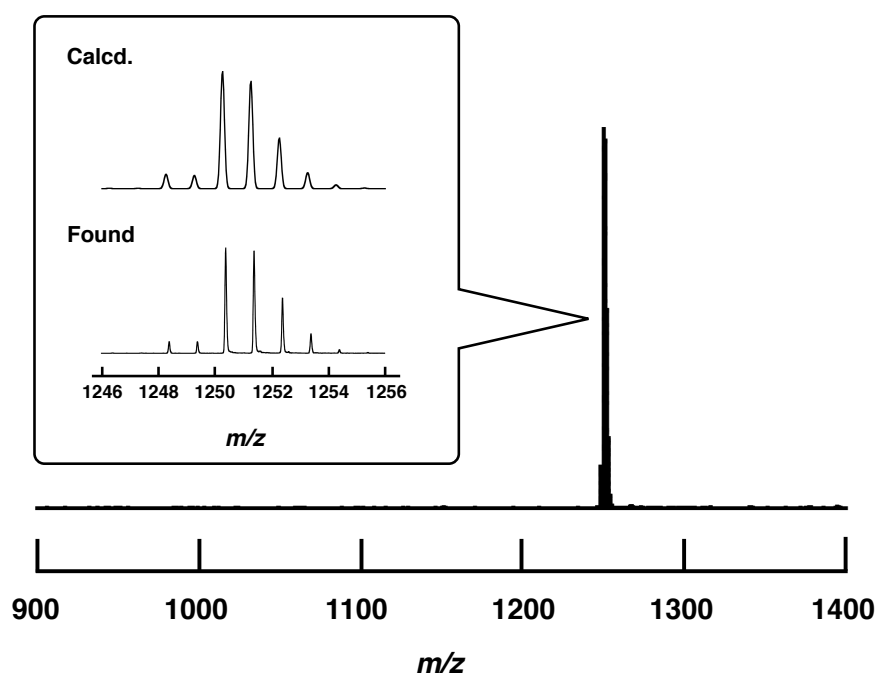


Figure S2. MALDI-TOF MS spectrum of $5^+ \cdot \text{I}_3^-$. Inset: Comparison of the calculated (top) and observed (bottom) spectrum of 5^+ .

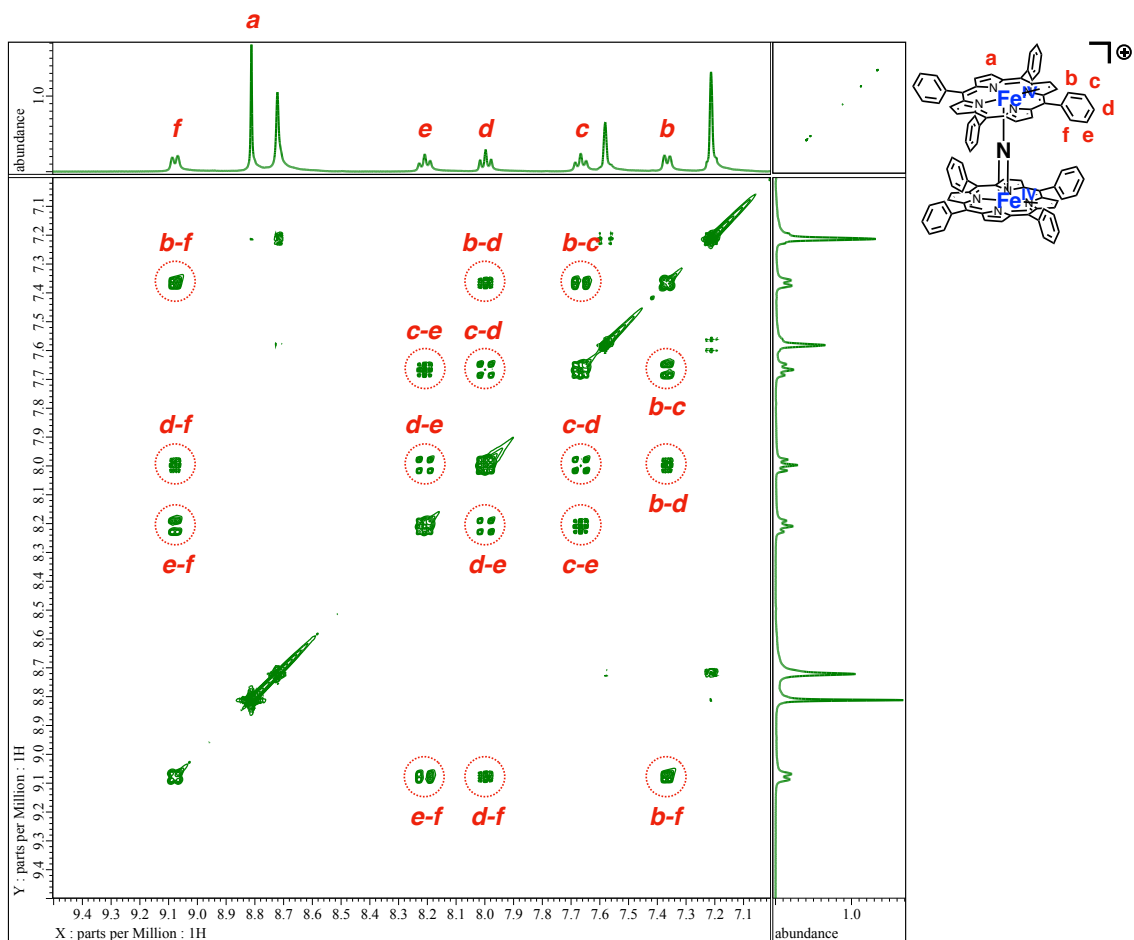


Figure S3. COSY spectrum of $4^+ \cdot \text{I}_3^-$ in pyridine- d_5 at 25°C.

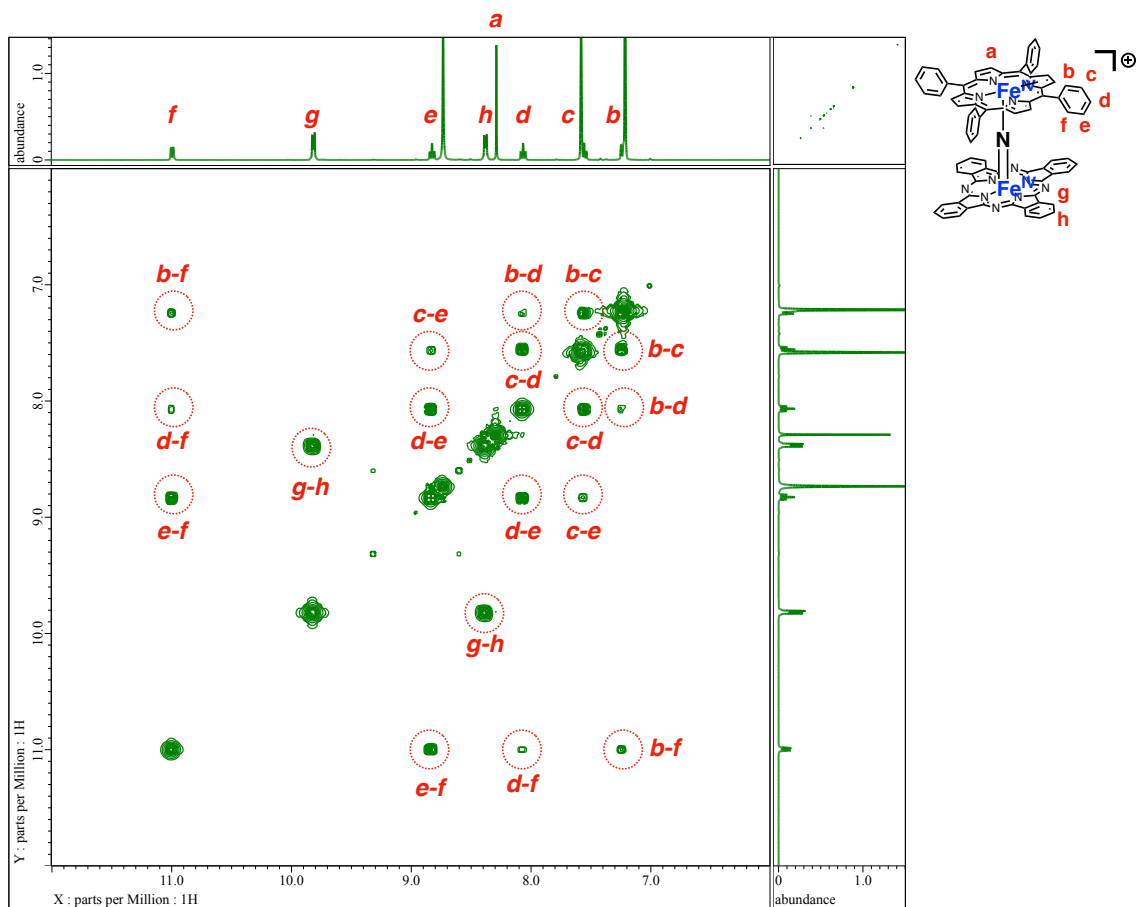


Figure S4. COSY spectrum of $5^+ \cdot \text{I}_3^-$ in pyridine- d_5 at 25°C.

Table S1. Summary of the results of methane oxidation reactions. Reactions were performed by using a silica gel-supported catalyst (30 mg, containing 57 μM of the catalyst molecule) in an aqueous solution (3.0 mL) containing H_2O_2 (189 mM) and TFA (51 mM) at 60 $^\circ\text{C}$ for 24 h under a CH_4 or N_2 atmosphere (1.0 MPa). The numbers in the parentheses indicate the standard deviation of each value.

Entry	Catalyst	Reaction Time / h	Gas	H_2O_2 / mM	Additive	$[\text{CH}_3\text{OH}]$ / mM	$[\text{HCHO}]$ / mM	$[\text{HCOOH}]$ / mM	TTN	$\text{TTN}_{\text{eff}}(\text{CH}_4)$
1	1 ⁺ -I-/SiO ₂	24	CH_4 (1.0 MPa)	189	...	0.14 (0.00)	0.20 (0.04)	1.69 (0.23)	99 (14)	75 (14)
2	1 ⁺ -I-/SiO ₂	24	N_2 (1.0 MPa)	189	...	0.08 (0.04)	0.03 (0.02)	0.41 (0.03)	24 (3)	...
3	4 ⁺ -I ₃ ⁻ /SiO ₂	24	CH_4 (1.0 MPa)	189	...	0.17 (0.02)	0.09 (0.02)	0.45 (0.06)	30 (4)	3 (2)
4	4 ⁺ -I ₃ ⁻ /SiO ₂	24	N_2 (1.0 MPa)	189	...	0.11 (0.07)	0.11 (0.10)	0.40 (0.04)	27 (2)	...
5	5 ⁺ -I ₃ ⁻ /SiO ₂	24	CH_4 (1.0 MPa)	189	...	0.13 (0.02)	0.13 (0.01)	0.41 (0.03)	28 (4)	5 (5)
6	5 ⁺ -I ₃ ⁻ /SiO ₂	24	N_2 (1.0 MPa)	189	...	0.26 (0.01)	0.13 (0.15)	0.27 (0.02)	23 (5)	...

Table S2. Summary of the results of ethane oxidation reactions. Reactions were performed by using a silica gel-supported catalyst (30 mg, containing 57 μM of the catalyst molecule) in an aqueous solution (3.0 mL) containing H_2O_2 (189 mM) and TFA (51 mM) at 60 $^\circ\text{C}$ for 8, 16, 24 or 48 h under a CH_3CH_3 or N_2 atmosphere (1.0 MPa). The numbers in the parentheses indicate the standard deviation of each value.

Entry	Catalyst	Reaction Time / h	Gas	H_2O_2 / mM	Additive	$[\text{EtOH}]$ / mM	$[\text{CH}_3\text{CHO}]$ / mM	$[\text{CH}_3\text{COOH}]$ / mM	$[\text{HCOOH}]$ / mM	TTN	$\text{TTN}_{\text{eff}}(\text{C}_2\text{H}_6)$
1	$\mathbf{1^+-I^-}/\text{SiO}_2$	8	C_2H_6 (1.0 MPa)	189	...	0.05	0.36	0.10	0.22	31	16
2	$\mathbf{1^+-I^-}/\text{SiO}_2$	8	N_2 (1.0 MPa)	189	...	0.01	0.00	0.08	0.20	15	...
3	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	8	C_2H_6 (1.0 MPa)	189	...	0.08	0.23	0.09	0.18	24	9
4	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	8	N_2 (1.0 MPa)	189	...	0.01	0.00	0.07	0.20	15	...
5	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	8	C_2H_6 (1.0 MPa)	189	...	0.03	0.04	0.06	0.15	13	0
6	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	8	N_2 (1.0 MPa)	189	...	0.01	0.00	0.07	0.16	13	...
7	$\mathbf{1^+-I^-}/\text{SiO}_2$	16	C_2H_6 (1.0 MPa)	189	...	0.15	1.57	0.47	0.34	101	76
8	$\mathbf{1^+-I^-}/\text{SiO}_2$	16	N_2 (1.0 MPa)	189	...	0.01	0.01	0.16	0.29	25	...
9	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	16	C_2H_6 (1.0 MPa)	189	...	0.13	0.83	0.22	0.25	57	36
10	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	16	N_2 (1.0 MPa)	189	...	0.02	0.02	0.11	0.26	21	...
11	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	16	C_2H_6 (1.0 MPa)	189	...	0.05	0.16	0.08	0.16	19	4
12	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	16	N_2 (1.0 MPa)	189	...	0.03	0.02	0.07	0.19	15	...
13	$\mathbf{1^+-I^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	...	0.17 (0.03)	3.44 (0.85)	0.87 (0.28)	0.43 (0.06)	194 (48)	152 (48)
14	$\mathbf{1^+-I^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	100mM Na_2SO_3	0.12 (0.01)	3.14 (0.75)	0.62 (0.27)	0.42 (0.09)	168 (46)	126 (46)
15	$\mathbf{1^+-I^-}/\text{SiO}_2$	24	N_2 (1.0 MPa)	189	...	0.01 (0.01)	0.18 (0.05)	0.26 (0.05)	0.41 (0.03)	42 (0)	...
16	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	...	0.13 (0.03)	0.84 (0.16)	0.15 (0.03)	0.32 (0.02)	57 (8)	17 (8)
17	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	100mM Na_2SO_3	0.03 (0.01)	0.49 (0.08)	0.08 (0.02)	0.35 (0.04)	41 (6)	1 (6)
18	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	24	N_2 (1.0 MPa)	189	...	0.01 (0.01)	0.27 (0.16)	0.16 (0.08)	0.40 (0.04)	40 (6)	...
19	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	...	0.08 (0.02)	1.00 (0.30)	0.24 (0.06)	0.31 (0.02)	66 (13)	34 (13)
20	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	24	C_2H_6 (1.0 MPa)	189	100mM Na_2SO_3	0.03 (0.00)	0.45 (0.02)	0.06 (0.01)	0.26 (0.01)	34 (1)	2 (6)
21	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	24	N_2 (1.0 MPa)	189	...	0.02 (0.01)	0.34 (0.12)	0.10 (0.02)	0.27 (0.02)	32 (6)	...
22	$\mathbf{1^+-I^-}/\text{SiO}_2$	48	C_2H_6 (1.0 MPa)	189	...	0.57	7.26	4.83	1.90	625	470
23	$\mathbf{1^+-I^-}/\text{SiO}_2$	48	N_2 (1.0 MPa)	189	...	0.00	0.04	1.62	1.26	155	...
24	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	48	C_2H_6 (1.0 MPa)	189	...	0.27	1.47	0.58	0.41	109	66
25	$\mathbf{4^+-I_3^-}/\text{SiO}_2$	48	N_2 (1.0 MPa)	189	...	0.01	0.01	0.30	0.51	43	...
26	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	48	C_2H_6 (1.0 MPa)	189	...	0.20	2.27	0.93	0.47	158	127
27	$\mathbf{5^+-I_3^-}/\text{SiO}_2$	48	N_2 (1.0 MPa)	189	...	0.00	0.01	0.22	0.35	31	...

