Electronic Supplementary Material (ESI) for Chemical Communications.

Supporting Information

Intermetal oxygen atom transfer from an $Fe^{V}O$ complex to a Mn^{III} complex: an experimental and theoretical approach

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Experimental Section

Materials. Commercially available chemicals were used without further purification unless otherwise indicated. Solvents were dried according to published procedures and distilled under Ar prior to use.[S1] Commercially available *meta*-chloroperoxybenzoic acid (*m*-CPBA, 55%) was purified by washing with phosphate buffer (pH 7.4) followed by water and was then dried under reduced pressure.[S1] The purity of *m*-CPBA was 94% based on the ratio of *m*-CPBA and *m*-CBA (*meta*-chlorobenzoic acid) in ^{1}H NMR spectrum.[S2]
$Na(H_2O)_x[Fe^{III}(TAML)(H_2O)]$ complex and TAML-H_4 ligand was purchased from Colin Horwitz, GreenOx Catalysts. Inc. The commercial complex was recrystallized from an isopropanol/H2O mixture for further use.[S3] $^{18}O_2$ (95% ^{18}O-enriched) and $H_2{}^{18}O$ (95% ^{18}O-enriched) were purchased from ICON Services Inc. (Summit, NJ, USA). Iron(V)-oxo complex, $[(TAML)Fe^{V}(O)]^{-}$ (**1**), manganese(V)-oxo complex, $[(TAML)Mn^{V}(O)]^{-}$ (**4**), μ-oxo bridged iron(IV) dimer complex, $[(TAML)_2Fe_2^{IV}(\mu\text{-}O)]^{2-}$ (**5**) and manganese(III) complex, $[Li(CH_3OH)_2][Mn^{III}(TAML)(CH_3OH)]$ was prepared according to the literature.[S4-S6]

Instrumentation. UV-Vis spectra were recorded on a Hewlett Packard Agilent 8453 UV-visible spectrophotometer equipped with a circulating water bath or with a UNISOKU cryostat system (USP-203; UNISOKU, Japan) for low-temperature experiments or on a UNISOKU RSP-601 stopped-flow spectrometer equipped with a MOS-type highly sensitive photodiode-array. Electrospray ionization mass (ESI-MS) spectra were collected on a Thermo Finnigan (San Jose, CA, USA) LCQ^{TM} Advantage MAX quadrupole ion trap instrument, by infusing samples directly into the source at 20 μL/min using a syringe pump. The spray voltage was set at 4.7 kV and the capillary temperature at 100 °C. Electron paramagnetic resonance (EPR) spectra were taken at 5.0 K using a X-band Bruker EMX-plus spectrometer equipped with a dual mode cavity (ER 4116DM). Low temperatures were achieved and controlled with an Oxford Instruments ESR900 liquid He quartz cryostat with an Oxford Instruments ITC503 temperature and gas flow controller. The experimental parameters for EPR spectra were as follows: Microwave frequency = 9.646 GHz, microwave power = 1.0 mW, modulation amplitude = 10 G, gain = 1×10^4, modulation frequency = 100 kHz, time constant = 40.96 ms and conversion time = 85.00 ms.

Reactivity Studies and Product Analysis. Reactions were run in a 1-cm UV cuvette and followed by monitoring UV-vis spectral changes of reaction solutions. Overall reaction rate constant and second-order rate constant (k_2) of the reaction between **5** and $[(TAML)Mn^{III}]^-$ (**3**) were determined under pseudo-first-order conditions (e.g., [substrate]/[**1** or **5**] > 10) by fitting the changes in absorbance at 830 nm due to **5** and compared in order to determine the rate-determining step of the intermetal oxygen atom transfer (OAT) reaction. The initial fast reaction traces such as the reaction between **1** and $[(TAML)M^{III}]^-$ (M = Fe or Mn) prior to the formation of **5**, were determined under second-order conditions, where both concentrations of **1** and $[(TAML)M^{III}]^-$ were maintained as the same (0.10 mM), because the OAT reaction rate from **1** to $[(TAML)M^{III}]^-$ were too fast to follow under pseudo-first-order conditions even with stopped-flow equipment. To explore the effect of ionic strength in the OAT reaction, the OAT reaction rates were determined with and without addition of tetrabutylammonium hexafluorophosphate (0.10 M, $TBAPF_6$). It has been confirmed that the OAT reaction rates didn't changed upon addition of $TBAPF_6$ suggesting that the effect of ionic strength was not pronounced in the present case. Moreover, due to fact that the charges did not change in the course of the reaction, especially, in polar-organic solvents, the ionic strength was constant in the course of the OAT reaction. The kinetic experiments were run at least in triplicate, and the data reported represent the average of these reactions. To determine the activation parameters, temperature-dependent kinetic experiments were performed with **5** and **3**.

Products formed in the intermetal OAT reaction from **1** to **3** were analyzed by UV-vis, ESI-MS, and EPR spectroscopic methods. Knowing the extinction coefficients of **4** (430 nm; ε = 4000 M^{-1} cm^{-1}) and $[(TAML)Fe^{III}]^-$ (**2**) (385 nm; ε = 6800 M^{-1} cm^{-1}), quantitative yields were determined by comparing the extinction coefficients obtained after the completion of the OAT reaction. The OAT reactions from **1** to **3** was titrated by the successive addition of **3** (0.10 – 0.60 equiv) to the solution of **1** (0.10 mM) in CH_3CN at –40 °C. The titration data were obtained by monitoring UV-vis spectral changes at 630 nm due to **1** and 830 nm due to **5**, respectively.

EPR measurements for the reaction of **1** (0.50 mM) with **3** were performed in CH_3CN at –40 °C. The EPR samples of the reaction solution were taken over time. Negative mode ESI-MS spectra taken after the completion of the reaction, exhibited two prominent peaks at *m/z*

of 426.1 and 441.1 due to **2** and **4**, respectively, which clearly indicated that the intermetal OAT reaction from **1** to **3** occurred with quantitative yield.

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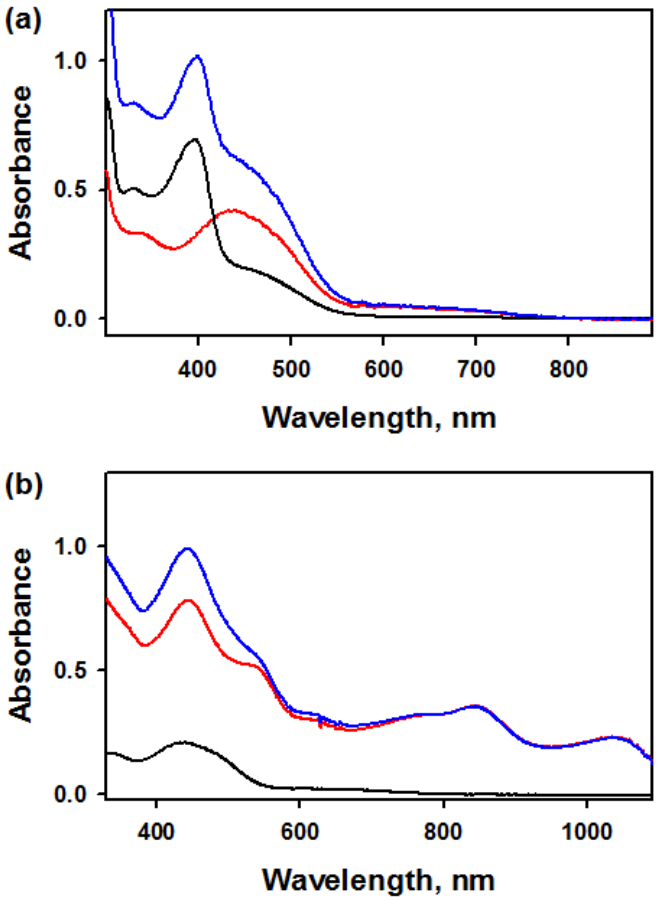

Figure S1. Simulated UV-vis spectra obtained from the sum (blue line) of (a) the spectra of **2** (0.10 mM, black line) and **4** (0.10 mM, red line) and (b) the spectra of **5** (0.05 mM, red line) and **4** (0.05 mM, black line).

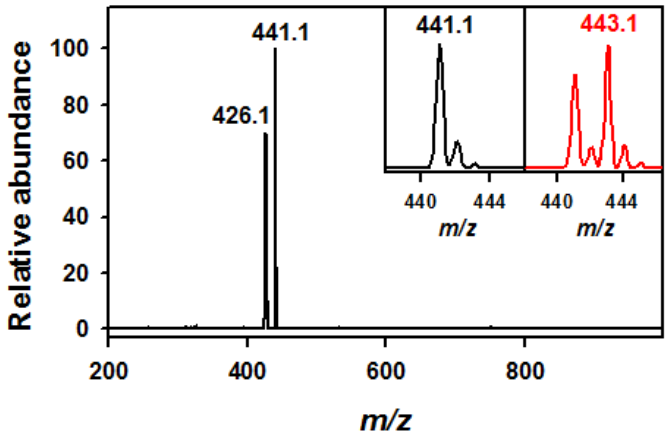

Figure S2. Negative mode ESI-MS spectrum obtained in the reaction of **1** (0.10 mM) and **3** (0.10 mM) in CH_3CN at –40 °C. The peaks at *m/z* of 426.1 and 441.1 correspond to **2** (calculated *m/z* of 426.1) and **4** (calculated *m/z* of 441.1), respectively. Insets show the observed isotopic distribution patterns for **4**-^{16}O (left panel) and **4**-^{18}O (right panel, obtained in the reaction with **1**-^{18}O and **3** in CH_3CN at –40 °C).

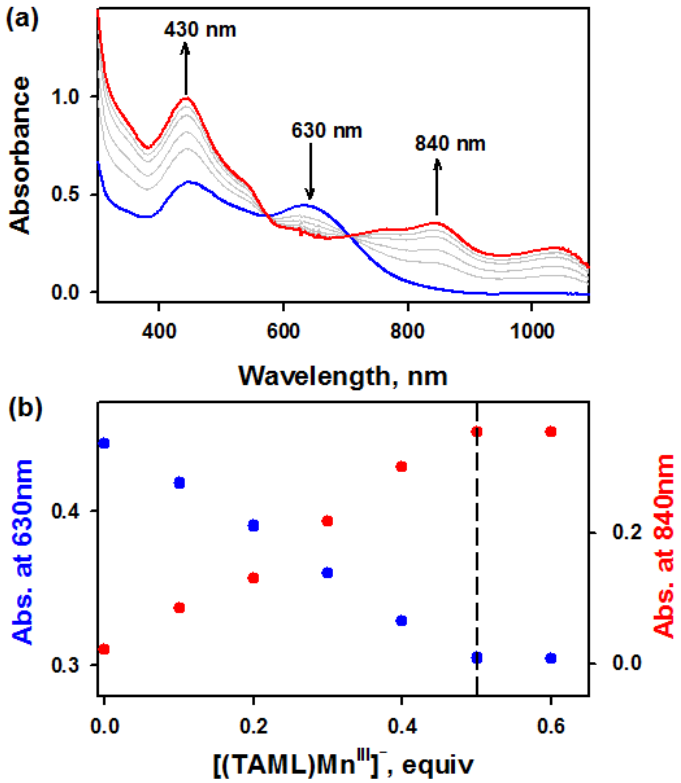

Figure S3. (a) UV-vis spectral changes showing the formation of **5** (red line) and disappearance of **1** (0.10 mM, blue line) upon addition of **3** to **1** in increment of 0.1 equiv in CH_3CN at –40 °C. (b) Plot of absorbance changes at 630 nm due to **1** (blue dot) and 840 nm due to **5** (red dot) against the equivalents of **3** added to **1** in CH_3CN at –40 °C.

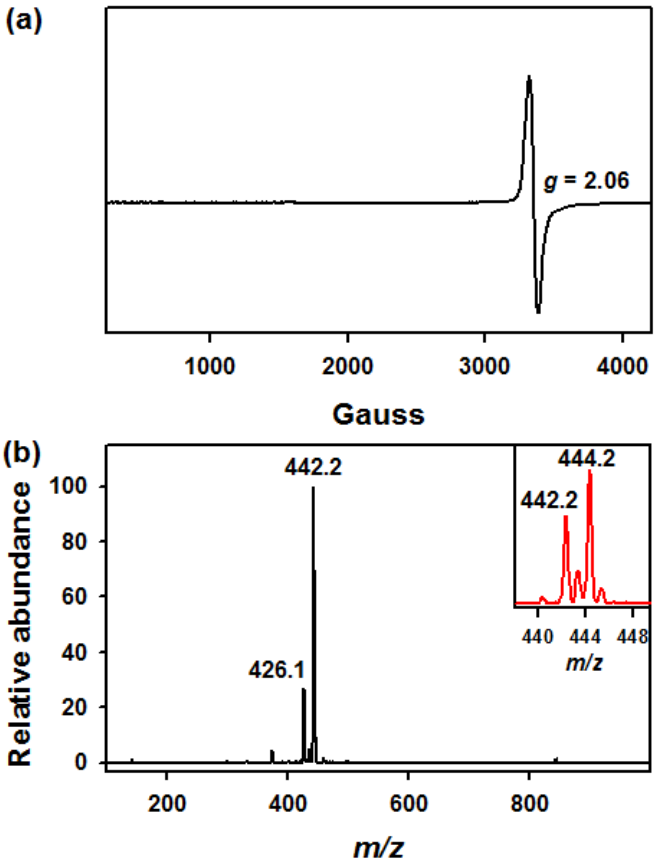

Figure S4. (a) X-band EPR spectrum of **1** (0.50 mM) at 5.0 K. (b) Negative mode ESI-MS of **1** (0.10 mM) in CH_3CN at –40 °C. The peaks at *m/z* of 426.1 and 442.2 correspond to **2** (calculated *m/z* of 426.1) and **1** (calculated *m/z* of 442.1), respectively. Insets show the observed isotopic distribution patterns for **1**-^{18}O in CH_3CN at –40 °C.[S2]

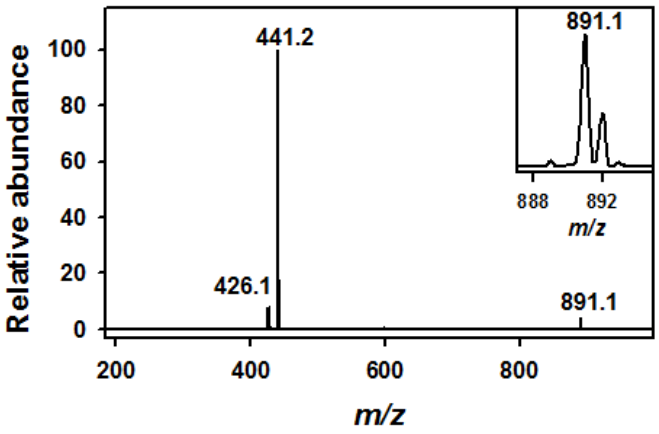

Figure S5. Negative mode ESI-MS obtained in the reaction of **1** (0.05 mM) and **3** (0.05 mM) in CH_3CN at –40 °C. The peaks at *m/z* of 426.1, 441.2 and 891.1 correspond to **2** (calculated *m/z* of 426.1), **4** (calculated *m/z* of 442.1) and $[(TAML)_2Fe_2^{IV}(O)Na]^-$ (calculated *m/z* of 891.1) respectively. Insets show the observed isotopic distribution patterns for $[(TAML)_2Fe_2^{IV}(O)Na]^-$ in CH_3CN at –40 °C.

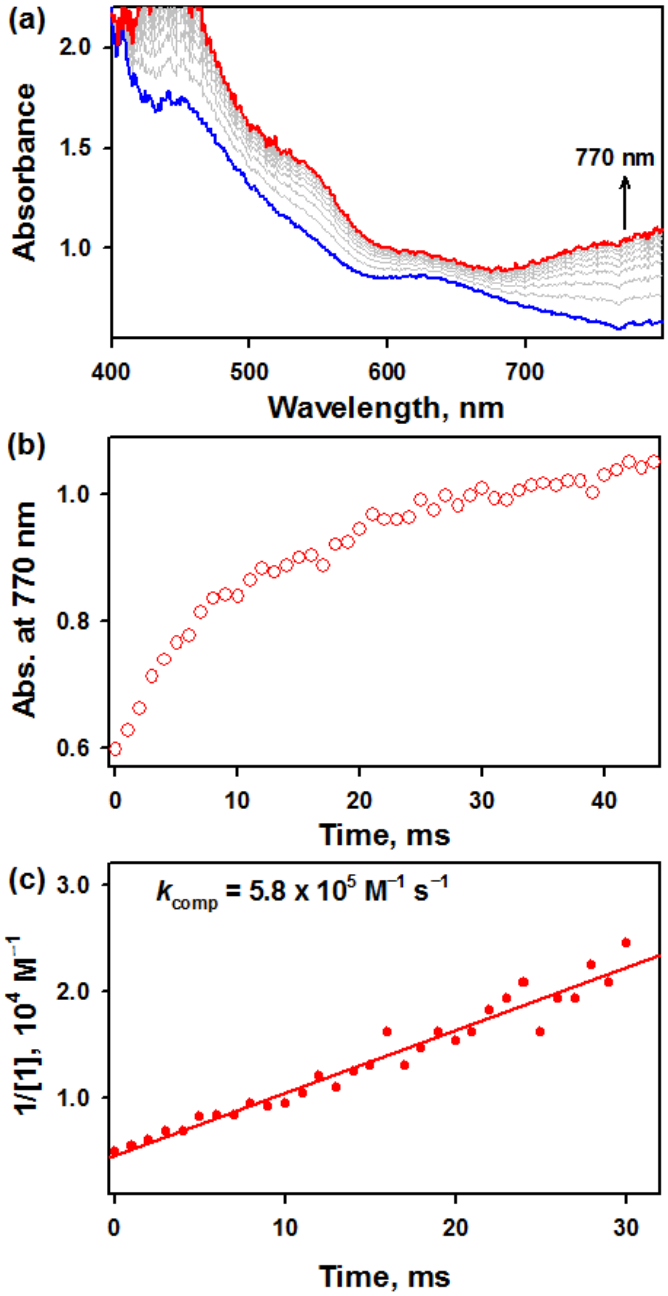

Figure S6. (a) UV-vis spectral changes showing the formation of **5** (red line) and disappearance of **1** (0.20 mM, blue line) upon addition of **2** (0.20 mM) in CH_3CN at –40 °C. (b) Time course monitored at 770 nm due to the formation of **5**. (c) Plot of 1/[**1**] against time to determine the comproportionation reaction rate (k_{comp}) in the reaction of **1** with **2** in CH_3CN at –40 °C.

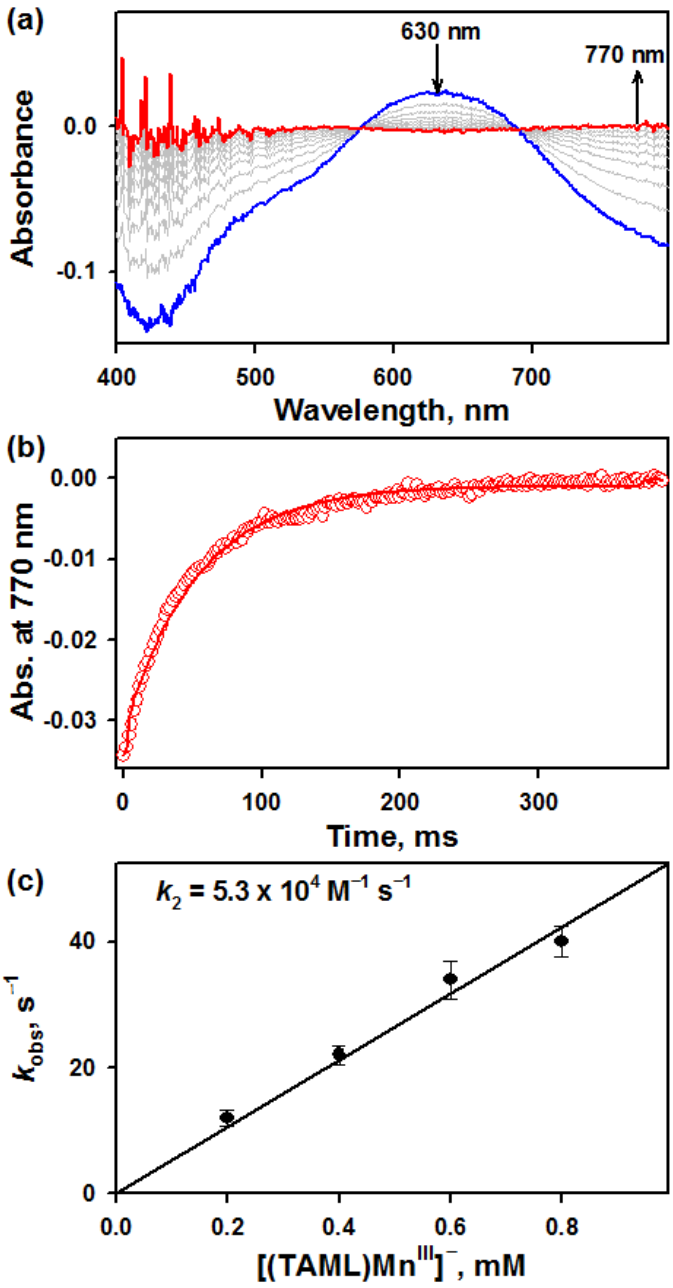

Figure S7. (a) UV-vis spectral changes showing the formation of **5** (red line) and disappearance of **1** (0.02 mM, blue line) upon addition of **3** (0.20 mM) in CH_3CN at –40 °C. (b) Time course monitored at 770 nm due to the formation of **5**. (c) Plot of pseudo-first order rate constants (k_{obs}) against the concentration of **3** to determine the second-order rate constant (k_2) in the OAT reaction between **1** and **3** in CH_3CN at –40 °C.

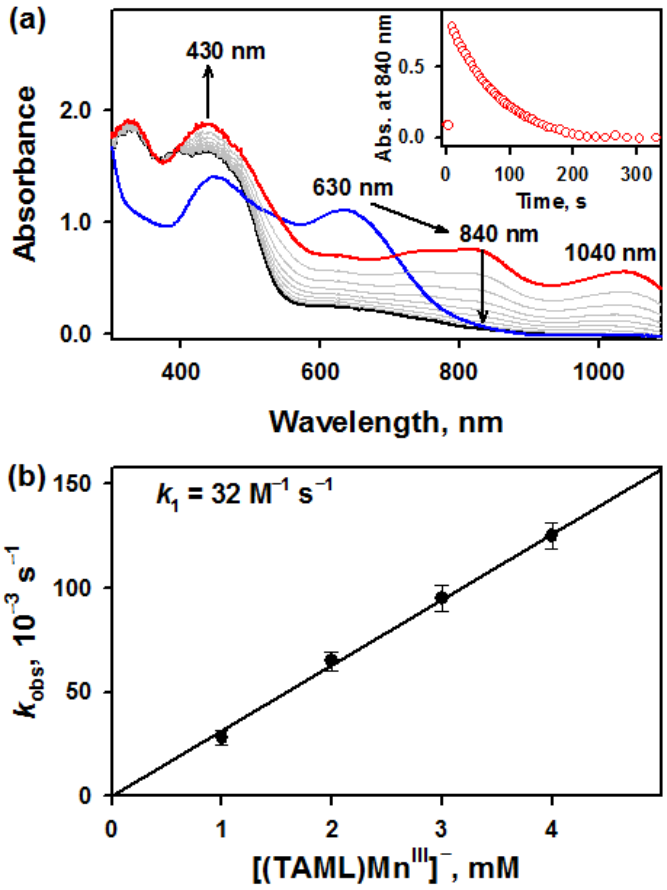

Figure S8. (a) UV-vis spectral changes observed in the reaction of **1** (0.20 mM, blue line) upon addition of **3** (1.0 mM) in CH_3CN at –40 °C. Inset shows the time course monitored at 840 nm due to the disappearance of **5** (red line). (b) Plot of pseudo-first order rate constants (k_{obs}) against the concentration of **3** to determine k_1 in the OAT reaction between **3** and **5** in CH_3CN at –40 °C.

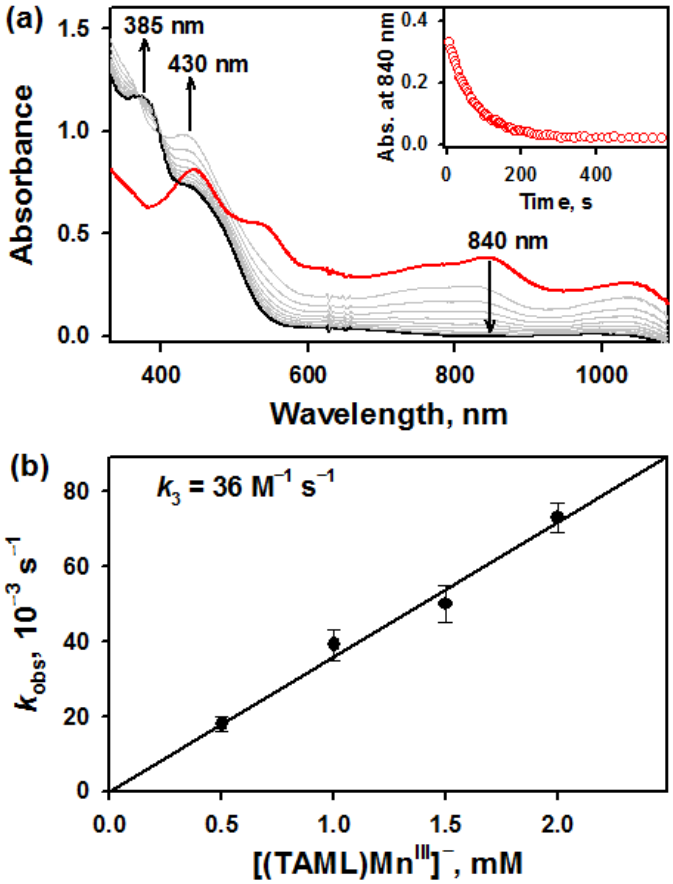

Figure S9. (a) UV-vis spectral changes observed in the reaction of **5** (0.05 mM, red line) upon addition of **3** (0.50 mM) in CH_3CN at –40 °C. Inset shows the time course monitored at 840 nm due to the disappearance of **5**. (b) Plot of pseudo-first order rate constants (k_{obs}) against the concentration of **3** to determine k_3 in the OAT reaction between **3** and **5** in CH_3CN at –40 °C.

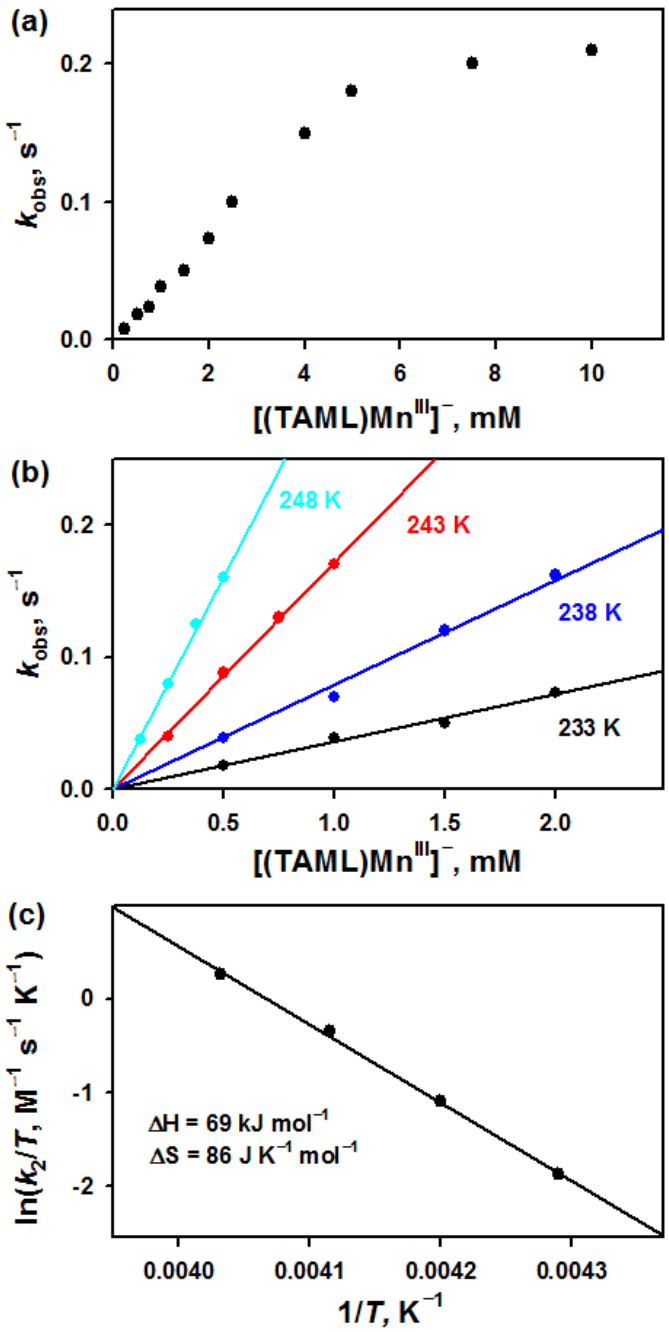

Figure S10. (a) Pseudo-first-order rate constants (k_{obs}) against **3** concentrations in the OAT reaction from **5** to **3** in CH_3CN at –40 °C. (b) Plots of k_{obs} against **3** concentrations in the OAT reaction from **5** to **3** in CH_3CN at different temperatures. (c) Eyring plots of ln(k_2/T) against 1/T in the OAT reactions from **5** to **3** to determine the thermodynamic parameters in CH_3CN at -40 °C.

