

# ELECTRONIC SUPPORTING INFORMATION

Fe(II) complexes of pyridine-substituted thiosemicarbazone ligands as catalysts for oxidations with hydrogen peroxide

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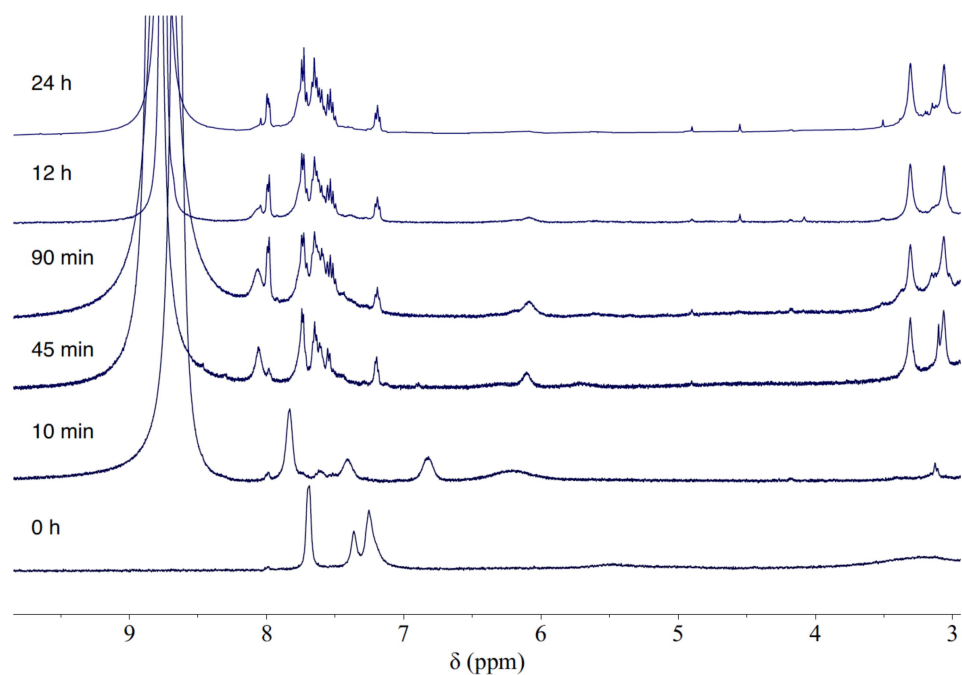
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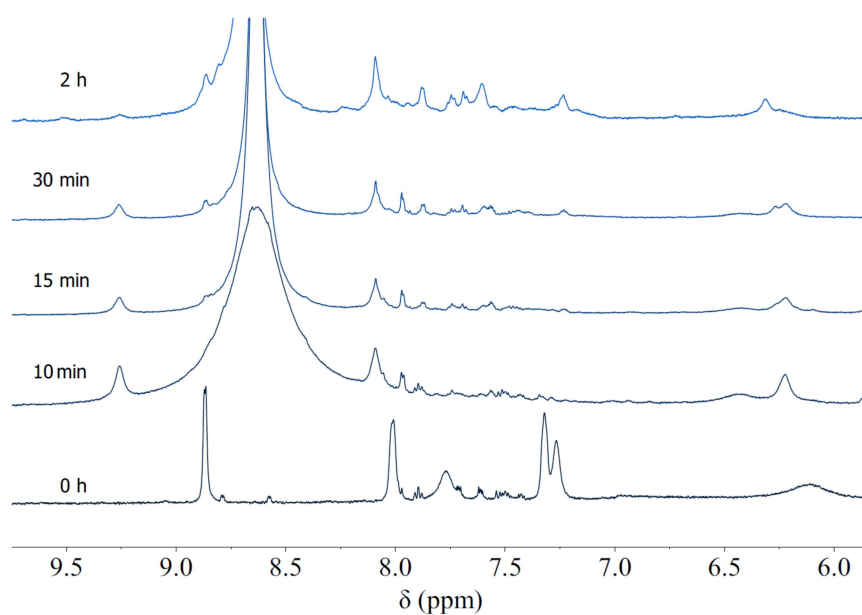
08028 Barcelona, Spain.