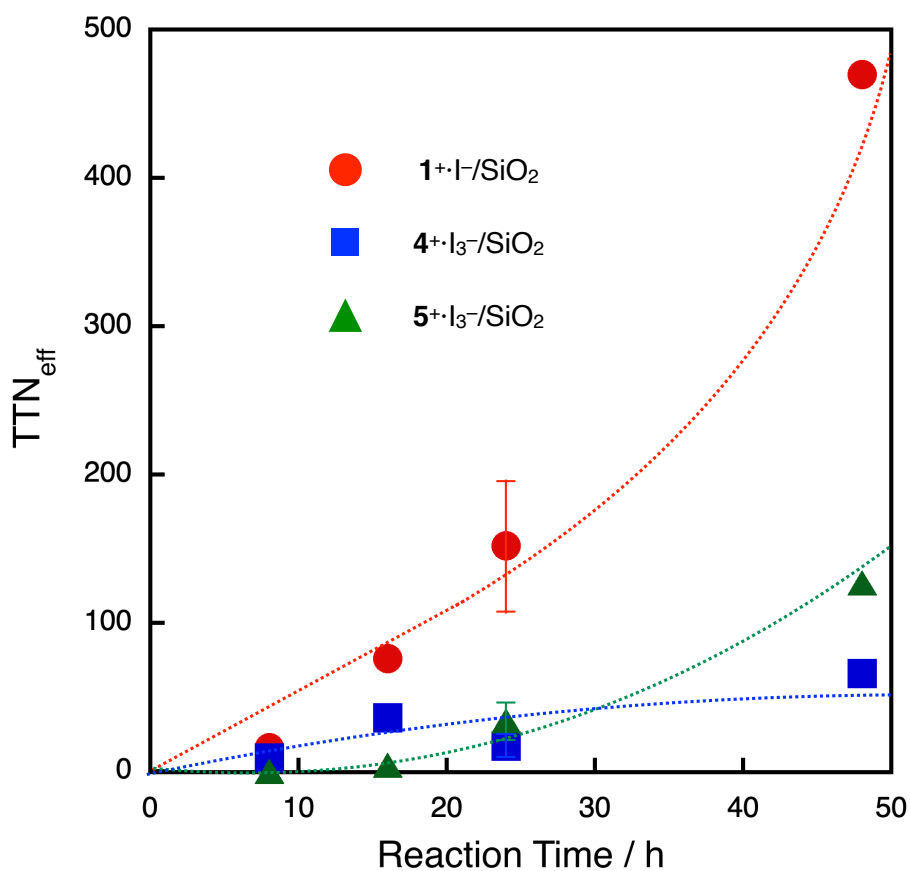


Figure S5. Time dependencies of TTN_{eff}s of CH₃CH₃ oxidation reactions by three catalysts (red filled circle: 1⁺·I⁻/SiO₂, blue filled square: 4⁺·I₃⁻/SiO₂, and green filled triangle: 5⁺·I₃⁻/SiO₂). Reactions were performed by using a silica gel-supported catalyst (30 mg, containing 57 μM of the catalyst molecule) in an aqueous solution (3.0 mL) containing H₂O₂ (189 mM) and TFA (51 mM) at 60 °C for 8, 16, 24 or 48 h under a CH₃CH₃ or N₂ atmosphere (1.0 MPa).

(a) Before Oxidation Reaction



1⁺·I⁻/SiO₂



4⁺·I₃⁻/SiO₂



5⁺·I₃⁻/SiO₂

(b) After Oxidation Reaction for 24 h at 60 °C



1⁺·I⁻/SiO₂



4⁺·I₃⁻/SiO₂



5⁺·I₃⁻/SiO₂

Figure S6. Comparison of the pictures of the reaction mixtures (a) before and (b) after oxidation reaction for 24 h at 60 °C. (a silica-gel supported catalyst (**1⁺·I⁻/SiO₂**, **4⁺·I₃⁻/SiO₂**, or **5⁺·I₃⁻/SiO₂**): 30 mg, TFA : 51 mM, H₂O₂ :189 mM)

DFT Calculation.

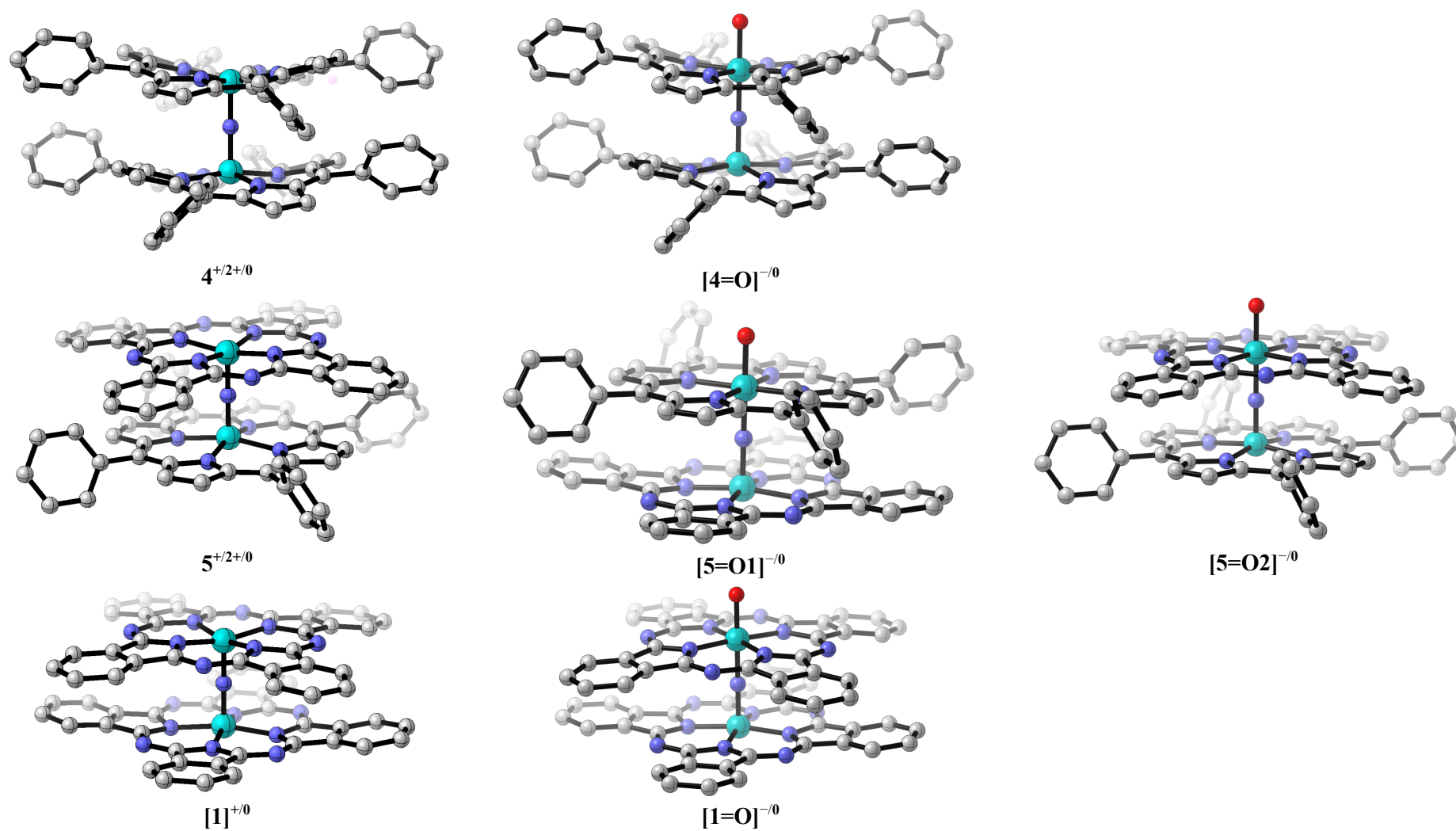


Figure S7. Complexes investigated with DFT. The superscripts denote the net charges. Hydrogens are omitted for clarity.

Table S3. Total energy, free energy (in E_h), and relative free energy (in eV), calculated at the BP86-D3BJ/def2-TZVP level of theory.

	$E(\text{gas})$	$G(\text{gas})$	$E(\text{COSMO})^a$	$G(\text{COSMO})^a$	$\Delta E(\text{COSMO})^c$	$\Delta G(\text{COSMO})^c$
1⁺	−5918.80978	−5918.07373	−5918.85839	−5918.12233		
1²⁺	−5918.50483	−5917.76888	−5918.65174	−5917.91580	5.62	5.62
1	−5919.02408	−5918.29034	−5919.04356	−5918.30983	−5.04	−5.10
5⁺	−6164.36488	−6163.45687	−6164.41250	−6163.50448		
5²⁺	−6164.05646	−6163.14987	−6164.19813	−6163.29154	5.83	5.79
5	−6164.56430	−6163.65961	−6164.58570	−6163.68101	−4.71	−4.80
4⁺	−6409.91160	−6408.83139	−6409.95959	−6408.87938		
4²⁺	−6409.60855	−6408.53103	−6409.74522	−6408.66770	5.83	5.76
4	−6410.09347	−6409.01767	−6410.11822	−6409.04242	−4.32	−4.44

^aCOSMO model with a dielectric constant of 12.5 to account for pyridine.

^bGibbs free energy corrections taken from calculations in the gas phase, calculated with the algorithm proposed by Grimme.¹

^cRelative energy with respect to the cationic complex.

Table S4. Average bond lengths (in Angstrom), spin population, total energy, and free energy (in E_h) of **1⁺**, **1²⁺**, and **1**, calculated at the BP86-D3BJ/def2-TZVP level of theory.

	Bond length (Å)				Spin population				
	Fe1–N(Pc)	Fe2–N(Pc)	Fe1–N(μ)	Fe2–N(μ)	Fe1	Fe2	N(μ)	Pc	Pc
1⁺	1.953	1.953	1.590	1.590	0.000	0.000	0.000	0.000	0.000
1²⁺	1.952	1.952	1.591	1.591	0.161	0.160	−0.018	0.348	0.348
1	1.958	1.958	1.616	1.616	0.499	0.499	−0.058	0.030	0.030

Table S5. Average bond lengths (in Angstrom), spin population, total energy, and free energy (in E_h) of **5⁺**, **5²⁺**, and **5**, calculated at the BP86-D3BJ/def2-TZVP level of theory.

	Bond length (Å)				Spin population				
	Fe1–N(P)	Fe2–N(Pc)	Fe1–N(μ)	Fe2–N(μ)	Fe1	Fe2	N(μ)	P	Pc
5⁺	2.001	1.954	1.587	1.600	0.000	0.000	0.000	0.000	0.000
5²⁺	2.001	1.950	1.581	1.605	0.048	0.008	−0.007	0.122	0.829
5	2.011	1.959	1.601	1.641	0.400	0.588	−0.055	0.030	0.037

Table S6. Average bond lengths (in Angstrom), spin population, total energy, and free energy (in E_h) of 4^+ , 4^{2+} , and **4**, calculated at the BP86-D3BJ/def2-TZVP level of theory.

	Bond length (Å)				Spin population				
	Fe1–N(P)	Fe2–N(P)	Fe1–N(μ)	Fe2–N(μ)	Fe1	Fe2	N(μ)	P	P
4^+	1.986	1.986	1.601	1.601	0.000	0.000	0.000	0.000	0.000
4^{2+}	1.989	1.989	1.598	1.598	−0.007	−0.007	0.003	0.506	0.506
4	2.000	2.000	1.626	1.626	0.478	0.502	−0.060	0.040	0.040

Table S7. Total energy, free energy (in E_h), and relative free energy (in eV) of oxo species, calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

	$E(\text{gas})$	$G(\text{gas})$	$E(\text{CPCM})^a$	$G(\text{CPCM})^a$	$\Delta E(\text{CPCM})$	$\Delta G(\text{CPCM})$
[1=O]	−5991.24079	−5990.48044	−5991.28316	−5990.52281		
[1=O] [−]	−5991.35983	−5990.60111	−5991.44961	−5990.69088	4.53	4.57
[5=O1]	−6236.58825	−6235.65248	−6236.63025	−6235.69448		
[5=O1] [−]	−6236.70941	−6235.77486	−6236.79933	−6235.86478	4.60	4.63
[5=O2]	−6236.59055	−6235.65510	−6236.63171	−6235.69625		
[5=O2] [−]	−6236.71472	−6235.77995	−6236.80311	−6235.86834	4.66	4.68
[4=O]	−6481.92751	−6480.81734	−6481.97569	−6480.86552		
[4=O] [−]	−6482.04558	−6480.93557	−6482.14352	−6481.03352	4.57	4.57

^aCPCM model with a dielectric constant of 80.4 to account for water.

^bGibbs free energy corrections taken from calculations in the gas phase, calculated with the algorithm proposed by Grimme.¹

^cRelative energy with respect to the neutral oxo complex.

Table S8. Average bond lengths (in Angstrom) and spin population of [**1=O**] and [**1=O**][−], calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

	Bond length (Å)					Spin population					
	Fe1–N(Pc)	Fe2–N(Pc)	Fe1–N(μ)	Fe2–N(μ)	Fe1–O	Fe1	Fe2	N(μ)	Pc	Pc	O
[1=O]	1.972	1.953	1.874	1.674	1.660	1.094	−0.593	−1.348	0.462	0.488	0.875
[1=O] [−]	1.975	1.956	1.888	1.679	1.661	1.129	−0.569	−1.364	−0.129	0.083	0.856

Table S9. Average bond lengths (in Angstrom) and spin population of $[\mathbf{5}=\mathbf{O1}]$ and $[\mathbf{5}=\mathbf{O1}]^-$, calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

	Bond length (Å)					Spin population					
	Fe1–N(P)	Fe2–N(Pc)	Fe1–N(μ)	Fe2–N(μ)	Fe1–O	Fe1	Fe2	N(μ)	P	Pc	O
$[\mathbf{5}=\mathbf{O1}]$	2.030	1.955	1.876	1.686	1.655	1.107	−0.581	−1.373	0.627	0.242	0.856
$[\mathbf{5}=\mathbf{O1}]^-$	2.029	1.955	1.910	1.699	1.651	1.175	−0.549	−1.470	0.000	0.000	0.841

Table S10. Average bond lengths (in Angstrom) and spin population of $[\mathbf{5}=\mathbf{O2}]$ and $[\mathbf{5}=\mathbf{O2}]^-$, calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

	Bond length (Å)					Spin population					
	Fe1–N(P)	Fe2–N(Pc)	Fe1–N(μ)	Fe2–N(μ)	Fe2–O	Fe1	Fe2	N(μ)	P	Pc	O
$[\mathbf{5}=\mathbf{O2}]$	2.011	1.969	1.654	1.863	1.671	−0.708	1.087	−1.123	0.262	0.755	0.816
$[\mathbf{5}=\mathbf{O2}]^-$	2.013	1.973	1.665	1.883	1.670	−0.658	1.133	−1.208	0.020	−0.142	0.817

Table S11. Average bond lengths (in Angstrom) and spin population of $[\mathbf{4}=\mathbf{O}]$ and $[\mathbf{4}=\mathbf{O}]^-$, calculated at the B3LYP-D3BJ/def2-TZVP level of theory.