Density Functional Theory Section

Geometry optimizations and energy evaluation. Density functional theory (DFT)[S7] calculations were performed using the BP86 functional[S8,S9] as implemented in the Gaussian 09 (G09) package.[S10] The geometries were optimized using the Def2-SVP basis set.[S11] The stationary points were confirmed by frequency calculations, and the transition states were connected with the ground states on both sides by performing IRC calculations and continuing relaxing the geometry down to the ground state from the end geometry obtained by IRC. The high molecular charge (2+) made it necessary to perform the optimizations in solvent to avoid artificial results (*vide infra*).[S12] Solvent (acetonitrile) effects were included using CPCM model[S13] with UFF cavity, per G09 default. Single-point energy evaluations on the optimized geometry were done with the Def2-TZVPP basis set.[S11] This resulting electronic energy (ΔE) was used throughout the text as the final energy due to sufficient accuracy (*vide infra*). MECP was found using a shell program to G09 that iterates to the same energy and geometry for two different electron configurations.[S14]

Functional and basis set evaluations. In a previous study, we noticed that a standard B3LYP[S8,S15]/LACVP (i.e. ECP basis set on Fe as tweaked by Jaguar and 6-31G on others)[S16] did not reproduce the correct electron configuration for low-spin **1**.[S2] This scheme yielded an antiferromagnetic coupled (TAML$^{\bullet+}$)Fe^{IV}O species, which was not seen by experiments. We found out that the quality of the geometry optimization would be the key to obtaining the correct electronic configuration, and that BP86/LACVP would be sufficient for this.[S2] We also found recently that B3LYP/Def2-SVP would be sufficient as well. For the current study, we have one additional benchmark; the crystal structure of species **5**.[S17] The crystal structure imply an $S = 0$ symmetrical Fe-O-Fe structure, where each of the Fe-O bonds are at 1.73Å. Using the B3LYP/Def2-SVP combination, the structure yielded an asymmetrical structure with Fe-O bonds of 1.70 Å and 1.91 Å (Table S18). This stems from a preference for an uneven spin density distribution of 1.57 and -2.57 on each of the iron centre (Table S12). Using BP86/Def2-SVP however, the obtained structure is symmetric with both Fe-O distances being 1.73 Å (Table S17), and the spins are equal but of opposite sign (±1.28, Table S11). Thus, we concluded that BP86/Def2-SVP would yield the most reliable geometry and electronic structure, and chose the BP86/Def2-TZVPP//BP86/Def2-SVP calculations as our primary source of information. However, we have also done B3LYP/Def2-TZVPP//B3LYP/Def2-SVP calculations which we present below (*vide infra*). While the individual numbers are different, it should be noted that this scheme does in fact not change any of the major conclusions drawn in the paper.

Free Energy Calculations. Free energy calculations were done and presented in the ESI tables below, albeit not used in the text (*vide infra*). Dispersion effects were added using DFT-D3 program with Becke-Johnson cutoff.[S18] In previous trials, we have found that using gas-phase optimizations in HAT reactions for highly charged species such as the current system (2+) can cause a hydride transfer (i.e. one proton and two electrons) rather than a net hydrogen atom transfer from the substrate to the metal-oxo species, possibly due to self-interaction errors (SIE). Most of the time, performing optimizations in solvent avoids these artificial results;[S12] hence the solvent effects were included during optimizations. However, in doing so, other problems may arise. Adding thermal contributions then becomes in principle inaccurate since the standard solvent models are parameterized to yield good solvation free energies and not any other property. This means that thermal effects are already included, to a certain extent, in the obtained electronic energies, hence possibly double counting the thermal contributions[S19] (the same consideration applies to the dispersion correction as well). On the other hand, gas-phase frequency calculations on the so obtained structure may not be meaningful either since the structure may not be in a stationary point without the solvent. This leaves us in principle with no easily available options to calculate in a uniform manner the free energies and at the same time avoid SIE, for highly charged systems, unless one is prepared to enlarge the model system to include counter ions,[S20] which may be more time consuming and sometimes leading to 'reactions' between the transition metal complex and the counter ions, which may or may not be realistic.

Assuming though that the above described errors are negligible in the cases where no hydride transfers are seen, the free energies (ΔG) can still be calculated by adding zero-point vibration energy (ΔZ_0), thermal corrections to Z_0 (ΔE(Thermal)) and entropy ($-T\Delta S$). Relatively recent consensus is that dispersion effects are needed as well (ΔDisp). Also, if the energy of separated reactants in solvent is evaluated, there is a correction factor of $RT \bullet \ln(24.5)$ due to change of standard states (either subtracted from the complexed states or added to the non-complexed states, depending on the reference state).[S21] Each of these "corrections" are plagued by its own error margins, and at least in our type of systems, we have frequently observed resulting ΔG that are not consistent with experiments. We chose therefore to base our discussions on ΔE values without any correction factors (except for solvent modeling, which is included by default on all calculations) due to its simplicity, both in calculation and analysis. Its accuracy is proven by many, many early days DFT ΔE calculations that gave surprisingly good agreement with experiments without any corrections (albeit possibly due to fortuitous cancelation of these "corrections"). Our approach is ultimately validated by the good agreement with experiments, typically within the expected error margins (3-5 kcal mol^{-1}). We do however list the calculated ΔG as well below.

B3LYP results vs BP86. While we consider the B3LYP results less accurate in the current study specifically due to mismatch to experiments (*vide supra*), it is of interest to know exactly how much the difference is. The Mulliken spin density distributions indicate that B3LYP has a preference of making ligand TAML radicals when possible (Table S10 and S12). Different spin distribution often leads to different geometries, which in turn affects energies. As shown in the energy graph in Fig. S11, the B3LYP calculated potential energy surface resembles the one calculated for BP86, but conceptual differences do exist. While the BP86 graph identify the first intermediate formation in the reaction of **1** with **3** as the rate-limiting step (4.2 kcal mol^{-1}), the B3LYP energies implicate the MECP as the *de facto* rate-limiting transition state, with the $S = 1/2$ intermediate (on the reactant side) being more stable than the $S = 3/2$ state. Hence, the total energy barrier is calculated as the difference between the MECP and the $S = 1/2$ intermediate (11.6 kcal mol^{-1}), which should correspond to k_2. As in the case of BP86, the comproportionation reaction also occurs without a barrier on the $S = 1$ surface (Fig. S12), with a potential rate-limiting barrier of 0.7 kcal mol^{-1}. The rate-limiting barrier is taken as the difference between the $S = 1 \rightarrow S = 0$ MECP and the $S = 1$ dimer (Fig. S12b). The reverse reaction, i.e. the disproportionation reaction, goes against a complexation energy of 6.3 kcal mol^{-1} (Table S6 and Fig. 12b). Considering that the highest point in the reaction of **1** with **3** is the MECP (6.8 kcal mol^{-1}), it adds to the rate-limiting barrier starting from **5**, and therefore the rate-limiting barrier becomes 6.3 + 6.8 = 13.1 kcal mol^{-1}. Hence, even with B3LYP, the conclusion is that $k_{comp} > k_2 > k_1$.

Effects of dispersion on geometry optimizations. Although dispersion effects[S18] were included in the free energy calculations below, its effect on the quality of the geometry optimizations were investigated as well. The results for selected structures are shown in Table S19. The RMSD of the both geometries (with or without dispersion) for structures **1**-**4** was in the range of 0.037 - 0.052 Å (Table S19). For representative intermediate di-metal complexes, the range was 0.271 – 0.347 Å (with H) or 0.217 – 0.263 Å (without H). The absolute metal-oxygen distance fluctuations were in the range 0.01 – 0.05 Å. Hence, we do not find dispersion effects being significant for the current investigation.

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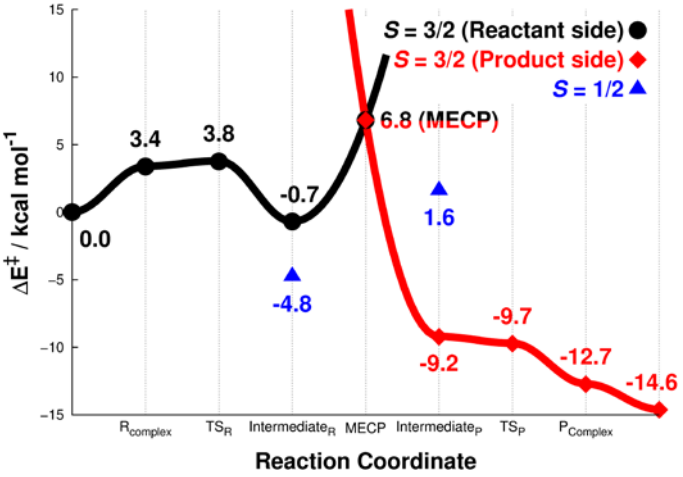

Figure S11. The reaction energy profile for the reaction of **1** with **3**, calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level. The potential rate limiting step in this particular graph would be the energy difference between the lowest intermediate on the reactant side (*S* = 1/2, -4.8 kcal mol^{-1}) and minimum energy crossing point (MECP, 6.8 kcal mol^{-1}), i.e. 11.6 kcal mol^{-1}.

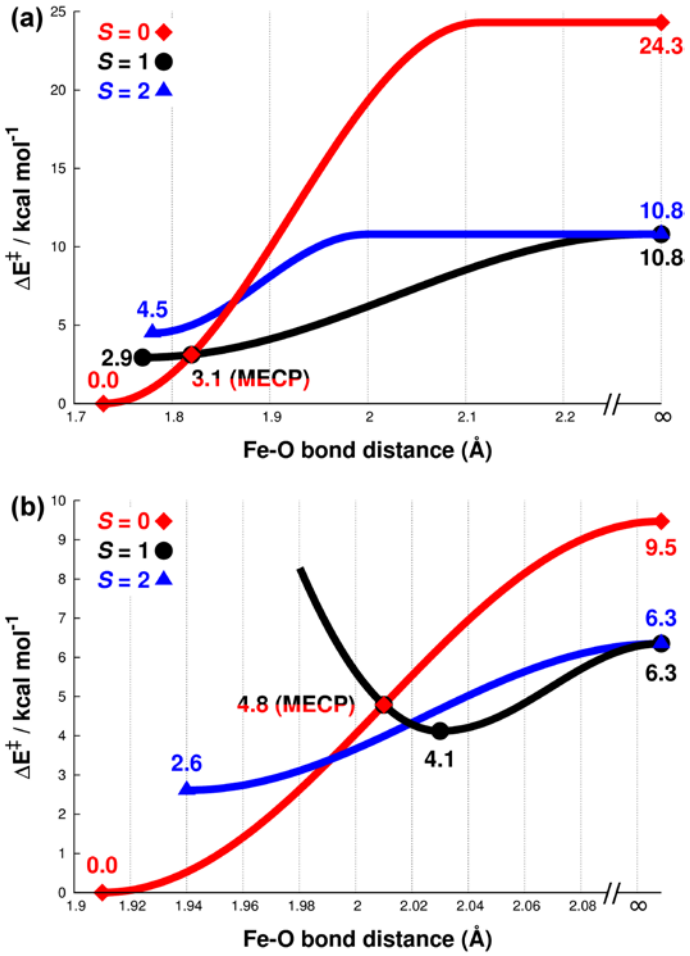

Figure S12. The reaction energy profile for the reaction of **1** with **2**, calculated at a) BP86/Def2-TZVPP//BP86/Def2-SVP level and b) B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level. The x-axis features the Fe-O distance between the iron in **2** and the oxo atom in **1**, and goes toward infinite separation. Thus, the complexation energy is the energy shown at infinite separation, which should correspond to the disproportionation rate k_3. Calculated minimum energy crossing point (MECP) between the S = 0 and 1 states are also shown.

Table S1. Relative Energies of constituent species calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*[a]**	ΔZ_0	Δ*E*(Thermal)[b]	-*T*Δ*S*[b]	ΔDisp	**Δ*G*[c]**
[(TAML)Fe^{V}O]$^{-}$ (1)								
S = 1/2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 3/2	14.01	-0.51	**13.49**	-0.74	+0.13	-0.63	+0.20	**12.45**
[(TAML)Fe^{III}]$^{-}$ (2)								
S = 1/2	10.31	+0.10	**10.40**	-0.36	+0.06	+0.14	-0.10	**10.14**
S = 3/2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 5/2	31.52	+0.30	**31.82**	-1.28	+0.35	-1.21	+0.50	**30.19**
[(TAML)Mn^{III}]$^{-}$ (3)								
S = 0	27.79	+0.10	**27.88**	+0.24	-0.12	+1.27	-0.34	**28.93**
S = 1	22.89	+0.15	**23.04**	-0.17	-0.03	+0.37	-0.19	**23.01**
S = 2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
[(TAML)Mn^{V}O]$^{-}$ (4)								
S = 0	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 1	19.37	-1.01	**18.36**	-0.85	+0.18	-0.73	+0.28	**17.24**

[a] Sum of the two previous columns. [b] *T* = 298.15 K. [c] Sum of the five previous columns, not considered in this study, see "Free energy calculations" section above.

Table S2. Relative Energies of constituent species calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*[a]**	ΔZ_0	Δ*E*(Thermal)[b]	-*T*Δ*S*[b]	ΔDisp	**ΔG**[c]
[(TAML)$Fe^{V}O$]$^{-}$ (1)								
S = 1/2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 3/2	2.76	+0.36	**3.12**	-0.88	+0.24	-1.40	+0.37	**1.45**
[(TAML)Fe^{III}]$^{-}$ (2)								
S = 1/2	20.31	+1.24	**21.55**	-0.38	-0.04	+0.55	-0.09	**21.60**
S = 3/2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 5/2	24.19	-0.87	**23.32**	-1.17	+0.26	-0.64	+0.34	**22.12**
[(TAML)Mn^{III}]$^{-}$ (3)								
S = 0	43.80	+0.55	**44.35**	+0.47	-0.19	+1.59	-0.48	**45.74**
S = 1	30.15	+0.02	**30.17**	+0.14	-0.11	+0.79	-0.24	**30.76**
S = 2	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
[(TAML)$Mn^{V}O$]$^{-}$ (4)								
S = 0	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	**0.00**
S = 1	14.38	-1.40	**12.98**	-1.01	+0.21	-0.86	+0.37	**11.69**

[a] Sum of the two previous columns. [b] *T* = 298.15 K. [c] Sum of the five previous columns, not considered in this study, see "Free energy calculations" section above.

Table S3. Relative Energies of **1** reacting with **3** calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*** [a]	ΔZ_0	Δ*E*(Thermal) [b]	-*T*Δ*S* [b]	ΔDisp	ΔCplx [b,c]	**Δ*G*** [d]
***S* = 3/2**									
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
1 + **3** (complex)	0.68	+1.87	**2.55**	+0.63	+0.77	+10.95	-10.32	-1.89	**2.68**
TS_R	1.16	+3.07	**4.23**	+0.46	+0.26	+13.12	-15.86	-1.89	**0.31**
$Intermediate_R$	-12.14	+5.26	**-6.89**	+0.78	+0.29	+15.32	-29.04	-1.89	**-21.42**
MECP (Reactant side) [e]	-12.01	+5.20	**-6.81**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
MECP (Product side) [e]	-11.99	+5.21	**-6.78**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
$Intermediate_P$	-21.97	+5.77	**-16.20**	+1.67	+0.19	+15.08	-31.94	-1.89	**-33.10**
TS_P	-18.09	+4.14	**-13.95**	+1.55	-0.07	+14.30	-22.37	-1.89	**-22.43**
2 + **4** (complex)	-18.19	+3.73	**-14.46**	+1.60	+0.53	+11.50	-20.14	-1.89	**-22.87**
2 (*S* = 3/2) + **4** (*S* = 0) (separated)	-19.86	+1.04	**-18.82**	+0.86	-0.21	+0.63	-4.27	+0.00	**-21.81**
***S* = 1/2**									
$Intermediate_R$	-14.97	+5.43	**-9.53**	+1.13	+0.14	+16.55	-30.50	-1.89	**-24.12**
$Intermediate_P$	-13.29	+5.60	**-7.69**	+1.33	+0.12	+16.24	-32.71	-1.89	**-24.61**
***S* = 5/2**									
Intermediate	-11.49	+5.11	**-6.38**	+0.49	+0.41	+14.89	-28.73	-1.89	**-21.22**

[a] Sum of the two previous columns. [b] T = 298.15 K. [c] Correction for change of standard state for complexation in solvent. [d] Sum of the six previous columns, see "Free energy calculations" section above. [e] The MECP geometries and Def2-SVP energies are the same (within convergence errors) for both the S = 3/2 states. The Def2-TZVPP energies are slightly different as this is an Def2-SVP optimized MECP. The value used in the text is -6.79 kcal mol^{-1}, which is the average Def2-TZVPP value. [f] Frequency calculations not possible since MECP is not in a stationary state in the respective electron configurations.

Table S4. Relative Energies of **1** reacting with **3** calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*** [a]	ΔZ_0	Δ*E*(Thermal) [b]	-*T*Δ*S* [b]	ΔDisp	ΔCplx [b,c]	**Δ*G*** [d]
***S* = 3/2**									
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
1 + **3** (complex)	-0.89	+4.27	**3.38**	-0.08	+0.86	+11.76	-12.91	-1.89	**1.11**
TS_R	-0.80	+4.54	**3.75**	-0.06	+0.29	+13.63	-13.54	-1.89	**2.16**
$Intermediate_R$	-8.07	+7.38	**-0.69**	+0.78	+0.38	+15.43	-23.02	-1.89	**-9.01**
MECP (Reactant side) [e]	-0.32	+6.99	**6.67**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
MECP (Product side) [e]	-0.33	+7.29	**6.96**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
$Intermediate_P$	-15.81	+6.60	**-9.22**	+1.94	+0.31	+14.31	-26.73	-1.89	**-21.28**
TS_P	-15.07	+5.33	**-9.73**	+1.60	-0.01	+14.23	-22.34	-1.89	**-18.15**
2 + **4** (complex)	-16.24	+3.51	**-12.74**	+1.64	+0.55	+11.73	-15.44	-1.89	**-16.16**
2 (*S* = 3/2) + **4** (*S* = 0) (separated)	-15.55	+0.94	**-14.62**	+1.19	-0.30	+1.08	-4.06	+0.00	**-16.71**
***S* = 1/2**									
$Intermediate_R$	-11.90	+7.14	**-4.76**	+0.52	+0.38	+15.86	-24.62	-1.89	**-14.52**
$Intermediate_P$	-5.86	+7.45	**1.60**	+1.03	+0.25	+16.13	-27.68	-1.89	**-10.57**
***S* = 5/2**									
$Intermediate_R$*	-11.70	+7.00	**-4.70**	+0.37	+0.44	+15.07	-25.85	-1.89	**-16.58**

[a] Sum of the two previous columns. [b] *T* = 298.15 K. [c] Correction for change of standard state for complexation in solvent. [d] Sum of the six previous columns, see "Free energy calculations" section above. [e] The MECP geometries and Def2-SVP energies are the same (within convergence errors) for both the *S* = 3/2 states. The Def2-TZVPP energies are slightly different as this is an Def2-SVP optimized MECP. The the average Def2-TZVPP value is 6.81 kcal mol^{-1}. [f] Frequency calculations not possible since MECP is not in a stationary state in the respective electron configurations.

Table S5. Relative Energies of **1** reacting with **2** calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*** [a]	ΔZ_0	Δ*E*(Thermal) [b]	-*T*Δ*S* [b]	ΔDisp	ΔCplx [b,c]	**Δ*G*** [d]
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	16.30	-5.49	**10.80**	-1.40	+0.01	-17.64	+25.58	+1.89	**19.25**
5 (*S* = 0)	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
MECP (*S* = 0) [e]	3.43	-0.37	**3.07**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
MECP (*S* = 1) [e]	3.46	-0.29	**3.17**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
5 (*S* = 1)	3.15	-0.21	**2.94**	-0.30	+0.15	-1.41	-2.19	+0.00	**-0.81**
5 (*S* = 2)	4.74	-0.23	**4.50**	-0.75	+0.31	-2.26	+1.89	+0.00	**3.69**

[a] Sum of the two previous columns. [b] *T* = 298.15 K. [c] Correction for change of standard state for complexation in solvent. [d] Sum of the six previous columns, see "Free energy calculations" section above. [e] The MECP geometries and Def2-SVP energies are the same (within convergence errors) for both the spin states. The Def2-TZVPP energies are slightly different as this is an Def2-SVP optimized MECP. The value used in the text is 3.12 kcal mol^{-1}, which is the average Def2-TZVPP value. [f] Frequency calculations not possible since MECP is not in a stationary state in the respective electron configurations.

Table S6. Relative Energies of **1** reacting with **2** calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level in kcal mol^{-1}

	ΔDef2-SVP	ΔDef2-TZVPP	**Δ*E*** [a]	ΔZ_0	Δ*E*(Thermal) [b]	-*T*Δ*S* [b]	ΔDisp	ΔCplx [b,c]	**Δ*G*** [d]
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	13.52	-7.17	**6.35**	-0.37	-0.51	-15.23	+22.78	+1.89	**14.91**
5 (*S* = 0)	0.00	+0.00	**0.00**	+0.00	+0.00	+0.00	+0.00	+0.00	**0.00**
MECP (*S* = 0) [e]	4.50	+0.46	**4.97**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
MECP (*S* = 1) [e]	4.52	+0.09	**4.61**	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]	---- [f]
5 (*S* = 1)	4.08	+0.04	**4.12**	+0.15	-0.03	-0.13	-1.13	+0.00	**2.98**
5 (*S* = 2)	2.57	+0.04	**2.61**	-0.36	+0.09	-0.98	+0.02	+0.00	**1.38**

[a] Sum of the two previous columns. [b] *T* = 298.15 K. [c] Correction for change of standard state for complexation in solvent. [d] Sum of the six previous columns, see "Free energy calculations" section above. [e] The MECP geometries and Def2-SVP energies are the same (within convergence errors) for both the spin states. The Def2-TZVPP energies are slightly different as this is an Def2-SVP optimized MECP. The average Def2-TZVPP value is 4.79 kcal mol^{-1}. [f] Frequency calculations not possible since MECP is not in a stationary state in the respective electron configurations.

Table S7. Mulliken spin density distribution of constituent species calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level

	M (Mn or Fe)	O	4 x N	Rest
[(TAML)Fe^{V}O]$^{-}$ (1)				
S = 1/2	0.71	0.28	0.01	0.00
S = 3/2	1.91	0.63	0.10	0.36
[(TAML)Fe^{III}]$^{-}$ (2)				
S = 1/2	1.02	----	-0.04	0.02
S = 3/2	2.71	----	0.05	0.24
S = 5/2	4.01	----	0.59	0.40
[(TAML)Mn^{III}]$^{-}$ (3)				
S = 0	-0.03	----	0.01	0.02
S = 1	2.19	----	-0.18	0.00
S = 2	3.93	----	-0.19	0.26
[(TAML)Mn^{V}O]$^{-}$ (4)				
S = 0	0.00	0.00	0.00	0.00
S = 1	1.87	0.13	-0.12	0.12

Table S8. Mulliken spin density distribution of constituent species calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level

	M (Mn or Fe)	O	4 x N	Rest
[(TAML)Fe^{V}O]$^{-}$ (1)				
S = 1/2	0.81	0.23	-0.02	-0.02
S = 3/2	1.43	0.57	0.37	0.62
[(TAML)Fe^{III}]$^{-}$ (2)				
S = 1/2	1.68	----	-0.43	-0.26
S = 3/2	2.88	----	-0.03	0.15
S = 5/2	4.17	----	0.59	0.24
[(TAML)Mn^{III}]$^{-}$ (3)				
S = 0	-0.02	----	0.00	0.02
S = 1	2.13	----	-0.17	0.04
S = 2	4.02	----	-0.20	0.18
[(TAML)Mn^{V}O]$^{-}$ (4)				
S = 0	0.00	0.00	0.00	0.00
S = 1	2.16	-0.04	-0.16	0.05

Table S9. Mulliken spin density distribution of **1** reacting with **3** calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level

	[(TAML)Fe]			Bridge	[(TAML)Mn]		
	Fe	4 x N	Rest	O	Mn	4 x N	Rest
***S* = 3/2**							
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	-0.71	-0.01	0.00	-0.28	3.93	-0.19	0.26
1 + **3** (complex)	-0.71	-0.01	0.00	-0.27	3.94	-0.20	0.26
TS_R	-0.70	-0.01	0.00	-0.27	3.92	-0.20	0.26
$Intermediate_R$	-0.03	0.05	0.12	-0.19	2.94	-0.10	0.20
MECP (Reactant side)	0.03	0.05	0.12	-0.18	2.88	-0.10	0.20
MECP (Product side)	1.69	0.16	0.21	-0.10	0.92	0.01	0.11
$Intermediate_P$	2.37	0.13	0.26	-0.06	0.22	0.04	0.05
TS_P	2.69	0.04	0.25	0.00	0.01	0.00	0.00
2 + **4** (complex)	2.70	0.04	0.25	0.00	0.01	0.00	0.00
2 (*S* = 3/2) + **4** (*S* = 0) (separated)	2.71	0.05	0.24	0.00	0.00	0.00	0.00
***S* = 1/2**							
$Intermediate_R$	-1.30	-0.10	-0.11	-0.08	2.59	-0.12	0.12
$Intermediate_P$	1.06	0.15	0.15	-0.01	-0.32	0.01	-0.04
***S* = 5/2**							
Intermediate	1.73	0.14	0.19	0.01	2.84	-0.09	0.19

Table S10. Mulliken spin density distribution of **1** reacting with **3** calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level

	[(TAML)Fe]			Bridge	[(TAML)Mn]		
	Fe	4 x N	Rest	O	Mn	4 x N	Rest
***S* = 3/2**							
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	-0.81	0.02	0.02	-0.23	4.02	-0.20	0.18
1 + **3** (complex)	-1.26	0.29	0.44	-0.47	4.02	-0.21	0.17
TS_R	-1.27	0.30	0.46	-0.47	4.02	-0.21	0.17
$Intermediate_R$	-1.33	0.31	0.55	-0.39	3.88	-0.17	0.15
MECP (Reactant side)	-0.82	0.31	0.55	-0.06	3.07	-0.13	0.09
MECP (Product side)	2.59	-0.32	-0.46	0.09	1.11	-0.01	0.01
$Intermediate_P$	2.81	0.00	0.15	-0.02	0.04	0.01	0.01
TS_P	2.86	-0.03	0.15	0.00	0.01	0.00	0.00
2 + **4** (complex)	2.89	-0.04	0.14	0.00	0.00	0.00	0.00
2 (*S* = 3/2) + **4** (*S* = 0) (separated)	2.88	-0.03	0.15	0.00	0.00	0.00	0.00
***S* = 1/2**							
$Intermediate_R$	-1.52	-0.07	-0.06	-0.21	3.62	-0.43	-0.32
$Intermediate_P$	2.62	-0.32	-0.47	-0.04	-0.78	0.01	-0.03
***S* = 5/2**							
Intermediate	2.59	-0.32	-0.45	0.18	3.07	-0.14	0.07

Table S11. Mulliken spin density distribution of **1** reacting with **2** calculated at BP86/Def2-TZVPP//BP86/Def2-SVP level

	[(TAML)Fe^{V}O]$^{-}$ (**1**)^{a}				[(TAML)Fe^{III}]$^{-}$ (**2**)		
	Fe	4 x N	Rest	O	Fe	4 x N	Rest
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	0.71	0.01	0.00	0.28	2.71	0.05	0.24
5 (*S* = 0)	-1.28	-0.09	-0.10	0.00	1.28	0.09	0.10
MECP (*S* = 0)	-1.22	-0.11	-0.14	-0.05	1.29	0.11	0.12
MECP (*S* = 1)	-0.20	0.05	0.11	-0.14	1.83	0.13	0.22
5 (*S* = 1)	-0.07	0.06	0.12	-0.12	1.66	0.14	0.21
5 (*S* = 2)	1.62	0.15	0.19	0.07	1.62	0.15	0.19

[a] **1** is here defined as the sub-compound containing the iron with the shortest distance to the bridging O.

Table S12. Mulliken spin density distribution of **1** reacting with **2** calculated at B3LYP/Def2-TZVPP//B3LYP/Def2-SVP level

	[(TAML)Fe^{V}O]$^{-}$ (**1**)^{a}				[(TAML)Fe^{III}]$^{-}$ (**2**)		
	Fe	4 x N	Rest	O	Fe	4 x N	Rest
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	0.81	-0.02	-0.02	0.23	2.88	-0.03	0.15
5 (*S* = 0)	-1.57	-0.04	-0.04	-0.14	2.57	-0.32	-0.46
MECP (*S* = 0)	-1.45	-0.25	-0.40	-0.31	2.67	-0.14	-0.11
MECP (*S* = 1)	-1.37	0.31	0.55	-0.33	2.71	0.00	0.13
5 (*S* = 1)	-1.38	0.31	0.55	-0.33	2.72	0.00	0.13
5 (*S* = 2)	1.87	0.00	0.02	0.26	2.62	-0.32	-0.46

[a] **1** is here defined as the sub-compound containing the iron with the shortest distance to the bridging O.