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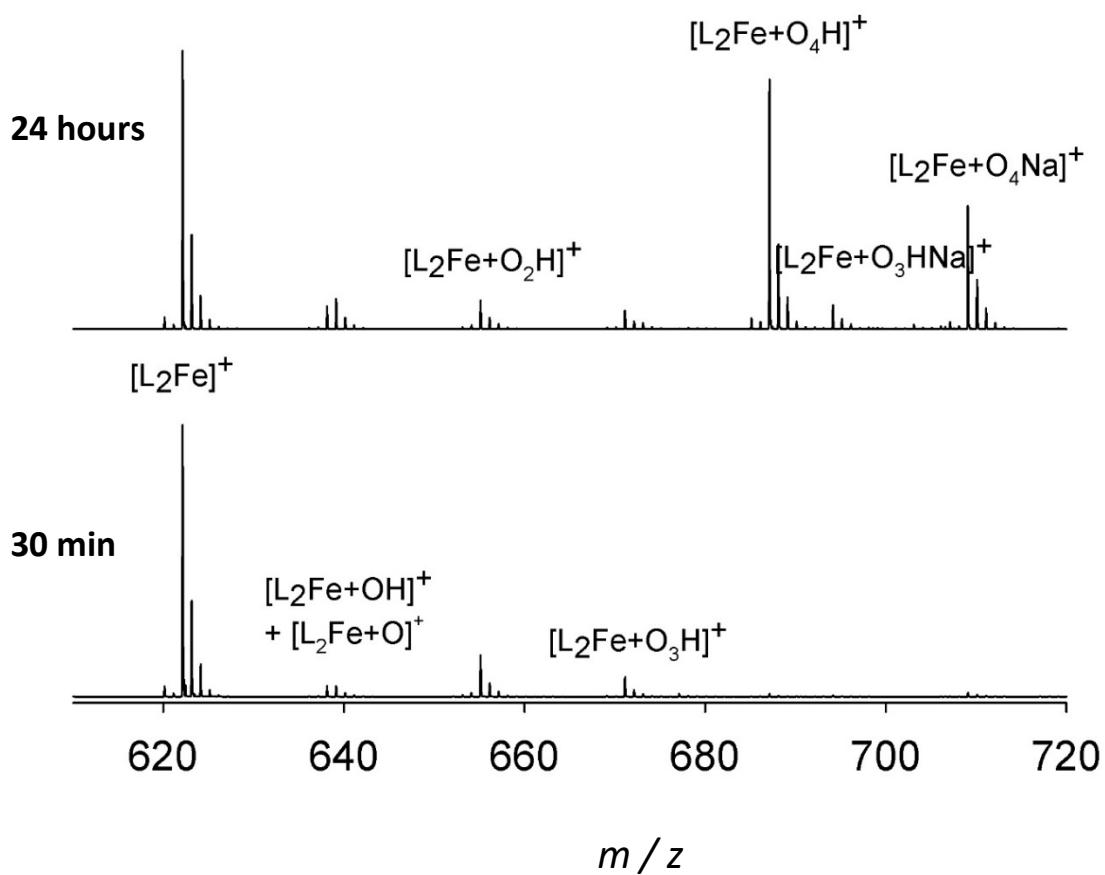
## Experimental Results