	Bond length (Å)					Spin population					
	Fe1–N(P)	Fe2–N(P)	Fe1–N(μ)	Fe2–N(μ)	Fe2–O	Fe1	Fe2	N(μ)	P	P	O
$[\mathbf{4}=\mathbf{O}]$	2.006	2.022	1.669	1.862	1.670	−0.632	1.080	−1.172	0.081	0.865	0.814
$[\mathbf{4}=\mathbf{O}]^-$	2.007	2.024	1.687	1.905	1.660	−0.547	1.166	−1.361	0.000	−0.047	0.814

Table S12. Decomposition analysis of Wiberg bond order in NAO basis, calculated at the BP86-D3BJ/def2-TZVP level of theory.

	5+		1 ⁺		4 ⁺	
	Fe1–N(μ)	Fe2–N(μ)	Fe1–N(μ)	Fe2–N(μ)	Fe1–N(μ)	Fe2–N(μ)
Fe(4s)–N(2s)	0.0677	0.0687	0.0683	0.0683	0.0685	0.0685
Fe(4p _z)–N(2s)	0.1568	0.1465	0.1505	0.1505	0.1567	0.1568
Fe(3d _{xz})–N(2p _x)	0.4493	0.3825	0.4136	0.4137	0.4120	0.4123
Fe(3d _{yz})–N(2p _y)	0.4482	0.3838	0.4137	0.4136	0.4202	0.4202
Fe(3d _{z2})–N(2s)	0.1362	0.1485	0.1442	0.1442	0.1331	0.1331
Fe(3d _{z2})–N(2p _z)	0.2990	0.3477	0.3216	0.3217	0.3250	0.3251
Total	1.6606	1.5769	1.6144	1.6145	1.6171	1.6175

- (1) Grimme, S. Supramolecular Binding Thermodynamics by Dispersion-Corrected Density Functional Theory. *Chem. - A Eur. J.* **2012**, *18* (32), 9955–9964. <https://doi.org/10.1002/chem.201200497>.

Cartesian coordinates of the complexes, calculated with BP86-D3(BJ)/def2-TZVP

1⁺

Fe	-0.0059356	0.0191794	1.5845153
Fe	0.0055962	-0.0188948	-1.5949951
C	0.0008050	-2.9609902	1.7497600
C	-2.9681239	-0.0015406	-1.7257356
N	0.7338326	-1.7729375	1.8196206
N	-1.7903267	0.7153082	-1.8202867
C	2.0737971	-2.1052898	1.7550522
C	-2.1175115	2.0731679	-1.7649816
C	2.2179382	-3.5484874	1.6833603
C	-3.5590615	2.2159570	-1.6792090
C	3.3414469	-4.3701323	1.5987176
C	-4.3809655	3.3402395	-1.5942303
H	4.3441526	-3.9453002	1.5982179
H	-3.9573751	4.3432114	-1.6192528
C	3.1231218	-5.7461045	1.5040880
C	-5.7535657	3.1222600	-1.4650537
H	3.9755672	-6.4221797	1.4334301
H	-6.4296879	3.9745182	-1.3936843
C	1.8208759	-6.2834432	1.5023240
C	-6.2872811	1.8190390	-1.4297059
C	0.6971137	-5.4609389	1.5961989
C	-5.4653314	0.6941843	-1.5247520
H	-0.3139666	-5.8655942	1.5937681
H	-5.8685807	-0.3169753	-1.4959895
C	0.9154222	-4.0856415	1.6836913
C	-4.0934630	0.9127336	-1.6456203
N	3.1102663	-1.2808542	1.7254344
N	-1.2918906	3.0973951	-1.7395415
C	2.9757948	0.0279325	1.7449119
C	0.0248307	2.9536263	-1.7653293
N	1.7876981	0.7623335	1.7952584
N	0.7430100	1.7744973	-1.8281319
C	2.1197166	2.1002450	1.6952509
C	2.0998208	2.1027126	-1.7550126
C	3.5628391	2.2426687	1.6187844
C	2.2413650	3.5454853	-1.6915935
C	4.3840018	3.3633078	1.4986659
C	3.3641341	4.3683279	-1.5961508
H	3.9586911	4.3653090	1.4667153
H	4.3671733	3.9441019	-1.5939210
C	5.7599852	3.1426640	1.4097002
C	3.1443229	5.7427947	-1.4926453
H	6.4356357	3.9927027	1.3114730
H	3.9952822	6.4197110	-1.4137466
C	6.2978849	1.8412465	1.4487523
C	1.8409539	6.2773602	-1.4933829
H	7.3782488	1.7114825	1.3812653
H	1.7107584	7.3569071	-1.4135432
C	5.4757858	0.7205566	1.5768047
C	0.7177898	5.4542082	-1.5977581
H	5.8808024	-0.2900063	1.6047608
H	-0.2935482	5.8580803	-1.5955891
C	4.1004155	0.9409156	1.6580076
C	0.9379542	4.0804093	-1.6913649
N	1.2950364	3.1357300	1.6455342
N	3.1233990	1.2778857	-1.6992275
C	-0.0134747	3.0023882	1.6846827
C	2.9802155	-0.0390900	-1.7113777
N	-0.7473552	1.8161119	1.7722226

N	1.8026785	-0.7581554	-1.7903565
C	-2.0865646	2.1466519	1.6854023
C	2.1295263	-2.1141605	-1.6985728
C	-2.2297151	3.5878700	1.5799233
C	3.5705604	-2.2545252	-1.6015871
C	-3.3517897	4.4069652	1.4592793
C	4.3917710	-3.3760183	-1.4806417
H	-4.3542744	3.9817158	1.4516512
H	3.9676331	-4.3790577	-1.4747475
C	-3.1321761	5.7806302	1.3378773
C	5.7644723	-3.1548920	-1.3583881
H	-3.9834276	6.4544581	1.2376392
H	6.4400966	-4.0048723	-1.2602910
C	-1.8302502	6.3186238	1.3470549
C	6.2990498	-1.8515351	-1.3650993
H	-1.7013212	7.3973363	1.2557131
H	7.3773735	-1.7203957	-1.2714863
C	-0.7080012	5.4988040	1.4759807
C	5.4775373	-0.7296285	-1.4929763
H	0.3029178	5.9038536	1.4817604
H	5.8813885	0.2817274	-1.4956903
C	-0.9273561	4.1253951	1.5875133
C	4.1053340	-0.9510301	-1.6052402
N	-3.1227916	1.3215790	1.6662201
N	1.3037795	-3.1376162	-1.6551484
C	-2.9888234	0.0137300	1.7208265
C	-0.0127184	-2.9947623	-1.6943304
N	-1.8011185	-0.7191245	1.7982423
N	-0.7304813	-1.8173999	-1.7872987
C	-2.1323961	-2.0590275	1.7265964
C	-2.0876829	-2.1438266	-1.7114825
C	-3.5747686	-2.2034862	1.6421372
C	-2.2296147	-3.5847788	-1.6161032
C	-4.3949321	-3.3270170	1.5446985
C	-3.3530218	-4.4064500	-1.5181441
H	-3.9690821	-4.3292780	1.5377500
H	-4.3560193	-3.9822139	-1.5274158
C	-5.7707797	-3.1092598	1.4469909
C	-3.1341020	-5.7799430	-1.4007910
H	-6.4457733	-3.9617070	1.3667448
H	-3.9856631	-6.4561557	-1.3224356
C	-6.3094292	-1.8075877	1.4552380
C	-1.8308037	-6.3146271	-1.3882234
C	-5.4881154	-0.6837662	1.5587407
C	-0.7068597	-5.4923881	-1.4912281
H	-5.8937151	0.3269303	1.5628390
H	0.3043964	-5.8963350	-1.4794708
C	-4.1128204	-0.9013535	1.6482255
C	-0.9262874	-4.1196802	-1.6010296
N	-1.3073290	-3.0951980	1.7034169
N	-3.1112750	-1.3177630	-1.6791924
N	0.0002855	0.0013882	-0.0052852
H	1.6928583	-7.3637713	1.4310089
H	-7.3653105	1.6902579	-1.3296046
H	-7.3897695	-1.6800546	1.3831960
H	-1.7013356	-7.3935700	-1.2995617

1²⁺

Fe	-0.0056528	0.0178636	1.5864308
Fe	0.0056802	-0.0176941	-1.5952579
C	0.0041157	-2.9620755	1.7316331
C	-2.9684568	0.0023309	-1.7074739
N	0.7346877	-1.7748909	1.8066010
N	-1.7896533	0.7191541	-1.8051484
C	2.0752613	-2.1063807	1.7286626
C	-2.1165524	2.0747902	-1.7390333
C	2.2210696	-3.5513283	1.6558889
C	-3.5601665	2.2199222	-1.6560830
C	3.3443403	-4.3697504	1.5707203
C	-4.3792749	3.3442622	-1.5796846
H	4.3479794	-3.9474606	1.5764247
H	-3.9582435	4.3479984	-1.6116332
C	3.1257228	-5.7504524	1.4817183
C	-5.7576265	3.1262901	-1.4655528
H	3.9785358	-6.4261178	1.4161772
H	-6.4337645	3.9791875	-1.4073190
C	1.8270239	-6.2870773	1.4888991
C	-6.2914761	1.8266996	-1.4385782
C	0.6996394	-5.4622698	1.5844504
C	-5.4666704	0.6979394	-1.5259608
H	-0.3097161	-5.8705904	1.6010569
H	-5.8741020	-0.3118099	-1.5165014
C	0.9193341	-4.0887695	1.6624082
C	-4.0956415	0.9176306	-1.6296678
N	3.1108557	-1.2808297	1.6907464
N	-1.2895549	3.0997765	-1.7085716
C	2.9754124	0.0293392	1.7166561
C	0.0272315	2.9557550	-1.7390120
N	1.7884478	0.7612643	1.7816051
N	0.7453786	1.7757510	-1.8091981
C	2.1195829	2.1001294	1.6770567
C	2.0997640	2.1034241	-1.7236866
C	3.5643231	2.2444909	1.5969246
C	2.2438102	3.5479452	-1.6577695
C	4.3826364	3.3659150	1.4892858
C	3.3670590	4.3677123	-1.5733958
H	3.9603791	4.3695202	1.4761045
H	4.3709192	3.9457816	-1.5805836
C	5.7632931	3.1456580	1.4034711
C	3.1479395	5.7477487	-1.4848306
H	6.4388524	3.9970552	1.3207733
H	4.0000353	6.4244600	-1.4218068
C	6.3000242	1.8473965	1.4358862
C	1.8483842	6.2823297	-1.4901682
H	7.3807978	1.7182053	1.3789925
H	1.7190235	7.3629608	-1.4299472
C	5.4753202	0.7220683	1.5540058
C	0.7208431	5.4565643	-1.5845726
H	5.8836751	-0.2867642	1.5902489
H	-0.2886396	5.8645071	-1.5997612
C	4.1018919	0.9431950	1.6289845
C	0.9415102	4.0839688	-1.6626403
N	1.2937670	3.1348071	1.6229240
N	3.1239792	1.2770227	-1.6647597
C	-0.0161114	3.0002263	1.6635913
C	2.9807533	-0.0399783	-1.6869158
N	-0.7472847	1.8148985	1.7602012
N	1.8024984	-0.7588159	-1.7766837
C	-2.0873262	2.1444768	1.6666918
C	2.1286277	-2.1125418	-1.6773609
C	-2.2325668	3.5874363	1.5611634

C	3.5714529	-2.2558232	-1.5800969
C	-3.3553459	4.4037614	1.4525036
C	4.3894257	-3.3783368	-1.4718180
H	-4.3590182	3.9815959	1.4614907
H	3.9680358	-4.3823636	-1.4833510
C	-3.1362439	5.7823594	1.3363145
C	5.7670338	-3.1582544	-1.3530551
H	-3.9886848	6.4564383	1.2523030
H	6.4423132	-4.0097674	-1.2699682
C	-1.8375818	6.3191193	1.3391832
C	6.3013228	-1.8585829	-1.3534983
H	-1.7091243	7.3984584	1.2584007
H	7.3802858	-1.7285281	-1.2695159
C	-0.7107626	5.4965916	1.4580584
C	5.4777017	-0.7318907	-1.4731189
H	0.2984975	5.9052919	1.4715711
H	5.8856916	0.2776163	-1.4848155
C	-0.9308786	4.1250408	1.5641956
C	4.1072127	-0.9533885	-1.5803384
N	-3.1227866	1.3182282	1.6409707
N	1.3013502	-3.1366697	-1.6300930
C	-2.9876232	0.0090233	1.6974023
C	-0.0151174	-2.9935344	-1.6737365
N	-1.8010356	-0.7210420	1.7862664
N	-0.7327420	-1.8155181	-1.7749197
C	-2.1314920	-2.0619587	1.7103773
C	-2.0876495	-2.1414066	-1.6911932
C	-3.5756785	-2.2084116	1.6253405
C	-2.2321709	-3.5841973	-1.5941836
C	-4.3930390	-3.3323490	1.5388872
C	-3.3557972	-4.4020661	-1.4972338
H	-3.9703707	-4.3357914	1.5509998
H	-4.3596694	-3.9806725	-1.5191158
C	-5.7732885	-3.1146697	1.4408960
C	-3.1370511	-5.7797306	-1.3764362
H	-6.4482214	-3.9679982	1.3745968
H	-3.9894497	-6.4550125	-1.3030377
C	-6.3104544	-1.8161741	1.4401693
C	-1.8374619	-6.3140462	-1.3620435
C	-5.4866211	-0.6880560	1.5358681
C	-0.7094728	-5.4902995	-1.4678378
H	-5.8954576	0.3211837	1.5459562
H	0.3001820	-5.8981006	-1.4669683
C	-4.1135784	-0.9068613	1.6238070
C	-0.9298463	-4.1199539	-1.5789064
N	-1.3054845	-3.0975988	1.6852097
N	-3.1120600	-1.3138839	-1.6571325
N	0.0001682	-0.0005357	-0.0044485
H	1.6989108	-7.3678725	1.4299920
H	-7.3709228	1.6981392	-1.3586401
H	-7.3909549	-1.6887358	1.3747525
H	-1.7083726	-7.3930269	-1.2768368

1

Fe	-0.0001356	-0.0002376	1.6103818
Fe	0.0000153	-0.0000775	-1.6209762
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C	-2.7518645	-1.1368976	-1.7470348
N	1.3862167	-1.3679083	1.8111146
N	-1.9475398	-0.0124173	-1.8207578
C	2.7502236	-1.1412483	1.7413774
C	-2.7661177	1.1017264	-1.7487602
C	3.4489503	-2.4134454	1.6489129
C	-4.1540937	0.6782851	-1.6524343
C	4.8018013	-2.7314290	1.5304475
C	-5.3444751	1.3950243	-1.5317129
H	5.5568499	-1.9463897	1.5184335
H	-5.3372721	2.4842156	-1.5218978
C	5.1378847	-4.0809999	1.4081029
C	-6.5265522	0.6632531	-1.4036925
H	6.1853482	-4.3680874	1.3076278
H	-7.4768463	1.1888135	-1.3016047
C	4.1483752	-5.0837153	1.4095141
C	-6.5173667	-0.7454619	-1.4001053
C	2.7946138	-4.7652042	1.5322490
C	-5.3259555	-1.4624365	-1.5253432
H	2.0194665	-5.5304298	1.5217501
H	-5.3046507	-2.5513782	-1.5108120
C	2.4590282	-3.4164579	1.6487928
C	-4.1450301	-0.7309215	-1.6502224
N	3.3775755	0.0224394	1.7104656
N	-2.4033196	2.3729888	-1.7166813
C	2.7345293	1.1775763	1.7398916
C	-1.1366967	2.7518848	-1.7475373
N	1.3675896	1.3860709	1.8099982
N	-0.0121889	1.9476525	-1.8209157
C	1.1407920	2.7499860	1.7394842
C	1.1019042	2.7663705	-1.7490274
C	2.4129431	3.4487592	1.6475266
C	0.6782706	4.1543316	-1.6522695
C	2.7308166	4.8018640	1.5317644
C	1.3946293	5.3449705	-1.5315864
H	1.9456634	5.5568052	1.5202902
H	2.4838355	5.3382873	-1.5226430
C	4.0805097	5.1383806	1.4120870
C	0.6625058	6.5266501	-1.4017303
H	4.3676247	6.1861040	1.3144851
H	1.1878113	7.4770477	-1.2992590
C	5.0833255	4.1489666	1.4126948
C	-0.7461978	6.5170011	-1.3971089
H	6.1271611	4.4500809	1.3155849
H	-1.2838122	7.4600116	-1.2902991
C	4.7648836	2.7949193	1.5325798
C	-1.4628043	5.3255347	-1.5237991
H	5.5302932	2.0199447	1.5217382
H	-2.5517373	5.3038300	-1.5093993
C	3.4160998	2.4589817	1.6478048
C	-0.7309268	4.1449608	-1.6496221
N	-0.0229145	3.3773009	1.7088201
N	2.3732046	2.4036451	-1.7182783
C	-1.1780335	2.7342956	1.7401486
C	2.7520563	1.1370039	-1.7489581
N	-1.3864623	1.3673930	1.8113084
N	1.9477210	0.0124366	-1.8207188
C	-2.7504684	1.1406638	1.7418495
C	2.7663272	-1.1016219	-1.7471091
C	-3.4492933	2.4127272	1.6491818