Table S13. Selected geometries of constituent species calculated at BP86/Def2-SVP level in Å

	M - O	M – N_1	M – N_2	M – N_3	M – N_4
[(TAML)$Fe^{V}O$]$^{-}$ (1)					
S = 1/2	1.60	1.87	1.91	1.87	1.92
S = 3/2	1.65	1.91	1.91	1.90	1.90
[(TAML)Fe^{III}]$^{-}$ (2)					
S = 1/2	----	1.86	1.86	1.86	1.87
S = 3/2	----	1.87	1.88	1.87	1.88
S = 5/2	----	2.03	1.96	2.03	1.96
[(TAML)Mn^{III}]$^{-}$ (3)					
S = 0	----	1.90	1.89	1.89	1.88
S = 1	----	1.91	1.91	1.89	1.88
S = 2	----	1.92	1.90	1.92	1.90
[(TAML)$Mn^{V}O$]$^{-}$ (4)					
S = 0	1.56	1.90	1.90	1.91	1.91
S = 1	1.61	1.95	1.90	1.94	1.88

Table S14. Selected geometries of constituent species calculated at B3LYP/Def2-SVP level in Å

	M - O	M – N_1	M – N_2	M – N_3	M – N_4
[(TAML)$Fe^{V}O$]$^{-}$ (1)					
S = 1/2	1.57	1.86	1.90	1.86	1.92
S = 3/2	1.63	1.93	1.93	1.89	1.89
[(TAML)Fe^{III}]$^{-}$ (2)					
S = 1/2	----	1.87	1.88	1.87	1.88
S = 3/2	----	1.87	1.88	1.87	1.88
S = 5/2	----	2.01	1.96	2.01	1.97
[(TAML)Mn^{III}]$^{-}$ (3)					
S = 0	----	1.89	1.89	1.89	1.89
S = 1	----	1.91	1.91	1.90	1.89
S = 2	----	1.92	1.91	1.92	1.91
[(TAML)$Mn^{V}O$]$^{-}$ (4)					
S = 0	1.53	1.89	1.89	1.91	1.91
S = 1	1.59	1.94	1.89	1.94	1.88

Table S15. Selected geometries of **1** reacting with **3** calculated at BP86/Def2-SVP level in Å and °

	Fe-O	Mn-O	Fe-Mn	Fe-O-Mn	Fe-N(avg)	Mn-N(avg)
***S* = 3/2**						
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	1.60	∞	∞	∞	1.89	1.91
1 + **3** (complex)	1.60	3.65	5.18	158.76	1.89	1.91
TS_R	1.61	3.13	4.65	157.67	1.89	1.92
$Intermediate_R$	1.71	1.81	3.46	159.31	1.91	1.94
MECP	1.73	1.79	3.46	159.70	1.91	1.94
$Intermediate_P$	2.02	1.62	3.59	161.32	1.91	1.91
TS_P	2.94	1.57	4.48	167.96	1.88	1.91
2 + **4** (complex)	3.12	1.56	4.65	167.08	1.88	1.91
2 (*S* = 3/2) + **4** (*S* = 0) (separated)	∞	1.56	∞	∞	1.87	1.90
***S* = 1/2**						
$Intermediate_R$	1.74	1.76	3.42	156.57	1.91	1.94
$Intermediate_P$	1.85	1.66	3.44	157.13	1.90	1.92
***S* = 5/2**						
Intermediate	1.79	1.80	3.51	156.41	1.91	1.93

Table S16. Selected geometries of **1** reacting with **3** calculated at B3LYP/Def2-SVP level in Å and °

	Fe-O	Mn-O	Fe-Mn	Fe-O-Mn	Fe-N(avg)	Mn-N(avg)
***S* = 3/2**						
1 (*S* = 1/2) + **3** (*S* = 2) (separated)	1.57	∞	∞	∞	1.89	1.91
1 + **3** (complex)	1.61	3.46	4.90	147.62	1.90	1.92
TS_R	1.62	3.26	4.77	153.78	1.90	1.92
$Intermediate_R$	1.66	2.09	3.68	157.74	1.91	1.95
MECP	1.87	1.73	3.55	160.08	1.92	1.94
$Intermediate_P$	2.31	1.57	3.84	162.19	1.90	1.90
TS_P	2.81	1.55	4.31	163.48	1.88	1.90
2 + **4** (complex)	3.57	1.53	5.02	157.27	1.88	1.90
2 (*S* = 3/2) **+ 4** (*S* = 0) (separated)	∞	1.53	∞	∞	1.88	1.90
***S* = 1/2**						
$Intermediate_R$	1.70	1.93	3.54	154.17	1.91	1.96
$Intermediate_P$	1.96	1.67	3.55	156.33	1.92	1.93
***S* = 5/2**						
Intermediate	1.91	1.77	3.60	155.98	1.93	1.94

Table S17. Selected geometries of **1** reacting with **2** calculated at BP86/Def2-SVP level in Å and °

	Fe_1-O[a]	Fe_2-O	Fe_1-Fe_2	Fe_1-O-Fe_2	Fe_1-N(avg)[a]	Fe_2-N(avg)
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	1.60	∞	∞	∞	1.89	1.87
5 (*S* = 0)	1.73	1.73	3.39	156.78	1.91	1.91
MECP (*S* = 0, 1)	1.69	1.82	3.37	162.43	1.90	1.92
5 (*S* = 1)	1.71	1.77	3.43	160.30	1.91	1.91
5 (*S* = 2)	1.78	1.78	3.49	157.51	1.91	1.91

[a] Fe_1 is here defined as the iron with the shortest distance to the bridging O.

Table S18. Selected geometries of **1** reacting with **2** calculated at B3LYP/Def2-SVP level in Å and °

	Fe_1-O	Fe_2-O	Fe_1-Fe_2	Fe_1-O-Fe_2	Fe_1-N(avg)	Fe_2-N(avg)
1 (*S* = 1/2) + **2** (*S* = 3/2) (separated)	1.57	∞	∞	∞	1.89	1.88
5 (*S* = 0)	1.70	1.91	3.52	155.07	1.91	1.93
MECP (*S* = 0, 1)	1.67	2.01	3.60	157.08	1.91	1.92
5 (*S* = 1)	1.66	2.03	3.61	156.23	1.91	1.92
5 (*S* = 2)	1.73	1.94	3.59	156.64	1.91	1.93

[a] Fe_1 is here defined as the iron with the shortest distance to the bridging O.

Table S19. Comparison of geometries obtained with and without dispersion (BP86/Def2-SVP/D3-BJ) in Å.

	Fe-O (Without dispersion)	Fe-O (With dispersion)	Mn-O (Without dispersion)	Mn-O (With dispersion)	**Total RMSD (without H)**	**Total RMSD (with H)**
***S* = 3/2**						
1 (*S* = 1/2)	1.60	1.60	----	----	**0.041**	**0.052**
3 (*S* = 2)	----	----	----	----	**0.030**	**0.047**
$Intermediate_R$	1.71	1.70	1.81	1.76	**0.217**	**0.271**
$Intermediate_P$	2.02	2.05	1.62	1.60	**0.257**	**0.347**
2 (*S* = 3/2)	----	----	----	----	**0.042**	**0.048**
4 (*S* = 0)	----	----	1.56	1.56	**0.025**	**0.037**
***S* = 1/2**						
$Intermediate_R$	1.74	1.72	1.76	1.74	**0.247**	**0.309**
	Fe_1-O (Without dispersion)	Fe_1-O (With dispersion)	Fe_2-O (Without dispersion)	Fe_2-O (With dispersion)	**Total RMSD (without H)**	**Total RMSD (with H)**
***S* = 0**						
5 (BP86)	1.73	1.71	1.73	1.71	**0.263**	**0.333**
5 (B3LYP)	1.70	1.68	1.91	1.93	**0.187**	**0.236**

Coordinates

Coordinates are given in xyz-format with charge/multiplicity given in parenthesis at the comment line.

BP86

51
Species 1 (-1/2)
Fe 0.01927 -0.00343 -0.01665
O 0.06906 0.03949 1.58274
N -0.00629 1.77802 -0.57296
N -1.85825 0.15504 -0.34055
N -0.24475 -1.76305 -0.59060
N 1.86896 0.06436 -0.54416
C -1.26579 2.40601 -0.55186
C 1.20850 2.40095 -0.78599
C -2.57816 -0.98569 -0.54837
C -2.33375 1.46523 -0.40345
C 0.75604 -2.71014 -0.70280
C -1.66044 -2.21569 -0.74555
C 2.40132 1.42925 -0.76644
C 2.73795 -0.98123 -0.54476
C 2.18305 -2.38996 -0.19777
O 1.34622 3.61507 -0.97220
O -3.81170 -1.06348 -0.64228
O 0.51184 -3.86369 -1.09672
O 3.96433 -0.86459 -0.75482
C -1.95936 -2.73107 -2.17531
C -2.03974 -3.26061 0.32789
C 3.33045 1.86853 0.39193
C 3.10339 1.57748 -2.13958
C -1.55117 3.78383 -0.68599
C -2.89183 4.20912 -0.66352
C -3.67545 1.90683 -0.39409
C -3.94305 3.28140 -0.52117
C 3.14908 -3.45069 -0.76340
C 2.15952 -2.51039 1.35713
H -0.72273 4.49246 -0.80193
H -3.11574 5.28390 -0.75568
H -4.47803 1.16531 -0.29319
H -4.98735 3.63245 -0.50472
H -1.64399 -1.98080 -2.92988
H -1.42326 -3.67747 -2.36518
H -3.05242 -2.88609 -2.27572
H -1.49514 -4.20833 0.16170
H -1.80060 -2.87896 1.34200
H -3.13119 -3.44750 0.27470
H 2.80771 1.75934 1.36447
H 4.23779 1.23614 0.39856
H 3.61607 2.93178 0.26201
H 4.02989 0.97686 -2.15724
H 2.43459 1.23008 -2.95441
H 3.33859 2.64689 -2.31276
H 2.83009 -4.46272 -0.45158
H 3.17284 -3.42656 -1.87192
H 4.17239 -3.25077 -0.39595
H 3.18783 -2.37356 1.75153
H 1.50141 -1.74770 1.81786
H 1.80589 -3.51924 1.65561

51
Species 1 (-1/4)
Fe 0.02338 -0.02663 -0.12815
O -0.12526 0.14000 1.50572
N 0.02313 1.84299 -0.52971
N -1.83786 0.15236 -0.53050
N -0.23878 -1.84685 -0.60904
N 1.86391 0.06137 -0.60102
C -1.23255 2.43248 -0.44205
C 1.23456 2.44530 -0.76734
C -2.55257 -0.99532 -0.77191
C -2.30421 1.45873 -0.44360
C 0.75119 -2.79300 -0.64535
C -1.65327 -2.25749 -0.84672
C 2.40578 1.43037 -0.84182
C 2.71047 -1.01406 -0.64133
C 2.16817 -2.38554 -0.13734
O 1.40867 3.66079 -0.92623
O -3.77887 -1.05269 -0.93295
O 0.55287 -3.97666 -0.98349
O 3.90791 -0.92959 -0.97928
C -1.85548 -2.84512 -2.26571
C -2.13565 -3.23903 0.24574
C 3.43153 1.82022 0.24686
C 3.00813 1.57263 -2.26195
C -1.53622 3.81457 -0.39928
C -2.87853 4.21917 -0.36449
C -3.65106 1.89253 -0.40401
C -3.92603 3.26729 -0.36719
C 3.16614 -3.48622 -0.53978
C 2.09248 -2.30628 1.41685
H -0.71189 4.53909 -0.40197
H -3.11820 5.29370 -0.32642
H -4.45090 1.14101 -0.41064
H -4.97284 3.60844 -0.33147
H -1.48603 -2.13388 -3.03352
H -1.30049 -3.79527 -2.36260
H -2.93674 -3.01657 -2.43886
H -1.57489 -4.18982 0.17321
H -1.97528 -2.80086 1.25244
H -3.21870 -3.43684 0.11634
H 2.98367 1.70554 1.25544
H 4.32458 1.17176 0.17336
H 3.73111 2.87907 0.11326
H 3.89889 0.92639 -2.35777
H 2.26332 1.27325 -3.02849
H 3.28531 2.63144 -2.43717
H 2.83366 -4.46200 -0.13858
H 3.24306 -3.57949 -1.64171
H 4.17217 -3.24625 -0.14751
H 3.09508 -2.07327 1.83312
H 1.37957 -1.52494 1.75194
H 1.76748 -3.28441 1.82963

50
Species 2 (-1/2)
Fe -0.47073 4.33293 -0.27085
O -3.77643 3.40687 1.73432
N 0.91838 4.18638 0.95594
O 3.22110 4.49151 1.19526
O 1.30031 6.17213 -3.40106
N -2.04291 4.57447 -1.24239
N -1.55098 3.80070 1.14560
N 0.79412 5.00822 -1.46416
C -3.30031 4.38871 -0.45658
C -2.91486 3.79072 0.93270
C -0.86825 3.46864 2.32716
C 0.55241 3.69228 2.21878
C 2.17489 4.57777 0.53947
C 2.15330 5.22254 -0.88180
C 0.52043 5.47327 -2.72463
C -0.81163 4.97745 -3.38283
C -2.11216 5.07823 -2.51658
O -3.15480 5.51095 -3.04528
C -0.61231 3.46810 -3.71826
H 0.27019 3.33382 -4.37881
H -1.50226 3.07212 -4.25146
H -0.45848 2.86923 -2.79919
C -1.03104 5.75384 -4.69313
H -0.15036 5.64233 -5.35352
H -1.17510 6.83622 -4.50205
H -1.93434 5.37873 -5.21038
C 3.25129 4.54497 -1.72947
H 3.00723 3.47501 -1.89630
H 4.21905 4.60105 -1.19196
H 3.34184 5.04667 -2.71082
C 2.46633 6.72673 -0.67404
H 2.51772 7.23771 -1.65311
H 3.43231 6.83864 -0.14106
H 1.67220 7.20498 -0.06286
C 1.39270 3.42622 3.32356
H 2.47139 3.60402 3.22467
C 0.82941 2.93959 4.51724
H 1.48514 2.72774 5.37719
C -0.55973 2.71907 4.62242
H -0.98450 2.33505 5.56396
C -1.41419 2.98162 3.53621
H -2.49757 2.81661 3.59952
C -4.26684 3.40506 -1.15042
H -4.64250 3.84048 -2.09508
H -5.11956 3.18771 -0.47648
H -3.75069 2.44897 -1.37782
C -4.00413 5.73799 -0.16159
H -3.30325 6.43590 0.34287
H -4.87289 5.57071 0.50704
H -4.34350 6.19676 -1.10846

50
Species 2 (-1/4)
Fe -0.47190 4.34098 -0.27446
O -3.79023 3.44610 1.74731
N 0.93312 4.18360 0.95289
O 3.22492 4.53721 1.20762
O 1.29089 6.18430 -3.41303
N -2.05546 4.59064 -1.24692
N -1.56316 3.78972 1.14277
N 0.80041 5.02799 -1.46979
C -3.30615 4.40757 -0.45282
C -2.92098 3.80614 0.93830
C -0.86518 3.45359 2.32145
C 0.55347 3.67839 2.21398
C 2.17697 4.59811 0.54588
C 2.15389 5.24369 -0.87844
C 0.52084 5.47868 -2.73164
C -0.80950 4.96184 -3.38396
C -2.11613 5.08125 -2.52368
O -3.15348 5.51829 -3.06033
C -0.60684 3.44785 -3.68891
H 0.27892 3.30074 -4.34246
H -1.49364 3.03969 -4.21833
H -0.45645 2.86088 -2.76129
C -1.02583 5.71115 -4.71031
H -0.14358 5.58607 -5.36634
H -1.17024 6.79703 -4.54195
H -1.92774 5.32538 -5.22225
C 3.25602 4.56943 -1.72333
H 3.01562 3.49863 -1.89044
H 4.22138 4.62839 -1.18170
H 3.34865 5.07063 -2.70500
C 2.46023 6.74892 -0.67386
H 2.51375 7.25795 -1.65412
H 3.42322 6.86440 -0.13617
H 1.66207 7.22604 -0.06692
C 1.39255 3.40064 3.31430
H 2.47081 3.58198 3.21437
C 0.83254 2.90109 4.50751
H 1.49151 2.68167 5.36324
C -0.55349 2.68071 4.61199
H -0.98014 2.28832 5.54936
C -1.40793 2.95576 3.52526
H -2.49214 2.79372 3.58669
C -4.27934 3.42847 -1.14365
H -4.65718 3.86518 -2.08709
H -5.12955 3.21496 -0.46521
H -3.76824 2.47008 -1.37302
C -4.00253 5.76043 -0.15991
H -3.29767 6.45649 0.34171
H -4.86999 5.59802 0.51168
H -4.34166 6.21866 -1.10750

50
Species 2 (-1/6)
Fe -0.40823 3.78091 -0.58623
O -3.77670 3.49776 1.76949
N 0.96996 3.96490 0.88904
O 3.19096 4.59222 1.24043
O 1.20036 6.30605 -3.36130
N -2.10387 4.40907 -1.33523
N -1.54869 3.54417 1.07451
N 0.88955 4.86778 -1.56987
C -3.29277 4.37410 -0.45563
C -2.89562 3.72412 0.92044
C -0.85888 3.31830 2.26685
C 0.56806 3.55607 2.16148
C 2.16709 4.52387 0.53636
C 2.15261 5.20951 -0.87947
C 0.52917 5.44719 -2.75489
C -0.80336 4.91069 -3.42275
C -2.11306 5.05045 -2.54332
O -3.08810 5.67014 -3.01323
C -0.60496 3.40814 -3.76433
H 0.27077 3.27282 -4.43327
H -1.50108 3.00393 -4.28034
H -0.43134 2.77909 -2.86625
C -1.02363 5.68004 -4.73643
H -0.14338 5.56476 -5.39786
H -1.16954 6.76129 -4.55054
H -1.92414 5.29885 -5.25551
C 3.36619 4.70352 -1.68984
H 3.26120 3.62005 -1.90754
H 4.29659 4.85501 -1.10707
H 3.43657 5.25296 -2.64877
C 2.27759 6.72947 -0.59689
H 2.32422 7.28762 -1.55016
H 3.19112 6.92050 0.00103
H 1.40032 7.08731 -0.01787
C 1.38443 3.39857 3.30616
H 2.46087 3.59289 3.20799
C 0.81256 3.01035 4.53254
H 1.45907 2.88512 5.41664
C -0.57363 2.78152 4.63534
H -1.01221 2.47765 5.60002
C -1.40904 2.93616 3.51285
H -2.49340 2.77299 3.57415
C -4.41925 3.53435 -1.09644
H -4.79122 4.03356 -2.01217
H -5.25267 3.41386 -0.37597
H -4.04326 2.52585 -1.36827
C -3.80099 5.79580 -0.10021
H -2.98263 6.39343 0.35388
H -4.62795 5.72203 0.63415
H -4.15027 6.31060 -1.01421

50
Species 3 (-1/1)
Mn -0.44364 4.09767 -0.37661
O -3.77275 3.48157 1.76682
N 0.94636 4.05489 0.91243
O 3.21301 4.52712 1.21430
O 1.26509 6.21792 -3.37661
N -2.05259 4.51340 -1.27163
N -1.54194 3.68914 1.10984
N 0.81330 4.95169 -1.48982
C -3.29446 4.38594 -0.45357
C -2.90541 3.78308 0.93461
C -0.85586 3.40763 2.31045
C 0.56403 3.61552 2.19705
C 2.17664 4.54250 0.53442
C 2.14889 5.21394 -0.87702
C 0.51518 5.46246 -2.73153
C -0.80967 4.95317 -3.40260
C -2.11324 5.05481 -2.53191
O -3.14399 5.52869 -3.04573
C -0.60553 3.45052 -3.75888
H 0.27682 3.32717 -4.42169
H -1.49511 3.05910 -4.29597
H -0.44804 2.83024 -2.85366
C -1.02956 5.74241 -4.70506
H -0.14894 5.63764 -5.36695
H -1.17532 6.82220 -4.50393
H -1.93158 5.36995 -5.22656
C 3.28521 4.60451 -1.72552
H 3.09025 3.52890 -1.91847
H 4.24276 4.69133 -1.17402
H 3.36662 5.13167 -2.69471
C 2.38887 6.72521 -0.63242
H 2.43666 7.26161 -1.59789
H 3.33797 6.86464 -0.07668
H 1.56281 7.15327 -0.02642
C 1.39606 3.39871 3.31574
H 2.47590 3.56719 3.21198
C 0.82664 2.97416 4.53340
H 1.48011 2.79937 5.40350
C -0.56125 2.77063 4.64389
H -0.99493 2.43631 5.60031
C -1.40878 2.98778 3.53859
H -2.49435 2.83840 3.60515
C -4.31240 3.43793 -1.12314
H -4.68867 3.88390 -2.06307
H -5.16020 3.25908 -0.43187
H -3.83856 2.46117 -1.35451
C -3.93801 5.76338 -0.15404
H -3.19957 6.43934 0.32599
H -4.79229 5.63083 0.54011
H -4.28715 6.22773 -1.09456

50
Species 3 (-1/3)
Mn -0.44857 4.16511 -0.35736
O -3.77586 3.52315 1.78118
N 0.96574 4.05453 0.92025
O 3.23106 4.53710 1.21467
O 1.24412 6.25273 -3.37081
N -2.07453 4.53094 -1.28112
N -1.54510 3.71801 1.11959
N 0.82347 4.96046 -1.49480
C -3.30719 4.40128 -0.45326
C -2.91152 3.81476 0.94291
C -0.85218 3.41510 2.30998
C 0.57428 3.60295 2.19329
C 2.19089 4.54353 0.53817
C 2.15878 5.22140 -0.87661
C 0.51028 5.47513 -2.73192
C -0.81073 4.94833 -3.40013
C -2.13171 5.04779 -2.54316
O -3.16231 5.50262 -3.08163
C -0.59516 3.44282 -3.73375
H 0.29045 3.31267 -4.39119
H -1.48037 3.03774 -4.26796
H -0.43796 2.83746 -2.81902
C -1.02530 5.71723 -4.71551
H -0.14350 5.60162 -5.37447
H -1.17000 6.80027 -4.53193
H -1.92692 5.33765 -5.23233
C 3.29483 4.62142 -1.73117
H 3.10485 3.54593 -1.92976
H 4.25417 4.71014 -1.18305
H 3.37084 5.15415 -2.69804
C 2.39515 6.73226 -0.62602
H 2.43607 7.27308 -1.58943
H 3.34598 6.87293 -0.07358
H 1.57024 7.15502 -0.01454
C 1.40412 3.36027 3.30992
H 2.48605 3.51583 3.20530
C 0.83184 2.93161 4.52344
H 1.48463 2.73786 5.39012
C -0.55966 2.74625 4.63623
H -0.99493 2.40690 5.59010
C -1.40596 2.98807 3.53677
H -2.49345 2.85361 3.60479
C -4.32168 3.43772 -1.10703
H -4.69175 3.86787 -2.05692
H -5.17361 3.26813 -0.41845
H -3.84413 2.45863 -1.32039
C -3.96189 5.77705 -0.17091
H -3.23060 6.46329 0.30568
H -4.82210 5.65048 0.51713
H -4.30369 6.22654 -1.12173

50
Species 3 (-1/5)
Mn -0.45953 4.20955 -0.36433
O -3.78896 3.54046 1.79238
N 0.95487 4.09356 0.92924
O 3.21653 4.56918 1.23115
O 1.27298 6.21380 -3.42109
N -2.09410 4.54128 -1.28008
N -1.56149 3.73164 1.13299
N 0.84862 4.98079 -1.51286
C -3.32158 4.41390 -0.44487
C -2.91997 3.82746 0.95422
C -0.85752 3.41041 2.31308
C 0.56413 3.61531 2.19819
C 2.18170 4.57831 0.54647
C 2.16917 5.24281 -0.87532
C 0.53315 5.46550 -2.75231
C -0.80711 4.93920 -3.40252
C -2.13118 5.05389 -2.54773
O -3.15653 5.51447 -3.08724
C -0.59967 3.42946 -3.72025
H 0.28217 3.29088 -4.38079
H -1.48865 3.01949 -4.24441
H -0.43691 2.83017 -2.80234
C -1.02444 5.69493 -4.72496
H -0.14117 5.57493 -5.38058
H -1.17198 6.77917 -4.55138
H -1.92439 5.30821 -5.23942
C 3.31548 4.62821 -1.70600
H 3.13040 3.54806 -1.88215
H 4.27077 4.73299 -1.15384
H 3.39340 5.13999 -2.68404
C 2.40466 6.75630 -0.64458
H 2.45085 7.28028 -1.61755
H 3.35245 6.90716 -0.08957
H 1.57561 7.18895 -0.04588
C 1.40008 3.35629 3.30507
H 2.47973 3.52647 3.20059
C 0.83652 2.89516 4.51236
H 1.49459 2.69144 5.37269
C -0.55126 2.69394 4.62389
H -0.98221 2.33196 5.57151
C -1.40318 2.95061 3.53029
H -2.48972 2.80759 3.59792
C -4.33572 3.44989 -1.09701
H -4.71190 3.87882 -2.04521
H -5.18370 3.27979 -0.40385
H -3.85810 2.47128 -1.31198
C -3.97292 5.79103 -0.16735
H -3.23972 6.47825 0.30466
H -4.83024 5.66606 0.52438
H -4.31860 6.23811 -1.11807

51
Species 4 (-1/1)
Mn 0.35322 9.48816 7.55819
O 3.89474 9.79651 9.42178
C -0.17535 8.70879 10.20743
N 1.65841 9.40975 8.93629
O -0.17616 10.95288 7.51643
O -2.61530 7.41270 9.29161
O -1.41414 7.78917 4.29166
O 2.91871 9.27443 4.38470
N -0.64403 8.56974 8.88944
N -0.71109 8.42157 6.38479
N 1.89378 9.35383 6.43875
C -1.77726 7.89136 8.51625
C 2.97525 9.61998 8.61193
C 1.87833 9.25077 5.06965
C 1.82777 9.38571 11.46586
H 2.85995 9.75629 11.46528
C -1.89654 7.75115 6.98879
O 0.51927 9.21208 4.33143
C 3.21439 9.57429 7.09295
C 1.16311 9.19937 10.23481
C -0.59856 8.39013 5.01704
C -0.17601 8.60355 12.63412
H -0.69901 8.37787 13.57734
C -1.93198 6.22929 6.70160
H -2.12764 6.04456 5.63072
H -2.72889 5.76748 7.31847
H -0.96375 5.76159 6.97676
C 3.83761 10.92913 6.68173
H 4.11831 10.91315 5.61259
H 4.73763 11.11881 7.30059
H 3.11658 11.75523 6.85332
C -3.21705 8.43809 6.56675
H -3.17012 9.52688 6.77627
H -4.05574 8.00649 7.14914
H -3.39740 8.28704 5.48665
C 1.14518 9.08833 12.66107
H 1.65569 9.24193 13.62538
C 0.74857 8.63767 2.91704
H 1.50679 9.24134 2.38491
H -0.20124 8.64489 2.35121
H 1.11322 7.59108 2.95924
C -0.84605 8.40521 11.41156
H -1.87280 8.02213 11.36999
C 4.19944 8.40168 6.85653
H 3.72450 7.43712 7.13230
H 5.09070 8.54670 7.49951
H 4.50115 8.36241 5.79516
C 0.01367 10.68016 4.19096
H -0.17046 11.15308 5.17453
H -0.93091 10.69531 3.60858
H 0.76729 11.28367 3.64384

51
Species 4 (-1/3)
Mn 0.37378 9.42800 7.51846
O 3.94381 9.76872 9.42136
C -0.14328 8.72393 10.19288
N 1.68141 9.52905 8.96103
O -0.19446 10.93544 7.57241
O -2.50670 7.27283 9.28321
O -1.45137 7.83213 4.20375
O 2.88849 9.11570 4.37297
N -0.57812 8.48922 8.86974
N -0.78429 8.43942 6.32340
N 1.91054 9.32187 6.43664
C -1.70690 7.78928 8.49443
C 2.99979 9.63576 8.62801
C 1.85639 9.20171 5.05715
C 1.76332 9.60268 11.48327
H 2.76692 10.04699 11.49706
C -1.88840 7.68364 6.96377
C 0.48163 9.28265 4.33263
C 3.23932 9.50233 7.10001
C 1.15392 9.32676 10.24109
C -0.66892 8.43785 4.96278
C -0.20739 8.70725 12.62267
H -0.74049 8.47352 13.55812
C -1.84412 6.17360 6.62276
H -2.04211 6.02384 5.54620
H -2.60802 5.64211 7.22475
H -0.84785 5.75052 6.86759
C 3.93626 10.79415 6.61650
H 4.22534 10.70614 5.55299
H 4.84199 10.96349 7.23250
H 3.26376 11.66828 6.73755
C -3.26347 8.29926 6.61218
H -3.27691 9.38017 6.86203
H -4.05930 7.79283 7.19393
H -3.45923 8.17864 5.53039
C 1.07300 9.29117 12.66975
H 1.54159 9.51202 13.64222
C 0.67964 8.82363 2.87513
H 1.44199 9.45306 2.37904
H -0.27880 8.90139 2.32937
H 1.01841 7.76967 2.82332
C -0.82384 8.41598 11.39025
H -1.81564 7.95084 11.33780
C 4.14801 8.26380 6.91324
H 3.62296 7.34367 7.24356
H 5.05560 8.38922 7.53658
H 4.43238 8.15409 5.85144
C 0.03240 10.77515 4.33014
H -0.16226 11.15499 5.35266
H -0.89922 10.87697 3.73552
H 0.81423 11.40510 3.85668