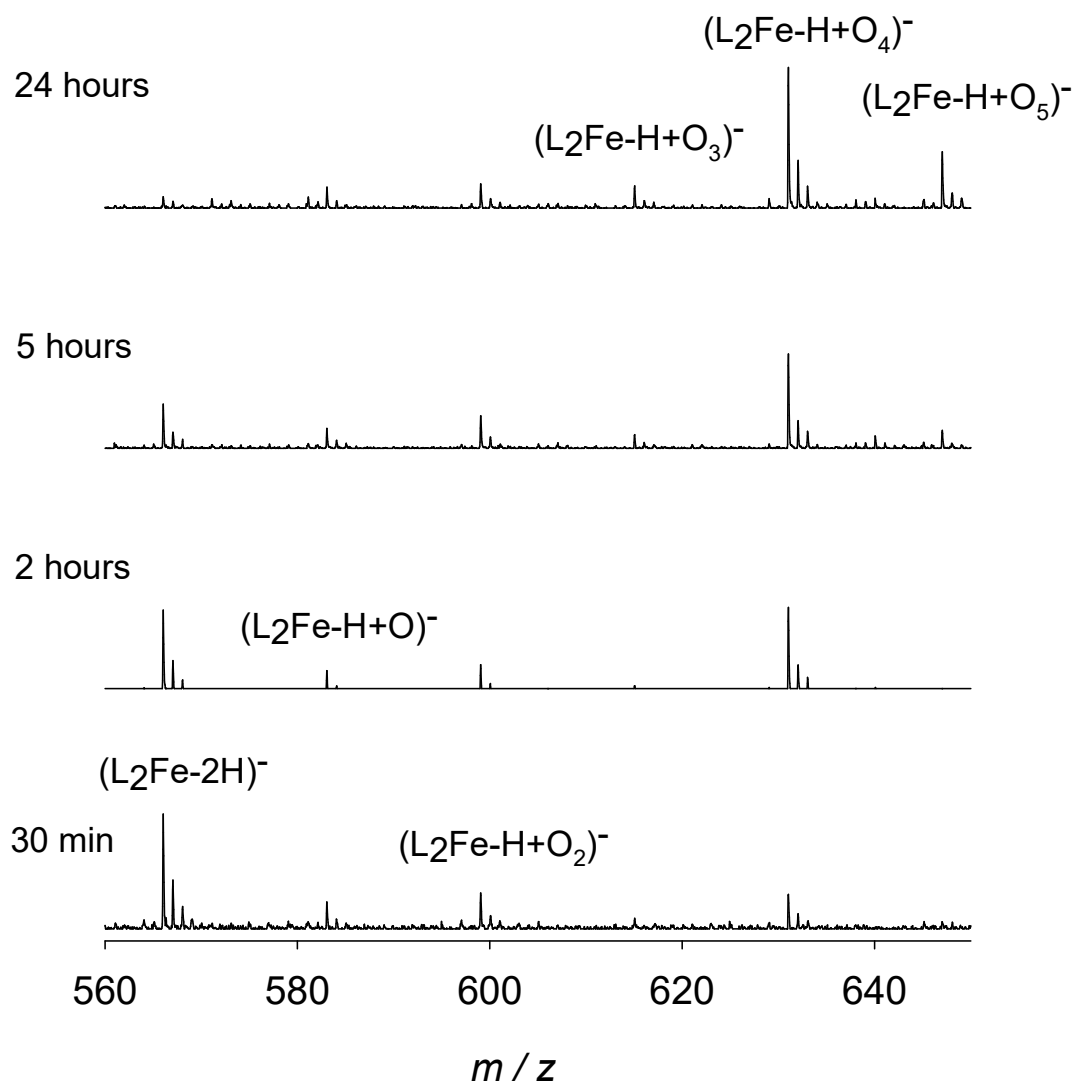
**Figure S1.** <sup>1</sup>H NMR spectra recorded during the reaction of complex [Fe(Bp44mT)<sub>2</sub>] ( $2 \times 10^{-3}$  M) with an excess of H<sub>2</sub>O<sub>2</sub> (0.10 M) in CD<sub>3</sub>CN solution at 25 °C (the broad signal centred at *ca.* 8.5 ppm corresponds to the added H<sub>2</sub>O<sub>2</sub>).



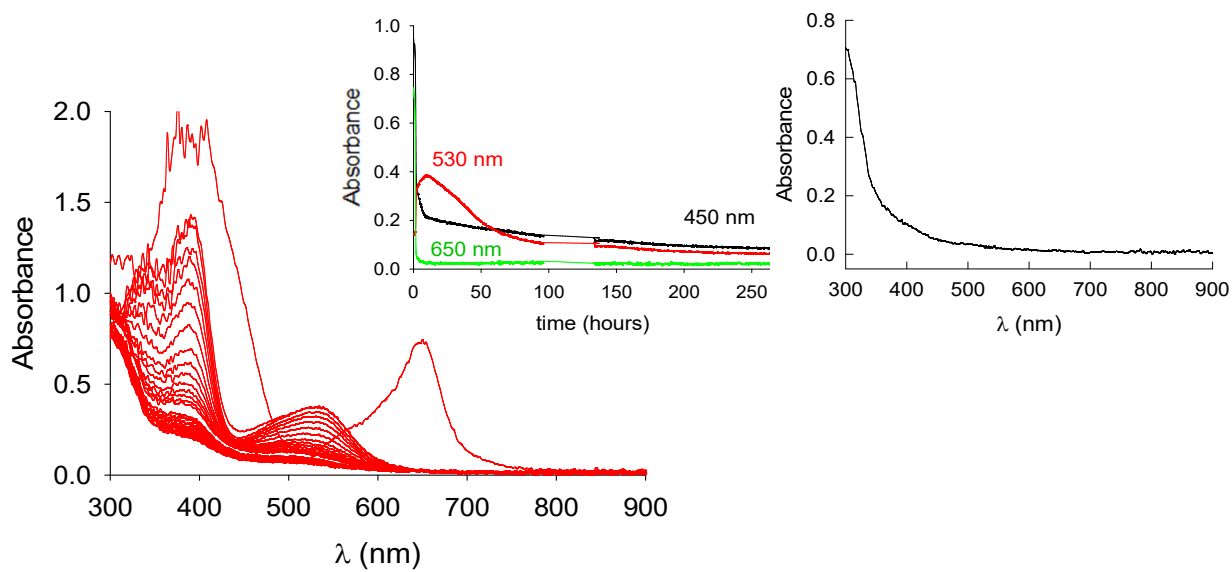
**Figure S2.** <sup>1</sup>H NMR spectra recorded during the reaction of complex [Fe(DpT)<sub>2</sub>] ( $3.1 \times 10^{-3}$  M) with an excess of H<sub>2</sub>O<sub>2</sub> (0.05 M) in CD<sub>3</sub>CN solution at 25 °C (the broad signal centred at *ca.* 8.5 ppm corresponds to the added H<sub>2</sub>O<sub>2</sub>).