C	4.1542792	-0.6779354	-1.6505135
C	-4.8023805	2.7304875	1.5327426
C	5.3446611	-1.3941220	-1.5265609
H	-5.5574428	1.9454218	1.5232711
H	5.3374060	-2.4832446	-1.5113548
C	-5.1386455	4.0798315	1.4085334
C	6.5269197	-0.6618428	-1.4030900
H	-6.1862781	4.3667716	1.3094498
H	7.4772481	-1.1870019	-1.2992158
C	-4.1490623	5.0824707	1.4060014
C	6.5180566	0.7468760	-1.4075058
H	-4.4499277	6.1259813	1.3046689
H	7.4617019	1.2846337	-1.3072807
C	-2.7951742	4.7642518	1.5281946
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H	5.3052892	2.5523555	-1.5249560
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N	-3.3778405	-0.0230156	1.7121708
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C	1.1369958	-2.7519196	-1.7472970
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N	0.0124107	-1.9476900	-1.8205013
C	-1.1411042	-2.7504828	1.7407422
C	-1.1016537	-2.7662956	-1.7475866
C	-2.4132641	-3.4491995	1.6481168
C	-0.6780403	-4.1541843	-1.6503360
C	-2.7309365	-4.8018266	1.5263702
C	-1.3944277	-5.3443946	-1.5260233
H	-1.9457331	-5.5566636	1.5128969
H	-2.4835893	-5.3372705	-1.5143764
C	-4.0803213	-5.1378273	1.4019049
C	-0.6623565	-6.5261089	-1.3963278
H	-4.3671535	-6.1850899	1.2986396
H	-1.1876849	-7.4761552	-1.2907472
C	-5.0831640	-4.1484612	1.4046715
C	0.7463552	-6.5170164	-1.3966624
C	-4.7649617	-2.7949341	1.5308250
C	1.4630139	-5.3259195	-1.5265335
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H	2.5519992	-5.3046352	-1.5151272
C	-3.4163865	-2.4594146	1.6495462
C	0.7311764	-4.1450803	-1.6503992
N	0.0225734	-3.3777807	1.7093682
N	-2.3729739	-2.4035115	-1.7155303
N	-0.0000318	-0.0003768	-0.0052558
H	4.4491712	-6.1274738	1.3105870
H	-7.4607227	-1.2828232	-1.2951100
H	-6.1267525	-4.4491281	1.3035550
H	1.2839660	-7.4601810	-1.2912396

5⁺

Fe	-0.7152258	0.4665024	-0.8654320
Fe	1.1551678	-0.7589063	1.4052848
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N	1.8508346	-2.2411201	0.3390105
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5

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H	-1.3266515	-7.5215371	-3.5705099
C	0.6242616	-5.4906808	1.7262981
H	-0.3901156	-5.8843281	1.7063720
C	-3.0421026	5.8087020	1.5905947
H	-3.8845496	6.4903536	1.4682385
C	6.3246739	1.7301225	1.5706854
H	7.3955819	1.5790532	1.4312880
C	5.2917480	-2.0213544	-0.4667031
H	4.6592705	-2.1804539	0.4073433
C	5.5638928	-1.1232719	-2.6935755
H	5.1391992	-0.6262603	-3.5667352
C	-2.4101783	-6.6323127	-0.4662654
C	6.9038863	-1.5142803	-2.6885265
H	7.5278101	-1.3184662	-3.5615543
C	6.6313496	-2.4128954	-0.4632324
H	7.0466405	-2.9100987	0.4150433
C	7.4420500	-2.1610576	-1.5728494
H	8.4887318	-2.4679291	-1.5695761
C	-0.0333651	-2.9794533	1.9848149
H	-3.7861120	-3.6248172	-1.5676492
C	-4.0196869	-1.4335309	-1.5686497
H	-7.3970484	-1.5832165	1.4393126
C	-4.7437328	1.3756960	-1.5827693
H	1.5804823	-7.3983317	1.4350581
C	-2.1623714	-7.4404015	-1.5787025
H	-2.9045885	-7.0495733	0.4126469
H	-5.0879204	-1.2564981	-1.5225424
C	-5.5598550	1.1371856	-2.6987762
C	-5.2943452	2.0150516	-0.4629542
H	-2.4688037	-8.4871523	-1.5765718
H	-5.1328054	0.6468579	-3.5745725

C	-6.8997402	1.5286546	-2.6944585
H	-4.6639326	2.1673813	0.4138762
C	-6.6339132	2.4069038	-0.4602200
C	-7.4411764	2.1654097	-1.5746440
H	-7.5212994	1.3398228	-3.5706792
H	-7.0513599	2.8979225	0.4205202
H	-8.4877204	2.4725111	-1.5716805

4⁺

Fe	0.0003049	1.6014014	-0.0001314
Fe	-0.0002978	-1.6002592	0.0000945
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N	-1.8899306	1.9645167	0.4616993
N	-0.0002699	0.0005214	0.0001404
N	-0.5138019	-1.8242582	1.9124512
C	-2.9754024	-1.9753086	0.3556084
C	-2.9673842	1.9766734	-0.4099138
C	-0.3937577	1.8483423	2.9971719
C	-1.7280441	1.5454637	-2.4656715
C	-4.1479028	-2.4157361	-0.3497762
H	-5.1165283	-2.5807302	0.1088504
C	-0.3058101	1.5324127	-4.2128686
H	0.1574810	1.4618316	-5.1897383
C	-2.3930480	-2.2684930	-1.7559288
C	-2.9296418	1.6417395	-1.7674146
C	-1.6830248	-1.3174070	3.8515170
H	-2.5073959	-1.0327137	4.4936002
C	-2.4359104	-2.3217091	-4.2392257
C	-1.7735653	-1.5432664	2.4331436
C	-0.3834652	-1.5290776	4.2058905
C	-1.6116806	1.3207662	-3.8824007
H	-2.4242420	1.0365431	-4.5395970
C	-2.9623864	-1.6399042	1.7134716
C	-2.6936572	-3.4106977	-6.3975134
C	-2.0116187	-3.2659373	-5.1894162
H	-1.1523590	-3.8990349	-4.9657299
C	-4.2615430	-1.4624703	2.4059646
C	-3.6411703	1.5285704	4.4617491
H	-3.9655440	0.7928787	3.7278602
H	-0.0633608	-1.4595404	-5.1910112
C	-4.2160783	1.4634343	-2.4830778
C	-3.7831741	-2.6153866	-1.6502309
H	-4.3956579	-2.9652596	-2.4730224
C	-3.5599580	-1.5296018	-4.5279199
H	-3.8979284	-0.7936975	-3.8004318
C	-4.2347514	-1.6686961	-5.7400818
H	-5.0980044	-1.0358192	-5.9472284
C	-0.3401527	-1.8473620	-3.0036419
C	-1.7010027	-2.1558901	-2.9609757
C	-3.8037876	-2.6094288	-6.6788974
C	-4.3382380	1.6670074	5.6613086
H	-5.2049105	1.0337174	5.8522647
C	-4.5929529	-2.2016616	3.5543308
H	-3.8990362	-2.9570240	3.9226710
C	-5.1519250	0.5287247	-2.0097634
H	-4.9089369	-0.0642587	-1.1301937
C	-5.1897296	-0.5288862	1.9157453
H	-4.9317597	0.0641688	1.0404879
C	-5.8072192	-1.9900208	4.2072682
H	-6.0525280	-2.5764522	5.0930707
C	-6.3511350	0.3126571	-2.6867854
H	-7.0544482	-0.4329043	-2.3147884
C	-6.6420716	1.0395146	-3.8437737
H	-7.5792440	0.8725367	-4.3752260
C	-6.7116331	-1.0404224	3.7232827
H	-7.6583049	-0.8742739	4.2378970
C	-6.4009717	-0.3137735	2.5713032
H	-7.0983143	0.4309605	2.1866376
N	1.8909992	1.9627378	-0.4620368
N	0.4789332	1.8252355	1.9216911
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N	1.8809538	-1.9627056	0.4962224
C	0.3946679	1.8487512	-2.9975297
C	-2.4238021	2.2691826	1.7121232
C	0.3389057	-1.8469794	3.0038454
C	-4.1529834	2.4154629	0.2742610
C	-1.7537911	2.1561914	2.9295415
C	0.3064105	1.5306552	4.2123690
H	0.0619095	-1.4579783	5.1910128
H	-2.3604483	-4.1563935	-7.1197883
C	-2.5122613	2.3211082	4.1940812
C	-4.5277855	2.2027080	-3.6368827
C	0.3821519	-1.5302559	-4.2059208
H	-4.3326466	-2.7215888	-7.6256838
C	-3.9250718	2.6076306	6.6082099
C	-5.7301245	1.9901809	-4.3112968
C	2.9684501	1.9740942	0.4095721
C	2.4250192	2.2675867	-1.7123285
C	1.7287949	1.5438947	2.4653109
C	1.7724147	-1.5436589	-2.4333115
C	2.9741080	-1.9753811	-0.3556533
C	2.3918340	-2.2678265	1.7561187
C	1.7548870	2.1557400	-2.9297704
C	-3.8121582	2.6146372	1.5813076
C	1.6998904	-2.1550174	2.9612275
H	-5.1133036	2.5797657	-0.2017307
H	-0.1570355	1.4596680	5.1891289
C	1.6121576	1.3183386	3.8818646
C	-2.1060171	3.2652770	5.1522198
H	-3.8282801	2.9590059	-3.9925178
C	1.6817623	-1.3185300	-3.8517827
C	-2.8103231	3.4094949	6.3475420
H	-4.4714266	2.7193270	7.5450644
H	-5.9602482	2.5767342	-5.2010771
C	2.9304687	1.6391913	1.7670723
C	4.1543240	2.4123497	-0.2744847
C	3.8135706	2.6122768	-1.5814262
C	2.9611841	-1.6401399	-1.7135645
C	4.1466514	-2.4154131	0.3498711
C	3.7819674	-2.6146970	1.6504108
C	2.5135308	2.3207953	-4.1941760
H	-4.4400062	2.9631768	2.3930128
C	2.4349936	-2.3199138	4.2394307
H	2.4245147	1.0333083	4.5389659
H	-1.2430069	3.8987742	4.9446012
H	2.5060493	-1.0341154	-4.4940896
H	-2.4909827	4.1553356	7.0759219
C	4.2166498	1.4602332	2.4829939
H	5.1145992	2.5764282	0.2016813
H	4.4415649	2.9608069	-2.3930220
C	4.2604123	-1.4626517	-2.4059038
H	5.1152658	-2.5806268	-0.1086911
H	4.3944953	-2.9644254	2.4732239
C	2.1086673	3.2663537	-5.1515019
C	3.6414570	1.5270293	-4.4623888
C	2.0102521	-3.2625058	5.1910610
C	3.5597879	-1.5283277	4.5267888
C	5.1521862	0.5251325	2.0097706
C	4.5285238	2.1993418	3.6368552
C	4.5919682	-2.2011207	-3.5546978
C	5.1885675	-0.5293301	-1.9150744
H	1.2463968	3.9007349	-4.9434878
C	2.8135087	3.4109127	-6.3464734
C	4.3390470	1.6658188	-5.6615982
H	3.9647318	0.7902512	-3.7291006
H	1.1504671	-3.8952853	4.9684951

C	2.6927686	-3.4064622	6.3989785
H	3.8978306	-0.7932740	3.7984807
C	4.2349576	-1.6664789	5.7388331
H	4.9088662	-0.0680144	1.1303916
C	6.3512478	0.3085735	2.6869032
H	3.8292302	2.9558224	3.9925220
C	5.7307982	1.9864520	4.3112623
H	3.8981573	-2.9563089	-3.9235898
C	5.8061420	-1.9887860	-4.2075797
C	6.3997184	-0.3135314	-2.5705604
H	4.9304252	0.0633185	-1.0396069
H	2.4953223	4.1578923	-7.0741918
C	3.9273236	2.6079206	-6.6076592
H	5.2049808	1.0316356	-5.8529334
H	2.3593052	-4.1510777	7.1222497
C	3.8036905	-2.6057881	6.6789355
H	5.0987277	-1.0339480	5.9448827
H	7.0542644	-0.4373216	2.3150161
C	6.6424361	1.0354546	3.8438195
H	5.9610850	2.5729408	5.2010445
H	6.0515208	-2.5745870	-5.0937814
C	6.7104035	-1.0393049	-3.7230790
H	7.0969219	0.4310983	-2.1854439
H	4.4741885	2.7200168	-7.5441677
H	4.3329316	-2.7173328	7.6255803
H	7.5796109	0.8683158	4.3752174
H	7.6570095	-0.8726543	-4.2376517

4²⁺

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Fe	0.0005441	-1.5984184	0.0001311
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N	-1.8908042	1.9458245	0.4799379
N	0.0001668	0.0000431	0.0002115
N	-0.4878891	-1.8210347	1.9225170
C	-2.9729296	-1.9602568	0.3977317
C	-2.9760761	1.9597057	-0.3841508
C	-0.3680229	1.8454862	3.0038138
C	-1.7460775	1.5281256	-2.4530284
C	-4.1522391	-2.4130807	-0.2868917
H	-5.1112368	-2.5914241	0.1863225
C	-0.3402299	1.5152382	-4.2109207
H	0.1126958	1.4432022	-5.1922680
C	-2.4193827	-2.2610112	-1.7173447
C	-2.9493380	1.6237110	-1.7423555
C	-1.6246865	-1.2965672	3.8748106
H	-2.4369784	-0.9999484	4.5267874
C	-2.4902637	-2.3252673	-4.2018055
C	-1.7337728	-1.5284462	2.4611246
C	-0.3197697	-1.5161796	4.2125558
C	-1.6436095	1.2959650	-3.8671010
H	-2.4590105	0.9994361	-4.5152304
C	-2.9402277	-1.6238120	1.7557844
C	-2.7456358	-3.3926567	-6.3707392
C	-2.0464506	-3.2403285	-5.1750900
H	-1.1674828	-3.8529398	-4.9728772
C	-4.2248745	-1.4475553	2.4652841
C	-3.6297640	1.5660205	4.4746279
H	-3.9832165	0.8510774	3.7335454
H	-0.1361248	-1.4444272	-5.1916719
C	-4.2369925	1.4477556	-2.4465667
C	-3.8040344	-2.6180330	-1.5922813
H	-4.4240340	-2.9867942	-2.4008132
C	-3.6481550	-1.5673237	-4.4582309
H	-3.9980526	-0.8519623	-3.7158547
C	-4.3322508	-1.7077559	-5.6634903
H	-5.2174889	-1.1005439	-5.8519641
C	-0.3802017	-1.8455537	-3.0019992
C	-1.7409534	-2.1539331	-2.9394225
C	-3.8852542	-2.6221656	-6.6219085
C	-4.3082580	1.7059165	5.6831066
H	-5.1927557	1.0987897	5.8752939
C	-4.5242146	-2.1589911	3.6419808
H	-3.8165947	-2.8970754	4.0184978
C	-5.1886046	0.5447030	-1.9383076
H	-4.9504547	-0.0288399	-1.0448411
C	-5.1794676	-0.5463107	1.9592816
H	-4.9456683	0.0255730	1.0636205
C	-5.7351242	-1.9552561	4.3009193
H	-5.9617072	-2.5262044	5.2013229
C	-6.3948409	0.3319091	-2.6019387
H	-7.1105615	-0.3890546	-2.2065896
C	-6.6810745	1.0367568	-3.7741423
H	-7.6275966	0.8780894	-4.2909652
C	-6.6635226	-1.0354735	3.8026809
H	-7.6079075	-0.8763995	4.3232731
C	-6.3829192	-0.3329362	2.6277324
H	-7.1008750	0.3866709	2.2339651
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N	0.4963974	1.8211804	1.9201453
N	0.4890907	-1.8204568	-1.9222569