1 + 3

101
1 + 3 Reactant complex (-2/4)
Fe 4.95794 9.48097 14.97362
O 5.76013 9.22758 16.33993
O 2.84838 12.73283 15.83985
O 1.33064 7.76831 15.86993
O 4.51134 5.87691 13.19724
O 7.97735 9.60429 12.31482
N 4.44678 11.27517 15.01295

N 3.11265 9.15323 15.41534
N 5.11651 7.98251 13.86144
N 6.34025 10.18450 13.85592
C 5.43172 12.19839 14.61735
C 6.53174 11.56264 13.95860
C 7.60143 12.33495 13.45319
C 7.57325 13.73098 13.61785
C 6.49277 14.35732 14.27090
C 5.41520 13.60357 14.76991
C 3.22218 11.58529 15.57446
C 2.34386 10.34939 15.83259
C 2.01414 10.31978 17.34455
C 1.06339 10.55599 14.98220
C 2.50863 7.93635 15.48899
C 3.35732 6.68208 15.14513
C 4.18913 6.31593 16.41220
C 2.40270 5.51405 14.82535
C 4.34843 6.83861 13.96828
C 6.27389 7.96226 12.91710
C 7.30285 6.87447 13.29882
C 5.81824 7.82522 11.44284
C 6.98439 9.33286 13.00502
H 8.42651 11.82729 12.93800
H 8.40958 14.33721 13.23445
H 6.48797 15.45139 14.39983
H 4.56619 14.07610 15.27733
H 2.93935 10.17601 17.93920
H 1.31709 9.48812 17.55725
H 1.55046 11.28096 17.64438
H 1.31419 10.55476 13.90095
H 0.34150 9.74470 15.18275
H 0.61365 11.53696 15.23573
H 4.87509 7.13436 16.70527
H 4.78423 5.39804 16.22453
H 3.50016 6.11314 17.25823
H 2.97973 4.58568 14.65613
H 1.70026 5.36891 15.66665
H 1.80551 5.71632 13.91312
H 6.88853 5.86451 13.12416
H 7.58727 6.96919 14.36704
H 8.21361 7.01420 12.68239
H 6.69551 7.97757 10.78270
H 5.38021 6.82685 11.26783
H 5.06114 8.59960 11.19991
Mn 7.70633 9.98557 19.33120
O 9.65776 13.21536 17.92499
O 11.31433 8.24532 18.71016
O 8.02814 6.35869 21.10489
O 4.44379 10.21593 21.67920
N 8.03362 11.81363 18.83535
N 9.48703 9.66039 18.72895
N 7.30056 8.40454 20.31453
N 6.16058 10.73701 20.19130
C 7.00441 12.71733 19.17591
C 5.94629 12.10927 19.94124
C 4.85853 12.89406 20.37941
C 4.81669 14.26742 20.06356
C 5.85026 14.86148 19.31686
C 6.94603 14.09395 18.87182
C 9.27231 12.10263 18.31704
C 10.24581 10.87323 18.31479
C 10.81341 10.70728 16.88908
C 11.37234 11.21605 19.32100
C 10.09148 8.44066 18.85917
C 9.14561 7.20093 19.10682
C 8.32754 6.97703 17.80073
C 10.02950 5.96497 19.34874
C 8.11367 7.30520 20.29725
C 6.17181 8.53134 21.27801
C 5.12285 7.42231 21.05268
C 6.66911 8.53066 22.74511
C 5.47725 9.92007 21.05876
H 4.06742 12.41219 20.96862
H 3.96328 14.87505 20.40590
H 5.80831 15.93561 19.07352
H 7.76803 14.53936 18.29655
H 10.00153 10.45199 16.17687
H 11.56920 9.89900 16.87459
H 11.27981 11.65780 16.56123
H 10.95463 11.32769 20.34381
H 12.12389 10.40482 19.32999
H 11.85230 12.17282 19.03270
H 7.66622 7.83267 17.55481
H 7.69194 6.07156 17.89702
H 9.01421 6.82059 16.94184
H 9.39766 5.06456 19.46900
H 10.72164 5.82011 18.49760
H 10.63897 6.07665 20.26715
H 5.55734 6.43377 21.29430
H 4.78678 7.41637 19.99505
H 4.24177 7.60983 21.69839
H 5.81670 8.71744 23.42892
H 7.13441 7.55568 22.98209
H 7.42217 9.33243 22.89701

101
TS_R (-2/4)
Fe 5.05359 9.50802 15.19381
O 5.82140 9.25796 16.58655
O 3.00157 12.82020 15.95986
O 1.37100 7.89336 16.04603
O 4.51763 5.91783 13.41111
O 8.14140 9.51276 12.61370
N 4.58261 11.31294 15.18956
N 3.19216 9.22977 15.60151
N 5.19461 7.99387 14.09973
N 6.47737 10.16010 14.09817
C 5.59125 12.20802 14.79039
C 6.69454 11.53570 14.17455
C 7.78766 12.27591 13.67055
C 7.77740 13.67648 13.79142
C 6.69138 14.33918 14.39791
C 5.59175 13.61767 14.89569
C 3.35389 11.66022 15.72182
C 2.44307 10.44949 15.98436
C 2.08305 10.45365 17.48950
C 1.18380 10.66988 15.10599
C 2.55784 8.02852 15.68040
C 3.37943 6.75052 15.35774
C 4.18864 6.37274 16.63550
C 2.39969 5.60405 15.03612
C 4.38385 6.87777 14.18947
C 6.35678 7.93957 13.16267
C 7.33911 6.80466 13.52673
C 5.90170 7.84688 11.68389
C 7.11853 9.27995 13.27318
H 8.61525 11.74074 13.18843
H 8.63148 14.25794 13.40888
H 6.70012 15.43679 14.49143
H 4.73905 14.11838 15.36845
H 2.99184 10.29796 18.10588
H 1.36171 9.64285 17.70169
H 1.63745 11.43096 17.76343
H 1.45424 10.64362 14.02984
H 0.43995 9.87888 15.30743
H 0.75211 11.66512 15.33387
H 4.89189 7.17525 16.93140
H 4.76306 5.43935 16.46027
H 3.48560 6.19181 17.47484
H 2.95515 4.66045 14.87913
H 1.68614 5.48201 15.87176
H 1.81641 5.81426 14.11685
H 6.89029 5.81505 13.32444
H 7.61811 6.86351 14.59867
H 8.25953 6.92601 12.92088
H 6.78755 7.96414 11.02805
H 5.41579 6.87354 11.49390
H 5.18449 8.66082 11.44953
Mn 7.58724 9.93160 19.07534
O 9.48994 13.23923 17.77912
O 11.28346 8.33088 18.56914
O 8.01725 6.34360 20.90988
O 4.26591 10.04309 21.35087
N 7.88605 11.78164 18.63532
N 9.40160 9.67166 18.54150
N 7.22093 8.34019 20.06283
N 6.01143 10.63523 19.92475
C 6.83235 12.65627 18.97634
C 5.77061 12.00722 19.70084
C 4.65948 12.75896 20.13908
C 4.59977 14.14043 19.86452
C 5.63886 14.77545 19.16065
C 6.75674 14.04095 18.71506
C 9.12670 12.11091 18.14709
C 10.13252 10.90977 18.15008
C 10.72906 10.77062 16.73334
C 11.23074 11.28001 19.17819
C 10.05119 8.47742 18.69370
C 9.15532 7.20133 18.93292
C 8.39268 6.92456 17.60474
C 10.08466 6.00990 19.22401
C 8.08388 7.27886 20.08756
C 6.07363 8.43179 21.00877
C 5.07477 7.27734 20.78759
C 6.54940 8.47494 22.48333
C 5.32982 9.78851 20.76447
H 3.86585 12.24656 20.69819
H 3.72864 14.72227 20.20698
H 5.58349 15.85592 18.95047
H 7.58209 14.51827 18.17133
H 9.93764 10.49668 16.00515
H 11.50828 9.98479 16.72712
H 11.17306 11.73655 16.41974
H 10.79269 11.36835 20.19475
H 12.00976 10.49561 19.19339
H 11.68074 12.25564 18.90552
H 7.70514 7.75004 17.33021
H 7.79290 5.99409 17.69159
H 9.11521 6.78824 16.77242
H 9.49031 5.08230 19.32802
H 10.81803 5.89000 18.40410
H 10.64909 6.15746 20.16592
H 5.54423 6.31144 21.05398
H 4.75587 7.23942 19.72556
H 4.17642 7.44107 21.41574
H 5.67994 8.63672 23.15190
H 7.05088 7.52417 22.74294
H 7.26608 9.30972 22.63291

101
Intermediate$_R$ (-2/4)
Fe 5.36379 9.56111 15.53649
O 6.22315 9.35819 17.00640
O 3.17732 12.81167 16.34024
O 1.65970 7.87156 16.16692
O 4.88670 5.97873 13.62974
O 8.41854 9.68125 12.92778
N 4.83291 11.36911 15.58589
N 3.50415 9.23153 15.91651
N 5.56736 8.02390 14.43372
N 6.71413 10.27284 14.39413
C 5.75061 12.29741 15.07827
C 6.84428 11.66253 14.40200
C 7.83001 12.44667 13.75789
C 7.72280 13.84750 13.79069
C 6.64642 14.47222 14.45349
C 5.65818 13.70883 15.09796
C 3.58682 11.66956 16.09349
C 2.69604 10.42647 16.27404
C 2.21103 10.38019 17.74038
C 1.50454 10.64600 15.30159
C 2.86923 8.02397 15.89030
C 3.71316 6.75692 15.58077
C 4.46762 6.37577 16.88576
C 2.75772 5.60556 15.21022
C 4.75687 6.91143 14.44649
C 6.66148 8.06098 13.41870
C 7.68616 6.92160 13.59260
C 6.09883 8.08093 11.96979
C 7.39212 9.41169 13.56939
H 8.65223 11.94015 13.23795
H 8.49399 14.45991 13.29609
H 6.57854 15.57174 14.47701
H 4.81361 14.17631 15.61667
H 3.06499 10.21316 18.42744
H 1.47930 9.56141 17.86902
H 1.73794 11.34799 18.00302
H 1.86211 10.66194 14.25057
H 0.76676 9.83234 15.41534
H 1.03056 11.62328 15.52276
H 5.13849 7.18761 17.22358
H 5.07149 5.45822 16.72673
H 3.73097 6.16610 17.68897
H 3.32985 4.67072 15.06001
H 2.01448 5.46259 16.01643
H 2.20698 5.82062 14.27232
H 7.23319 5.94629 13.33929
H 8.05743 6.88683 14.63557
H 8.54865 7.11950 12.92458
H 6.93244 8.24161 11.25700
H 5.59470 7.12356 11.74691
H 5.37062 8.90987 11.84898
Mn 7.11518 9.79166 18.51471
O 9.21766 13.07216 17.43078
O 10.91780 8.22267 18.22858
O 7.65747 6.36498 20.71846
O 4.17009 10.17177 21.27849
N 7.56845 11.65504 18.25100
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C 6.61121 12.59428 18.67742
C 5.57166 12.00077 19.46530
C 4.56661 12.81354 20.03472
C 4.59907 14.20520 19.82130
C 5.62028 14.78814 19.04818
C 6.62821 13.99115 18.47197
C 8.82251 11.94695 17.77123
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C 10.39052 10.56236 16.37197
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C 9.68519 8.34694 18.38616
C 8.85394 7.07306 18.74273
C 8.15364 6.60014 17.43930
C 9.82757 5.97086 19.20232
C 7.76489 7.24980 19.84624
C 5.86003 8.48185 20.80815
C 4.81175 7.35268 20.72006
C 6.45312 8.57451 22.23983
C 5.14251 9.83816 20.58306
H 3.78807 12.34128 20.64635
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H 5.63499 15.87793 18.88474
H 7.43722 14.42637 17.87372
H 9.60675 10.29417 15.63438
H 11.15907 9.76694 16.38584
H 10.85223 11.51909 16.05495
H 10.43357 11.20431 19.82851
H 11.65081 10.30751 18.84800
H 11.33802 12.06602 18.53416
H 7.46400 7.36535 17.03361
H 7.57579 5.67174 17.62896
H 8.92086 6.37400 16.66949
H 9.27341 5.03327 19.39611
H 10.59236 5.79709 18.42249
H 10.35164 6.25526 20.13656
H 5.27042 6.38224 20.98528
H 4.39633 7.28669 19.69464
H 3.98023 7.57657 21.41807
H 5.64009 8.80933 22.95545
H 6.93183 7.61758 22.51491
H 7.21019 9.38466 22.29310

101
MECP (-2/4)
Fe 5.39771 9.55545 15.59085
O 6.25754 9.35780 17.07427
O 3.32817 12.90828 16.29823
O 1.61962 8.02781 16.18604
O 4.80758 5.92665 13.79572
O 8.42658 9.51179 12.94497
N 4.93839 11.38613 15.60163
N 3.52389 9.30829 15.95939
N 5.54769 7.97895 14.52874
N 6.77258 10.18787 14.43207
C 5.89589 12.26493 15.07987
C 6.96019 11.57222 14.41416
C 7.97815 12.30255 13.75788
C 7.93219 13.70723 13.76794
C 6.88494 14.38852 14.42064
C 5.86512 13.67895 15.07767
C 3.69809 11.74636 16.08046
C 2.75308 10.54328 16.26074
C 2.21479 10.55477 17.70883
C 1.60497 10.78517 15.24191
C 2.84307 8.12505 15.94746
C 3.64825 6.81799 15.70757
C 4.37855 6.46947 17.03513
C 2.66106 5.68113 15.37828
C 4.70508 6.89321 14.57639
C 6.63741 7.95384 13.50984
C 7.63426 6.79534 13.72171
C 6.06959 7.93669 12.06304
C 7.40601 9.28785 13.61314
H 8.77625 11.75256 13.24486
H 8.72808 14.27734 13.26217
H 6.86381 15.49006 14.42560
H 5.04228 14.19037 15.58978
H 3.03413 10.36534 18.43142
H 1.44034 9.77513 17.83047
H 1.78050 11.55079 17.92984
H 1.99827 10.76539 14.20389
H 0.83403 10.00163 15.34622
H 1.16029 11.78366 15.42590
H 5.07833 7.26936 17.34128
H 4.94787 5.52334 16.92259
H 3.62946 6.32443 17.84133
H 3.20635 4.72442 15.27241
H 1.90903 5.59280 16.18429
H 2.12199 5.87038 14.42834
H 7.15345 5.82284 13.51220
H 8.01204 6.79321 14.76304
H 8.49675 6.94245 13.04072
H 6.90299 8.05423 11.34175
H 5.54225 6.98453 11.87453
H 5.35944 8.77703 11.91605
Mn 7.14734 9.78146 18.56549
O 9.35164 12.98347 17.45111
O 10.90525 8.10074 18.29599
O 7.61239 6.41145 20.87099
O 4.19706 10.29135 21.29970
N 7.66166 11.62490 18.28606
N 9.04078 9.45585 18.26750
N 6.92523 8.36528 19.86374
N 5.80284 10.66131 19.65925
C 6.73149 12.59933 18.69180
C 5.66531 12.04724 19.47280
C 4.67931 12.89545 20.02313
C 4.76102 14.28337 19.80044
C 5.81062 14.82685 19.03673
C 6.79791 13.99331 18.47647
C 8.92436 11.87448 17.80468
C 9.84519 10.62874 17.82559
C 10.43066 10.42258 16.41180
C 10.96716 10.97511 18.84066
C 9.68034 8.26439 18.47330
C 8.82148 7.02447 18.87368
C 8.10637 6.52671 17.58763
C 9.76976 9.91568 19.36917
C 7.73977 7.26387 19.96975
C 5.85878 8.55795 20.88893
C 4.79047 7.44573 20.83378
C 6.45136 8.68214 22.31838
C 5.16888 9.91960 20.62321
H 3.87813 12.45262 20.62750
H 3.98915 14.94446 20.22683
H 5.86299 15.91431 18.86589
H 7.62695 14.39719 17.88382
H 9.63013 10.16847 15.68763
H 11.17640 9.60591 16.42882
H 10.91663 11.36093 16.07641
H 10.54147 11.11305 19.85676
H 11.71202 10.16028 18.87194
H 11.45315 11.92231 18.53352
H 7.43720 7.29712 17.15845
H 7.50478 5.62084 17.80935
H 8.86601 6.25521 16.82508
H 9.19433 4.99840 19.59547
H 10.52887 5.69903 18.59474
H 10.30102 6.22073 20.29295
H 5.22969 6.47693 21.13522
H 4.37859 7.35281 19.80924
H 3.95983 7.70837 21.51924
H 5.63997 8.94902 23.02429
H 6.91396 7.72582 22.62127
H 7.22083 9.48154 22.35107

101
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Fe 5.30214 9.67784 15.41901
O 6.32391 9.40658 17.14581
O 3.21888 12.95340 16.44724
O 1.56670 8.05478 15.89652
O 4.81549 6.10248 13.47682
O 8.39436 9.82535 12.86193
N 4.84943 11.51167 15.61880
N 3.45910 9.37662 15.82013
N 5.54268 8.11841 14.33667
N 6.69499 10.39772 14.34807
C 5.81820 12.42691 15.17150
C 6.88102 11.78727 14.44968
C 7.91516 12.56357 13.88093
C 7.89003 13.96433 14.02718
C 6.84428 14.59258 14.72931
C 5.80577 13.83306 15.30290
C 3.61359 11.82062 16.12455
C 2.67169 10.58923 16.18661
C 2.08622 10.48606 17.61166
C 1.55171 10.89152 15.15430
C 2.79531 8.18612 15.70798
C 3.63828 6.90342 15.42848
C 4.36385 6.52742 16.74920
C 2.67815 5.75797 15.05459
C 4.71242 7.03218 14.30578
C 6.63278 8.19769 13.32130
C 7.66203 7.05829 13.46781
C 6.06896 8.24125 11.87399
C 7.36395 9.55317 13.50041
H 8.71156 12.05375 13.32451
H 8.69960 14.56859 13.58646
H 6.83470 15.68930 14.83839
H 4.97895 14.30384 15.84846
C 2.88210 10.24779 18.34667
H 1.31615 9.69303 17.64876
H 1.63442 11.45854 17.89383
H 1.97829 10.95520 14.13101
H 0.79133 10.09056 15.17509
H 1.08337 11.86654 15.39701
H 5.04507 7.33167 17.08533
H 4.95700 5.59886 16.61332
H 3.61612 6.34041 17.54841
H 3.24572 4.81862 14.91465
H 1.92311 5.62232 15.85172
H 2.14007 5.97119 14.10925
H 7.19658 6.08634 13.22096
H 8.05193 7.01681 14.50446
H 8.51424 7.25128 12.78539
H 6.89809 8.42307 11.16070
H 5.57033 7.28446 11.63487
H 5.33285 9.06611 11.77148
Mn 7.09871 9.71328 18.53193
O 9.26039 12.99320 17.70087
O 10.85774 8.12351 18.10703
O 7.60363 6.18843 20.57949
O 4.11243 9.91333 21.20088
N 7.62417 11.54055 18.47972
N 8.98271 9.43995 18.30339
N 6.95534 8.22877 19.74078
N 5.80878 10.45763 19.71138
C 6.68112 12.47805 18.92937
C 5.61771 11.84591 19.63843
C 4.58826 12.61938 20.21891
C 4.63177 14.01933 20.08743
C 5.68610 14.64486 19.39430
C 6.71702 13.88501 18.81214
C 8.87289 11.85572 17.99529
C 9.79337 10.62892 17.91644
C 10.33368 10.52524 16.47199
C 10.93827 10.91513 18.92479
C 9.64438 8.23554 18.36393
C 8.84010 6.95167 18.66830
C 8.14713 6.49901 17.35143
C 9.82285 5.84732 19.10817
C 7.76015 7.11345 19.76065
C 5.86282 8.28017 20.75449
C 4.82956 7.14578 20.58931
C 6.41949 8.32117 22.20474
C 5.13797 9.62059 20.57338
H 3.78287 12.11358 20.76414
H 3.82751 14.62745 20.53163
H 5.70622 15.74223 19.29756
H 7.54573 14.35449 18.27029
H 9.51456 10.28804 15.76339
H 11.10494 9.73642 16.40832
H 10.77205 11.50104 16.18116
H 10.53852 10.97219 19.95871
H 11.69814 10.11553 18.87672
H 11.40116 11.89102 18.67619
H 7.45239 7.26583 16.96111
H 7.57783 5.56274 17.52605
H 8.91846 6.29317 16.58076
H 9.27440 4.90277 19.28162
H 10.58919 5.69453 18.32579
H 10.34288 6.11739 20.04927
H 5.27817 6.17180 20.85397
H 4.46371 7.10292 19.54459
H 3.96562 7.35474 21.25160
H 5.58395 8.50384 22.90992
H 6.91096 7.36245 22.44861
H 7.15621 9.14387 22.31464

101
TS_P (-2/4)
Fe 5.04364 9.62201 14.94202
O 6.47179 9.55786 17.50571
O 3.18604 12.86402 16.35749
O 1.38277 7.99339 15.62758
O 4.61142 5.97568 13.20824
O 8.27958 9.67235 12.59928
N 4.73155 11.42305 15.37141
N 3.27699 9.31628 15.52442
N 5.34814 8.02040 13.99665
N 6.54894 10.28597 14.03689
C 5.76134 12.30733 14.99167
C 6.79672 11.66001 14.23133
C 7.88311 12.41478 13.73865
C 7.94304 13.79847 14.00006
C 6.93051 14.43171 14.74444
C 5.83699 13.69435 15.24163
C 3.52737 11.74370 15.94628
C 2.54475 10.53356 15.98411
C 2.03549 10.37025 17.43250
C 1.38276 10.91024 15.02944
C 2.60719 8.12636 15.42631
C 3.46596 6.84370 15.16077
C 4.24041 6.53527 16.47501
C 2.51517 5.66964 14.86438
C 4.51898 6.93151 14.00522
C 6.48726 8.06478 13.03282
C 7.49677 6.92556 13.28618
C 5.99754 8.05004 11.56123
C 7.22743 9.42567 13.20966
H 8.65750 11.90364 13.15221
H 8.79375 14.38467 13.61628
H 6.98821 15.51398 14.94427
H 5.03316 14.16459 15.81833
H 2.87162 10.09476 18.10812
H 1.26308 9.57963 17.47774
H 1.60609 11.32995 17.78402
H 1.75756 11.01682 13.98952
H 0.60718 10.12324 15.04945
H 0.94752 11.88018 15.34407
H 4.92696 7.35859 16.75082
H 4.83739 5.60588 16.36276
H 3.52654 6.38349 17.31188
H 3.09335 4.73372 14.74613
H 1.78527 5.55480 15.68789
H 1.94662 5.83570 13.92752
H 7.03705 5.94677 13.05366
H 7.82242 6.92551 14.34691
H 8.39047 7.07935 12.64844
H 6.86076 8.19957 10.88154
H 5.50445 7.08642 11.33714
H 5.27143 8.87245 11.38936
Mn 7.24383 9.85033 18.83810
O 9.39287 13.14051 18.02029
O 10.95218 8.23733 18.21808
O 7.65230 6.19580 20.63143
O 4.32381 10.00981 21.58231
N 7.76856 11.67606 18.79706
N 9.11417 9.57414 18.55376
N 7.10641 8.33290 19.99133
N 5.98151 10.57392 20.05908
C 6.81465 12.60296 19.25076
C 5.77286 11.96138 19.98253
C 4.73338 12.72378 20.55813
C 4.74173 14.12169 20.39264
C 5.77169 14.75564 19.67209
C 6.81688 14.00654 19.09939
C 9.00486 11.99706 18.29126
C 9.90598 10.76263 18.12923
C 10.31423 10.67509 16.63990
C 11.13376 11.01937 19.04009
C 9.75293 8.35806 18.53225
C 8.93765 7.07291 18.80406
C 8.23017 6.67398 17.47450
C 9.91622 9.54530 19.19428
C 7.85876 7.18664 19.90545
C 5.97824 8.33250 20.96507
C 4.90208 7.28241 20.60709
C 6.46384 8.17039 22.42876
C 5.31634 9.71832 20.90288
H 3.94571 12.21289 21.12458
H 3.92795 14.72062 20.83198

H 5.76370 15.85043 19.54839
H 7.63099 14.48215 18.54002
H 9.42452 10.48642 16.00457
H 11.04364 9.85819 16.49026
H 10.76514 11.63853 16.32819
H 10.82562 11.04755 20.10606
H 11.88557 10.22222 18.90590
H 11.57230 12.00336 18.77918
H 7.52579 7.45336 17.12698
H 7.66809 5.72796 17.61667
H 8.99143 6.50817 16.68438
H 9.36085 5.00029 19.33924
H 10.67474 5.81560 18.40035
H 10.44677 6.17833 20.13987
H 5.29564 6.26114 20.76008
H 4.59022 7.39414 19.54836
H 4.01407 7.44218 21.25108
H 5.60707 8.33300 23.11298
H 6.88243 7.16019 22.58202
H 7.24447 8.92402 22.66243

101
2 + 4 Product complex (-2/4)
Fe 4.92746 9.63170 14.89525
O 6.60239 9.55110 17.52247
O 3.00036 12.84436 16.28343
O 1.28922 7.93825 15.52984
O 4.57423 5.98883 13.14311
O 8.23761 9.72165 12.66159
N 4.59149 11.42339 15.34156
N 3.15817 9.29845 15.45014
N 5.27580 8.03872 13.95187
N 6.45073 10.31554 14.03751
C 5.62306 12.32016 14.99493
C 6.68355 11.68848 14.25594
C 7.77959 12.45511 13.80488
C 7.82416 13.83567 14.08546
C 6.78599 14.45409 14.80652
C 5.68281 13.70443 15.26276
C 3.36793 11.72829 15.88365
C 2.40207 10.50331 15.90230
C 1.87728 10.32850 17.34399
C 1.24742 10.86299 14.93292
C 2.51334 8.09569 15.34589
C 3.40358 6.83115 15.09427
C 4.17978 6.54829 16.41392
C 2.48265 5.63362 14.79917
C 4.46191 6.93849 13.94467
C 6.44231 8.09812 13.02313
C 7.45279 6.96595 13.30348
C 5.99812 8.08478 11.53745
C 7.16531 9.46460 13.23150
H 8.57368 11.95487 13.23556
H 8.68268 14.43109 13.73471
H 6.83115 15.53415 15.02086
H 4.85983 14.16843 15.82129
H 2.71018 10.06752 18.02957
H 1.11893 9.52373 17.37839
H 1.42562 11.27943 17.69140
H 1.63454 10.97580 13.89816
H 0.48401 10.06387 14.94215
H 0.79270 11.82584 15.24170
H 4.85741 7.38240 16.68074
H 4.78847 5.62516 16.31276
H 3.46745 6.39727 17.25224
H 3.08406 4.71195 14.68427
H 1.75384 5.50193 15.62123
H 1.91228 5.78365 13.86077
H 7.00822 5.98447 13.05314
H 7.74550 6.96412 14.37392
H 8.36467 7.12873 12.69440
H 6.87960 8.24440 10.88385
H 5.52104 7.11732 11.29557
H 5.26964 8.90077 11.34636
Mn 7.34863 9.84878 18.86444
O 9.53172 13.11052 18.03285
O 11.05134 8.19574 18.32599
O 7.68806 6.20260 20.68696
O 4.37383 10.05405 21.54488
N 7.88939 11.66971 18.81629
N 9.22013 9.55332 18.61184
N 7.17442 8.34125 20.02503
N 6.07156 10.59380 20.05715
C 6.93470 12.60838 19.24350
C 5.87590 11.98216 19.96417
C 4.83272 12.75819 20.51411
C 4.85371 14.15420 20.33346
C 5.89999 14.77291 19.62336
C 6.94938 14.01009 19.07669
C 9.13291 11.97438 18.31909
C 10.02872 10.73154 18.19040
C 10.47053 10.62412 16.71211
C 11.23763 10.98992 19.12588
C 9.84648 8.33098 18.61206
C 9.01068 7.05621 18.87401
C 8.31694 6.66073 17.53563
C 9.96911 5.91813 19.28262
C 7.91613 7.18707 19.95864
C 6.02447 8.35677 20.97248
C 4.94623 7.31654 20.59236
C 6.47310 8.19458 22.44780
C 5.37877 9.74953 20.88959
H 4.03168 12.25864 21.07194
H 4.03683 14.76352 20.75230
H 5.90170 15.86625 19.48713
H 7.77579 14.47360 18.52514
H 9.59539 10.43096 16.05813
H 11.19942 9.80232 16.58920
H 10.93267 11.58204 16.39973
H 10.90489 11.03758 20.18374
H 11.98328 10.18240 19.02147
H 11.69376 11.96484 18.86098
H 7.62311 7.44507 17.17753
H 7.74540 5.71961 17.67310
H 9.08629 6.48629 16.75522
H 9.39971 4.98104 19.42481
H 10.73680 5.77482 18.49992
H 10.48971 6.14912 20.23418
H 5.32593 6.29180 20.75683
H 4.65988 7.42833 19.52639
H 4.04505 7.48634 21.21520
H 5.60229 8.37011 23.11086
H 6.87585 7.18008 22.61478
H 7.25685 8.93986 22.69722