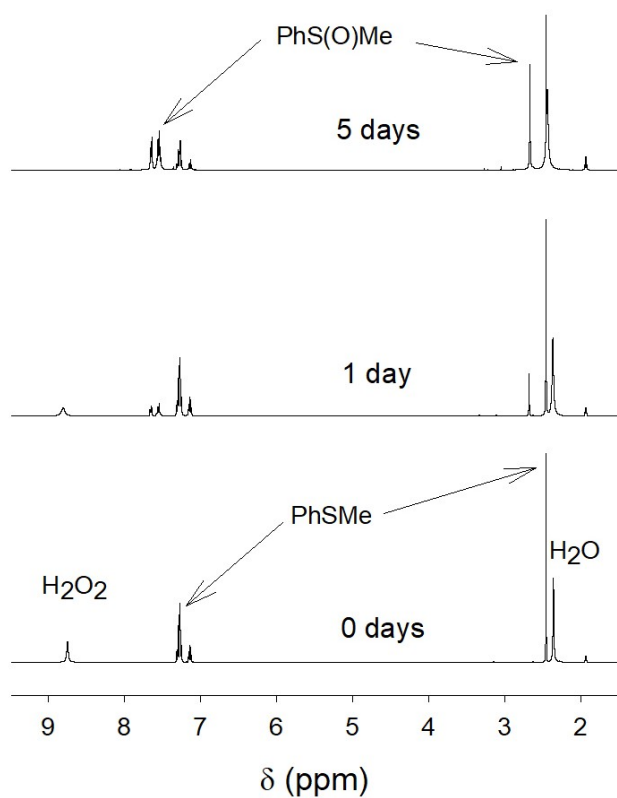
**Figure S3.** ESI-MS spectra recorded during the reaction of complex  $[Fe(Bp44mT)_2]$  ( $2.2 \times 10^{-3}$  M) with an excess of  $H_2O_2$  (0.25 M) in  $CH_3CN$  solution at  $25^\circ C$ . The bottom spectrum was obtained 30 min after mixing and the top one after 24 hours.