N	1.8927429	-1.9465303	0.4713706
C	0.3667240	1.8454442	-3.0038909
C	-2.4132570	2.2598688	1.7285000
C	0.3815275	-1.8460234	3.0021835
C	-4.1525403	2.4117235	0.3058694
C	-1.7292506	2.1530201	2.9475136
C	0.3390643	1.5157863	4.2108904
H	0.1377118	-1.4447663	5.1918478
H	-2.4050553	-4.1205461	-7.1070688
C	-2.4728371	2.3238131	4.2133181
C	-4.5417981	2.1613152	-3.6205392
C	0.3212369	-1.5157425	-4.2123209
H	-4.4265758	-2.7395576	-7.5606820
C	-3.8565775	2.6195521	6.6400679
C	-5.7554498	1.9581169	-4.2746087
C	2.9746820	1.9613283	0.3840675
C	2.4118631	2.2607220	-1.7286955
C	1.7449210	1.5291581	2.4529994
C	1.7350021	-1.5276767	-2.4607277
C	2.9741670	-1.9601953	-0.3975511
C	2.4206639	-2.2612240	1.7174411
C	1.7278666	2.1534204	-2.9476972
C	-3.7985741	2.6164373	1.6097444
C	1.7422723	-2.1542935	2.9395181
H	-5.1137503	2.5896388	-0.1630091
H	-0.1138454	1.4436876	5.1922452
C	1.6425465	1.2970516	3.8671060
C	-2.0243937	3.2382237	5.1851158
H	-3.8361065	2.9003820	-3.9987798
C	1.6260992	-1.2959751	-3.8744301
C	-2.7179913	3.3899841	6.3840716
H	-4.3935243	2.7364609	7.5814110
H	-5.9862762	2.5306267	-5.1729430
C	2.9480971	1.6251885	1.7422602
C	4.1509097	2.4140179	-0.3059062
C	3.7969474	2.6181764	-1.6098745
C	2.9414178	-1.6232999	-1.7554275
C	4.1536108	-2.4127082	0.2870435
C	3.8054095	-2.6179180	1.5923998
C	2.4713828	2.3242367	-4.2135152
H	-4.4151130	2.9846596	2.4211590
C	2.4916923	-2.3253617	4.2018929
H	2.4580899	1.0010076	4.5152766
H	-1.1462393	3.8507689	4.9792234
H	2.4385651	-0.9996474	-4.5263326
H	-2.3738312	4.1173319	7.1192680
C	4.2358913	1.4494518	2.4462513
H	5.1119517	2.5926760	0.1630361
H	4.4133104	2.9867421	-2.4212656
C	4.2260810	-1.4470068	-2.4649858
H	5.1127054	-2.5905489	-0.1861722
H	4.4254866	-2.9864209	2.4009970
C	2.0221779	3.2376980	-5.1858750
C	3.6291137	1.5674789	-4.4743086
C	2.0487887	-3.2411951	5.1748302
C	3.6485980	-1.5660551	4.4586737
C	5.1875476	0.5466698	1.9375769
C	4.5407500	2.1626722	3.6204142
C	4.5260655	-2.1600164	-3.6405281
C	5.1798552	-0.5442969	-1.9601426
H	1.1435232	3.8496456	-4.9803510
C	2.7157935	3.3895301	-6.3848036
C	4.3076178	1.7073894	-5.6827724
H	3.9831703	0.8532385	-3.7328382
H	1.1704607	-3.8546487	4.9723700

C	2.7479568	-3.3929872	6.3705691
H	3.9978745	-0.8502636	3.7164174
C	4.3326572	-1.7059859	5.6640190
H	4.9493194	-0.0266333	1.0439726
C	6.3938331	0.3336853	2.6010519
H	3.8350324	2.9015438	3.9989854
C	5.7544829	1.9593309	4.2742895
H	3.8188896	-2.8990009	-4.0161385
C	5.7369216	-1.9563372	-4.2996108
C	6.3832443	-0.3309943	-2.6287664
H	4.9455511	0.0285983	-1.0652475
H	2.3710864	4.1162484	-7.1203663
C	3.8551810	2.6201000	-6.6402589
H	5.1927618	1.1010582	-5.8744992
H	2.4081132	-4.1214513	7.1066714
C	3.8865640	-2.6211394	6.6221496
H	5.2171544	-1.0977871	5.8527921
H	7.1095434	-0.3871335	2.2054228
C	6.6800956	1.0381396	3.7734837
H	5.9853652	2.5315786	5.1727775
H	5.9640782	-2.5283816	-5.1991739
C	6.6645266	-1.0350775	-3.8026271
H	7.1006348	0.3896927	-2.2359423
H	4.3921794	2.7371097	-7.5815596
H	4.4278650	-2.7381175	7.5609868
H	7.6266673	0.8793673	4.2901835
H	7.6088609	-0.8760640	-4.3233300

4

Fe	-0.0002130	1.6278291	-0.0003340
Fe	0.0001439	-1.6244072	0.0001802
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N	-0.5016554	1.8397287	-1.9291346
N	-1.9055525	1.9640654	0.4911038
N	-0.0001272	0.0019855	-0.0000463
N	-0.4925899	-1.8378862	1.9313805
C	-2.9819450	-1.9936924	0.3852841
C	-2.9840626	1.9955292	-0.3721302
C	-0.3612017	1.8513063	3.0090067
C	-1.7602025	1.5937052	-2.4549025
C	-4.1723440	-2.4060757	-0.3146666
H	-5.1383481	-2.5697394	0.1505412
C	-0.3592191	1.5502719	-4.2212149
H	0.0918035	1.4598973	-5.2023521
C	-2.4296325	-2.2427479	-1.7367032
C	-2.9539378	1.6896798	-1.7377033
C	-1.6484956	-1.3709880	3.8849972
H	-2.4694438	-1.1019618	4.5382781
C	-2.4937698	-2.2776787	-4.2195633
C	-1.7488983	-1.5931879	2.4628898
C	-0.3403265	-1.5511136	4.2231661
C	-1.6657872	1.3697259	-3.8770992
H	-2.4893166	1.0992871	-4.5265172
C	-2.9457823	-1.6888783	1.7509395
C	-2.7979174	-3.3553005	-6.3806924
C	-2.1014251	-3.2269357	-5.1784289
H	-1.2487333	-3.8727972	-4.9662597
C	-4.2369163	-1.5157605	2.4608710
C	-3.5876290	1.4663047	4.5109901
H	-3.9065256	0.7278252	3.7780588
H	-0.1148357	-1.4602826	-5.2019628
C	-4.2481048	1.5148593	-2.4416114
C	-3.8264534	-2.5765454	-1.6244999
H	-4.4552633	-2.8970995	-2.4473239
C	-3.6068235	-1.4665345	-4.4964009
H	-3.9219418	-0.7264174	-3.7634575
C	-4.3012293	-1.5918348	-5.6993241
H	-5.1560569	-0.9424718	-5.8916235
C	-0.3741111	-1.8502959	-3.0077529
C	-1.7418429	-2.1291764	-2.9472963
C	-3.8984094	-2.5358823	-6.6474119
C	-4.2763693	1.5895484	5.7173739
H	-5.1306317	0.9402359	5.9123424
C	-4.5623121	-2.2644665	3.6048252
H	-3.8657416	-3.0249332	3.9575261
C	-5.1742472	0.5685736	-1.9707159
H	-4.9154163	-0.0352674	-1.1029214
C	-5.1652836	-0.5685593	1.9962484
H	-4.9101557	0.0377882	1.1290740
C	-5.7655525	-2.0502451	4.2779270
H	-6.0008423	-2.6417604	5.1636486
C	-6.3793619	0.3514387	-2.6373223
H	-7.0713183	-0.4053569	-2.2658226
C	-6.6868682	1.0842710	-3.7863102
H	-7.6263495	0.9123756	-4.3128945
C	-6.6705180	-1.0899811	3.8163761
H	-7.6080899	-0.9201270	4.3470104
C	-6.3678492	-0.3537831	2.6682440
H	-7.0616404	0.4036852	2.3015598
N	1.9050001	1.9647651	-0.4917367
N	0.5012337	1.8397815	1.9284849
N	0.4929842	-1.8372733	-1.9310617

N	1.9077091	-1.9612396	0.4830731
C	0.3607091	1.8520911	-3.0097214
C	-2.4222733	2.2448734	1.7473769
C	0.3744773	-1.8509935	3.0081156
C	-4.1713154	2.4079935	0.3330968
C	-1.7291446	2.1303639	2.9548264
C	0.3587308	1.5492120	4.2204173
H	0.1149024	-1.4617538	5.2024520
H	-2.4831873	-4.1029753	-7.1099712
C	-2.4753607	2.2772984	4.2306176
C	-4.5785528	2.2605422	-3.5861143
C	0.3404936	-1.5496315	-4.2227181
H	-4.4402151	-2.6355422	-7.5887858
C	-3.8685635	2.5314110	6.6655019
C	-5.7842757	2.0438210	-4.2539453
C	2.9834915	1.9967004	0.3715296
C	2.4216278	2.2459873	-1.7479564
C	1.7598305	1.5939692	2.4542272
C	1.7491274	-1.5915954	-2.4624874
C	2.9823124	-1.9924561	-0.3850411
C	2.4300795	-2.2424230	1.7368872
C	1.7285680	2.1315922	-2.9554645
C	-3.8195733	2.5786424	1.6413747
C	1.7423193	-2.1293483	2.9475628
H	-5.1394218	2.5714825	-0.1277981
H	-0.0923352	1.4582810	5.2014814
C	1.6654210	1.3694413	3.8763388
C	-2.0781159	3.2245214	5.1895007
H	-3.8838881	3.0205726	-3.9434886
C	1.6485611	-1.3688245	-3.8844868
C	-2.7689192	3.3508189	6.3952619
H	-4.4058385	2.6293943	7.6096460
H	-6.0233500	2.6328258	-5.1403289
C	2.9535234	1.6905788	1.7370384
C	4.1705354	2.4098825	-0.3335968
C	3.8187399	2.5805223	-1.6418597
C	2.9460454	-1.6869438	-1.7505595
C	4.1728277	-2.4047155	0.3147812
C	3.8269673	-2.5758395	1.6245387
C	2.4749735	2.2785917	-4.2311402
H	-4.4446822	2.8993052	2.4669846
C	2.4945710	-2.2765280	4.2198033
H	2.4890015	1.0990423	4.5257028
H	-1.2260728	3.8703754	4.9746762
H	2.4693192	-1.0989529	-4.5376563
H	-2.4503928	4.0968728	7.1245570
C	4.2477445	1.5155922	2.4407859
H	5.1385341	2.5738397	0.1273654
H	4.4436983	2.9016694	-2.4673932
C	4.2371450	-1.5132320	-2.4603990
H	5.1388964	-2.5678836	-0.1504640
H	4.4558580	-2.8965807	2.4472297
C	2.0776608	3.2252718	-5.1905222
C	3.5874485	1.4676854	-4.5110069
C	2.1026773	-3.2244783	5.1801489
C	3.6072747	-1.4644812	4.4954317
C	5.1737853	0.5694654	1.9693975
C	4.5781756	2.2604559	3.5858292
C	4.5627438	-2.2615614	-3.6045479
C	5.1655573	-0.5663934	-1.9951571
H	1.2255144	3.8711254	-4.9761039
C	2.7684939	3.3509773	-6.3963408
C	4.2763327	1.5904704	-5.7173424
H	3.9062510	0.7294697	-3.7777656
H	1.2504935	-3.8713092	4.9688974

C	2.7988613	-3.3502006	6.3828852
H	3.9223073	-0.7256615	3.7611680
C	4.3012903	-1.5870455	5.6988413
H	4.9148585	-0.0338967	1.1013138
C	6.3787731	0.3516510	2.6359917
H	3.8835561	3.0202970	3.9437018
C	5.7837647	2.0430354	4.2536838
H	3.8661340	-3.0217574	-3.9577494
C	5.7663339	-2.0474909	-4.2770640
C	6.3684988	-0.3517958	-2.6665326
H	4.9102757	0.0397186	-1.1278731
H	2.4498058	4.0964832	-7.1261257
C	3.8683496	2.5316745	-6.6660464
H	5.1307793	0.9412609	-5.9118492
H	2.4844062	-4.0967909	7.1133933
C	3.8985933	-2.5294411	6.6486130
H	5.1556380	-0.9367741	5.8901903
H	7.0706036	-0.4050586	2.2640864
C	6.6862480	1.0836312	3.7855278
H	6.0228115	2.6313579	5.1405288
H	6.0017982	-2.6387666	-5.1628994
C	6.6714687	-1.0877658	-3.8147299
H	7.0624108	0.4052651	-2.2992374
H	4.4056487	2.6292263	-7.6102218
H	4.4399511	-2.6268357	7.5904823
H	7.6256114	0.9111829	4.3121411
H	7.6093797	-0.9181251	-4.3448321

Cartesian coordinates of the oxo complexes, calculated with B3LYP-D3(BJ)/def2-

TZVP

[1=O]

Fe	0.0000000	0.0000000	1.8864919
Fe	0.0000000	0.0000000	-1.6609018
C	1.1613268	-2.7327153	1.7086768
C	-2.7497374	-1.1116361	-1.7350958
N	1.3921634	-1.3922742	1.7837787
N	-1.9483861	0.0000000	-1.7934502
C	2.7328942	-1.1613269	1.7150460
C	-2.7497374	1.1116361	-1.7350958
C	3.4327286	-2.4416128	1.6166847
C	-4.1460415	0.7003366	-1.6609939
C	4.7742288	-2.7651411	1.5090090
C	-5.3269984	1.4205007	-1.5701423
H	5.5305523	-1.9927846	1.5047437
H	-5.3156647	2.5013632	-1.5606969
C	5.1041714	-4.1146242	1.3954368
C	-6.5138385	0.6999026	-1.4728134
H	6.1436015	-4.4052166	1.3108596
H	-7.4553984	1.2285135	-1.3952898
C	4.1155336	-5.1028943	1.3893448
C	-6.5138385	-0.6999026	-1.4728134
C	2.7655306	-4.7731932	1.4976795
C	-5.3269984	-1.4205007	-1.5701423
H	1.9930261	-5.5292912	1.4845248
H	-5.3156647	-2.5013632	-1.5606969
C	2.4418888	-3.4322378	1.6118586
C	-4.1460415	-0.7003366	-1.6609939
N	3.3583238	0.0000000	1.6943129
N	-2.3731941	2.3733018	-1.7173532
C	2.7328942	1.1613269	1.7150460
C	-1.1116131	2.7497324	-1.7399467
N	1.3921634	1.3922742	1.7837787
N	0.0000000	1.9480904	-1.7942203
C	1.1613268	2.7327153	1.7086768
C	1.1116131	2.7497324	-1.7399467
C	2.4418888	3.4322378	1.6118586
C	0.7003512	4.1466001	-1.6761947
C	2.7655306	4.7731932	1.4976795
C	1.4204969	5.3282766	-1.5956503
H	1.9930261	5.5292912	1.4845248
H	2.5013791	5.3169389	-1.5853638
C	4.1155336	5.1028943	1.3893448
C	0.6998700	6.5162771	-1.5129339
H	4.4061993	6.1418871	1.2999049
H	1.2284705	7.4586745	-1.4462871
C	5.1041714	4.1146242	1.3954368
C	-0.6998700	6.5162771	-1.5129339
H	6.1436015	4.4052166	1.3108596
H	-1.2284705	7.4586745	-1.4462871
C	4.7742288	2.7651411	1.5090090
C	-1.4204969	5.3282766	-1.5956503
H	5.5305523	1.9927846	1.5047437
H	-2.5013791	5.3169389	-1.5853638
C	3.4327286	2.4416128	1.6166847
C	-0.7003512	4.1466001	-1.6761947
N	0.0000000	3.3580703	1.6834067
N	2.3731941	2.3733018	-1.7173532
C	-1.1613268	2.7327153	1.7086768
C	2.7497374	1.1116361	-1.7350958
N	-1.3921634	1.3922742	1.7837787