101
Intermediate$_R$ (-2/2)
Fe 5.37713 9.57798 15.54381
O 6.22809 9.32430 17.03926
O 3.20818 12.88223 16.26051
O 1.64977 7.94683 16.16121
O 4.85132 5.93986 13.70357
O 8.41909 9.62069 12.92871
N 4.88808 11.40990 15.60521
N 3.51592 9.27883 15.91569
N 5.57610 7.98457 14.48176
N 6.70910 10.26125 14.37305
C 5.83098 12.31147 15.10217
C 6.89310 11.64475 14.40102
C 7.90659 12.40079 13.76378
C 7.85334 13.80285 13.82096
C 6.80610 14.45854 14.50427
C 5.79540 13.72531 15.14695
C 3.63280 11.73351 16.07170
C 2.72627 10.49418 16.25087
C 2.21137 10.46964 17.70755
C 1.55487 10.71566 15.25481
C 2.86828 8.07618 15.90989
C 3.70189 6.78811 15.64787
C 4.43994 6.43971 16.96955
C 2.73338 5.63755 15.30975
C 4.75688 6.89078 14.51037
C 6.65062 8.02125 13.45103
C 7.67392 6.87662 13.59259
C 6.05195 8.04177 12.01459
C 7.38973 9.37183 13.57364
H 8.70179 11.87217 13.22430
H 8.63938 14.39453 13.32451
H 6.77889 15.55964 14.53834
H 4.97083 14.21794 15.67470
H 3.04780 10.29520 18.41378
H 1.46364 9.66421 17.82938
H 1.74964 11.44772 17.95181
H 1.93165 10.71504 14.21034
H 0.80762 9.91018 15.36560
H 1.08977 11.70141 15.45610
H 5.12193 7.25192 17.28381
H 5.03086 5.50816 16.84522
H 3.69548 6.26613 17.77471
H 3.29630 4.69291 15.18798
H 1.98626 5.52480 16.11758
H 2.18751 5.82932 14.36416
H 7.19595 5.90532 13.37080
H 8.08704 6.84789 14.61956
H 8.51109 7.05455 12.88792
H 6.86703 8.18554 11.27684
H 5.52915 7.08829 11.81778
H 5.33034 8.87839 11.90790
Mn 7.09333 9.77931 18.49807
O 9.15198 13.11122 17.48470
O 10.90359 8.26427 18.13982
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C 4.47483 14.11472 19.81708
C 5.48815 14.72837 19.05188
C 6.51885 13.96409 18.47801
C 8.76628 11.97208 17.77976
C 9.73645 10.76298 17.75610
C 10.33420 10.62762 16.33890
C 10.83834 11.12207 18.79002
C 9.67277 8.36652 18.31902
C 8.86794 7.07875 18.68176
C 8.14975 6.60223 17.39007
C 9.86758 5.99015 19.11736
C 7.79926 7.23668 19.80751
C 5.88592 8.43018 20.79463
C 4.87194 7.26824 20.75746
C 6.51123 8.56957 22.21060
C 5.12791 9.76138 20.56889
H 3.70754 12.23123 20.63420
H 3.67078 14.72679 20.25659
H 5.47454 15.81918 18.89626
H 7.31920 14.42407 17.88722
H 9.54985 10.35373 15.60474
H 11.11856 9.84795 16.33529
H 10.77350 11.59812 16.03215
H 10.40025 11.20711 19.80653
H 11.61599 10.33783 18.79895
H 11.28499 12.09921 18.51899
H 7.43906 7.35753 17.00262
H 7.59192 5.66315 17.58707
H 8.90630 6.39148 16.60565
H 9.33077 5.04468 19.32152
H 10.61666 5.82670 18.32012
H 10.40850 6.27994 20.04012
H 5.36930 6.32019 21.03289
H 4.43481 7.16520 19.74484
H 4.05084 7.48095 21.47096
H 5.70900 8.78281 22.94507
H 7.03271 7.63426 22.48276
H 7.23834 9.40786 22.23259

101
Intermediate$_P$ (-2/2)
Fe 5.36623 9.72528 15.49105
O 6.23567 9.33861 17.07540
O 3.25842 13.01521 16.39369
O 1.61949 8.11957 15.99129
O 4.84777 6.14560 13.54100
O 8.44754 9.82688 12.93322
N 4.90422 11.55468 15.63121
N 3.51275 9.42990 15.85519
N 5.57278 8.16127 14.39575
N 6.73077 10.43030 14.38604
C 5.86052 12.46769 15.16574
C 6.92330 11.81602 14.45580
C 7.95457 12.58136 13.86379
C 7.92101 13.98246 13.97783
C 6.87310 14.62374 14.66961
C 5.84064 13.87753 15.26529
C 3.65869 11.87414 16.12127
C 2.72606 10.64329 16.21442
C 2.15592 10.56377 17.64793
C 1.59577 10.92665 15.18680
C 2.84506 8.23756 15.77560
C 3.66534 6.94729 15.48554
C 4.37660 6.53980 16.80487
C 2.68620 5.82428 15.09035
C 4.74283 7.07495 14.37097
C 6.66526 8.22199 13.38418
C 7.68232 7.07116 13.52602
C 6.09948 8.27698 11.93635
C 7.40932 9.56530 13.55866
H 8.75269 12.06332 13.31828
H 8.72478 14.58136 13.51988
H 6.86013 15.72273 14.75009
H 5.01459 14.35919 15.80141
H 2.95950 10.33873 18.37809
H 1.38616 9.77207 17.70519
H 1.70727 11.54128 17.91735
H 2.01214 10.97264 14.15855
H 0.83635 10.12606 15.23046
H 1.13119 11.90600 15.41842
H 5.07105 7.32552 17.15662
H 4.95083 5.60137 16.65661
H 3.61822 6.35446 17.59423
H 3.23860 4.87801 14.93791
H 1.92769 5.68902 15.88400
H 2.15422 6.06125 14.14706
H 7.20723 6.10609 13.27240
H 8.06897 7.02020 14.56278
H 8.53727 7.26053 12.84621
H 6.93097 8.44320 11.22203
H 5.58473 7.32795 11.70092
H 5.37770 9.11421 11.83487
Mn 7.04955 9.64887 18.48924
O 9.18435 12.97724 17.64566
O 10.84223 8.13044 18.12821
O 7.63280 6.13732 20.58245
O 4.09630 9.84418 21.19272
N 7.53364 11.50229 18.35958
N 8.93652 9.41481 18.26117
N 6.92392 8.15173 19.71170
N 5.78005 10.39694 19.68821
C 6.58340 12.42096 18.82353
C 5.56144 11.78052 19.59019
C 4.54475 12.54839 20.20188
C 4.55660 13.94667 20.04826
C 5.56846 14.57912 19.29920
C 6.58505 13.82682 18.68355
C 8.78840 11.83382 17.91736
C 9.73170 10.61624 17.87354
C 10.31154 10.50179 16.44587
C 10.84834 10.93502 18.90370
C 9.62033 8.22358 18.35459
C 8.83310 6.92270 18.65107
C 8.14560 6.47188 17.33194
C 9.83254 5.82921 19.07832
C 7.75015 7.05882 19.74955
C 5.85843 8.22238 20.74930
C 4.82900 7.07809 20.63760
C 6.45000 8.29384 22.18543
C 5.12321 9.55851 20.56142
H 3.77391 12.03742 20.79064
H 3.76245 14.54799 20.51943
H 5.56571 15.67539 19.18694
H 7.38470 14.30064 18.10306
H 9.51688 10.24293 15.71719
H 11.09733 9.72516 16.41221
H 10.74213 11.48095 16.15393
H 10.42291 10.99835 19.92719
H 11.62222 10.14768 18.88456
H 11.29979 11.91578 18.65381
H 7.43893 7.23278 16.95087
H 7.58927 5.52602 17.49799
H 8.91777 6.28276 16.55748
H 9.29669 4.87680 19.24901
H 10.59781 5.68980 18.29210
H 10.35339 6.09927 20.01888
H 5.29769 6.11344 20.90292
H 4.43028 7.01352 19.60607
H 3.98383 7.28833 21.32338
H 5.63239 8.48212 22.91005
H 6.95620 7.34321 22.43170
H 7.18309 9.12373 22.26198

101
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Fe 5.35515 9.57221 15.50690
O 6.22966 9.30465 17.04572
O 3.21216 12.87631 16.25530
O 1.62561 7.95120 16.11633
O 4.83448 5.96167 13.64588
O 8.41591 9.62540 12.90485
N 4.86545 11.40009 15.55855
N 3.49528 9.28070 15.87964
N 5.54504 8.00980 14.42442
N 6.72310 10.25356 14.37070
C 5.81388 12.30651 15.05841
C 6.88917 11.64468 14.38146
C 7.90152 12.40248 13.74991
C 7.84024 13.80741 13.79612
C 6.78446 14.45834 14.46326
C 5.76899 13.71841 15.09698
C 3.61841 11.72558 16.03629
C 2.70279 10.49512 16.21256
C 2.19277 10.46996 17.67069
C 1.53071 10.72267 15.21950
C 2.84111 8.08029 15.85835
C 3.67225 6.79528 15.58474
C 4.41902 6.43953 16.90114
C 2.70491 5.64605 15.24047
C 4.72276 6.91076 14.44802
C 6.64115 8.03037 13.41392
C 7.65533 6.88356 13.60285
C 6.08201 8.03715 11.96372
C 7.38687 9.37621 13.55200
H 8.70710 11.87487 13.22487
H 8.63048 14.39910 13.30625
H 6.74930 15.55932 14.49584
H 4.93519 14.20683 15.61427
H 3.03272 10.29237 18.37218
H 1.44221 9.66772 17.79577
H 1.73572 11.44975 17.91668
H 1.90459 10.71883 14.17401
H 0.77551 9.92488 15.33170
H 1.07285 11.71179 15.42098
H 5.10247 7.25138 17.21469
H 5.00891 5.50873 16.76804
H 3.67957 6.26349 17.71025
H 3.26856 4.70314 15.10973
H 1.96099 5.52618 16.05007
H 2.15520 5.84527 14.29858
H 7.18984 5.90960 13.36668
H 8.02766 6.86156 14.64600
H 8.51901 7.06035 12.93049
H 6.91784 8.18267 11.25018
H 5.56995 7.08120 11.75256
H 5.36037 8.87026 11.83192
Mn 7.11140 9.76913 18.54108
O 9.13355 13.09356 17.48841
O 10.91889 8.25195 18.10948
O 7.80387 6.41342 20.77963
O 4.14748 10.05812 21.29579
N 7.52916 11.63382 18.31693
N 8.99972 9.52820 18.15981
N 6.98881 8.33872 19.81749
N 5.70532 10.54765 19.63996
C 6.54417 12.55090 18.73225
C 5.49718 11.92777 19.48497
C 4.46048 12.71128 20.03768
C 4.46917 14.10525 19.84067
C 5.49767 14.71765 19.10051
C 6.53742 13.94981 18.54189
C 8.76919 11.95463 17.81126
C 9.74635 10.75451 17.76584
C 10.33041 10.63799 16.34150
C 10.85713 11.10666 18.79231
C 9.69416 8.36011 18.32126
C 8.89831 7.08300 18.73494
C 8.13936 6.57571 17.47708
C 9.90564 6.00232 19.17210
C 7.85988 7.27205 19.88040
C 5.91888 8.44563 20.85311
C 4.93202 7.26074 20.79211
C 6.51497 8.59815 22.27813
C 5.13190 9.75776 20.60430
H 3.67643 12.21568 20.62321
H 3.65880 14.71656 20.26964
H 5.49384 15.80928 18.94990
H 7.35154 14.41024 17.97049
H 9.53947 10.36804 15.61302
H 11.11782 9.86178 16.32210
H 10.76221 11.61369 16.04091
H 10.42926 11.18047 19.81401
H 11.63852 10.32594 18.78619
H 11.29958 12.08730 18.52694
H 7.43233 7.33140 17.08267
H 7.57310 5.65214 17.71829
H 8.87267 6.32964 16.68110
H 9.37322 5.06242 19.41053
H 10.63471 5.82023 18.36077
H 10.46966 6.31294 20.07414
H 5.43438 6.32293 21.09212
H 4.52777 7.14192 19.76704
H 4.08572 7.46600 21.47791
H 5.69408 8.80354 22.99372
H 7.04421 7.67304 22.56872
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1 + 2
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Fe 5.41066 9.68643 15.56903
O 6.24446 9.34641 17.04662
O 3.27885 12.99237 16.38943
O 1.64118 8.09920 16.03250
O 4.84449 6.14597 13.55365
O 8.46613 9.80166 12.97284
N 4.94446 11.52041 15.69994
N 3.53655 9.40380 15.89676
N 5.59043 8.14139 14.43173
N 6.75300 10.40202 14.42974
C 5.90349 12.42953 15.24441
C 6.95803 11.77938 14.51793
C 7.98470 12.54753 13.91685
C 7.95195 13.94573 14.03753
C 6.91196 14.58573 14.74718
C 5.88787 13.84028 15.35276
C 3.68561 11.84541 16.15839
C 2.75424 10.61726 16.25552
C 2.17772 10.54361 17.68711
C 1.62709 10.90017 15.22325
C 2.86794 8.21451 15.81897
C 3.68315 6.92451 15.51897
C 4.39792 6.51015 16.83338
C 2.70126 5.80527 15.12058
C 4.75310 7.06054 14.40105
C 6.67325 8.20563 13.41168
C 7.68076 7.04291 13.51638
C 6.08926 8.29325 11.97148
C 7.42841 9.53810 13.59704
H 8.77456 12.03188 13.35758
H 8.74861 14.54749 13.57112
H 6.90151 15.68443 14.83095
H 5.06831 14.32088 15.89893
H 2.97534 10.31913 18.42342
H 1.40606 9.75349 17.74119
H 1.72864 11.52244 17.95140
H 2.04654 10.94293 14.19614
H 0.86797 10.09942 15.26761
H 1.16372 11.88069 15.45173
H 5.08833 7.29685 17.19180
H 4.97641 5.57557 16.67800
H 3.63939 6.31428 17.61988
H 3.25119 4.85825 14.96311
H 1.94436 5.66807 15.91547
H 2.16785 6.04726 14.17951
H 7.19348 6.08796 13.24871
H 8.08183 6.96647 14.54561
H 8.52777 7.23930 12.82862
H 6.91359 8.46084 11.24924
H 5.56027 7.35395 11.72863
H 5.37641 9.14039 11.89297
Fe 7.07578 9.70278 18.52194
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O 10.84963 8.11970 18.07733
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O 4.02000 9.83776 21.11698
N 7.53815 11.53615 18.37291
N 8.95105 9.42117 18.19840
N 6.89954 8.16921 19.67530
N 5.73119 10.42656 19.65317
C 6.57650 12.44756 18.81827
C 5.52318 11.80250 19.55086
C 4.49458 12.57443 20.14373
C 4.52435 13.97143 20.00911
C 5.56319 14.60653 19.29337
C 6.58902 13.85718 18.69559
C 8.79619 11.85949 17.91126
C 9.73090 10.63285 17.82834
C 10.30994 10.54604 16.39856
C 10.85557 10.92899 18.85960
C 9.62237 8.23432 18.28850
C 8.80974 6.94566 18.60090
C 8.09509 6.51713 17.29099
C 9.79375 5.83218 19.00983
C 7.74015 7.09124 19.71793
C 5.81708 8.24175 20.69517
C 4.81302 7.07490 20.60412
C 6.40146 8.34681 22.13408
C 5.05825 9.57000 20.49541
H 3.70562 12.06263 20.70780
H 3.72618 14.57607 20.46917
H 5.57135 15.70434 19.19854
H 7.40783 14.33393 18.14493
H 9.51383 10.31325 15.66318
H 11.08282 9.75653 16.35359
H 10.75805 11.52288 16.12541
H 10.43419 10.98141 19.88547
H 11.61638 10.12936 18.82476
H 11.31743 11.90799 18.62179
H 7.40371 7.29932 16.92455
H 7.51770 5.58351 17.45604
H 8.85363 6.31387 16.50636
H 9.24563 4.88575 19.17694
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H 10.32727 6.08447 19.94811
H 5.30294 6.12484 20.88417
H 4.41313 6.98405 19.57562
H 3.96482 7.27718 21.28870
H 5.57704 8.52011 22.85487
H 6.93299 7.41153 22.38673
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101
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Fe 5.35715 9.68965 15.54969
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O 3.16673 12.91845 16.51214
O 1.61620 8.01189 15.90901
O 4.96239 6.13207 13.53537
O 8.39355 9.96194 12.91790
N 4.83997 11.51468 15.71563
N 3.48725 9.36091 15.86243
N 5.59842 8.17480 14.39364
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C 5.76788 12.46257 15.25696
C 6.83774 11.85944 14.51735
C 7.82272 12.67210 13.91101
C 7.74205 14.07103 14.04379
C 6.69173 14.66391 14.77033
C 5.70201 13.86939 15.37849
C 3.58502 11.79361 16.19546
C 2.67009 10.54895 16.23528
C 2.07210 10.42019 17.65348
C 1.55496 10.84317 15.19435
C 2.84519 8.16302 15.73188
C 3.70458 6.89791 15.44459
C 4.39868 6.50030 16.77592
C 2.76576 5.75152 15.02144
C 4.80163 7.06268 14.35458
C 6.69835 8.27388 13.39121
C 7.76538 7.17324 13.56406
C 6.15485 8.28440 11.93549
C 7.38063 9.65020 13.56651
H 8.62562 12.19038 13.33932
H 8.51534 14.70327 13.57745
H 6.64292 15.76021 14.87365
H 4.87276 14.31179 15.94316
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H 1.32094 9.60878 17.67446
H 1.59260 11.37915 17.93640
H 1.99081 10.92859 14.17665
H 0.81083 10.02708 15.19750
H 1.06485 11.80540 15.44488
H 5.05761 7.30616 17.15137
H 5.00838 5.58371 16.63461
H 3.62954 6.28332 17.54658
H 3.34564 4.82054 14.87697
H 1.99194 5.59405 15.79596
H 2.25007 5.98103 14.06733
H 7.33884 6.18215 13.32360
H 8.14497 7.15907 14.60488
H 8.61689 7.38982 12.88784
H 6.98859 8.49273 11.23522
H 5.69710 7.30808 11.69468

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Fe 7.11768 9.70244 18.53714
O 9.27329 12.89786 17.55376
O 10.84694 7.99805 18.04155
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C 4.61515 12.66852 20.13349
C 4.72395 14.06562 20.02902
C 5.81603 14.65527 19.35991
C 6.82138 13.86088 18.78362
C 8.89231 11.77152 17.89313
C 9.79574 10.53376 17.79575
C 10.31986 10.42055 16.34688
C 10.95971 10.81565 18.78691
C 9.63297 8.15667 18.29473
C 8.79473 6.90823 18.67485
C 8.05438 6.43527 17.39232
C 9.75048 5.78886 19.13347
C 7.74200 7.13598 19.78341
C 5.81138 8.32073 20.72566
C 4.80069 7.16434 20.58137
C 6.34587 8.41456 22.18185
C 5.06982 9.65351 20.49801
H 3.78263 12.18802 20.66141
H 3.94037 14.70274 20.46993
H 5.88340 15.75200 19.27720
H 7.67642 14.30318 18.26015
H 9.48857 10.20849 15.64487
H 11.06342 9.60506 16.28268
H 10.78952 11.37985 16.04978
H 10.57357 10.89271 19.82481
H 11.70083 9.99837 18.73968
H 11.43934 11.77875 18.52032
H 7.38786 7.21996 16.98782
H 7.44933 5.53069 17.60916
H 8.80181 6.16984 16.61632
H 9.18181 4.86213 19.33726
H 10.50363 5.59823 18.34683
H 10.28893 6.06877 20.06129
H 5.25209 6.20566 20.89361
H 4.45624 7.07604 19.53250
H 3.92069 7.38837 21.21730
H 5.49685 8.60941 22.86727
H 6.84613 7.47158 22.46546
H 7.06882 9.25131 22.27622

101
Species 5 (-2/3)
Fe 5.37359 9.69666 15.56249
O 6.26571 9.39848 17.06716
O 3.17753 12.91983 16.51494
O 1.63051 8.01610 15.92502
O 4.97542 6.13892 13.54924
O 8.39800 9.96595 12.92257
N 4.85345 11.51574 15.72434
N 3.50260 9.36223 15.87538
N 5.60424 8.18386 14.40464
N 6.70699 10.47190 14.43712
C 5.77915 12.46466 15.26671
C 6.84975 11.86205 14.52802
C 7.83613 12.67412 13.92240
C 7.75242 14.07244 14.05257
C 6.69972 14.66527 14.77760
C 5.71140 13.87159 15.38764
C 3.59729 11.79407 16.20651
C 2.68504 10.54927 16.24681
C 2.08136 10.42212 17.66268
C 1.57477 10.84192 15.19941
C 2.85980 8.16468 15.74793
C 3.71469 6.89872 15.45679
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C 2.77327 5.75693 15.02606
C 4.81153 7.06671 14.36965
C 6.70346 8.27963 13.40197
C 7.76849 7.17682 13.57369
C 6.15612 8.29355 11.94751
C 7.38877 9.65326 13.57533
H 8.63949 12.19232 13.35193
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H 1.60016 11.38121 17.94227
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H 1.08443 11.80518 15.44512
H 5.06515 7.29505 17.16875
H 5.01157 5.57494 16.64269
H 3.63207 6.27396 17.55385
H 3.35102 4.82512 14.87857
H 1.99810 5.59788 15.79881
H 2.25944 5.99183 14.07222
H 7.34032 6.18699 13.33170
H 8.14690 7.16097 14.61478
H 8.62062 7.39337 12.89830
H 6.98839 8.50455 11.24634
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H 5.39092 9.08944 11.83112
Fe 7.10611 9.69539 18.52416
O 9.27816 12.90666 17.55554
O 10.83752 8.00429 18.04843
O 7.59201 6.24109 20.65107
O 4.03337 9.94759 21.10482
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N 5.74470 10.46486 19.61855
C 6.70669 12.45200 18.83712
C 5.60957 11.85096 19.53718
C 4.61686 12.66426 20.13247
C 4.72140 14.06135 20.02698
C 5.80076 14.65359 19.33886
C 6.79563 13.86093 18.74246
C 8.87937 11.77880 17.87237
C 9.78336 10.53701 17.78530
C 10.31562 10.41593 16.33993
C 10.94280 10.82196 18.78057
C 9.62211 8.15956 18.29647
C 8.78704 6.90616 18.67313
C 8.05191 6.43492 17.38741
C 9.74799 5.79029 19.12852
C 7.72807 7.12271 19.78105
C 5.80032 8.31184 20.71515
C 4.78363 7.15935 20.58560
C 6.34230 8.41121 22.16877
C 5.06429 9.64738 20.48476
H 3.79244 12.18304 20.67245
H 3.94587 14.69694 20.48403
H 5.86584 15.75052 19.25824
H 7.64182 14.30367 18.20518
H 9.48878 10.20238 15.63311
H 11.05942 9.60011 16.28179
H 10.78794 11.37369 16.04154
H 10.55166 10.90021 19.81664
H 11.68492 10.00531 18.73894
H 11.42226 11.78527 18.51482
H 7.38164 7.21836 16.98642
H 7.45030 5.52689 17.59976
H 8.80054 6.17553 16.61042
H 9.18253 4.86165 19.33253
H 10.50132 5.60270 18.34121
H 10.28615 6.07119 20.05622
H 5.23875 6.20002 20.89092
H 4.42440 7.07258 19.54162
H 3.91262 7.38405 21.23363
H 5.49791 8.61162 22.85835
H 6.84159 7.46748 22.45182
H 7.06946 9.24530 22.25497

101
Species 5 (-2/5)
Fe 5.37840 9.67915 15.52782
O 6.24469 9.33985 17.04678
O 3.28808 12.98430 16.39195
O 1.61066 8.10157 16.03030
O 4.78258 6.18505 13.48262
O 8.45236 9.78884 12.93837
N 4.91533 11.50789 15.63814
N 3.50945 9.40270 15.88181
N 5.53819 8.17171 14.36922
N 6.76766 10.38316 14.42805
C 5.88335 12.41893 15.18746
C 6.95611 11.76828 14.49579
C 7.98600 12.53454 13.90350
C 7.94516 13.93674 14.00542
C 6.89240 14.57690 14.68859
C 5.85910 13.82904 15.28194
C 3.67041 11.83627 16.12452
C 2.72924 10.61920 16.23422
C 2.16506 10.55705 17.67087
C 1.59577 10.90187 15.20934
C 2.83234 8.21817 15.79684
C 3.64272 6.93391 15.46798
C 4.38970 6.50795 16.76230
C 2.65821 5.81594 15.07430
C 4.69034 7.09014 14.33530
C 6.64038 8.21250 13.36576
C 7.62541 7.03376 13.50880
C 6.09310 8.29941 11.91342
C 7.41644 9.53165 13.57046
H 8.78891 12.01563 13.36593
H 8.74894 14.53559 13.54743
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H 4.97058 5.57932 16.58285
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H 5.38922 9.15201 11.81483
Fe 7.10829 9.69511 18.56373
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O 10.87990 8.12050 18.07940
O 7.71118 6.22353 20.64437
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N 6.95061 8.19879 19.73663
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C 4.53230 13.96237 20.04221
C 5.58477 14.59784 19.35425
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C 9.75625 10.63349 17.84954
C 10.32308 10.55799 16.41465
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C 7.80134 7.11978 19.78219
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H 10.76175 11.53945 16.14315
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H 8.84482 6.29810 16.56300
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H 10.38678 6.10369 19.98234
H 5.35193 6.11948 20.90620
H 4.50413 6.97403 19.56602
H 3.99116 7.25969 21.26274
H 5.55106 8.51839 22.88862
H 6.92525 7.41781 22.46132
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B3LYP

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Fe 0.01697 0.00099 -0.02051
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N -0.00850 1.76668 -0.59211
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N -0.24532 -1.75466 -0.58735
N 1.86644 0.06254 -0.54995
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C 1.19811 2.38217 -0.82313
C -2.56867 -0.97986 -0.53027
C -2.32594 1.46278 -0.40405
C 0.75160 -2.69355 -0.70460
C -1.65848 -2.20418 -0.73455
C 2.39328 1.42377 -0.77018
C 2.73192 -0.97350 -0.51712
C 2.17678 -2.38247 -0.19905
O 1.33321 3.57882 -1.04206
O -3.79166 -1.06166 -0.60754
O 0.51389 -3.83302 -1.10485
O 3.95350 -0.85618 -0.68174
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H -1.42882 -3.64689 -2.36140
H -3.04743 -2.87382 -2.25634
H -1.48772 -4.18897 0.16787
H -1.79418 -2.87276 1.33996
H -3.11307 -3.44348 0.28252
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H 3.57231 2.93833 0.26450
H 4.04955 0.97615 -2.11749
H 2.48221 1.20550 -2.94318
H 3.35595 2.62349 -2.30161
H 2.81944 -4.43968 -0.50386
H 3.16376 -3.37764 -1.88676
H 4.15375 -3.24476 -0.41567
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N -0.25769 -1.84159 -0.56780
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C 1.23970 2.47249 -0.60571
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C -2.30888 1.45276 -0.52245
C 0.71580 -2.77710 -0.67936
C -1.68157 -2.25052 -0.68821
C 2.40491 1.45609 -0.70394
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C 2.16851 -2.38946 -0.26613
O 1.43120 3.67911 -0.66513
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O 3.90342 -0.88235 -0.95682
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C 3.12975 -3.44792 -0.83179
C 2.21568 -2.45612 1.28760
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H -4.95166 3.59699 -0.74448
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H -1.45203 -3.76100 -2.24110
H -3.08779 -3.02093 -2.16579
H -1.52042 -4.17530 0.31342
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H -3.15729 -3.44654 0.38090
H 2.90139 1.60082 1.41569
H 4.27064 1.12838 0.36707
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H 3.94433 1.07240 -2.19529
H 2.34864 1.47188 -2.89066
H 3.34448 2.76670 -2.16853
H 2.82148 -4.44772 -0.50245
H 3.13048 -3.44150 -1.93291
H 4.15317 -3.24543 -0.49301
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H 1.54187 -1.71468 1.73832
H 1.92093 -3.46176 1.62858