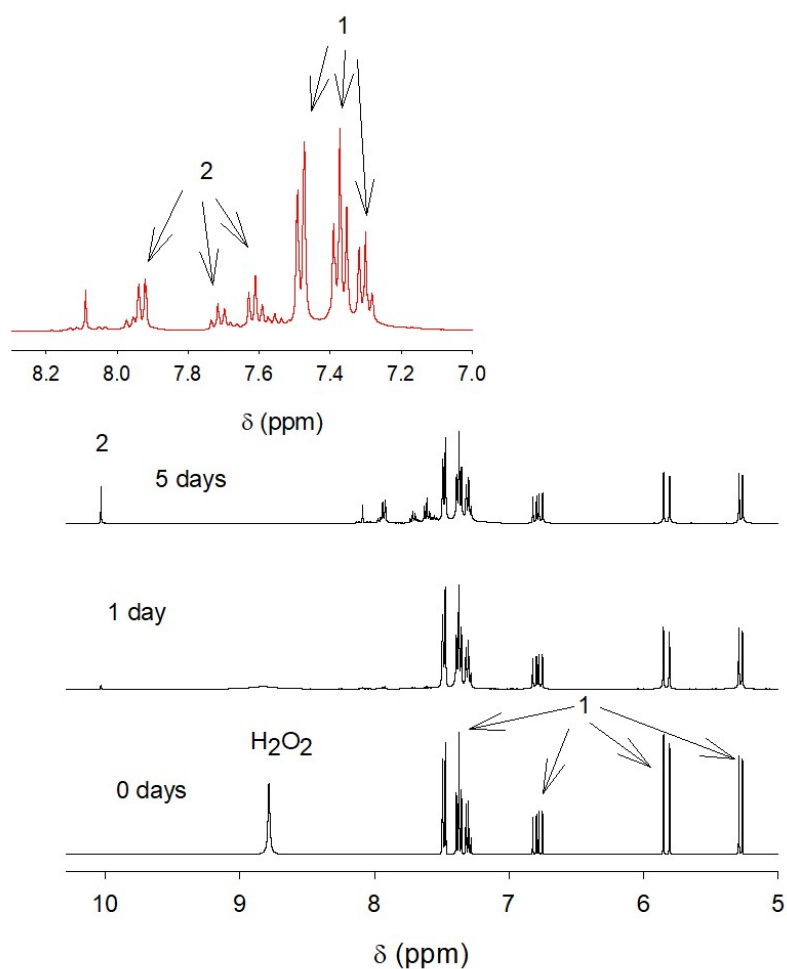
**Figure S4.** ESI-MS spectra recorded during the reaction of complex  $[Fe(DpT)_2]$  ( $2.2 \times 10^{-3}$  M) with an excess of  $H_2O_2$  (0.25 M) in  $CH_3CN$  solution at 25 °C.



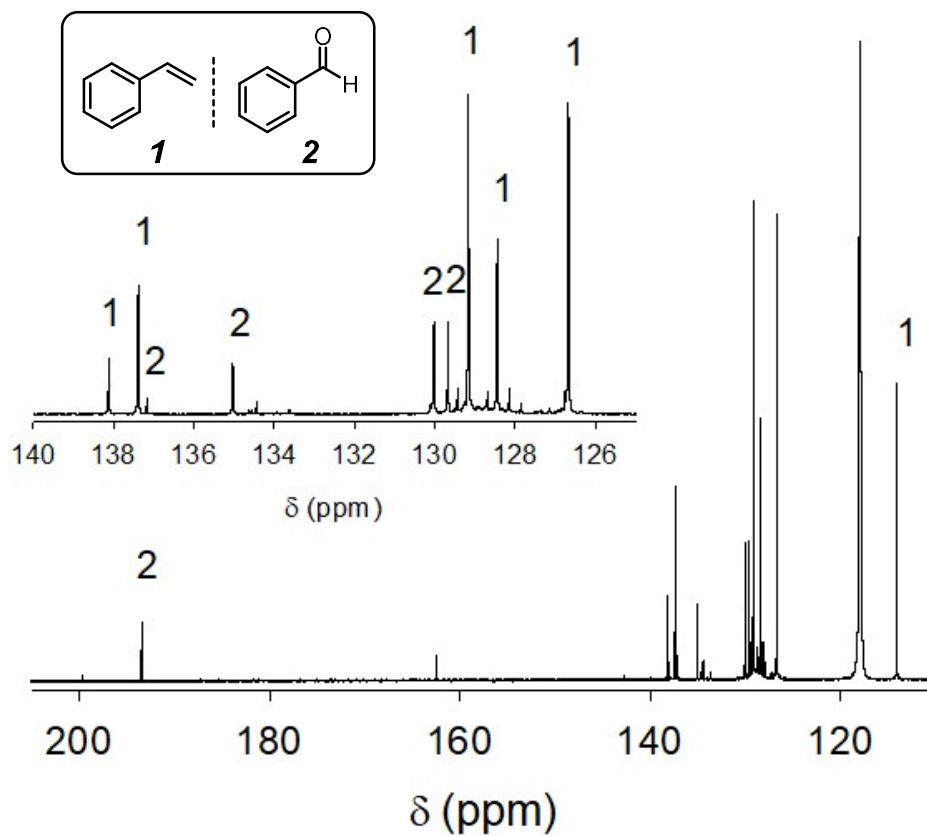
**Figure S5.** Spectral changes observed during the reaction of the  $[\text{Fe}(\text{Dp44mT})_2]$  complex ( $3 \times 10^{-5}$  M) with  $\text{H}_2\text{O}_2$  (0.02 M) in acetonitrile solution at 25 °C. The insets show the traces at selected wavelengths and the final spectrum.