N	1.9483861	0.0000000	-1.7934502
C	-2.7328942	1.1613269	1.7150460
C	2.7497374	-1.1116361	-1.7350958
C	-3.4327286	2.4416128	1.6166847
C	4.1460415	-0.7003366	-1.6609939
C	-4.7742288	2.7651411	1.5090090
C	5.3269984	-1.4205007	-1.5701423
H	-5.5305523	1.9927846	1.5047437
H	5.3156647	-2.5013632	-1.5606969
C	-5.1041714	4.1146242	1.3954368
C	6.5138385	-0.6999026	-1.4728134
H	-6.1436015	4.4052166	1.3108596
H	7.4553984	-1.2285135	-1.3952898
C	-4.1155336	5.1028943	1.3893448
C	6.5138385	0.6999026	-1.4728134
H	-4.4061993	6.1418871	1.2999049
H	7.4553984	1.2285135	-1.3952898
C	-2.7655306	4.7731932	1.4976795
C	5.3269984	1.4205007	-1.5701423
H	-1.9930261	5.5292912	1.4845248
H	5.3156647	2.5013632	-1.5606969
C	-2.4418888	3.4322378	1.6118586
C	4.1460415	0.7003366	-1.6609939
N	-3.3583238	0.0000000	1.6943129
N	2.3731941	-2.3733018	-1.7173532
C	-2.7328942	-1.1613269	1.7150460
C	1.1116131	-2.7497324	-1.7399467
N	-1.3921634	-1.3922742	1.7837787
N	0.0000000	-1.9480904	-1.7942203
C	-1.1613268	-2.7327153	1.7086768
C	-1.1116131	-2.7497324	-1.7399467
C	-2.4418888	-3.4322378	1.6118586
C	-0.7003512	-4.1466001	-1.6761947
C	-2.7655306	-4.7731932	1.4976795
C	-1.4204969	-5.3282766	-1.5956503
H	-1.9930261	-5.5292912	1.4845248
H	-2.5013791	-5.3169389	-1.5853638
C	-4.1155336	-5.1028943	1.3893448
C	-0.6998700	-6.5162771	-1.5129339
H	-4.4061993	-6.1418871	1.2999049
H	-1.2284705	-7.4586745	-1.4462871
C	-5.1041714	-4.1146242	1.3954368
C	0.6998700	-6.5162771	-1.5129339
C	-4.7742288	-2.7651411	1.5090090
C	1.4204969	-5.3282766	-1.5956503
H	-5.5305523	-1.9927846	1.5047437
H	2.5013791	-5.3169389	-1.5853638
C	-3.4327286	-2.4416128	1.6166847
C	0.7003512	-4.1466001	-1.6761947
N	0.0000000	-3.3580703	1.6834067
N	-2.3731941	-2.3733018	-1.7173532
N	0.0000000	0.0000000	0.0127395
H	4.4061993	-6.1418871	1.2999049
H	-7.4553984	-1.2285135	-1.3952898
H	-6.1436015	-4.4052166	1.3108596
H	1.2284705	-7.4586745	-1.4462871
O	0.0000000	0.0000000	3.5464283

[1=O]⁻

Fe	0.0000000	0.0000000	1.9270097
Fe	0.0000000	0.0000000	-1.6393081
C	1.1618013	-2.7356103	1.7619600
C	-2.7506994	-1.1124281	-1.7526123
N	1.3946553	-1.3945421	1.8280666
N	-1.9496718	0.0000000	-1.7922678
C	2.7356020	-1.1618190	1.7581083
C	-2.7506994	1.1124281	-1.7526123
C	3.4314327	-2.4394366	1.6546504
C	-4.1451957	0.7010693	-1.6962460
C	4.7737323	-2.7674944	1.5270085
C	-5.3305165	1.4198873	-1.6156385
H	5.5282671	-1.9930492	1.5061330
H	-5.3167775	2.5008661	-1.5939477
C	5.1028454	-4.1128409	1.4059275
C	-6.5170121	0.7013536	-1.5364146
H	6.1414361	-4.4028665	1.3017875
H	-7.4595186	1.2303672	-1.4646086
C	4.1114895	-5.1040889	1.4087743
C	-6.5170121	-0.7013536	-1.5364146
C	2.7665585	-4.7744481	1.5328679
C	-5.3305165	-1.4198873	-1.6156385
H	1.9919249	-5.5289295	1.5166043
H	-5.3167775	-2.5008661	-1.5939477
C	2.4391132	-3.4317384	1.6576564
C	-4.1451957	-0.7010693	-1.6962460
N	3.3599409	0.0000000	1.7347888
N	-2.3740854	2.3740721	-1.7389749
C	2.7356020	1.1618190	1.7581083
C	-1.1124288	2.7506638	-1.7527643
N	1.3946553	1.3945421	1.8280666
N	0.0000000	1.9496245	-1.7918211
C	1.1618013	2.7356103	1.7619600
C	1.1124288	2.7506638	-1.7527643
C	2.4391132	3.4317384	1.6576564
C	0.7010784	4.1452371	-1.6983542
C	2.7665585	4.7744481	1.5328679
C	1.4199082	5.3307250	-1.6201557
H	1.9919249	5.5289295	1.5166043
H	2.5008811	5.3169872	-1.5975931
C	4.1114895	5.1040889	1.4087743
C	0.7013596	6.5175509	-1.5460870
H	4.4010934	6.1430194	1.3069086
H	1.2303540	7.4603454	-1.4780280
C	5.1028454	4.1128409	1.4059275
C	-0.7013596	6.5175509	-1.5460870
H	6.1414361	4.4028665	1.3017875
H	-1.2303540	7.4603454	-1.4780280
C	4.7737323	2.7674944	1.5270085
C	-1.4199082	5.3307250	-1.6201557
H	5.5282671	1.9930492	1.5061330
H	-2.5008811	5.3169872	-1.5975931
C	3.4314327	2.4394366	1.6546504
C	-0.7010784	4.1452371	-1.6983542
N	0.0000000	3.3600303	1.7414106
N	2.3740854	2.3740721	-1.7389749
C	-1.1618013	2.7356103	1.7619600
C	2.7506994	1.1124281	-1.7526123
N	-1.3946553	1.3945421	1.8280666
N	1.9496718	0.0000000	-1.7922678
C	-2.7356020	1.1618190	1.7581083
C	2.7506994	-1.1124281	-1.7526123
C	-3.4314327	2.4394366	1.6546504

C	4.1451957	-0.7010693	-1.6962460
C	-4.7737323	2.7674944	1.5270085
C	5.3305165	-1.4198873	-1.6156385
H	-5.5282671	1.9930492	1.5061330
H	5.3167775	-2.5008661	-1.5939477
C	-5.1028454	4.1128409	1.4059275
C	6.5170121	-0.7013536	-1.5364146
H	-6.1414361	4.4028665	1.3017875
H	7.4595186	-1.2303672	-1.4646086
C	-4.1114895	5.1040889	1.4087743
C	6.5170121	0.7013536	-1.5364146
H	-4.4010934	6.1430194	1.3069086
H	7.4595186	1.2303672	-1.4646086
C	-2.7665585	4.7744481	1.5328679
C	5.3305165	1.4198873	-1.6156385
H	-1.9919249	5.5289295	1.5166043
H	5.3167775	2.5008661	-1.5939477
C	-2.4391132	3.4317384	1.6576564
C	4.1451957	0.7010693	-1.6962460
N	-3.3599409	0.0000000	1.7347888
N	2.3740854	-2.3740721	-1.7389749
C	-2.7356020	-1.1618190	1.7581083
C	1.1124288	-2.7506638	-1.7527643
N	-1.3946553	-1.3945421	1.8280666
N	0.0000000	-1.9496245	-1.7918211
C	-1.1618013	-2.7356103	1.7619600
C	-1.1124288	-2.7506638	-1.7527643
C	-2.4391132	-3.4317384	1.6576564
C	-0.7010784	-4.1452371	-1.6983542
C	-2.7665585	-4.7744481	1.5328679
C	-1.4199082	-5.3307250	-1.6201557
H	-1.9919249	-5.5289295	1.5166043
H	-2.5008811	-5.3169872	-1.5975931
C	-4.1114895	-5.1040889	1.4087743
C	-0.7013596	-6.5175509	-1.5460870
H	-4.4010934	-6.1430194	1.3069086
H	-1.2303540	-7.4603454	-1.4780280
C	-5.1028454	-4.1128409	1.4059275
C	0.7013596	-6.5175509	-1.5460870
C	-4.7737323	-2.7674944	1.5270085
C	1.4199082	-5.3307250	-1.6201557
H	-5.5282671	-1.9930492	1.5061330
H	2.5008811	-5.3169872	-1.5975931
C	-3.4314327	-2.4394366	1.6546504
C	0.7010784	-4.1452371	-1.6983542
N	0.0000000	-3.3600303	1.7414106
N	-2.3740854	-2.3740721	-1.7389749
N	0.0000000	0.0000000	0.0394982
H	4.4010934	-6.1430194	1.3069086
H	-7.4595186	-1.2303672	-1.4646086
H	-6.1414361	-4.4028665	1.3017875
H	1.2303540	-7.4603454	-1.4780280
O	0.0000000	0.0000000	3.5884657

[5=O1]

Fe	0.0000000	0.0000000	1.5091406
Fe	0.0000000	-0.0000000	-2.0531619
N	-1.9950874	0.3688387	1.4314914
N	0.0742523	1.9476380	-2.2016923
N	1.9950874	-0.3688387	1.4314914
N	-0.0742523	-1.9476380	-2.2016923
N	-0.3690306	-1.9944804	1.4294651
N	2.4617677	2.2796919	-2.1383527
N	1.9476164	-0.0743201	-2.2010792
N	-1.9476164	0.0743201	-2.2010792
N	-2.4617677	-2.2796919	-2.1383527
N	0.0000000	0.0000000	-0.3671522
N	-2.2795954	2.4616889	-2.1308802
N	0.3690306	1.9944804	1.4294651
N	2.2795954	-2.4616889	-2.1308802
C	-1.2160294	-2.7047616	-2.1578965
C	4.1157918	-0.8616242	-2.0849629
C	2.7847555	-4.0609312	1.4460817
C	-0.8616623	-4.1159356	-2.0869414
C	1.2160294	2.7047616	-2.1578965
C	1.9490571	-2.8303399	1.4239181
C	0.5528574	-2.9916535	1.4201894
C	1.0037354	-2.7918073	-2.1457121
C	0.5385630	-4.1711338	-2.0722613
C	-2.5986438	1.6017930	1.4186578
C	-4.1714732	-0.5386573	-2.0773508
C	-2.7046003	1.2159953	-2.1532465
C	-4.0325145	1.4377801	1.4048210
C	2.7919398	1.0037828	-2.1501098
C	-2.9923851	-0.5530022	1.4198453
C	1.6019443	2.5980740	1.4099738
C	-2.7919398	-1.0037828	-2.1501098
C	2.7046003	-1.2159953	-2.1532465
C	-5.2692562	1.6273815	-1.9953054
H	-5.2206061	2.7075482	-2.0047886
C	2.5986438	-1.6017930	1.4186578
C	-0.1065833	-4.2754628	1.3822507
H	0.3890180	-5.2281482	1.3311971
C	-1.4378046	-4.0318462	1.3929272
H	-2.2383523	-4.7490044	1.3747699
C	2.8307358	1.9490773	1.4165304
C	5.2692562	-1.6273815	-1.9953054
H	5.2206061	-2.7075482	-2.0047886
C	0.8616623	4.1159356	-2.0869414
C	2.7628600	-4.9064145	2.5573856
H	2.1320960	-4.6564991	3.4005862
C	-5.3834774	-1.2066361	-1.9715329
H	-5.4241458	-2.2857390	-1.9581334
C	-1.6019443	-2.5980740	1.4099738
C	-6.5386124	-0.4400339	-1.8661546
C	4.2762092	-0.1065631	1.3878684
H	5.2289706	0.3890303	1.3368904
C	-1.9490571	2.8303399	1.4239181
C	-2.7847555	4.0609312	1.4460817
C	1.2067219	-5.3824879	-1.9605179
H	2.2858041	-5.4224064	-1.9421018
C	-4.1157918	0.8616242	-2.0849629
C	2.9923851	0.5530022	1.4198453
C	-0.5528574	2.9916535	1.4201894
C	-1.6273132	-5.2692071	-1.9934607
H	-2.7074647	-5.2210438	-2.0060184
C	-0.5385630	4.1711338	-2.0722613
C	4.1714732	0.5386573	-2.0773508

C	4.0325145	-1.4377801	1.4048210
H	4.7496731	-2.2384454	1.3926976
C	0.4401550	-6.5373078	-1.8517760
H	0.9313361	-7.4965048	-1.7502480
C	5.3834774	1.2066361	-1.9715329
H	5.4241458	2.2857390	-1.9581334
C	3.5507412	-6.0495473	2.5895537
H	3.5297961	-6.6909553	3.4613877
C	-2.8307358	-1.9490773	1.4165304
C	1.6273132	5.2692071	-1.9934607
H	2.7074647	5.2210438	-2.0060184
C	4.0604792	2.7862948	1.4369305
C	1.4378046	4.0318462	1.3929272
H	2.2383523	4.7490044	1.3747699
C	-6.4827950	0.9591760	-1.8802583
H	-7.4009835	1.5266070	-1.7980879
C	4.3905661	-5.5314062	0.3977068
H	5.0181681	-5.7751653	-0.4507199
C	3.6061476	-4.3854767	0.3653860
H	3.5992032	-3.7465215	-0.5065511
C	4.3673244	-6.3660485	1.5091447
H	4.9809605	-7.2575383	1.5343199
C	-2.7628600	4.9064145	2.5573856
H	-2.1320960	4.6564991	3.4005862
C	0.1065833	4.2754628	1.3822507
H	-0.3890180	5.2281482	1.3311971
C	-0.4401550	6.5373078	-1.8517760
C	-3.6061476	4.3854767	0.3653860
H	-3.5992032	3.7465215	-0.5065511
C	0.9590288	6.4820566	-1.8716916
H	1.5264520	7.3999699	-1.7864527
C	6.4827950	-0.9591760	-1.8802583
H	7.4009835	-1.5266070	-1.7980879
C	-3.5507412	6.0495473	2.5895537
H	-3.5297961	6.6909553	3.4613877
C	-1.2067219	5.3824879	-1.9605179
H	-2.2858041	5.4224064	-1.9421018
C	-0.9590288	-6.4820566	-1.8716916
H	-1.5264520	-7.3999699	-1.7864527
C	6.5386124	0.4400339	-1.8661546
H	7.4984187	0.9312341	-1.7707980
C	4.3882540	3.6000556	0.3515569
H	3.7532173	3.5852067	-0.5231687
C	4.8999709	2.7754805	2.5528775
H	4.6471295	2.1508829	3.3997912
C	-4.3905661	5.5314062	0.3977068
C	6.0405339	3.5671401	2.5850087
H	6.6770489	3.5552816	3.4605977
C	5.5319655	4.3877190	0.3836651
H	5.7784866	5.0093129	-0.4683918
C	6.3605111	4.3759824	1.4998271
H	7.2499027	4.9926619	1.5249810
C	-1.0037354	2.7918073	-2.1457121
H	-4.7496731	2.2384454	1.3926976
C	-4.2762092	0.1065631	1.3878684
H	-7.4984187	-0.9312341	-1.7707980
C	-4.0604792	-2.7862948	1.4369305
H	-0.9313361	7.4965048	-1.7502480
C	-4.3673244	6.3660485	1.5091447
H	-5.0181681	5.7751653	-0.4507199
H	-5.2289706	-0.3890303	1.3368904
C	-4.8999709	-2.7754805	2.5528775
C	-4.3882540	-3.6000556	0.3515569
H	-4.9809605	7.2575383	1.5343199
H	-4.6471295	-2.1508829	3.3997912