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O 1.31613 6.13124 -3.40603
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C 2.16105 5.19991 -0.88371
O 0.53223 5.46772 -2.71441
C -0.81485 5.00678 -3.36748
C -2.12231 5.06347 -2.50648
O -3.16212 5.45559 -3.05250
C -0.61843 3.51623 -3.76383
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H -1.50706 3.14478 -4.29941
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H -0.16996 5.73881 -5.31042
H -1.18070 6.89422 -4.41862
H -1.93873 5.47395 -5.16798
C 3.23880 4.48595 -1.72176
H 2.97726 3.42421 -1.85796
H 4.20974 4.53971 -1.20834
H 3.32034 4.95677 -2.70917
C 2.52181 6.69119 -0.69006
H 2.57320 7.18977 -1.66547
H 3.49104 6.78267 -0.17708
H 1.75586 7.19398 -0.07753
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H 2.45384 3.63831 3.23960
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H -0.98440 2.39023 5.55439
C -1.41620 3.01893 3.54322
H -2.48903 2.85053 3.61236
C -4.24292 3.35399 -1.14548
H -4.60567 3.76539 -2.09549
H -5.09861 3.13265 -0.49125
H -3.71065 2.41107 -1.35008
C -4.04263 5.68844 -0.16830
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Species 2 (-1/4)
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O 1.31698 6.11819 -3.41769
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C -0.86528 3.48755 2.33944
C 0.54429 3.71542 2.23415
C 2.16562 4.60777 0.55781
C 2.15727 5.21982 -0.87665
O 0.52990 5.46572 -2.72279
C -0.81391 4.99582 -3.37464
C -2.12029 5.06446 -2.51400
O -3.15998 5.44760 -3.06203
C -0.61865 3.50379 -3.76573
H 0.24980 3.39802 -4.43549
H -1.50744 3.13314 -4.30116
H -0.45522 2.86368 -2.88741
C -1.03776 5.80942 -4.65865
H -0.16784 5.71652 -5.32091
H -1.17785 6.87799 -4.43570
H -1.93676 5.45395 -5.17761
C 3.23280 4.48952 -1.70195
H 2.96414 3.42822 -1.82793
H 4.19784 4.54091 -1.17734
H 3.32951 4.94774 -2.69421
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H 2.58913 7.19601 -1.69032
H 3.47478 6.80700 -0.17655
H 1.74113 7.22830 -0.11824
C 1.37681 3.44097 3.32824
H 2.44629 3.62071 3.23391
C 0.82145 2.94280 4.51606
H 1.47588 2.72783 5.36524
C -0.55436 2.71987 4.61844
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H -1.17832 6.80465 -4.48524
H -1.92570 5.37456 -5.22758
C 3.34468 4.65885 -1.67965
H 3.23093 3.57928 -1.86961
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H 2.34630 7.25508 -1.55991
H 3.19360 6.89017 -0.01690
H 1.41924 7.07840 -0.04454
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H 2.44377 3.59798 3.21455
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C -0.56861 2.81101 4.63811
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C -4.38092 3.49070 -1.08001
H -4.75109 3.95341 -2.00498
H -5.21354 3.37361 -0.37135
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Species 3 (-1/1)
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N 0.93877 4.05496 0.92432
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C 3.30132 4.57779 -1.69186
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H 1.63894 7.20289 -0.08750
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H 2.45570 3.56038 3.21378
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H 1.48438 2.68406 5.35147
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H -0.97380 2.30938 5.54250
C -1.39656 2.96591 3.52787
H -2.47205 2.81116 3.59592
C -4.30794 3.41526 -1.09729
H -4.67850 3.82306 -2.04676
H -5.15500 3.23424 -0.42000
H -3.81166 2.45197 -1.29696
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H -4.85947 5.61834 0.50572
H -4.35232 6.19872 -1.11716

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O -0.16269 10.92395 7.52106
O -2.58590 7.40130 9.27947
O -1.41445 7.81860 4.30542
O 2.90035 9.29706 4.39703
N -0.63721 8.56332 8.88585
N -0.70834 8.42183 6.38689
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C -1.76010 7.88689 8.51326
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H 2.84422 9.74438 11.45634
C -1.88963 7.75775 6.99233
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C 3.20553 9.57294 7.09576
C 1.16186 9.18780 10.22719
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H -2.13131 6.06319 5.63301
H -2.72537 5.78221 7.30453
H -0.97437 5.77288 6.96336
C 3.81673 10.93429 6.70336
H 4.08821 10.94068 5.64111
H 4.71340 11.12020 7.31243
H 3.09636 11.74628 6.89210
C -3.20710 8.45163 6.58694
H -3.15656 9.52911 6.81087
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H -3.39393 8.32059 5.51467
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H 1.64616 9.24305 13.59687
C 0.75507 8.61620 2.93883
H 1.50875 9.20762 2.40519
H -0.18385 8.61528 2.37239
H 1.11714 7.57832 2.99816
C -0.83829 8.40965 11.39712
H -1.85710 8.03200 11.36164
C 4.19757 8.41485 6.84616
H 3.73288 7.45143 7.11043
H 5.08159 8.55770 7.48425
H 4.49909 8.38575 5.79404
C 0.01768 10.67049 4.17306
H -0.17208 11.16133 5.13648
H -0.91587 10.67506 3.58932
H 0.76944 11.25862 3.62423

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Species 4 (-1/3)
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O 3.91458 9.85206 9.41093
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O -0.21911 10.88578 7.52895
O -2.46778 7.23407 9.27040
O -1.49328 7.90771 4.21823
O 2.88464 9.11077 4.39984
N -0.56381 8.45948 8.87337
N -0.76902 8.41417 6.32426
N 1.90893 9.31948 6.44260
C -1.68566 7.76690 8.49343
C 2.98259 9.67879 8.62967
C 1.85935 9.18697 5.07426
C 1.76304 9.57267 11.47787
H 2.75041 10.02971 11.49610
C -1.89373 7.70224 6.96911
C 0.49550 9.24553 4.33624
C 3.22544 9.54321 7.10948
C 1.15785 9.29904 10.24282
C -0.67660 8.44617 4.97351
C -0.17819 8.64409 12.60988
H -0.70007 8.39469 13.53736
C -1.92790 6.20478 6.59556
H -2.16082 6.08355 5.53183
H -2.69045 5.69751 7.20402
H -0.95177 5.73733 6.80126
C 3.88674 10.84572 6.62004
H 4.17534 10.76305 5.56521
H 4.78158 11.04264 7.22824
H 3.19589 11.69576 6.73587
C -3.24276 8.38696 6.66315
H -3.20253 9.45141 6.94338
H -4.04573 7.90416 7.23903
H -3.46370 8.31152 5.59137
C 1.08552 9.24286 12.65761
H 1.55106 9.45990 13.62257
C 0.70738 8.72876 2.90290
H 1.47844 9.32302 2.39706
H -0.23425 8.79643 2.34516
H 1.03140 7.67718 2.89847
C -0.79061 8.35738 11.38327
H -1.76771 7.88335 11.33581
C 4.16559 8.33108 6.93681
H 3.66573 7.40830 7.27161
H 5.06045 8.48344 7.55707
H 4.45596 8.21665 5.88672
C 0.06755 10.73842 4.26053
H -0.12769 11.16790 5.25202
H -0.85098 10.82306 3.65908
H 0.85545 11.32928 3.76752

1 + 3

101
1 + 3 Reactant complex (-2/4)
Fe 4.99171 9.31126 15.13747
O 5.74031 8.96136 16.52398
O 3.51189 12.84696 16.23342
O 1.09469 8.30154 15.71536
O 4.05745 5.76286 13.38012
O 8.15714 8.86530 12.76116
N 4.84936 11.20045 15.32185
N 3.12301 9.33208 15.49465
N 4.98744 7.73372 14.07161
N 6.49426 9.78787 14.07044
C 5.93324 11.91191 14.88987
C 6.88741 11.09257 14.16680
C 8.02966 11.69612 13.58387
C 8.22440 13.05957 13.73270
C 7.29310 13.86012 14.44038
C 6.15517 13.30702 15.00464
C 3.68689 11.69072 15.87569
C 2.57536 10.62682 15.97173
C 2.12577 10.54838 17.44504
C 1.43153 11.14901 15.06986
C 2.30481 8.25003 15.45996
C 2.92875 6.85281 15.19107
C 3.56716 6.37873 16.52757
C 1.79944 5.88056 14.81339
C 4.03827 6.76436 14.10765
C 6.17616 7.53873 13.20396
C 7.00972 6.31777 13.64059
C 5.79847 7.44900 11.70547
C 7.07149 8.78794 13.31872
H 8.73676 11.07178 13.04304
H 9.11511 13.52550 13.30444
H 7.48025 14.93117 14.54819
H 5.43470 13.91247 15.54889
H 2.94611 10.17348 18.07658
H 1.26747 9.87209 17.54042
H 1.84390 11.54938 17.80283
H 1.76379 11.19762 14.02027
H 0.56767 10.47904 15.13545
H 1.14444 12.16140 15.38980
H 4.38430 7.04217 16.84216
H 3.96473 5.35798 16.40979
H 2.80264 6.35703 17.32052
H 2.20326 4.86887 14.68460
H 1.03211 5.87566 15.59715
H 1.31598 6.17432 13.86904
H 6.43556 5.39608 13.48702
H 7.27529 6.39888 14.70647
H 7.93865 6.27246 13.05360
H 6.71324 7.41861 11.09529
H 5.20027 6.54953 11.52426
H 5.21040 8.33182 11.40676
Mn 7.65455 10.09029 19.17964
O 9.17173 13.59275 17.97301
O 11.46115 8.88698 18.52774
O 8.37201 6.40249 20.68607
O 4.32644 9.70158 21.36954
N 7.74354 11.96861 18.78833
N 9.47280 10.02255 18.59273
N 7.44422 8.39199 20.03240
N 6.00232 10.56830 20.03476
C 6.60129 12.70019 19.17030
C 5.62496 11.91520 19.86637
C 4.44630 12.52093 20.32481
C 4.23123 13.88858 20.09922
C 5.18398 14.65414 19.42249
C 6.36967 14.06648 18.95723
C 8.92902 12.43284 18.30598
C 10.05658 11.34844 18.25770
C 10.65956 11.34432 16.84210
C 11.10626 11.78964 19.30153
C 10.23350 8.90278 18.67634
C 9.49021 7.52627 18.86085
C 8.80561 7.19319 17.50628
C 10.55134 6.45101 19.14028
C 8.38327 7.41517 19.97640
C 6.25776 8.29679 20.92367
C 5.36750 7.10486 20.52951
C 6.66530 8.21132 22.41075
C 5.40672 9.60317 20.78730
H 3.71773 11.91302 20.85815
H 3.30877 14.35299 20.45838
H 5.00973 15.71978 19.25030
H 7.12462 14.65047 18.43406
H 9.90751 11.01891 16.10603
H 11.51630 10.65946 16.79721
H 10.98717 12.35942 16.57465
H 10.66318 11.79143 20.31086
H 11.95775 11.09845 19.29383
H 11.45263 12.80843 19.07368
H 8.01057 7.90369 17.24062
H 8.35784 6.18698 17.55023
H 9.55274 7.19384 16.69604
H 10.07735 5.46370 19.20751
H 11.30055 6.44578 18.33869
H 11.07430 6.63957 20.08944
H 5.90528 6.16172 20.69167
H 5.08629 7.17357 19.46667
H 4.44815 7.11149 21.13280
H 5.76673 8.23253 23.04480
H 7.22659 7.28694 22.59354
H 7.30151 9.06970 22.68182

101
TS_R (-2/4)
Fe 5.05646 9.41057 15.14467
O 5.85830 9.12253 16.51850
O 3.41226 12.88062 16.21916
O 1.22964 8.20537 15.81312
O 4.26110 5.80271 13.44201
O 8.20275 9.08969 12.72622
N 4.81605 11.29248 15.30281
N 3.19731 9.33796 15.54377
N 5.11616 7.81735 14.10391
N 6.50988 9.94969 14.03976
C 5.85380 12.05228 14.84360
C 6.83673 11.27286 14.11281
C 7.93744 11.92633 13.50341
C 8.06538 13.29891 13.63456
C 7.10615 14.06030 14.34958
C 6.00718 13.45828 14.93940
C 3.63994 11.73002 15.87372
C 2.58718 10.61109 16.00333
C 2.15738 10.53793 17.48266
C 1.40829 11.05429 15.10423
C 2.43659 8.21394 15.53880
C 3.13022 6.84794 15.27855
C 3.82308 6.43214 16.60694
C 2.04804 5.80877 14.94371
C 4.21492 6.80483 14.16732
C 6.29085 7.67620 13.20708
C 7.19105 6.49641 13.62280
C 5.87971 7.56522 11.71855
C 7.12792 8.96740 13.29615
H 8.66573 11.33202 12.95695
H 8.92393 13.80445 13.18603
H 7.24079 15.14071 14.44135
H 5.26616 14.03301 15.48926
H 3.00217 10.21630 18.11127
H 1.33503 9.82173 17.60007
H 1.82949 11.53027 17.82502
H 1.72918 11.10877 14.05139
H 0.58599 10.33531 15.18530
H 1.06407 12.05196 15.41391
H 4.59969 7.15132 16.90040
H 4.28452 5.43815 16.49277
H 3.07567 6.36915 17.41391
H 2.50349 4.81773 14.82523
H 1.29970 5.77796 15.74501
H 1.52911 6.05649 14.00511
H 6.65835 5.54836 13.48073
H 7.47646 6.58960 14.68234
H 8.10755 6.49545 13.01488
H 6.77878 7.57355 11.08473
H 5.31825 6.63885 11.55582
H 5.24476 8.41947 11.43309
Mn 7.57921 10.01099 19.14681
O 9.18461 13.44082 17.84513
O 11.35328 8.69425 18.49235
O 8.22520 6.35675 20.76687
O 4.28644 9.78126 21.41283
N 7.72390 11.87930 18.72250
N 9.39446 9.88026 18.55549
N 7.33842 8.34464 20.05496
N 5.96278 10.56259 20.02710
C 6.61152 12.65476 19.10596
C 5.62330 11.91601 19.83450
C 4.47138 12.56742 20.29827
C 4.29475 13.93586 20.04616
C 5.25964 14.65682 19.33842
C 6.41891 14.02287 18.86734
C 8.91351 12.29641 18.20872
C 10.00624 11.17773 18.16317
C 10.56653 11.11040 16.73122
C 11.09898 11.62094 19.16073
C 10.12914 8.74519 18.66192
C 9.35790 7.39330 18.90120
C 8.66080 7.02991 17.56138
C 10.39666 6.30550 19.21432
C 8.25485 7.34538 20.02438
C 6.16768 8.30933 20.97144
C 5.23732 7.13145 20.63136
C 6.60155 8.25782 22.45294
C 5.35224 9.63517 20.81418
H 3.73339 11.99386 20.85607
H 3.39298 14.43632 20.40938
H 5.11559 15.72350 19.14595
H 7.18298 14.57171 18.32002
H 9.78463 10.78239 16.02786
H 11.40162 10.39926 16.68539
H 10.91550 12.10585 16.42047
H 10.68714 11.66659 20.18222
H 11.93044 10.90620 19.14946
H 11.46458 12.62224 18.88980
H 7.90284 7.76676 17.26193
H 8.16741 6.04812 17.64735
H 9.40916 6.96146 16.75518
H 9.90250 5.33077 19.31226
H 11.14497 6.26000 18.41326
H 10.92366 6.51253 20.15749
H 5.75137 6.17894 20.81447
H 4.93829 7.17352 19.57203
H 4.32948 7.18286 21.24982
H 5.71644 8.33042 23.10189
H 7.13527 7.32170 22.65660
H 7.27077 9.10282 22.68360

101
Intermediate$_R$ (-2/4)
Fe 5.28350 9.50400 15.47376
O 6.11419 9.30654 16.89469
O 3.16665 12.74144 16.47175
O 1.61599 7.83618 16.07649
O 4.80758 5.97918 13.50367
O 8.50798 9.57842 13.14476
N 4.79282 11.34777 15.60713
N 3.43887 9.19668 15.83674
N 5.53290 7.96386 14.37726
N 6.67250 10.24132 14.38150
C 5.68567 12.23906 15.09936
C 6.78592 11.59322 14.39546
C 7.76220 12.38628 13.73528
C 7.64954 13.76200 13.77953
C 6.57214 14.39325 14.46194
C 5.60009 13.65603 15.11029
C 3.55440 11.62783 16.15760
C 2.66213 10.38019 16.28805
C 2.22781 10.25739 17.76253
C 1.44645 10.66508 15.37143
C 2.80986 7.99120 15.79533
C 3.64763 6.72753 15.46338
C 4.39025 6.32195 16.76489
C 2.68698 5.59323 15.07267
C 4.70715 6.88175 14.34177
C 6.66718 8.01632 13.41706
C 7.65770 6.85296 13.59451
C 6.17264 8.09705 11.94812
C 7.41688 9.34197 13.63711
H 8.57988 11.89360 13.21485
H 8.40277 14.38033 13.28565
H 6.51967 15.48435 14.47906
H 4.77768 14.13061 15.63820
H 3.09980 10.06453 18.40507
H 1.51351 9.43288 17.87398
H 1.75642 11.19527 18.09111
H 1.77010 10.74873 14.32141
H 0.71633 9.85308 15.45129
H 0.98134 11.61631 15.66778
H 5.06716 7.11322 17.10907
H 4.97622 5.40471 16.59505
H 3.65571 6.11400 17.55881
H 3.24946 4.66652 14.90202
H 1.95181 5.43426 15.87108
H 2.13947 5.82973 14.14799
H 7.18236 5.90447 13.31977
H 7.99700 6.79255 14.63816
H 8.53646 7.02118 12.95544
H 7.03000 8.23948 11.27349
H 5.64818 7.17172 11.68492
H 5.48261 8.94609 11.81991
Mn 7.19287 9.85957 18.60013
O 9.28269 13.09485 17.39017
O 10.95656 8.24464 18.29638
O 7.66758 6.37310 20.72265
O 4.22168 10.23275 21.31357
N 7.63835 11.72744 18.26439
N 9.08049 9.55611 18.20005
N 6.95166 8.35258 19.82073
N 5.80521 10.68887 19.69426
C 6.68130 12.65781 18.70810
C 5.65076 12.07399 19.51121
C 4.65721 12.89321 20.06938
C 4.68127 14.27674 19.83982
C 5.68870 14.84709 19.05795
C 6.68878 14.04373 18.49040
C 8.87327 11.99395 17.76823
C 9.83642 10.76966 17.79429
C 10.46469 10.60196 16.39937
C 10.91830 11.14593 18.83571
C 9.73105 8.39261 18.42579
C 8.88041 7.12354 18.78215
C 8.18708 6.65610 17.47778
C 9.84379 6.01455 19.23501
C 7.77365 7.28109 19.88322
C 5.86633 8.52266 20.82191
C 4.79027 7.43057 20.68314
C 6.41909 8.55887 22.26674
C 5.18869 9.90978 20.61776
H 3.88784 12.43482 20.68733
H 3.90221 14.90727 20.27756
H 5.70223 15.92629 18.88117
H 7.48489 14.47259 17.88589
H 9.69931 10.32889 15.65639
H 11.22685 9.81230 16.42390
H 10.92788 11.54861 16.08407
H 10.46134 11.26584 19.83187
H 11.67913 10.35913 18.89118
H 11.38597 12.10047 18.55384
H 7.50587 7.41589 17.07301
H 7.60961 5.73574 17.66237
H 8.94936 6.42819 16.71517
H 9.28713 5.08759 19.42226
H 10.60308 5.83910 18.46254
H 10.36530 6.28736 20.16444
H 5.21985 6.44698 20.91280
H 4.39151 7.41063 19.65728
H 3.95867 7.63901 21.37225
H 5.60350 8.79149 22.96672
H 6.86818 7.59310 22.52490
H 7.18888 9.34244 22.36059

101
MECP (-2/4)
Fe 5.32414 9.52336 15.52698
O 6.27614 9.37391 17.12655
O 3.16783 12.77153 16.46898
O 1.64319 7.84881 16.11344
O 4.83690 5.98988 13.54591
O 8.53185 9.59927 13.16318
N 4.81219 11.38121 15.62648
N 3.46992 9.21198 15.89335
N 5.58439 7.96213 14.43656
N 6.69761 10.26693 14.40372
C 5.69508 12.26998 15.09621
C 6.79556 11.62155 14.39417
C 7.76312 12.41277 13.72050
C 7.64461 13.78905 13.74878
C 6.56935 14.42231 14.43094
C 5.60471 13.68608 15.09290
C 3.57151 11.65799 16.16815
C 2.68234 10.40407 16.30431
C 2.21509 10.30643 17.77068
C 1.48390 10.66853 15.35904
C 2.84060 8.01057 15.84038
C 3.68315 6.74484 15.50983
C 4.41976 6.33778 16.81224
C 2.72192 5.61186 15.11612
C 4.74910 6.89382 14.38811
C 6.69034 8.03823 13.44578
C 7.69189 6.87823 13.57823
C 6.15735 8.13637 11.99135
C 7.44073 9.36680 13.66059
H 8.58015 11.91782 13.20096
H 8.39000 14.40479 13.24039
H 6.50947 15.51297 14.43423
H 4.78146 14.16069 15.61923
H 3.07373 10.14012 18.43846
H 1.51007 9.47360 17.88225
H 1.72285 11.24369 18.06909
H 1.82928 10.73199 14.31417
H 0.75547 9.85479 15.44032
H 1.00909 11.62387 15.62667
H 5.09688 7.12859 17.15782
H 5.00669 5.42031 16.64554
H 3.68357 6.13054 17.60506
H 3.28326 4.68461 14.94436
H 1.98382 5.45308 15.91189
H 2.17701 5.85028 14.19043
H 7.20445 5.93002 13.32366
H 8.07783 6.81733 14.60592
H 8.54207 7.04734 12.90183
H 6.99465 8.29517 11.29497
H 5.63252 7.21043 11.73016
H 5.45709 8.98164 11.89539
Mn 7.14794 9.83201 18.55421
O 9.23328 13.05810 17.36042
O 10.91298 8.23762 18.24206
O 7.62388 6.36177 20.68327
O 4.20858 10.20721 21.28136
N 7.61571 11.68670 18.27656
N 9.03360 9.54306 18.20758
N 6.96023 8.36891 19.81090
N 5.81299 10.66385 19.68409
C 6.66176 12.62340 18.69610
C 5.63304 12.04029 19.49596
C 4.63174 12.85606 20.04909
C 4.65487 14.23644 19.81318
C 5.66458 14.80818 19.03191
C 6.66881 14.00934 18.47045
C 8.84289 11.95810 17.75171
C 9.79800 10.74064 17.77729
C 10.41464 10.56275 16.37880
C 10.88444 11.12268 18.81291
C 9.69128 8.37295 18.40086
C 8.86366 7.10306 18.76659
C 8.18286 6.60533 17.46582
C 9.83871 6.01330 19.24304
C 7.75783 7.27322 19.85436
C 5.86555 8.50872 20.80418
C 4.79726 7.41119 20.65207

C 6.41381 8.54456 22.25106
C 5.18315 9.88260 20.60163
H 3.85884 12.39954 20.66332
H 3.87113 14.86744 20.24174
H 5.67297 15.88698 18.85111
H 7.46195 14.44028 17.86424
H 9.64617 10.28001 15.64339
H 11.18281 9.77990 16.40198
H 10.86712 11.51084 16.05312
H 10.43088 11.25006 19.80961
H 11.64509 10.33603 18.87070
H 11.34913 12.07543 18.52043
H 7.49084 7.34928 17.05169
H 7.62318 5.67707 17.66346
H 8.95353 6.37906 16.71185
H 9.29098 5.08502 19.44874
H 10.59903 5.82948 18.47361
H 10.35772 6.31206 20.16633
H 5.22615 6.42938 20.88559
H 4.40887 7.39148 19.62292
H 3.95818 7.61877 21.33194
H 5.59265 8.76701 22.94780
H 6.87027 7.58222 22.50770
H 7.17505 9.33550 22.35099

101
Intermediate$_P$ (-2/4)
Fe 5.21544 9.69874 15.26595
O 6.38273 9.43456 17.24729
O 3.19634 12.92536 16.45191
O 1.55831 8.02480 15.88835
O 4.81750 6.07862 13.46214
O 8.35636 9.82804 12.81253
N 4.79811 11.52025 15.55658
N 3.41055 9.36903 15.77388
N 5.52300 8.10273 14.27069
N 6.65614 10.40674 14.26718
C 5.78104 12.42727 15.12110
C 6.83805 11.79526 14.39748
C 7.88119 12.56879 13.86736
C 7.87478 13.95951 14.04776
C 6.83637 14.57894 14.74825
C 5.78745 13.81979 15.28701
C 3.58551 11.81173 16.09758
C 2.64568 10.57861 16.17918
C 2.12333 10.46084 17.62289
C 1.48776 10.88964 15.20148
C 2.76811 8.17849 15.67334
C 3.62006 6.90439 15.37383
C 4.34249 6.52092 16.69044
C 2.66451 5.76022 14.99884
C 4.70452 7.02084 14.25754
C 6.62755 8.19028 13.27766
C 7.67295 7.07837 13.46943
C 6.09459 8.19049 11.82415
C 7.33199 9.56259 13.44288
H 8.67482 12.07199 13.31312
H 8.69099 14.55822 13.63413
H 6.83787 15.66395 14.88437
H 4.97117 14.28768 15.83272
H 2.95014 10.23684 18.31484
H 1.37848 9.65800 17.69219
H 1.66593 11.41262 17.93089
H 1.87084 10.96868 14.17075
H 0.73565 10.09359 15.23643
H 1.02715 11.85096 15.47234
H 5.01436 7.31572 17.03749
H 4.93599 5.60374 16.54784
H 3.60005 6.32500 17.48019
H 3.22865 4.82955 14.85821
H 1.91638 5.62165 15.78932
H 2.12992 5.97385 14.06123
H 7.22939 6.09731 13.25900
H 8.05359 7.08117 14.50173
H 8.52077 7.25261 12.79093
H 6.92575 8.37136 11.12664
H 5.62073 7.22943 11.59345
H 5.35075 8.99305 11.69136
Mn 7.12898 9.73863 18.59012
O 9.27727 12.97440 17.72241
O 10.84474 8.12528 18.12326
O 7.57048 6.19417 20.56149
O 4.17643 9.95206 21.25307
N 7.66186 11.54905 18.53787
N 9.00302 9.44967 18.35156
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C 5.66375 11.86737 19.68295
C 4.63049 12.63903 20.23831
C 4.66787 14.02880 20.08554
C 5.71927 14.64505 19.39640
C 6.75261 13.88548 18.83829
C 8.89624 11.85238 18.03147
C 9.80621 10.62815 17.93954
C 10.30876 10.51543 16.48598
C 10.97213 10.91504 18.91626
C 9.64837 8.24526 18.39565
C 8.84773 6.96803 18.70660
C 8.17469 6.49566 17.39038
C 9.82824 5.87477 19.16686
C 7.75613 7.12869 19.77936
C 5.87238 8.29952 20.77560
C 4.81762 7.19988 20.55057
C 6.39860 8.28066 22.23204
C 5.18211 9.65280 20.62107
H 3.82591 12.14807 20.77914
H 3.86344 14.63506 20.50992
H 5.73508 15.73220 19.28400
H 7.57202 14.35187 18.29885
H 9.47634 10.28346 15.80456
H 11.06569 9.72724 16.40317
H 10.74521 11.47759 16.18074
H 10.59767 10.98278 19.95022
H 11.72245 10.11951 18.86181
H 11.43196 11.87815 18.65173
H 7.48730 7.24428 16.97893
H 7.61110 5.56744 17.57181
H 8.95072 6.28411 16.63897
H 9.28634 4.93796 19.34533
H 10.59519 5.71582 18.39926
H 10.33512 6.15745 20.10175
H 5.23729 6.21166 20.76862
H 4.46120 7.21555 19.51052
H 3.95984 7.39054 21.21150
H 5.56111 8.46509 22.92044
H 6.85586 7.31185 22.45988
H 7.14911 9.07364 22.37873

101
TS$_P$ (-2/4)
Fe 5.08465 9.72062 14.98831
O 6.45155 9.46397 17.42467
O 3.25163 12.93926 16.42456
O 1.47827 8.07159 15.80603
O 4.70079 6.04173 13.34919
O 8.30393 9.74942 12.66028
N 4.78001 11.52065 15.42638
N 3.33729 9.39953 15.62856
N 5.40542 8.09493 14.08035
N 6.59563 10.37580 14.08656
C 5.80263 12.39984 15.02093
C 6.83020 11.75250 14.26630
C 7.90584 12.50111 13.76758
C 7.96369 13.88088 14.01238
C 6.95803 14.51422 14.74742
C 5.87522 13.78043 15.25367
C 3.59395 11.82906 16.01885
C 2.62117 10.61714 16.09771
C 2.15827 10.46998 17.55897
C 1.43261 10.98049 15.17875
C 2.68091 8.21273 15.55404
C 3.51862 6.92839 15.24653
C 4.26641 6.55614 16.55539
C 2.54554 5.78792 14.90704
C 4.58941 7.00993 14.11054
C 6.54332 8.14176 13.12205
C 7.56786 7.02576 13.39229
C 6.05851 8.09592 11.65447
C 7.26573 9.51083 13.27606
H 8.67657 11.99474 13.18974
H 8.80507 14.46013 13.62233
H 7.01078 15.59027 14.93420
H 5.08313 14.25908 15.82563
H 3.01014 10.21108 18.20748
H 1.40087 9.68015 17.63965
H 1.73414 11.42162 17.91127
H 1.77452 11.08258 14.13570
H 0.66640 10.19792 15.22184
H 1.00222 11.94154 15.49638
H 4.96312 7.34201 16.87557
H 4.83809 5.62484 16.41500
H 3.54033 6.38895 17.36680
H 3.09894 4.85154 14.76312
H 1.81489 5.66373 15.71595
H 1.99080 5.99670 13.97986
H 7.12409 6.04265 13.19145
H 7.90111 7.05628 14.44119
H 8.44692 7.17094 12.74760
H 6.91337 8.23994 10.97729
H 5.57848 7.13288 11.44457
H 5.33016 8.90209 11.46829
Mn 7.19073 9.76604 18.74852
O 9.31111 13.04555 17.94609
O 10.89061 8.18012 18.14625
O 7.63035 6.15472 20.57965
O 4.26693 9.91428 21.45373
N 7.70130 11.58647 18.71015
N 9.06277 9.50046 18.48299
N 7.05855 8.25699 19.91040
N 5.91325 10.48007 19.94606
C 6.73695 12.50471 19.14885
C 5.69541 11.86171 19.85947
C 4.64189 12.61151 20.40508
C 4.63979 14.00078 20.23482
C 5.67279 14.63744 19.53788
C 6.72918 13.89924 18.99178
C 8.93093 11.91134 18.21411
C 9.83903 10.69042 18.05343
C 10.24462 10.60559 16.56718
C 11.06289 10.95872 18.95902
C 9.70463 8.29581 18.46574
C 8.91132 7.00837 18.76172
C 8.22809 6.56204 17.43997
C 9.90386 5.91128 19.18713
C 7.82339 7.12778 19.84638
C 5.93420 8.26198 20.88056
C 4.87207 7.19361 20.55466
C 6.42486 8.14110 22.34261
C 5.25844 9.63117 20.79051
H 3.85087 12.10511 20.95210
H 3.81832 14.58917 20.65177
H 5.65802 15.72306 19.41103
H 7.53771 14.38091 18.44864
H 9.36163 10.41328 15.93804
H 10.97231 9.79999 16.41483
H 10.68672 11.56306 16.25536
H 10.75611 10.99052 20.01682
H 11.81572 10.17399 18.83251
H 11.49367 11.93546 18.69574
H 7.52528 7.31268 17.05723
H 7.67885 5.62190 17.60348
H 8.99670 6.38184 16.67272
H 9.36966 4.96736 19.34981
H 10.66497 5.77565 18.40938
H 10.41748 6.17664 20.12377
H 5.27565 6.18754 20.71623
H 4.54651 7.28397 19.50720
H 3.99704 7.34810 21.20251
H 5.57513 8.30108 23.02200
H 6.85935 7.15158 22.51959
H 7.18644 8.90855 22.55463