**Figure S6.** <sup>1</sup>H NMR spectra showing the conversion of thioanisole to methyl phenyl sulfoxide catalyzed by the  $[\text{Fe}(\text{Dp44mT})_2]$  complex. The spectra were recorded for a mixture containing the complex ( $2.1 \times 10^{-3}$  M) with an excess of  $\text{H}_2\text{O}_2$  (0.32 M) and thioanisole (0.32 M) in  $\text{CD}_3\text{CN}$  solution that was maintained at 50 °C during the times indicated.

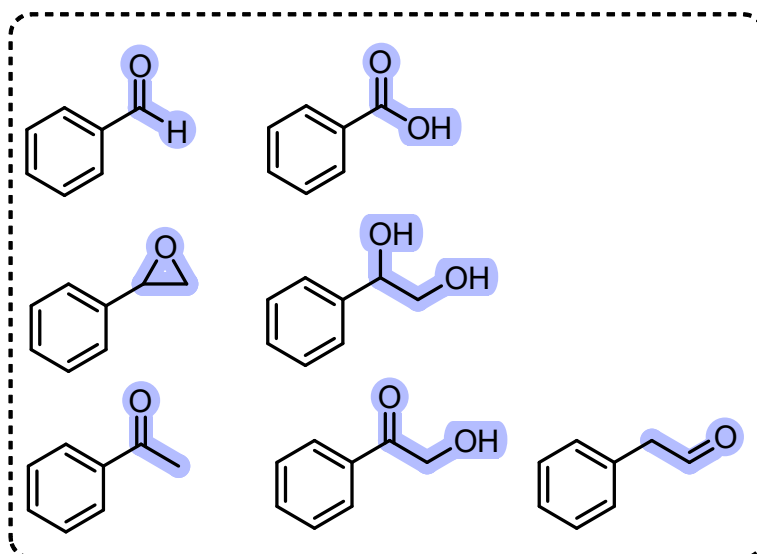


**Figure S7.** <sup>1</sup>H NMR spectra showing the conversion of styrene to benzaldehyde catalyzed by the [Fe(Dp44mT)<sub>2</sub>] complex. The spectra were recorded for a mixture containing the complex ( $2.1 \times 10^{-3}$  M) with an excess of H<sub>2</sub>O<sub>2</sub> (0.32 M) and styrene (0.32 M) in CD<sub>3</sub>CN solution that was maintained at 50 °C during the times indicated. The spectrum in red corresponds to an expansion of the spectrum recorded after 5 days. The signals labeled with 1 correspond to styrene and those labeled with 2 to benzaldehyde.