C	-6.0405339	-3.5671401	2.5850087
H	-3.7532173	-3.5852067	-0.5231687
C	-5.5319655	-4.3877190	0.3836651
C	-6.3605111	-4.3759824	1.4998271
H	-6.6770489	-3.5552816	3.4605977
H	-5.7784866	-5.0093129	-0.4683918
H	-7.2499027	-4.9926619	1.5249810
O	0.0000000	-0.0000000	3.1638964

[5=O1]⁻

Fe	0.0000000	0.0000000	1.5446152
Fe	0.0000000	-0.0000000	-2.0642158
N	-1.9952296	0.3623299	1.4603645
N	0.0893056	1.9473990	-2.2113415
N	1.9952296	-0.3623299	1.4603645
N	-0.0893056	-1.9473990	-2.2113415
N	-0.3625273	-1.9948326	1.4589804
N	2.4797362	2.2613147	-2.1587261
N	1.9475257	-0.0890970	-2.2108028
N	-1.9475257	0.0890970	-2.2108028
N	-2.4797362	-2.2613147	-2.1587261
N	-0.0000000	0.0000000	-0.3650790
N	-2.2610821	2.4794672	-2.1535304
N	0.3625273	1.9948326	1.4589804
N	2.2610821	-2.4794672	-2.1535304
C	-1.2363409	-2.6956917	-2.1723614
C	4.1080099	-0.8922367	-2.0976248
C	2.8053929	-4.0510282	1.4556675
C	-0.8923083	-4.1081892	-2.1023764
C	1.2363409	2.6956917	-2.1723614
C	1.9577795	-2.8252281	1.4497132
C	0.5741393	-2.9900751	1.4510458
C	0.9832814	-2.7990352	-2.1639084
C	0.5085684	-4.1734194	-2.0909432
C	-2.5993303	1.5878015	1.4463972
C	-4.1736420	-0.5086674	-2.0903409
C	-2.6955518	1.2361251	-2.1682321
C	-4.0342716	1.4182894	1.4304739
C	2.7993407	0.9834790	-2.1657166
C	-2.9905725	-0.5742026	1.4501715
C	1.5879362	2.5991041	1.4400387
C	-2.7993407	-0.9834790	-2.1657166
C	2.6955518	-1.2361251	-2.1682321
C	-5.2574929	1.6643606	-1.9945070
H	-5.1998994	2.7443416	-1.9935447
C	2.5993303	-1.5878015	1.4463972
C	-0.0861612	-4.2747842	1.4144569
H	0.4107037	-5.2274670	1.3625747
C	-1.4181073	-4.0340120	1.4220394
H	-2.2167980	-4.7540060	1.3979284
C	2.8255384	1.9578398	1.4435478
C	5.2574929	-1.6643606	-1.9945070
H	5.1998994	-2.7443416	-1.9935447
C	0.8923083	4.1081892	-2.1023764
C	2.8215234	-4.9004321	2.5641222
H	2.2099921	-4.6530236	3.4221806
C	-5.3904049	-1.1675610	-1.9719080
H	-5.4351052	-2.2466771	-1.9466470
C	-1.5879362	-2.5991041	1.4400387
C	-6.5393014	-0.3947049	-1.8572628
C	4.2752867	-0.0863883	1.4179736
H	5.2280891	0.4101986	1.3654069
C	-1.9577795	2.8252281	1.4497132
C	-2.8053929	4.0510282	1.4556675
C	1.1677045	-5.3899215	-1.9713377
H	2.2467287	-5.4340555	-1.9428512
C	-4.1080099	0.8922367	-2.0976248
C	2.9905725	0.5742026	1.4501715
C	-0.5741393	2.9900751	1.4510458
C	-1.6642650	-5.2580151	-2.0020336
H	-2.7442377	-5.2009140	-2.0042851
C	-0.5085684	4.1734194	-2.0909432
C	4.1736420	0.5086674	-2.0903409

C	4.0342716	-1.4182894	1.4304739
H	4.7541285	-2.2172356	1.4103450
C	0.3949993	-6.5391676	-1.8594926
H	0.8805354	-7.5006425	-1.7475555
C	5.3904049	1.1675610	-1.9719080
H	5.4351052	2.2466771	-1.9466470
C	3.6103988	-6.0445209	2.5733514
H	3.6101696	-6.6899489	3.4434012
C	-2.8255384	-1.9578398	1.4435478
C	1.6642650	5.2580151	-2.0020336
H	2.7442377	5.2009140	-2.0042851
C	4.0509724	2.8060164	1.4477985
C	1.4181073	4.0340120	1.4220394
H	2.2167980	4.7540060	1.3979284
C	-6.4741314	1.0052945	-1.8707088
H	-7.3871582	1.5795480	-1.7728142
C	4.3944669	-5.5161530	0.3654036
H	5.0015719	-5.7539040	-0.5002767
C	3.6011445	-4.3755882	0.3553867
H	3.5672122	-3.7361964	-0.5156850
C	4.4025156	-6.3563871	1.4735283
H	5.0194230	-7.2467572	1.4802869
C	-2.8215234	4.9004321	2.5641222
H	-2.2099921	4.6530236	3.4221806
C	0.0861612	4.2747842	1.4144569
H	-0.4107037	5.2274670	1.3625747
C	-0.3949993	6.5391676	-1.8594926
C	-3.6011445	4.3755882	0.3553867
H	-3.5672122	3.7361964	-0.5156850
C	1.0049815	6.4744390	-1.8771420
H	1.5791498	7.3877531	-1.7814667
C	6.4741314	-1.0052945	-1.8707088
H	7.3871582	-1.5795480	-1.7728142
C	-3.6103988	6.0445209	2.5733514
H	-3.6101696	6.6899489	3.4434012
C	-1.1677045	5.3899215	-1.9713377
H	-2.2467287	5.4340555	-1.9428512
C	-1.0049815	-6.4744390	-1.8771420
H	-1.5791498	-7.3877531	-1.7814667
C	6.5393014	0.3947049	-1.8572628
H	7.5008987	0.8802370	-1.7463247
C	4.3744618	3.6013691	0.3469355
H	3.7355503	3.5654247	-0.5243960
C	4.8996044	2.8253346	2.5568713
H	4.6528336	2.2144352	3.4156210
C	-4.3944669	5.5161530	0.3654036
C	6.0417627	3.6168999	2.5660726
H	6.6864105	3.6193276	3.4366955
C	5.5132075	4.3973151	0.3568803
H	5.7500414	5.0042307	-0.5092086
C	6.3523615	4.4088441	1.4657296
H	7.2410134	5.0282099	1.4726420
C	-0.9832814	2.7990352	-2.1639084
H	-4.7541285	2.2172356	1.4103450
C	-4.2752867	0.0863883	1.4179736
H	-7.5008987	-0.8802370	-1.7463247
C	-4.0509724	-2.8060164	1.4477985
H	-0.8805354	7.5006425	-1.7475555
C	-4.4025156	6.3563871	1.4735283
H	-5.0015719	5.7539040	-0.5002767
H	-5.2280891	-0.4101986	1.3654069
C	-4.8996044	-2.8253346	2.5568713
C	-4.3744618	-3.6013691	0.3469355
H	-5.0194230	7.2467572	1.4802869
H	-4.6528336	-2.2144352	3.4156210

C	-6.0417627	-3.6168999	2.5660726
H	-3.7355503	-3.5654247	-0.5243960
C	-5.5132075	-4.3973151	0.3568803
C	-6.3523615	-4.4088441	1.4657296
H	-6.6864105	-3.6193276	3.4366955
H	-5.7500414	-5.0042307	-0.5092086
H	-7.2410134	-5.0282099	1.4726420
O	0.0000000	-0.0000000	3.1953200

[5=O2]

Fe	0.0000000	0.0000000	1.2770380
Fe	0.0000000	-0.0000000	-2.2396717
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N	0.5794479	1.8798815	-2.1641993
N	1.8238996	-0.8226929	1.4802473
N	-0.5794479	-1.8798815	-2.1641993
N	-0.8244419	-1.8236705	1.4743409
N	2.9671714	1.5676967	-2.1004446
N	1.8798878	-0.5797904	-2.1624851
N	-1.8798878	0.5797904	-2.1624851
N	-2.9671714	-1.5676967	-2.1004446
N	0.0000000	-0.0000000	-0.3767865
N	-1.5676275	2.9673009	-2.0879729
N	0.8244419	1.8236705	1.4743409
N	1.5676275	-2.9673009	-2.0879729
C	-1.8703959	-2.3018841	-2.1167609
C	3.7645227	-1.8953995	-2.0116118
C	1.7386539	-4.6081972	1.5005439
C	-1.8959568	-3.7653304	-2.0360331
C	1.8703959	2.3018841	-2.1167609
C	1.2147465	-3.2121785	1.4744328
C	-0.1657128	-3.0289083	1.4687040
C	0.2480972	-2.9571397	-2.1019915
C	-0.5585152	-4.1789546	-2.0188357
C	-2.1272695	2.1666518	1.4736233
C	-4.1783346	0.5578908	-2.0041628
C	-2.3017748	1.8704521	-2.1027386
C	-3.5581505	2.3486533	1.4765797
C	2.9569534	0.2481100	-2.1016187
C	-3.0298984	0.1649186	1.4705380
C	2.1679806	2.1279321	1.4575013
C	-2.9569534	-0.2481100	-2.1016187
C	2.3017748	-1.8704521	-2.1027386
C	-4.6761524	2.9300469	-1.9078676
H	-4.3523850	3.9614066	-1.9160068
C	2.1272695	-2.1666518	1.4736233
C	-1.1154892	-4.1141079	1.4491059
H	-0.8607195	-5.1586656	1.4208908
C	-2.3484268	-3.5592547	1.4553612
H	-3.2988926	-4.0623430	1.4500889
C	3.2142763	1.2157699	1.4618157
C	4.6761524	-2.9300469	-1.9078676
H	4.3523850	-3.9614066	-1.9160068
C	1.8959568	3.7653304	-2.0360331
C	1.5731327	-5.4048237	2.6348267
H	1.0590887	-4.9973738	3.4959191
C	-5.5140382	0.2206225	-1.8810713
H	-5.8293130	-0.8120319	-1.8634118
C	-2.1679806	-2.1279321	1.4575013
C	-6.4358267	1.2611872	-1.7650876
C	4.1140971	-1.1163374	1.4601767
H	5.1589192	-0.8636258	1.4287649
C	-1.2147465	3.2121785	1.4744328
C	-1.7386539	4.6081972	1.5005439
C	-0.2219999	-5.5153988	-1.9018803
H	0.8107276	-5.8302334	-1.8774480
C	-3.7645227	1.8953995	-2.0116118
C	3.0298984	-0.1649186	1.4705380
C	0.1657128	3.0289083	1.4687040
C	-2.9312039	-4.6776293	-1.9446851
H	-3.9625717	-4.3540383	-1.9597984
C	0.5585152	4.1789546	-2.0188357
C	4.1783346	-0.5578908	-2.0041628

C	3.5581505	-2.3486533	1.4765797
H	4.0599258	-3.2998905	1.4779197
C	-1.2631907	-6.4378071	-1.7984347
H	-1.0340680	-7.4906346	-1.6969049
C	5.5140382	-0.2206225	-1.8810713
H	5.8293130	0.8120319	-1.8634118
C	2.0649744	-6.7039027	2.6668070
H	1.9316199	-7.3068212	3.5560878
C	-3.2142763	-1.2157699	1.4618157
C	2.9312039	4.6776293	-1.9446851
H	3.9625717	4.3540383	-1.9597984
C	4.6100513	1.7399657	1.4791748
C	2.3484268	3.5592547	1.4553612
H	3.2988926	4.0623430	1.4500889
C	-6.0236645	2.5946516	-1.7784881
H	-6.7630720	3.3797690	-1.6870374
C	2.8995982	-6.4396452	0.4293198
H	3.4120657	-6.8402774	-0.4368460
C	2.4070916	-5.1406226	0.3978588
H	2.5134975	-4.5329425	-0.4897564
C	2.7313181	-7.2258759	1.5634281
H	3.1159411	-8.2375323	1.5883526
C	-1.5731327	5.4048237	2.6348267
H	-1.0590887	4.9973738	3.4959191
C	1.1154892	4.1141079	1.4491059
H	0.8607195	5.1586656	1.4208908
C	1.2631907	6.4378071	-1.7984347
C	-2.4070916	5.1406226	0.3978588
H	-2.5134975	4.5329425	-0.4897564
C	2.5966270	6.0260062	-1.8219785
H	3.3822805	6.7661084	-1.7413164
C	6.0236645	-2.5946516	-1.7784881
H	6.7630720	-3.3797690	-1.6870374
C	-2.0649744	6.7039027	2.6668070
H	-1.9316199	7.3068212	3.5560878
C	0.2219999	5.5153988	-1.9018803
H	-0.8107276	5.8302334	-1.8774480
C	-2.5966270	-6.0260062	-1.8219785
H	-3.3822805	-6.7661084	-1.7413164
C	6.4358267	-1.2611872	-1.7650876
H	7.4880014	-1.0311955	-1.6589760
C	5.1305375	2.4207559	0.3782041
H	4.5140714	2.5356798	-0.5019205
C	5.4198527	1.5625635	2.6025327
H	5.0220537	1.0407035	3.4634086
C	-2.8995982	6.4396452	0.4293198
C	6.7195897	2.0531879	2.6247710
H	7.3324661	1.9101907	3.5057819
C	6.4301683	2.9118250	0.3997170
H	6.8210331	3.4333423	-0.4656353
C	7.2297426	2.7301979	1.5223700
H	8.2421582	3.1132531	1.5394788
C	-0.2480972	2.9571397	-2.1019915
H	-4.0599258	3.2998905	1.4779197
C	-4.1140971	1.1163374	1.4601767
H	-7.4880014	1.0311955	-1.6589760
C	-4.6100513	-1.7399657	1.4791748
H	1.0340680	7.4906346	-1.6969049
C	-2.7313181	7.2258759	1.5634281
H	-3.4120657	6.8402774	-0.4368460
H	-5.1589192	0.8636258	1.4287649
C	-5.4198527	-1.5625635	2.6025327
C	-5.1305375	-2.4207559	0.3782041
H	-3.1159411	8.2375323	1.5883526
H	-5.0220537	-1.0407035	3.4634086