101
2 + 4 Product complex (-2/4)
Fe 4.95791 9.78004 14.60934
O 6.45739 9.32568 17.81253
O 3.33081 13.04433 16.17493
O 1.37672 8.22226 15.64383
O 4.48089 6.05003 13.12970
O 8.16184 9.66174 12.26808
N 4.76190 11.57726 15.10476
N 3.25200 9.50806 15.36137
N 5.22477 8.12651 13.74748
N 6.50082 10.36268 13.71613
C 5.82620 12.40774 14.70276
C 6.80724 11.72263 13.91794
C 7.92079 12.42089 13.43001
C 8.06511 13.78626 13.71721
C 7.10722 14.45550 14.48360
C 5.98534 13.77338 14.97746
C 3.61338 11.92587 15.74714
C 2.59994 10.74817 15.86286
C 2.20125 10.61387 17.34451
C 1.38303 11.15053 15.00047
C 2.57029 8.33415 15.33990
C 3.37396 7.02725 15.03050
C 4.17497 6.67896 16.31663
C 2.36856 5.89479 14.76821
C 4.40206 7.05178 13.85056
C 6.37349 8.10685 12.80245
C 7.37244 6.98779 13.15243
C 5.90913 7.98993 11.33392
C 7.12867 9.46571 12.90673
H 8.65554 11.88653 12.83062
H 8.93659 14.32557 13.33616
H 7.22738 15.51984 14.70333
H 5.22835 14.28199 15.57135
H 3.07298 10.31761 17.94962
H 1.41724 9.85496 17.46105
H 1.83426 11.58076 17.71872
H 1.67999 11.24739 13.94328
H 0.59821 10.38860 15.07596
H 0.99290 12.12153 15.33982
H 4.90741 7.45464 16.57806
H 4.71341 5.72743 16.17987
H 3.48575 6.55867 17.16805
H 2.89997 4.94635 14.62109
H 1.67663 5.80275 15.61460
H 1.77166 6.09042 13.86455
H 0.91377 6.00310 12.99671
H 7.68423 7.06989 14.20628
H 8.26696 7.08013 12.51934
H 6.77488 8.08452 10.66184
H 5.41579 7.02447 11.17007
H 5.19609 8.79584 11.09457
Mn 7.24963 9.70463 19.07126
O 9.15656 13.06861 18.08428
O 10.96163 8.27422 18.24506
O 7.89566 6.10809 20.84999
O 4.52331 9.79834 21.98425
N 7.65737 11.54788 18.94634
N 9.10974 9.52473 18.69531
N 7.25365 8.21383 20.25959
N 6.01107 10.38727 20.32836
C 6.65886 12.42230 19.39891
C 5.70447 11.74976 20.19998
C 4.63396 12.45622 20.76854
C 4.52268 13.83083 20.52530
C 5.46583 14.49542 19.73404
C 6.54235 13.80121 19.16821
C 8.84287 11.92209 18.38710
C 9.79663 10.74016 18.18989
C 10.09472 10.64159 16.67876
C 11.06869 11.08058 18.99744
C 9.79574 8.34699 18.64348
C 9.07666 7.02967 18.99866
C 8.34663 6.53261 17.71907
C 10.14086 5.98572 19.38489
C 8.03579 7.10370 20.13410
C 6.16310 8.17401 21.26646
C 5.10439 7.10384 20.92701
C 6.69626 8.00437 22.70667
C 5.45960 9.53424 21.23704
H 3.91271 11.92846 21.38752
H 3.68601 14.38459 20.95917
H 5.36593 15.56834 19.55017
H 7.28581 14.30639 18.55694
H 9.17579 10.39811 16.12222
H 10.84339 9.86414 16.48606
H 10.46947 11.60992 16.31645
H 10.83856 11.11848 20.07435
H 11.84548 10.32785 18.82828
H 11.43384 12.07049 18.68801
H 7.57325 7.23417 17.38006
H 7.87169 5.55957 17.91872
H 9.07632 6.39918 16.90536
H 9.66068 5.02075 19.58677
H 10.86694 5.87517 18.57063
H 10.68847 6.28902 20.29052
H 5.53004 6.09844 21.02655
H 4.74177 7.23716 19.89525
H 4.24910 7.21038 21.61015
H 5.86600 8.14143 23.41446
H 7.13763 7.01112 22.83900
H 7.46270 8.76619 22.92189

101
Intermediate$_R$ (-2/2)
Fe 5.32470 9.54905 15.47501
O 6.17478 9.27104 16.91754
O 3.17323 12.78877 16.39098
O 1.64426 7.86542 16.09065
O 4.91366 5.89458 13.67611
O 8.33987 9.67793 12.86519
N 4.81807 11.37562 15.59596
N 3.47315 9.22200 15.86837
N 5.54496 7.97182 14.39618
N 6.64027 10.27226 14.31173
C 5.75423 12.29002 15.10909
C 6.80714 11.65495 14.38297
C 7.81084 12.43299 13.77784
C 7.76040 13.82573 13.88784
C 6.72253 14.44952 14.59446
C 5.72002 13.69170 15.20757
C 3.59259 11.66483 16.11707
C 2.69013 10.42000 16.25670
C 2.18903 10.34167 17.71134
C 1.51161 10.67643 15.28491
C 2.84893 8.02015 15.83863
C 3.69336 6.74651 15.55405
C 4.41540 6.37273 16.87413
C 2.73608 5.60120 15.18382
C 4.77100 6.86127 14.44032
C 6.64807 8.02993 13.40572
C 7.71323 6.94186 13.62918
C 6.10818 7.97319 11.95407
C 7.32934 9.40953 13.51483
H 8.60048 11.93464 13.22040
H 8.53909 14.43044 13.41509
H 6.69350 15.53981 14.67157
H 4.90626 14.16269 15.75310
H 3.02598 10.14695 18.39795
H 1.45361 9.53446 17.81494
H 1.72667 11.29861 17.99563
H 1.87837 10.72814 14.24672
H 0.77724 9.86708 15.35910
H 1.03817 11.63796 15.53135
H 5.09063 7.17134 17.20448
H 5.00101 5.44949 16.73648
H 3.66936 6.18598 17.66308
H 3.30048 4.67023 15.04735
H 1.98893 5.46675 15.97581
H 2.20026 5.81029 14.24542
H 7.28496 5.94790 13.45309
H 8.09776 6.98613 14.65815
H 8.55401 7.10945 12.94032
H 6.93517 8.13467 11.24690
H 5.64178 6.99972 11.76493
H 5.35706 8.76391 11.79552
Mn 7.12621 9.81611 18.50659
O 9.23164 13.08979 17.42233
O 10.90204 8.23862 18.15908
O 7.70324 6.43048 20.75270
O 4.05748 10.10672 21.10106
N 7.58420 11.70766 18.27324
N 9.02827 9.54864 18.17080
N 9.91535 8.33443 19.76390
N 5.76055 10.65166 19.63500
C 6.65978 12.61702 18.71817
C 5.59774 12.00415 19.49332
C 4.59094 12.81649 20.06995
C 4.64292 14.18878 19.88633
C 5.68681 14.78914 19.13921
C 6.68587 14.02387 18.55972
C 8.84147 11.98254 17.75820
C 9.78236 10.75364 17.74073
C 10.35230 10.59544 16.31768
C 10.90504 11.11447 18.74627
C 9.68667 8.37838 18.35544
C 8.86648 7.11102 18.76124
C 8.16574 6.58655 17.48233
C 9.85549 6.03717 19.24334
C 7.77559 7.29241 19.86531
C 5.83142 8.48742 20.76783
C 4.81257 7.33575 20.70379
C 6.39706 8.63964 22.20415
C 5.08731 9.81737 20.51092
H 3.79870 12.34571 20.64672
H 3.86553 14.81988 20.32385
H 5.69951 15.87447 19.01321
H 7.48780 14.47474 17.98165
H 9.55369 10.34493 15.60318
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H 10.82114 11.53703 15.99593
H 10.48667 11.23686 19.75840
H 11.65411 10.31585 18.76818
H 11.37594 12.06213 18.44779
H 7.46575 7.32001 17.06157
H 7.60823 5.66358 17.70883
H 8.92383 6.34493 16.72057
H 9.31786 5.10812 19.47114
H 10.60723 5.84638 18.46764
H 10.38230 6.35377 20.15577
H 5.30244 6.39112 20.96912
H 4.39443 7.24716 19.69060
H 3.98669 7.53047 21.40324
H 5.57613 8.84454 22.90707
H 6.91300 7.71809 22.49539
H 7.11199 9.47672 22.24906

101
Intermediate$_P$ (-2/2)
Fe 5.34340 9.70873 15.48428
O 6.25634 9.30574 17.17359
O 3.24208 12.97880 16.46953
O 1.61965 8.09669 15.98867
O 4.80575 6.22133 13.42692
O 8.54449 9.79034 13.10222
N 4.86991 11.57216 15.61708
N 3.47857 9.42239 15.83985
N 5.58064 8.16233 14.35857
N 6.73797 10.45083 14.38855
C 5.78341 12.45766 15.13327
C 6.87932 11.80263 14.42902
C 7.88785 12.58777 13.81074
C 7.80862 13.96476 13.89083
C 6.73438 14.60496 14.56976
C 5.73293 13.87536 15.18151
C 3.62441 11.86374 16.15402
C 2.70754 10.62600 16.24579
C 2.19210 10.51853 17.69500
C 1.54459 10.93085 15.26792
C 2.82641 8.23757 15.74418
C 3.64633 6.96090 15.39413
C 4.36219 6.50190 16.69029
C 2.66412 5.85868 14.96556
C 4.72588 7.11303 14.28401
C 6.69298 8.24120 13.37683
C 7.68004 7.06746 13.50273
C 6.17253 8.36365 11.91944
C 7.46143 9.55585 13.61275
H 8.70225 12.08873 13.29126
H 8.58469 14.57712 13.42557
H 6.70642 15.69641 14.61047
H 4.91115 14.35636 15.70496
H 3.02359 10.30766 18.38426
H 1.45727 9.70772 17.76697
H 1.72345 11.46650 17.99785
H 1.92439 11.01652 14.23689
H 0.80559 10.12363 15.30526
H 1.07110 11.88442 15.54348
H 5.05831 7.26360 17.06228
H 4.92540 5.57340 16.50303
H 3.61520 6.29223 17.47244
H 3.20749 4.92383 14.77802
H 1.91647 5.69791 15.75208
H 2.13163 6.12894 14.04134
H 7.18056 6.12831 13.23819
H 8.05846 6.99173 14.53231
H 8.53608 7.23037 12.83208
H 7.01694 8.51691 11.23078
H 5.63486 7.44910 11.64547
H 5.48634 9.22056 11.82615
Mn 7.09179 9.64313 18.57398
O 9.20044 12.93774 17.52168
O 10.86198 8.13005 18.29511
O 7.56829 6.04991 20.56398
O 4.23482 9.92641 21.33918
N 7.55219 11.51857 18.30541
N 8.96958 9.41289 18.32647
N 6.93720 8.11577 19.79234
N 5.88022 10.43557 19.80040
C 6.61724 12.43071 18.79366
C 5.65446 11.81388 19.64510
C 4.66512 12.59574 20.26463
C 4.64286 13.97970 20.04976
C 5.59883 14.58777 19.22833
C 6.58605 13.82118 18.59761
C 8.78922 11.82125 17.85061
C 9.74167 10.60437 17.87690
C 10.33474 10.41722 16.46799
C 10.84614 10.98803 18.89131
C 9.64051 8.23149 18.46305
C 8.84555 6.92399 18.73197
C 8.20456 6.48547 17.38971
C 9.83874 5.83376 19.16801
C 7.71831 7.01571 19.79774
C 5.86351 8.22269 20.80324
C 4.76204 7.16341 20.60824
C 6.41790 8.17156 22.24858
C 5.21972 9.61502 20.67032
H 3.93900 12.11242 20.91333
H 3.87086 14.58486 20.53295
H 5.57632 15.66979 19.07098
H 7.34043 14.27817 17.96184
H 9.55121 10.13411 15.74893
H 11.10629 9.63768 16.47401
H 10.77784 11.36692 16.13329
H 10.41196 11.11351 19.89682
H 11.61400 10.20805 18.93367
H 11.29876 11.94397 18.59097
H 7.49678 7.23248 17.01033
H 7.66799 5.53271 17.52530
H 8.99171 6.32594 16.63543
H 9.30465 4.88879 19.32655
H 10.61144 5.69673 18.40105
H 10.34158 6.09907 20.11032
H 5.17223 6.16105 20.78170
H 4.36159 7.21028 19.58454
H 3.93697 7.35237 21.31054
H 5.60726 8.37963 22.96234
H 6.84864 7.18490 22.45315
H 7.20199 8.93449 22.38333

101
Intermediate (-2/6)
Fe 5.34183 9.69911 15.51226
O 6.25315 9.30074 17.14015
O 3.21884 12.96493 16.48759
O 1.61002 8.08173 15.96560
O 4.81444 6.22301 13.43019
O 8.52893 9.81740 13.10769
N 4.85594 11.56608 15.64114
N 3.46858 9.41159 15.84112
N 5.57655 8.16699 14.36577
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C 7.88891 12.60381 13.87550
C 7.81892 13.97993 13.98599
C 6.74688 14.61147 14.67434
C 5.73749 13.87396 15.26482
C 3.60840 11.85161 16.17130
C 2.69403 10.61114 16.24957
C 2.16847 10.49256 17.69421
C 1.53726 10.91980 15.26528
C 2.82027 8.22664 15.73739
C 3.64931 6.95372 15.39795
C 4.36214 6.50901 16.70048
C 2.67782 5.84191 14.97058
C 4.73007 7.11226 14.29043
C 6.68618 8.25814 13.38254
C 7.68027 7.08914 13.49504
C 6.15825 8.38639 11.92817
C 7.44855 9.57557 13.62300
H 8.70190 12.11118 13.34774
H 8.60123 14.59690 13.53743
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H 2.99580 10.27624 18.38671
H 1.43365 9.68068 17.75473
H 1.69715 11.43781 18.00148
H 1.92475 11.01357 14.23778
H 0.80061 10.11003 15.29148
H 1.05947 11.87039 15.54379
H 5.04837 7.28182 17.06911
H 4.93471 5.58443 16.52221
H 3.61155 6.29630 17.47860
H 3.22934 4.91032 14.79007
H 1.92799 5.67901 15.75470
H 2.14714 6.10293 14.04273
H 7.18432 6.14892 13.22763
H 8.06461 7.00936 14.52176

H 8.53154 7.26142 12.82064
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H 5.62397 7.47048 11.65183
H 5.46740 9.24037 11.84300
Mn 7.15369 9.66537 18.62091
O 9.26286 12.93348 17.58618
O 10.88880 8.03793 18.18432
O 7.61037 6.08934 20.57378
O 4.18659 9.91848 21.33033
N 7.62713 11.53401 18.42042
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N 6.93384 8.12660 19.78622
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C 5.64523 14.61165 19.26087
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C 8.85742 11.81747 17.90928
C 9.79921 10.58649 17.85489
C 10.38427 10.47247 16.43582
C 10.91428 10.89858 18.88287
C 9.67163 8.18237 18.36139
C 8.82381 6.90723 18.66768
C 8.11299 6.50334 17.35062
C 9.78496 5.77597 19.06748
C 7.73317 7.03102 19.77858
C 5.84298 8.23687 20.78874
C 4.77050 7.14901 20.60151
C 6.39810 8.21413 22.23368
C 5.16460 9.62281 20.64383
H 3.83324 12.13610 20.78374
H 3.83489 14.61829 20.44805
H 5.64943 15.69591 19.11963
H 7.46425 14.29699 18.11073
H 9.59494 10.23848 15.70591
H 11.14054 9.67809 16.40355
H 10.84559 11.42902 16.14924
H 10.48704 10.98116 19.89548
H 11.66363 10.09936 18.88009
H 11.38855 11.85750 18.62845
H 7.43319 7.28871 16.99551
H 7.53323 5.57880 17.50299
H 8.86714 6.30447 16.57243
H 9.22455 4.84491 19.21896
H 10.53717 5.62850 18.28247
H 10.31435 6.00721 20.00387
H 5.19985 6.15772 20.79256
H 4.37384 7.17229 19.57589
H 3.93907 7.33050 21.29812
H 5.58046 8.40893 22.94284
H 6.85249 7.24027 22.44832
H 7.16209 8.99807 22.36147

1 + 2

101
Species 5 (-2/1)
Fe 5.34362 9.66440 15.48190
O 6.18593 9.30504 16.91093
O 3.23799 12.88438 16.55462
O 1.62414 8.01601 15.94373
O 4.90694 6.09169 13.52673
O 8.35895 9.88026 12.87643
N 4.86045 11.48896 15.68639
N 3.48279 9.34674 15.84299
N 5.54733 8.13518 14.33042
N 6.66730 10.42438 14.35135
C 5.81180 12.41376 15.24714
C 6.85285 11.80137 14.48762
C 7.86475 12.59387 13.91737
C 7.83453 13.98076 14.09603
C 6.80935 14.58270 14.83749
C 5.79839 13.80852 15.41702
C 3.63747 11.77064 16.21578
C 2.70826 10.53926 16.26418
C 2.14832 10.40134 17.69192
C 1.57267 10.86609 15.26182
C 2.83875 8.15916 15.73711
C 3.67053 6.88583 15.41940
C 4.36976 6.45485 16.73387
C 2.70524 5.76675 14.99463
C 4.76354 7.03058 14.32455
C 6.65887 8.22170 13.35218
C 7.71589 7.12002 13.54719
C 6.13273 8.21881 11.89449
C 7.34784 9.59169 13.51694
H 8.64509 12.11242 13.33258
H 8.61993 14.59687 13.64973
H 6.79566 15.66811 14.96913
H 4.99327 14.26279 15.98903
H 2.95173 10.16148 18.40368
H 1.39587 9.60401 17.72751
H 1.68990 11.35259 18.00052
H 1.98118 10.96846 14.24323
H 0.82651 10.06410 15.26397
H 1.10059 11.81904 15.54190
H 5.04735 7.23298 17.10610
H 4.94889 5.53206 16.56896
H 3.60988 6.24387 17.50327
H 3.26146 4.83588 14.82713
H 1.94885 5.60897 15.77352
H 2.18077 6.01853 14.06043
H 7.28346 6.13537 13.33277
H 8.09117 7.12559 14.58056
H 8.56382 7.30633 12.87196
H 6.96722 8.40558 11.20262
H 5.66755 7.25367 11.66414
H 5.38405 9.01587 11.75767
Fe 7.11577 9.72450 18.52372
O 9.27274 12.96695 17.54239
O 10.85189 8.08681 18.12305
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N 8.99473 9.42132 18.20614
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C 5.80397 14.65601 19.40485
C 6.78814 13.90435 18.79127
C 8.87423 11.85795 17.85993
C 9.78360 10.61412 17.80678
C 10.34756 10.48716 16.37750
C 10.91688 10.92478 18.81856
C 9.63869 8.23683 18.33355
C 8.80467 6.96960 18.68042
C 8.09938 6.50965 17.38009
C 9.77112 5.86011 19.12556
C 7.71856 7.14261 19.78008
C 5.77781 8.30949 20.68440
C 4.76799 7.15311 20.57683
C 6.31226 8.43434 22.13674
C 5.03084 9.63451 20.44594
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H 3.96668 14.66744 20.56970
H 5.84632 15.74636 19.34897
H 7.60978 14.36727 18.25176
H 9.54243 10.26694 15.66053
H 11.08492 9.67613 16.34287
H 10.82686 11.43134 16.07927
H 10.50369 11.02844 19.83502
H 11.64860 10.11014 18.81667
H 11.40826 11.87003 18.54556
H 7.41875 7.27745 16.99149
H 7.52055 5.59089 17.56731
H 8.85467 6.28180 16.61116
H 9.21599 4.93231 19.31406
H 10.52465 5.68634 18.34736
H 10.29772 6.13067 20.05293
H 5.25435 6.20662 20.83979
H 4.37650 7.07946 19.55225
H 3.92309 7.33463 21.25686
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101
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Fe 5.32884 9.71939 15.48717
O 6.33810 9.32667 17.17915
O 3.18030 12.94996 16.49685
O 1.60527 8.05093 15.92067
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C 7.82429 12.66183 13.87388
C 7.77710 14.05300 14.02276
C 6.74596 14.65594 14.75407
C 5.74515 13.87778 15.34856
C 3.59954 11.83543 16.17931
C 2.67446 10.59460 16.23661
C 2.10228 10.47617 17.66150
C 1.54328 10.89559 15.22247
C 2.82289 8.20827 15.73234
C 3.67220 6.93668 15.42857
C 4.37084 6.52681 16.74860
C 2.72012 5.80174 15.01614
C 4.76893 7.07781 14.33081
C 6.66270 8.27167 13.35748
C 7.72781 7.17615 13.54241
C 6.12412 8.26490 11.90453
C 7.34839 9.64920 13.51808
H 8.61159 12.17752 13.30057
H 8.55615 14.66904 13.56462
H 6.71910 15.74349 14.86755
H 4.93344 14.33142 15.91197
H 2.90263 10.25358 18.38320
H 1.35930 9.66980 17.70153
H 1.62954 11.42546 17.95458
H 1.95687 10.98908 14.20476
H 0.80660 10.08478 15.22971
H 1.05620 11.84625 15.48456
H 5.03980 7.31465 17.11689
H 4.96148 5.60853 16.59881
H 3.61175 6.31782 17.51957
H 3.28613 4.87375 14.86487
H 1.96062 5.64811 15.79303
H 2.19800 6.03259 14.07533
H 7.29518 6.18879 13.33969
H 8.11433 7.18935 14.57236
H 8.56856 7.35908 12.85712
H 6.95021 8.45564 11.20353
H 5.66094 7.29793 11.67792
H 5.36945 9.05774 11.77275
Fe 7.16200 9.66340 18.59072
O 9.24883 12.89071 17.47535
O 10.88239 8.04781 18.17544
O 7.66502 6.22292 20.70731
O 3.98998 9.84605 21.00192
N 7.62185 11.50775 18.35693
N 9.02086 9.37456 18.26802
N 6.94441 8.18162 19.77305
N 5.77120 10.43880 19.65567
C 6.71447 12.41391 18.82296
C 5.63040 11.79079 19.56323
C 4.64163 12.60022 20.17931
C 4.73443 13.97622 20.06972
C 5.80261 14.58634 19.35895
C 6.78151 13.82824 18.74159
C 8.86941 11.78571 17.83041
C 9.79481 10.55547 17.80670
C 10.32479 10.38342 16.36976
C 10.94551 10.91004 18.78299
C 9.67284 8.18671 18.39159
C 8.84493 6.92251 18.74188
C 8.12036 6.47550 17.44487
C 9.81023 5.80760 19.17413
C 7.77127 7.10256 19.84552
C 5.80758 8.26265 20.72695
C 4.81307 7.09884 20.57110
C 6.29883 8.37427 22.19439
C 5.05816 9.58202 20.47109
H 3.83417 12.12230 20.72822
H 3.97297 14.60651 20.53595
H 5.84601 15.67600 19.29287
H 7.59883 14.28648 18.19142
H 9.50411 10.13014 15.68235
H 11.07493 9.58444 16.33715
H 10.78032 11.32562 16.03170
H 10.55554 11.04081 19.80546
H 11.69128 10.10817 18.78992
H 11.41498 11.85304 18.46755
H 7.44209 7.25208 17.07150
H 7.53726 5.56094 17.63621
H 8.86441 6.24885 16.66518
H 9.25410 4.88035 19.36290
H 10.55405 5.63431 18.38657
H 10.34848 6.07092 20.09696
H 5.28181 6.15341 20.86744
H 4.47964 7.01753 19.52719
H 3.93198 7.28497 21.20222
H 5.43884 8.53968 22.86015
H 6.81536 7.45115 22.47958
H 6.99506 9.22117 22.30507

101
Species 5 (-2/3)
Fe 5.31168 9.79644 15.48800
O 6.35225 9.31075 17.16339
O 3.16105 12.99003 16.59826
O 1.59801 8.10472 15.87806
O 4.97837 6.18704 13.56771
O 8.30197 10.08904 12.83104
N 4.81494 11.62393 15.73806
N 3.45203 9.45088 15.87387
N 5.56842 8.25650 14.35125
N 6.65552 10.58245 14.37548
C 5.74222 12.56685 15.26390
C 6.78812 11.97509 14.49204
C 7.76278 12.79124 13.89695
C 7.70052 14.18273 14.06113
C 6.67517 14.76235 14.81294
C 5.69472 13.96103 15.41622
C 3.58284 11.88615 16.24312
C 2.65578 10.64457 16.25612
C 2.03619 10.50348 17.65830
C 1.55926 10.96526 15.20988
C 2.81926 8.26713 15.71657
C 3.67656 7.00014 15.41184
C 4.34512 6.57098 16.74204
C 2.73076 5.87263 14.96487
C 4.80140 7.14419 14.33996
C 6.67844 8.37341 13.37136
C 7.77557 7.31793 13.60392
C 6.16626 8.31256 11.91200
C 7.31991 9.77682 13.51122
H 8.54605 12.32447 13.30354
H 8.46383 14.81304 13.59604
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H 4.88592 14.39738 15.99771
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H 1.28805 9.70077 17.66054
H 1.55870 11.45136 17.94809
H 2.00887 11.07232 14.20890
H 0.82025 10.15693 15.17843
H 1.06585 11.91364 15.46875
H 5.01071 7.35035 17.13420
H 4.93347 5.65117 16.59306
H 3.56907 6.35695 17.49472
H 3.29976 4.94845 14.80393
H 1.95960 5.70556 15.72724
H 2.22179 6.12304 14.02162
H 7.37876 6.31206 13.41867
H 8.14341 7.36788 14.64015
H 8.62233 7.51073 12.92873
H 6.99570 8.52261 11.22088
H 5.74409 7.32418 11.69811
H 5.38372 9.07274 11.75277
Fe 7.17497 9.59581 18.57924
O 9.28530 12.78314 17.42320
O 10.85343 7.91705 18.07866
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O 3.95538 9.78885 20.91282
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C 4.82623 13.93262 20.09244
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C 8.90098 11.68591 17.79215
C 9.79941 10.43853 17.73574
C 10.25088 10.24177 16.27471
C 11.00410 10.77727 18.64901
C 9.65965 8.07991 18.35440
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C 4.81703 7.04414 20.60291
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H 7.68677 14.20947 18.20105
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H 4.47760 6.93061 19.56386
H 3.93775 7.23778 21.23401
H 5.42309 8.55896 22.84768
H 6.81216 7.47671 22.50407
H 6.97150 9.24181 22.27480