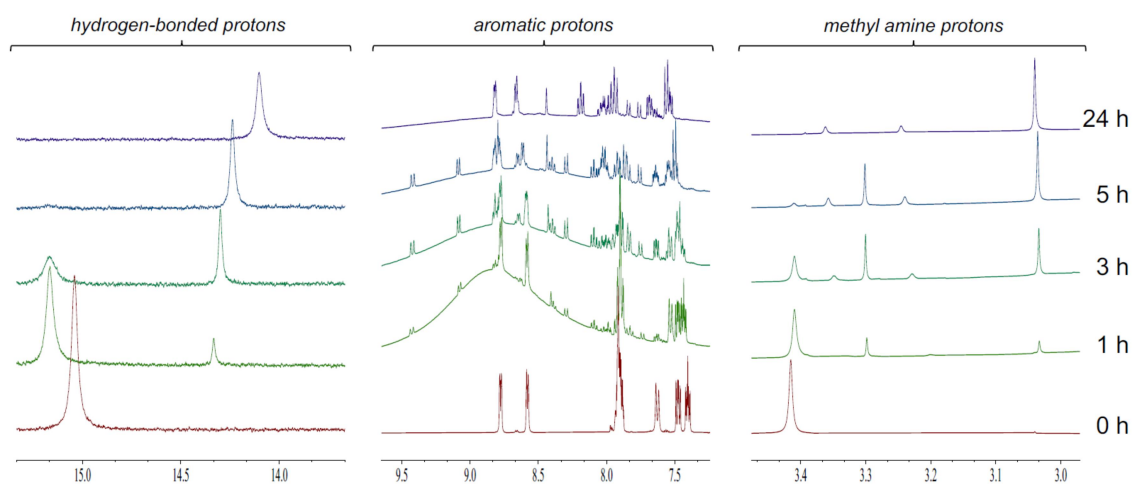


**Figure S8.**  $^{13}\text{C}$  NMR spectrum showing the conversion of styrene to benzaldehyde catalyzed by the  $[\text{Fe}(\text{Dp44mT})_2]$  complex. The spectrum was recorded for a mixture containing the complex ( $2.1 \times 10^{-3}$  M) with an excess of  $\text{H}_2\text{O}_2$  (0.32 M) and styrene (0.32 M) in  $\text{CD}_3\text{CN}$  solution that was maintained at  $50^\circ\text{C}$  during 5 days. The signals labeled with 1 correspond to styrene and those labeled with 2 to benzaldehyde.

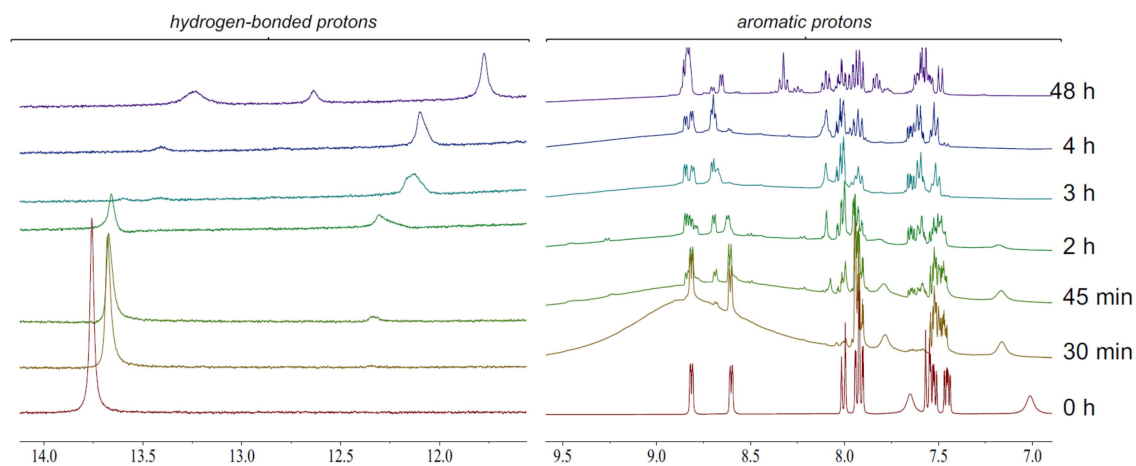




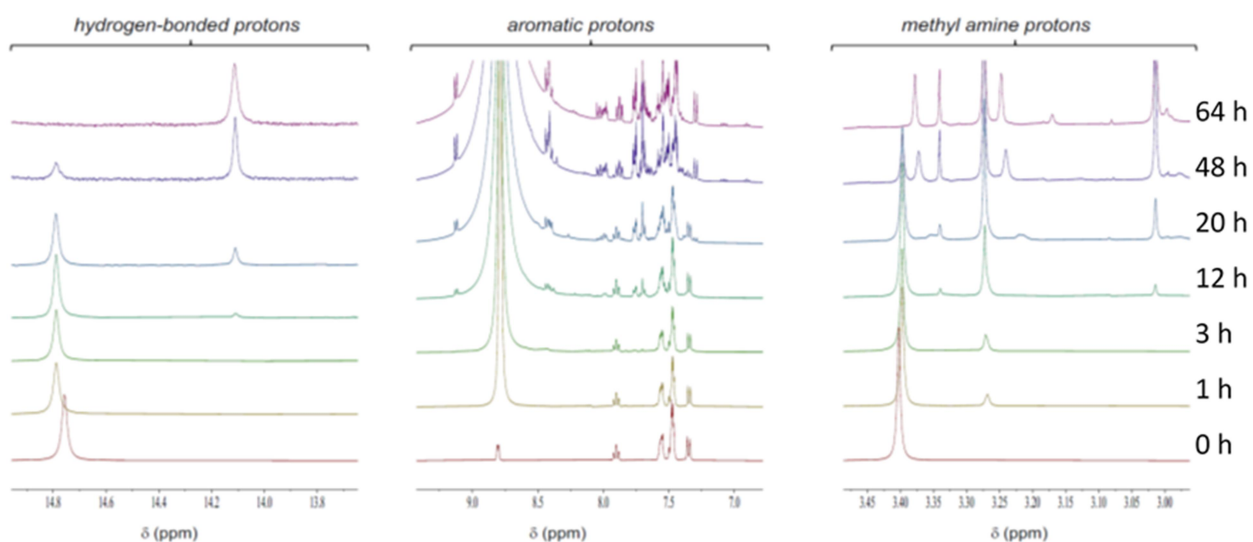
**Figure S9.** Oxidation products observed in catalytic oxidation of styrene using different catalysts and oxidants (not all products are usually observed in the same experiment).