C	-6.7195897	-2.0531879	2.6247710
H	-4.5140714	-2.5356798	-0.5019205
C	-6.4301683	-2.9118250	0.3997170
C	-7.2297426	-2.7301979	1.5223700
H	-7.3324661	-1.9101907	3.5057819
H	-6.8210331	-3.4333423	-0.4656353
H	-8.2421582	-3.1132531	1.5394788
O	0.0000000	-0.0000000	-3.9111152

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Fe	0.0000000	0.0000000	-2.2512355
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N	1.8274578	-0.8200744	1.4964393
N	-0.5911239	-1.8816944	-2.1739239
N	-0.8167622	-1.8278697	1.5102652
N	2.9774282	1.5524821	-2.0929680
N	1.8813844	-0.5909639	-2.1772239
N	-1.8813844	0.5909639	-2.1772239
N	-2.9774282	-1.5524821	-2.0929680
N	0.0000000	-0.0000000	-0.3681089
N	-1.5532339	2.9781557	-2.1254110
N	0.8167622	1.8278697	1.5102652
N	1.5532339	-2.9781557	-2.1254110
C	-1.8860153	-2.2945012	-2.1076553
C	3.7516600	-1.9174711	-2.0612689
C	1.7567306	-4.6018289	1.4777981
C	-1.9155509	-3.7499385	-2.0078021
C	1.8860153	2.2945012	-2.1076553
C	1.2244270	-3.2090814	1.4774032
C	-0.1541120	-3.0332572	1.5007254
C	0.2334074	-2.9630843	-2.1240744
C	-0.5768376	-4.1725742	-2.0148643
C	-2.1364181	2.1596869	1.4708008
C	-4.1737130	0.5787310	-2.0415810
C	-2.2949845	1.8866614	-2.1403655
C	-3.5672416	2.3365683	1.4581908
C	2.9627129	0.2329748	-2.1178469
C	-3.0314291	0.1554790	1.4910195
C	2.1571760	2.1350403	1.5096844
C	-2.9627129	-0.2329748	-2.1178469
C	2.2949845	-1.8866614	-2.1403655
C	-4.6652582	2.9575154	-1.9662964
H	-4.3341995	3.9871121	-1.9799135
C	2.1364181	-2.1596869	1.4708008
C	-1.1022731	-4.1190261	1.4953646
H	-0.8480700	-5.1633420	1.4533568
C	-2.3369177	-3.5649516	1.5135621
H	-3.2870496	-4.0692613	1.5059973
C	3.2054606	1.2227302	1.5028489
C	4.6652582	-2.9575154	-1.9662964
H	4.3341995	-3.9871121	-1.9799135
C	1.9155509	3.7499385	-2.0078021
C	1.6163545	-5.4167598	2.6025663
H	1.1131048	-5.0237368	3.4767652
C	-5.5179944	0.2554397	-1.9216185
H	-5.8384490	-0.7760608	-1.8942691
C	-2.1571760	-2.1350403	1.5096844
C	-6.4325674	1.2976952	-1.8179696
C	4.1189729	-1.1008749	1.4594037
H	5.1626006	-0.8431595	1.4178185
C	-1.2244270	3.2090814	1.4774032
C	-1.7567306	4.6018289	1.4777981
C	-0.2509889	-5.5149144	-1.8803872
H	0.7806288	-5.8357333	-1.8748060
C	-3.7516600	1.9174711	-2.0612689
C	3.0314291	-0.1554790	1.4910195
C	0.1541120	3.0332572	1.5007254
C	-2.9528301	-4.6610976	-1.8680833
H	-3.9822920	-4.3299096	-1.8581904
C	0.5768376	4.1725742	-2.0148643
C	4.1737130	-0.5787310	-2.0415810

C	3.5672416	-2.3365683	1.4581908
H	4.0739889	-3.2849249	1.4328108
C	-1.2901036	-6.4262177	-1.7284995
H	-1.0646178	-7.4785252	-1.6066817
C	5.5179944	-0.2554397	-1.9216185
H	5.8384490	0.7760608	-1.8942691
C	2.1151308	-6.7138433	2.6078362
H	1.9984355	-7.3311178	3.4903418
C	-3.2054606	-1.2227302	1.5028489
C	2.9528301	4.6610976	-1.8680833
H	3.9822920	4.3299096	-1.8581904
C	4.5994839	1.7530861	1.5162270
C	2.3369177	3.5649516	1.5135621
H	3.2870496	4.0692613	1.5059973
C	-6.0114858	2.6334134	-1.8417731
H	-6.7474604	3.4236037	-1.7569090
C	2.9102529	-6.4105756	0.3613188
H	3.4068955	-6.7953965	-0.5215024
C	2.4083101	-5.1149392	0.3556833
H	2.4884712	-4.4954650	-0.5270629
C	2.7666242	-7.2153808	1.4861212
H	3.1561997	-8.2260538	1.4884441
C	-1.6163545	5.4167598	2.6025663
H	-1.1131048	5.0237368	3.4767652
C	1.1022731	4.1190261	1.4953646
H	0.8480700	5.1633420	1.4533568
C	1.2901036	6.4262177	-1.7284995
C	-2.4083101	5.1149392	0.3556833
H	-2.4884712	4.4954650	-0.5270629
C	2.6257883	6.0045322	-1.7238308
H	3.4135532	6.7375721	-1.5999966
C	6.0114858	-2.6334134	-1.8417731
H	6.7474604	-3.4236037	-1.7569090
C	-2.1151308	6.7138433	2.6078362
H	-1.9984355	7.3311178	3.4903418
C	0.2509889	5.5149144	-1.8803872
H	-0.7806288	5.8357333	-1.8748060
C	-2.6257883	-6.0045322	-1.7238308
H	-3.4135532	-6.7375721	-1.5999966
C	6.4325674	-1.2976952	-1.8179696
H	7.4872959	-1.0750147	-1.7130099
C	5.1315426	2.3813773	0.3900266
H	4.5233284	2.4506410	-0.5016589
C	5.3965208	1.6275765	2.6549854
H	4.9882040	1.1398813	3.5310578
C	-2.9102529	6.4105756	0.3613188
C	6.6963927	2.1192934	2.6702808
H	7.3004883	2.0148164	3.5633682
C	6.4308277	2.8740512	0.4047578
H	6.8320312	3.3514837	-0.4813817
C	7.2181462	2.7462865	1.5438455
H	8.2312136	3.1294975	1.5536449
C	-0.2334074	2.9630843	-2.1240744
H	-4.0739889	3.2849249	1.4328108
C	-4.1189729	1.1008749	1.4594037
H	-7.4872959	1.0750147	-1.7130099
C	-4.5994839	-1.7530861	1.5162270
H	1.0646178	7.4785252	-1.6066817
C	-2.7666242	7.2153808	1.4861212
H	-3.4068955	6.7953965	-0.5215024
H	-5.1626006	0.8431595	1.4178185
C	-5.3965208	-1.6275765	2.6549854
C	-5.1315426	-2.3813773	0.3900266
H	-3.1561997	8.2260538	1.4884441
H	-4.9882040	-1.1398813	3.5310578

C	-6.6963927	-2.1192934	2.6702808
H	-4.5233284	-2.4506410	-0.5016589
C	-6.4308277	-2.8740512	0.4047578
C	-7.2181462	-2.7462865	1.5438455
H	-7.3004883	-2.0148164	3.5633682
H	-6.8320312	-3.3514837	-0.4813817
H	-8.2312136	-3.1294975	1.5536449
O	0.0000000	0.0000000	-3.9210852

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Fe	0.0000000	0.0000000	-1.8802128
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N	-1.9250643	-0.4605916	1.9554495
N	0.0000000	-0.0000000	-0.0178993
N	-0.5063129	-1.9556681	-1.8184411
C	-3.0052075	-0.3508164	-1.9473588
C	-2.9771004	0.4184552	2.0162125
C	-0.4053887	-2.9975765	1.8592681
C	-1.7210991	2.4862089	1.6467799
C	-4.2058306	0.3585678	-2.3209842
H	-5.1715060	-0.0896930	-2.4753720
C	-0.2990054	4.2271590	1.6033989
H	0.1589425	5.1971912	1.5256411
C	-2.4554008	1.7564903	-2.1623655
C	-2.9203654	1.7892163	1.7582108
C	-1.6764995	-3.8960699	-1.4301084
H	-2.4958172	-4.5481934	-1.1902286
C	-2.4556744	4.2237343	-2.2881314
C	-1.7627049	-2.4664325	-1.6195763
C	-0.3747131	-4.2335174	-1.5873007
C	-1.6066432	3.9116267	1.4525581
H	-2.4174051	4.5807262	1.2298622
C	-2.9473581	-1.7372255	-1.7091906
C	-2.7605048	6.2922866	-3.5061705
C	-2.0798569	5.0978245	-3.3124637
H	-1.2611641	4.8259930	-3.9654254
C	-4.2394334	-2.4561619	-1.5965276
C	-3.6055226	-4.5136558	1.4977321
H	-3.8971037	-3.8375595	0.7093566
H	-0.0691712	5.2088434	-1.5000946
C	-4.2029880	2.5330901	1.6560019
C	-3.8611937	1.6619241	-2.4668417
H	-4.4936995	2.4835235	-2.7519527
C	-3.5249436	4.5769804	-1.4608455
H	-3.8246525	3.9124609	-0.6652018
C	-4.1961428	5.7777540	-1.6466647
H	-5.0146587	6.0356942	-0.9869645
C	-0.3469318	3.0106525	-1.8440301
C	-1.7296359	2.9447989	-2.0931342
C	-3.8176097	6.6385920	-2.6709941
C	-4.3047399	-5.6994470	1.6809174
H	-5.1343854	-5.9341051	1.0260142
C	-4.5502936	-3.5373310	-2.4265691
H	-3.8461383	-3.8387225	-3.1898565
C	-5.1654284	2.1445962	0.7193978
H	-4.9576801	1.3065780	0.0715531
C	-5.1762545	-2.0548465	-0.6392964
H	-4.9373006	-1.2353069	0.0218333
C	-5.7568008	-4.2104732	-2.2877671
H	-5.9845181	-5.0417085	-2.9427216
C	-6.3543696	2.8479602	0.5810820
H	-7.0755928	2.5381536	-0.1647686
C	-6.6096297	3.9532680	1.3847052
H	-7.5340776	4.5060054	1.2758879
C	-6.6709646	-3.8167960	-1.3162451
H	-7.6078839	-4.3473477	-1.2043840
C	-6.3770855	-2.7345970	-0.4941543
H	-7.0776909	-2.4239836	0.2703613
N	1.9250643	0.4605916	1.9554495
N	0.4720631	-1.9423221	1.8385682
N	0.5063129	1.9556681	-1.8184411

N	1.9576407	-0.5083665	-1.8985029
C	0.4053887	2.9975765	1.8592681
C	-2.4518209	-1.7062155	2.2220514
C	0.3469318	-3.0106525	-1.8440301
C	-4.1747591	-0.2762359	2.4167406
C	-1.7703669	-2.9153770	2.1255299
C	0.2990054	-4.2271590	1.6033989
H	0.0691712	-5.2088434	-1.5000946
H	-2.4663388	6.9518939	-4.3125466
C	-2.5263025	-4.1819680	2.3200739
C	-4.4820526	3.6333988	2.4726686
C	0.3747131	4.2335174	-1.5873007
H	-4.3436676	7.5729732	-2.8197720
C	-3.9382104	-6.5770337	2.6951142
C	-5.6706024	4.3389808	2.3355671
C	2.9771004	-0.4184552	2.0162125
C	2.4518209	1.7062155	2.2220514
C	1.7210991	-2.4862089	1.6467799
C	1.7627049	2.4664325	-1.6195763
C	3.0052075	0.3508164	-1.9473588
C	2.4554008	-1.7564903	-2.1623655
C	1.7703669	2.9153770	2.1255299
C	-3.8468818	-1.5836430	2.5578518
C	1.7296359	-2.9447989	-2.0931342
H	-5.1290784	0.1884737	2.5945323
H	-0.1589425	-5.1971912	1.5256411
C	1.6066432	-3.9116267	1.4525581
C	-2.1694183	-5.0713084	3.3376594
H	-3.7613823	3.9307011	3.2223171
C	1.6764995	3.8960699	-1.4301084
C	-2.8686047	-6.2569666	3.5244953
H	-4.4822448	-7.5016839	2.8404136
H	-5.8665715	5.1880669	2.9782356
C	2.9203654	-1.7892163	1.7582108
C	4.1747591	0.2762359	2.4167406
C	3.8468818	1.5836430	2.5578518
C	2.9473581	1.7372255	-1.7091906
C	4.2058306	-0.3585678	-2.3209842
C	3.8611937	-1.6619241	-2.4668417
C	2.5263025	4.1819680	2.3200739
H	-4.4833269	-2.3955502	2.8630955
C	2.4556744	-4.2237343	-2.2881314
H	2.4174051	-4.5807262	1.2298622
H	-1.3418686	-4.8217305	3.9887291
H	2.4958172	4.5481934	-1.1902286
H	-2.5805324	-6.9292100	4.3229201
C	4.2029880	-2.5330901	1.6560019
H	5.1290784	-0.1884737	2.5945323
H	4.4833269	2.3955502	2.8630955
C	4.2394334	2.4561619	-1.5965276
H	5.1715060	0.0896930	-2.4753720
H	4.4936995	-2.4835235	-2.7519527
C	2.1694183	5.0713084	3.3376594
C	3.6055226	4.5136558	1.4977321
C	2.0798569	-5.0978245	-3.3124637
C	3.5249436	-4.5769804	-1.4608455
C	5.1654284	-2.1445962	0.7193978
C	4.4820526	-3.6333988	2.4726686
C	4.5502936	3.5373310	-2.4265691
C	5.1762545	2.0548465	-0.6392964
H	1.3418686	4.8217305	3.9887291
C	2.8686047	6.2569666	3.5244953
C	4.3047399	5.6994470	1.6809174
H	3.8971037	3.8375595	0.7093566
H	1.2611641	-4.8259930	-3.9654254

C	2.7605048	-6.2922866	-3.5061705
H	3.8246525	-3.9124609	-0.6652018
C	4.1961428	-5.7777540	-1.6466647
H	4.9576801	-1.3065780	0.0715531
C	6.3543696	-2.8479602	0.5810820
H	3.7613823	-3.9307011	3.2223171
C	5.6706024	-4.3389808	2.3355671
H	3.8461383	3.8387225	-3.1898565
C	5.7568008	4.2104732	-2.2877671
C	6.3770855	2.7345970	-0.4941543
H	4.9373006	1.2353069	0.0218333
H	2.5805324	6.9292100	4.3229201
C	3.9382104	6.5770337	2.6951142
H	5.1343854	5.9341051	1.0260142
H	2.4663388	-6.9518939	-4.3125466
C	3.8176097	-6.6385920	-2.6709941
H	5.0146587	-6.0356942	-0.9869645
H	7.0755928	-2.5381536	-0.1647686
C	6.6096297	-3.9532680	1.3847052
H	5.8665715	-5.1880669	2.9782356
H	5.9845181	5.0417085	-2.9427216
C	6.6709646	3.8167960	-1.3162451
H	7.0776909	2.4239836	0.2703613
H	4.4822448	7.5016839	2.8404136
H	4.3436676	-7.5729732	-2.8197720
H	7.5340776	-4.5060054	1.2758879
H	7.6078839	4.3473477	-1.2043840
O	0.0000000	-0.0000000	-3.5504645

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Fe	0.0000000	0.0000000	-1.9010374
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N	-1.9267322	-0.4685103	1.9808187
N	0.0000000	-0.0000000	0.0041284
N	-0.5149516	-1.9554469	-1.8316078
C	-3.0088268	-0.3446496	-1.9517462
C	-2.9811599	0.4075912	2.0434065
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