101
Species 5 (-2/5)
Fe 5.34817 9.70382 15.52887
O 6.28603 9.32854 17.18356
O 3.19887 12.95597 16.49001
O 1.63061 8.06025 15.97959
O 4.85734 6.20920 13.47460
O 8.53000 9.83776 13.11519
N 4.84896 11.56682 15.65270
N 3.48170 9.40137 15.86755
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C 6.85633 11.82265 14.46813
C 7.85849 12.62066 13.85651
C 7.76816 13.99679 13.94638
C 6.68943 14.62333 14.63003
C 5.69394 13.88059 15.23624
C 3.59693 11.84477 16.17917
C 2.69181 10.59801 16.25750
C 2.14708 10.48691 17.69534
C 1.54603 10.89025 15.25505
C 2.84117 8.21098 15.76132
C 3.68091 6.94275 15.43356
C 4.39386 6.51256 16.74042
C 2.71964 5.82013 15.01136
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C 7.71321 7.10270 13.53002
C 6.17421 8.37333 11.95672
C 7.45630 9.58703 13.63911
H 8.67675 12.13232 13.33302
H 8.53923 14.61847 13.48512
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H 1.41370 9.67341 17.75117
H 1.66807 11.43276 17.98851
H 1.94644 10.97819 14.23203
H 0.81453 10.07577 15.27854
H 1.05744 11.83948 15.51915
H 5.06974 7.29385 17.11044
H 4.97830 5.59440 16.56865
H 3.64225 6.29403 17.51559
H 3.27917 4.89175 14.83930
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H 8.09986 7.03443 14.55669
H 8.56137 7.27924 12.85282
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Fe 7.15420 9.69274 18.63432
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C 10.91982 10.90079 18.83951
C 9.65656 8.18835 18.37791
C 8.82192 6.91611 18.69505
C 8.11980 6.49083 17.38028
C 9.78488 5.79394 19.11647
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C 5.83803 8.25741 20.76762
C 4.77717 7.15843 20.57754
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C 5.15124 9.62958 20.60356
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H 3.84180 14.62581 20.39557
H 5.66046 15.69159 19.06460
H 7.48113 14.28635 18.07608
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H 11.09703 9.62390 16.38049
H 10.80424 11.37125 16.09823
H 10.51085 11.00811 19.85741
H 11.66697 10.09968 18.84204
H 11.39109 11.85281 18.55461
H 7.44378 7.27302 17.01285
H 7.53878 5.56877 17.54306
H 8.87839 6.27993 16.60947
H 9.22672 4.86386 19.28215
H 10.54041 5.63619 18.33667
H 10.31074 6.04208 20.05088
H 5.20916 6.17276 20.78838
H 4.39642 7.16589 19.54610
H 3.93321 7.34521 21.25760
H 5.53797 8.44420 22.91818
H 6.83239 7.28781 22.45283
H 7.12099 9.04899 22.35678

DISPERSION CORRECTED GEMETRIES

51
Species 1 (-1/2) BP86
Fe 0.02825 -0.00374 -0.03704
O 0.09957 0.04428 1.56105
N -0.00416 1.76970 -0.60459
N -1.85026 0.15354 -0.32960
N -0.24026 -1.75146 -0.61152
N 1.86518 0.05942 -0.57881
C -1.26127 2.39817 -0.57515
C 1.20794 2.39240 -0.82151
C -2.57215 -0.98883 -0.50579
C -2.32645 1.46066 -0.39961
C 0.75889 -2.69451 -0.75157
C -1.65321 -2.20923 -0.73057
C 2.39862 1.42367 -0.77364
C 2.73686 -0.98080 -0.56151
C 2.17491 -2.38472 -0.22620
O 1.34532 3.60416 -1.02066
O -3.80727 -1.07337 -0.56044
O 0.51642 -3.83683 -1.17574
O 3.96701 -0.86225 -0.74399
C -1.98606 -2.71533 -2.15305
C -1.98322 -3.25736 0.35110
C 3.27625 1.84465 0.42779
C 3.14674 1.58334 -2.11625
C -1.54617 3.77318 -0.72258
C -2.88629 4.19834 -0.68712
C -3.66708 1.90030 -0.37713
C -3.93549 3.27297 -0.51871
C 3.14461 -3.44752 -0.77253
C 2.11713 -2.49883 1.32588
H -0.71795 4.47776 -0.85914
H -3.11179 5.27143 -0.79020
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H -4.97891 3.62500 -0.49306
H -1.69455 -1.95334 -2.90498
H -1.44508 -3.65384 -2.36330
H -3.07997 -2.87698 -2.22527
H -1.43153 -4.19698 0.16510
H -1.70999 -2.86894 1.35358
H -3.07299 -3.45746 0.33654
H 2.70546 1.71986 1.37054
H 4.17751 1.20505 0.46450
H 3.57197 2.90775 0.32675
H 4.07890 0.99262 -2.10246
H 2.50827 1.22937 -2.95184
H 3.37294 2.65616 -2.27697
H 2.81764 -4.45712 -0.46218
H 3.18288 -3.42504 -1.88026
H 4.16191 -3.24723 -0.39004
H 3.13851 -2.37176 1.73962
H 1.45899 -1.72483 1.76591
H 1.74313 -3.50144 1.61872

50
Species 2 (-1/5) BP86
Mn -0.45912 4.20709 -0.37323
O -3.78517 3.53657 1.77930
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O 3.21290 4.56631 1.21944
O 1.25093 6.23525 -3.41156
N -2.08780 4.54455 -1.28253
N -1.55866 3.72370 1.11878
N 0.84248 4.98209 -1.51408
C -3.31001 4.42953 -0.44630
C -2.91547 3.82557 0.94316
C -0.85605 3.39813 2.29586
C 0.56443 3.60383 2.18153
C 2.17725 4.57668 0.53680
C 2.15443 5.25474 -0.87445
C 0.52416 5.46958 -2.74904
C -0.80346 4.92029 -3.39406
C -2.12244 5.06319 -2.54534
O -3.13905 5.54733 -3.07945
C -0.59406 3.40362 -3.66084
H 0.29549 3.24556 -4.30559
H -1.47890 2.98003 -4.18011
H -0.44307 2.83079 -2.72426
C -1.01514 5.63506 -4.73634
H -0.12928 5.49456 -5.38404
H -1.16215 6.72303 -4.59242
H -1.91311 5.23302 -5.24194
C 3.30209 4.66706 -1.71602
H 3.12193 3.58860 -1.90492
H 4.25795 4.77349 -1.16613
H 3.36690 5.19352 -2.68669
C 2.35621 6.76707 -0.62528
H 2.38363 7.30177 -1.59274
H 3.30163 6.93373 -0.07161
H 1.51652 7.16627 -0.01885
C 1.40119 3.34245 3.28522
H 2.47998 3.51437 3.17874
C 0.83742 2.87699 4.49030
H 1.49493 2.67011 5.34987
C -0.55010 2.67482 4.60130
H -0.97995 2.30918 5.54761
C -1.40261 2.93471 3.50944
H -2.48901 2.79216 3.57400
C -4.33484 3.49014 -1.10910
H -4.70098 3.93671 -2.05254
H -5.18497 3.32222 -0.41881
H -3.86441 2.51083 -1.33451
C -3.92815 5.81552 -0.15387
H -3.17349 6.47614 0.32152
H -4.78555 5.70416 0.53940
H -4.26324 6.27870 -1.10025

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Species 3 (-1/4) BP86
Fe -0.45971 4.23203 -0.31738
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N 0.93832 4.11487 0.91974
O 3.21680 4.52580 1.19682
O 1.25668 6.23449 -3.37787
N -2.04265 4.57643 -1.25259
N -1.55516 3.75129 1.11940

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C -3.28843 4.41531 -0.45505
C -2.91213 3.81309 0.93251
C -0.86104 3.42646 2.30116
C 0.55806 3.63356 2.18760
C 2.17221 4.56720 0.52904
C 2.13469 5.23689 -0.87818
C 0.50506 5.48912 -2.71930
C -0.80684 4.95396 -3.37891
C -2.10580 5.08446 -2.51975
O -3.13839 5.54433 -3.04558
C -0.59464 3.43967 -3.65816
H 0.29281 3.28868 -4.30756
H -1.48006 3.01666 -4.17694
H -0.43843 2.87143 -2.72072
C -1.02079 5.68280 -4.71301
H -0.13526 5.55125 -5.36311
H -1.16971 6.76922 -4.55744
H -1.91884 5.28531 -5.22227
C 3.24187 4.60348 -1.74175
H 3.01315 3.53386 -1.92922
H 4.20919 4.66663 -1.20490
H 3.31659 5.12813 -2.71226
C 2.39967 6.74170 -0.63821
H 2.43479 7.27367 -1.60638
H 3.35851 6.87035 -0.09720
H 1.58574 7.17505 -0.02010
C 1.39602 3.37577 3.29157
H 2.47480 3.54714 3.18501
C 0.83138 2.91201 4.49658
H 1.48797 2.70774 5.35744
C -0.55651 2.70850 4.60717
H -0.98579 2.34470 5.55442
C -1.40935 2.96496 3.51504
H -2.49526 2.81943 3.57934
C -4.26959 3.44948 -1.14678
H -4.63478 3.89099 -2.09255
H -5.12506 3.24620 -0.47244
H -3.76308 2.48802 -1.37168
C -3.95649 5.77843 -0.16082
H -3.23032 6.45805 0.33205
H -4.81858 5.63163 0.52027
H -4.29362 6.24014 -1.10663

51
Species 4 (-1/1) BP86
Mn 0.36049 9.47032 7.55166
O 3.89149 9.80749 9.41556
C -0.17247 8.70236 10.19965
N 1.66063 9.39637 8.92979
O -0.16669 10.93534 7.50297
O -2.62868 7.43965 9.28547
O -1.38946 7.74815 4.29812
O 2.92476 9.24280 4.38957
N -0.63864 8.56199 8.88327
N -0.69405 8.39979 6.38708
N 1.89532 9.32614 6.44018
C -1.77974 7.90041 8.51180
C 2.97367 9.61900 8.60716
C 1.88432 9.21975 5.07349
C 1.83152 9.37658 11.45559
H 2.86387 9.74539 11.45218
C -1.89069 7.75576 6.98742
C 0.52770 9.18803 4.34094
C 3.20826 9.57230 7.09090
C 1.16602 9.18976 10.22687
C -0.57973 8.35781 5.02181
C -0.17456 8.59976 12.62337
H -0.69772 8.37652 13.56665
C -1.95049 6.23652 6.70904
H -2.14394 6.05018 5.63874
H -2.75522 5.79213 7.32770
H -0.98837 5.76110 6.99091
C 3.78680 10.94046 6.67077
H 4.05241 10.92804 5.59811
H 4.68713 11.16082 7.27799
H 3.03750 11.73904 6.84934
C -3.18434 8.47656 6.55065
H -3.10044 9.56309 6.75870
H -4.04200 8.07285 7.12434
H -3.35430 8.32820 5.46884
C 1.14753 9.08159 12.65020
H 1.65746 9.23483 13.61444
C 0.74936 8.63922 2.91909
H 1.50458 9.25272 2.39481
H -0.20381 8.65587 2.35989
H 1.11450 7.59278 2.94466
C -0.84520 8.40158 11.40151
H -1.87262 8.02180 11.35728
C 4.21130 8.41942 6.85672
H 3.74631 7.45093 7.13431
H 5.09771 8.57999 7.50191
H 4.51219 8.38324 5.79572
C 0.01814 10.65505 4.23553
H -0.15938 11.10217 5.23134
H -0.93052 10.67809 3.66109
H 0.76786 11.27079 3.69779

1+3

101
Intermediate$_R$ (-2/4) BP86
Fe 5.39571 9.53700 15.59931
O 6.23826 9.24306 17.04782
O 3.15298 12.73449 16.44427
O 1.81414 7.73988 16.43920
O 4.93311 6.03318 13.59432
O 8.49330 9.75221 13.06490
N 4.86539 11.33407 15.73770
N 3.56627 9.17082 16.00185
N 5.62501 8.04344 14.47320
N 6.76986 10.29028 14.52990
C 5.77799 12.28299 15.26160
C 6.89454 11.67825 14.59891
C 7.89438 12.48396 14.01326
C 7.76713 13.88185 14.07186
C 6.65712 14.47790 14.70167
C 5.66233 13.68896 15.30332
C 3.61089 11.60399 16.23312
C 2.78096 10.33096 16.48476
C 2.53015 10.23234 18.00409
C 1.46325 10.52140 15.69818
C 2.97832 7.94432 16.03182
C 3.83272 6.71621 15.62196
C 4.66269 6.31510 16.87208
C 2.88914 5.55713 15.25706
C 4.82374 6.92862 14.45463
C 6.73398 8.11670 13.48527
C 7.75096 6.97514 13.66036
C 6.19707 8.17587 12.03175
C 7.45986 9.46236 13.68816
H 8.73843 11.99521 13.51295
H 8.54836 14.51439 13.62081
H 6.57172 15.57536 14.74369
H 4.79751 14.13191 15.80761
H 3.49570 10.11828 18.53115
H 1.88678 9.35962 18.22057
H 2.04218 11.15875 18.36672
H 1.66969 10.53337 14.60748
H 0.76307 9.69794 15.92059
H 1.01647 11.49510 15.97997
H 5.30455 7.14623 17.21761
H 5.30435 5.44078 16.63983
H 3.97559 6.03288 17.69499
H 3.47519 4.64241 15.04975
H 2.18765 5.37322 16.09126
H 2.29362 5.79202 14.35187
H 7.29457 6.00401 13.39734
H 8.10638 6.93701 14.70765
H 8.62176 7.17297 13.00420
H 7.04052 8.36541 11.33854
H 5.70117 7.22311 11.77525
H 5.46556 9.00434 11.93090
Mn 7.09038 9.84507 18.47092
O 9.22634 13.04078 17.24716
O 10.82622 8.19365 18.20360
O 7.30039 6.29589 20.48043
O 4.21614 10.40244 21.26433
N 7.53872 11.67733 18.08052
N 8.95724 9.53565 18.15862
N 6.84635 8.42206 19.73340
N 5.72787 10.72217 19.52872
C 6.60379 12.64433 18.48324
C 5.56416 12.09841 19.30014
C 4.56629 12.94117 19.83108
C 4.61735 14.32189 19.56258
C 5.65032 14.86117 18.77386
C 6.64492 14.02953 18.22766
C 8.79918 11.93325 17.60009
C 9.72696 10.69296 17.63329
C 10.22537 10.40870 16.20369
C 10.88956 11.08531 18.57588
C 9.59871 8.34919 18.37001
C 8.74334 7.09724 18.72446
C 8.14395 6.60523 17.37904
C 9.68383 6.00774 19.27174
C 7.56768 7.26066 19.73552
C 5.70606 8.57090 20.67539
C 4.56785 7.58123 20.34943
C 6.16840 8.44392 22.14349
C 5.12356 9.99751 20.52160
H 3.78494 12.50175 20.46191
H 3.83752 14.98126 19.97619
H 5.68013 15.94322 18.56863
H 7.45584 14.42306 17.60598
H 9.37966 10.12104 15.54971
H 10.96682 9.58802 16.22202
H 10.69252 11.32230 15.78566
H 10.50381 11.25826 19.60231
H 11.63964 10.27640 18.60525
H 11.34701 12.02530 18.21005
H 7.48596 7.36540 16.91782
H 7.55532 5.67977 17.53986
H 8.96953 6.37529 16.67473
H 9.11227 5.08015 19.45694
H 10.49473 5.81513 18.54605
H 10.14792 6.32166 20.22876
H 4.92651 6.54200 20.46384
H 4.21715 7.73166 19.31007
H 3.71631 7.76291 21.03477
H 5.32674 8.71321 22.81114
H 6.50428 7.41244 22.34952
H 7.00868 9.14241 22.33778

101
Intermediate$_P$ (-2/4) BP86
Fe 5.34522 9.73633 15.40780
O 6.26415 9.26822 17.18132
O 3.16786 12.91918 16.53947
O 1.74031 7.93924 16.08427
O 5.15038 6.10595 13.55022
O 8.42863 10.08681 12.85143
N 4.86927 11.54887 15.72785
N 3.53019 9.36917 15.81656
N 5.67462 8.21223 14.32830
N 6.74969 10.53392 14.40500
C 5.81201 12.50575 15.30862
C 6.89504 11.92487 14.56772
C 7.91716 12.74544 14.04968
C 7.85471 14.13721 14.25504
C 6.78271 14.70943 14.96410
C 5.75929 13.90148 15.49516
C 3.62373 11.80482 16.23824
C 2.76763 10.51536 16.38997
C 2.54275 10.28580 17.89873
C 1.44457 10.79001 15.64366
C 2.92719 8.14657 15.75221
C 3.80067 6.90871 15.38018
C 4.49232 6.47761 16.70250
C 2.86404 5.77668 14.91959
C 4.92608 7.07064 14.31291
C 6.82705 8.32549 13.38855
C 7.93049 7.30467 13.72642
C 6.37710 8.20815 11.91363
C 7.44187 9.74503 13.52368
H 8.73267 12.27646 13.48618
H 8.65576 14.77913 13.85451
H 6.74434 15.79958 15.11967
H 4.91765 14.32419 16.05502
H 3.51804 10.10632 18.39117
H 1.88925 9.40641 18.05264
H 2.07877 11.18126 18.35771
H 1.63459 10.87731 14.55312
H 0.72733 9.96905 15.81410
H 1.02798 11.75223 16.00194
H 5.13478 7.28460 17.10167
H 5.11841 5.57798 16.53351
H 3.72311 6.22922 17.46212
H 3.44806 4.85616 14.73677
H 2.09427 5.59213 15.69098
H 2.34616 6.04371 13.97550
H 7.55149 6.27554 13.58598
H 8.25473 7.43020 14.77814
H 8.80583 7.47663 13.06882
H 7.23363 8.44394 11.25128
H 6.00470 7.18874 11.70985
H 5.56410 8.93586 11.70838
Mn 7.03282 9.69058 18.52026
O 9.25321 12.88473 17.51869
O 10.68041 7.97369 17.96130
O 7.32689 6.17016 20.55566
O 4.13489 10.13582 21.26268
N 7.56609 11.49972 18.31059
N 8.88836 9.37499 18.27599
N 6.85841 8.28074 19.78329
N 5.76830 10.52975 19.66012
C 6.65038 12.47795 18.72388
C 5.59596 11.91252 19.49567
C 4.58712 12.73506 20.03697
C 4.64989 14.12199 19.81183
C 5.70280 14.68349 19.06518
C 6.70880 13.87038 18.51419
C 8.81949 11.76581 17.81566
C 9.67082 10.49500 17.68859
C 9.90377 10.25153 16.18177
C 10.98399 10.78119 18.44924
C 9.50320 8.14917 18.32682
C 8.67947 6.90972 18.72409
C 7.98805 6.41033 17.42405
C 9.64356 5.81752 19.22574
C 7.58136 7.11533 19.78533
C 5.72040 8.36979 20.73493
C 4.61536 7.34574 20.40288
C 6.18165 8.26763 22.20741
C 5.10249 9.76523 20.58653
H 3.78476 12.27684 20.62567
H 3.86129 14.77060 20.22513
H 5.73691 15.77096 18.89345
H 7.53139 14.28431 17.92275
H 8.93453 10.05803 15.68325
H 10.57081 9.38194 16.03789
H 10.35713 11.15198 15.72298
H 10.78311 10.86791 19.53731
H 11.71344 9.97102 18.28324
H 11.39184 11.74737 18.09213
H 7.33445 7.18544 16.98368
H 7.37527 5.51306 17.64352
H 8.76190 6.13403 16.68005
H 9.08036 4.89170 19.44269
H 10.41296 5.62095 18.45732
H 10.15728 6.13317 20.15649
H 4.98585 6.31768 20.56509
H 4.30215 7.45641 19.34659
H 3.73753 7.53709 21.05116
H 5.32809 8.51501 22.86902
H 6.54753 7.24909 22.42346
H 6.99777 8.99423 22.40074

101
Intermediate$_R$ (-2/2) BP86
Fe 5.39571 9.49599 15.59620
O 6.14197 9.22266 17.11934
O 3.19210 12.77256 16.26571
O 1.80845 7.78313 16.52199
O 4.81011 5.99104 13.61070
O 8.59256 9.53773 13.20156
N 4.91587 11.31984 15.69159
N 3.55089 9.18184 15.95610
N 5.63685 7.93180 14.53772
N 6.80288 10.18626 14.54205
C 5.87933 12.22388 15.24074
C 6.98706 11.56634 14.60729
C 8.03904 12.32594 14.04847
C 7.97919 13.72537 14.11667
C 6.88192 14.37272 14.72255
C 5.83014 13.63401 15.28488
C 3.65383 11.62978 16.14085
C 2.81268 10.36943 16.45274
C 2.65197 10.29548 17.98664
C 1.45648 10.56285 15.74123
C 2.96018 7.96022 16.06733
C 3.78991 6.70364 15.67884
C 4.61292 6.31026 16.93520
C 2.81681 5.56025 15.34271
C 4.77995 6.87073 14.49868
C 6.72105 8.00063 13.52663
C 7.67849 6.79945 13.58266
C 6.13349 8.16728 12.09736
C 7.51128 9.30492 13.76197
H 8.87105 11.80166 13.56456
H 8.80022 14.32280 13.68947
H 8.65029 15.47311 14.76518
H 4.96799 14.11639 15.75703
H 3.64730 10.15171 18.44731
H 1.99960 9.44252 18.25088
H 2.21583 11.23718 18.37476
H 1.59788 10.55104 14.64017
H 0.76051 9.75329 16.02089
H 1.04156 11.54908 16.02828
H 5.27377 7.13485 17.26102
H 5.23503 5.41706 16.72032
H 3.92286 6.05931 17.76589
H 3.37983 4.62717 15.15261
H 2.11505 5.41082 16.18370
H 2.22392 5.78856 14.43417
H 7.15241 5.87744 13.27702
H 8.07219 6.66854 14.60748
H 8.53364 6.99032 12.90440
H 6.95566 8.32356 11.37047
H 5.56032 7.26018 11.83345
H 5.45782 9.04671 12.06217
Mn 7.04909 9.88518 18.44821
O 9.09913 13.14329 17.23447
O 10.80820 8.32751 18.16832
O 7.31965 6.26675 20.31414
O 4.28414 10.35892 21.36247
N 7.45402 11.72905 18.07616
N 8.90243 9.61129 18.05591
N 6.86574 8.43162 19.69123
N 5.73248 10.73059 19.58358
C 6.51273 12.67147 18.50912
C 5.51476 12.09537 19.35967
C 4.49970 12.90691 19.91101
C 4.49620 14.28350 19.62860
C 5.49715 14.85521 18.81657
C 6.50799 14.05855 18.25391
C 8.70500 12.02222 17.57178
C 9.66538 10.80814 17.61911
C 10.29809 10.59633 16.23258
C 10.73092 11.20830 18.67201
C 9.56966 8.43796 18.27611
C 8.73717 7.15808 18.57617
C 8.14235 6.71023 17.21479
C 9.69881 6.06301 19.07418
C 7.57241 7.26741 19.61080
C 5.75319 8.54669 20.66774
C 4.60169 7.56852 20.35218
C 6.26639 8.37183 22.11388
C 5.16322 9.97471 20.57869
H 3.74822 12.44682 20.56303
H 3.70348 14.91975 20.05339
H 5.48486 15.93714 18.60955
H 7.29312 14.47639 17.61551
H 9.53725 10.27033 15.49806
H 11.09059 9.82789 16.29610
H 10.73241 11.55265 15.87991
H 10.25143 11.34343 19.66394
H 11.49722 10.41707 18.74726
H 11.19488 12.16820 18.37152
H 7.46713 7.47255 16.78359
H 7.57434 5.76635 17.33872
H 8.97342 6.52448 16.50392
H 9.13986 5.12261 19.23152
H 10.50442 5.90496 18.33394
H 10.17014 6.34811 20.03640
H 4.96704 6.52741 20.41443
H 4.21048 7.75412 19.33366
H 3.77905 7.72398 21.07798
H 5.44702 8.60923 22.82042
H 6.61511 7.33528 22.26798
H 7.10927 9.06811 22.30413

1 + 2

101
Species 5 (-2/1) BP86
Fe 5.43457 9.64293 15.62442
O 6.23708 9.27805 17.08580
O 3.21295 12.86543 16.48736
O 1.82357 7.88302 16.38455
O 4.91840 6.19197 13.50099
O 8.53087 9.88560 13.09606
N 4.93454 11.45391 15.81301
N 3.59491 9.29790 15.98107
N 5.66338 8.14411 14.46759
N 6.80569 10.40502 14.56859
C 5.88054 12.39170 15.39527
C 6.98579 11.77923 14.71669
C 8.03623 12.57369 14.20600
C 7.96774 13.96655 14.35406
C 6.86245 14.57274 14.98860
C 5.81745 13.79725 15.51237
C 3.67155 11.73395 16.28251
C 2.82193 10.46038 16.48336
C 2.53588 10.32741 17.99374
C 1.52388 10.68638 15.67404
C 2.99404 8.07501 15.98821
C 3.82464 6.83895 15.54807
C 4.62799 6.36569 16.78792
C 2.85107 5.72137 15.13293
C 4.83845 7.05925 14.39794
C 6.75358 8.25754 13.46658
C 7.76338 7.09979 13.55276
C 6.18227 8.39330 12.02912
C 7.49464 9.58682 13.70789
H 8.87059 12.08109 13.69404
H 8.78617 14.59240 13.96417
H 6.82214 15.66900 15.08929
H 4.95545 14.24623 16.01635
H 3.48522 10.17396 18.53903
H 1.86833 9.46474 18.17297
H 2.06362 11.25615 18.37093
H 1.75430 10.72492 14.58881
H 0.81160 9.86406 15.85976
H 1.08160 11.65736 15.97178
H 5.28327 7.16619 17.17798
H 5.25539 5.49073 16.52155
H 3.92759 6.05849 17.58993
H 3.41377 4.80002 14.89300
H 2.13914 5.52449 15.95537
H 2.26889 6.00681 14.23363
H 7.27613 6.14751 13.27595
H 8.16452 7.01631 14.58032
H 8.60782 7.30587 12.86555
H 7.00955 8.60049 11.32136
H 5.66465 7.45866 11.74915
H 5.46052 9.23510 11.98484
Fe 7.06266 9.78730 18.49648
O 9.23359 12.97218 17.39148
O 10.76361 8.09136 18.15855
O 7.15812 6.09721 20.23565
O 4.20001 10.21251 21.28260
N 7.54491 11.59115 18.20519
N 8.90548 9.44917 18.18878
N 6.80596 8.29273 19.65144
N 5.74374 10.59791 19.58707
C 6.62259 12.54825 18.62903
C 5.56534 11.97005 19.40411
C 4.54448 12.78973 19.93581
C 4.59991 14.17453 19.71578
C 5.66478 14.74897 18.98792
C 6.67685 13.94683 18.44019
C 8.80221 11.85705 17.70730
C 9.69782 10.60068 17.69077
C 10.18390 10.35844 16.24890
C 10.87546 10.94668 18.63670
C 9.53463 8.24758 18.33048
C 8.67272 6.98633 18.59238
C 8.10764 6.57354 17.20729
C 9.59225 5.86160 19.10518
C 7.47913 7.11241 19.57782
C 5.65231 8.38874 20.58014
C 4.48560 7.46414 20.17084
C 6.08599 8.13983 22.04277
C 5.10462 9.82800 20.52744
H 3.74477 12.32668 20.52482
H 3.80551 14.81885 20.12494
H 5.69721 15.83915 18.83299
H 7.50522 14.36597 17.85995
H 9.33138 10.09903 15.59309
H 10.91794 9.53140 16.23561
H 10.65333 11.28210 15.85589
H 10.50170 11.08995 19.67218
H 11.61336 10.12645 18.63169
H 11.34061 11.89335 18.29777
H 7.46023 7.36189 16.78016
H 7.51625 5.64059 17.30001
H 8.95047 6.38408 16.51133
H 9.00793 4.93170 19.22986
H 10.41973 5.69899 18.39076
H 10.03516 6.12206 20.08824
H 4.81933 6.41073 20.18216
H 4.13312 7.72349 19.15435
H 3.64268 7.60215 20.87698
H 5.24304 8.38719 22.71775
H 6.38591 7.08527 22.17365
H 6.94568 8.79330 22.29933

101
Species 5 (-2/1) B3LYP
Fe 5.35926 9.61032 15.46719
O 6.14872 9.15927 16.88447
O 3.31233 12.82075 16.64968
O 1.70907 7.93863 16.12336
O 4.89902 6.11385 13.43772
O 8.45101 9.84187 12.96720
N 4.92981 11.42716 15.77127
N 3.51761 9.30668 15.83396
N 5.56077 8.12723 14.29167
N 6.74149 10.37505 14.42422
C 5.91065 12.34155 15.38626
C 6.96207 11.73385 14.63850
C 8.02207 12.51572 14.15198
C 8.02651 13.89011 14.39791
C 6.98195 14.49041 15.11298
C 5.92217 13.72591 15.60728
C 3.71364 11.70869 16.30975
C 2.80576 10.46545 16.41620
C 2.51144 10.23486 17.90750
C 1.52498 10.81134 15.63216
C 2.88968 8.11050 15.78534
C 3.70801 6.85838 15.37640
C 4.45857 6.39101 16.64908
C 2.73074 5.75521 14.94807
C 4.76993 7.03170 14.26146
C 6.70676 8.20967 13.36105
C 7.72682 7.08586 13.59732
C 6.23779 8.23477 11.88955
C 7.41967 9.55846 13.57682
H 8.81324 12.03316 13.58444
H 8.85402 14.49983 14.02651
H 6.99608 15.56767 15.29742
H 5.10602 14.17595 16.16407
H 3.44337 9.97628 18.42439
H 1.79617 9.41256 18.02850
H 2.10656 11.15172 18.35935
H 1.76122 10.93918 14.56338
H 0.78907 10.00781 15.73750
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C 4.64114 14.14326 19.91441
C 5.71945 14.74177 19.21013
C 6.70627 13.97367 18.62320
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C 10.88231 11.00174 18.58661
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C 8.73736 7.03747 18.67010
C 8.07805 6.54768 17.35697
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