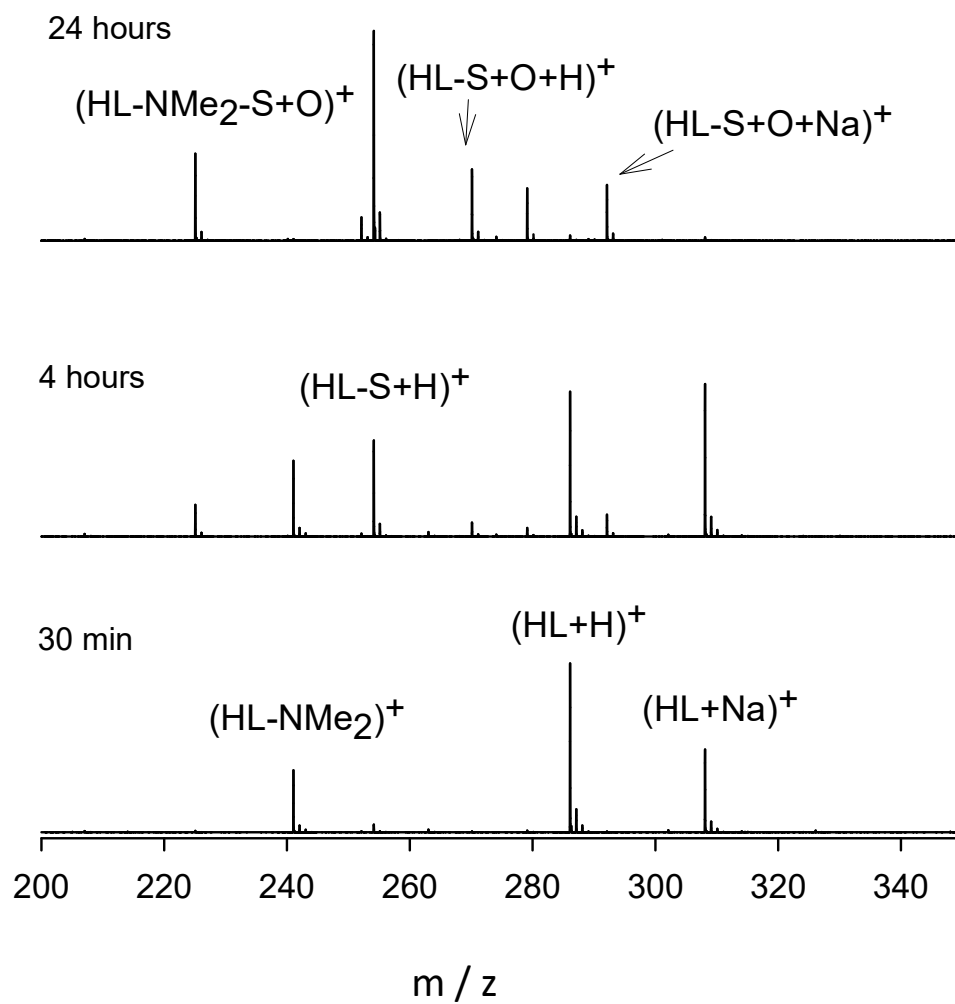
**Figure S10.** Time-resolved  $^1\text{H}$  NMR spectra of ligand HDp44mT (bottom spectrum) after addition of  $0.25\text{ M H}_2\text{O}_2$  to a  $3 \times 10^{-3}\text{ M CD}_3\text{CN}$  solution. The signal intensity has been set independently between sections (the broad signal centred at 8.8 ppm corresponds to the added  $\text{H}_2\text{O}_2$ ).



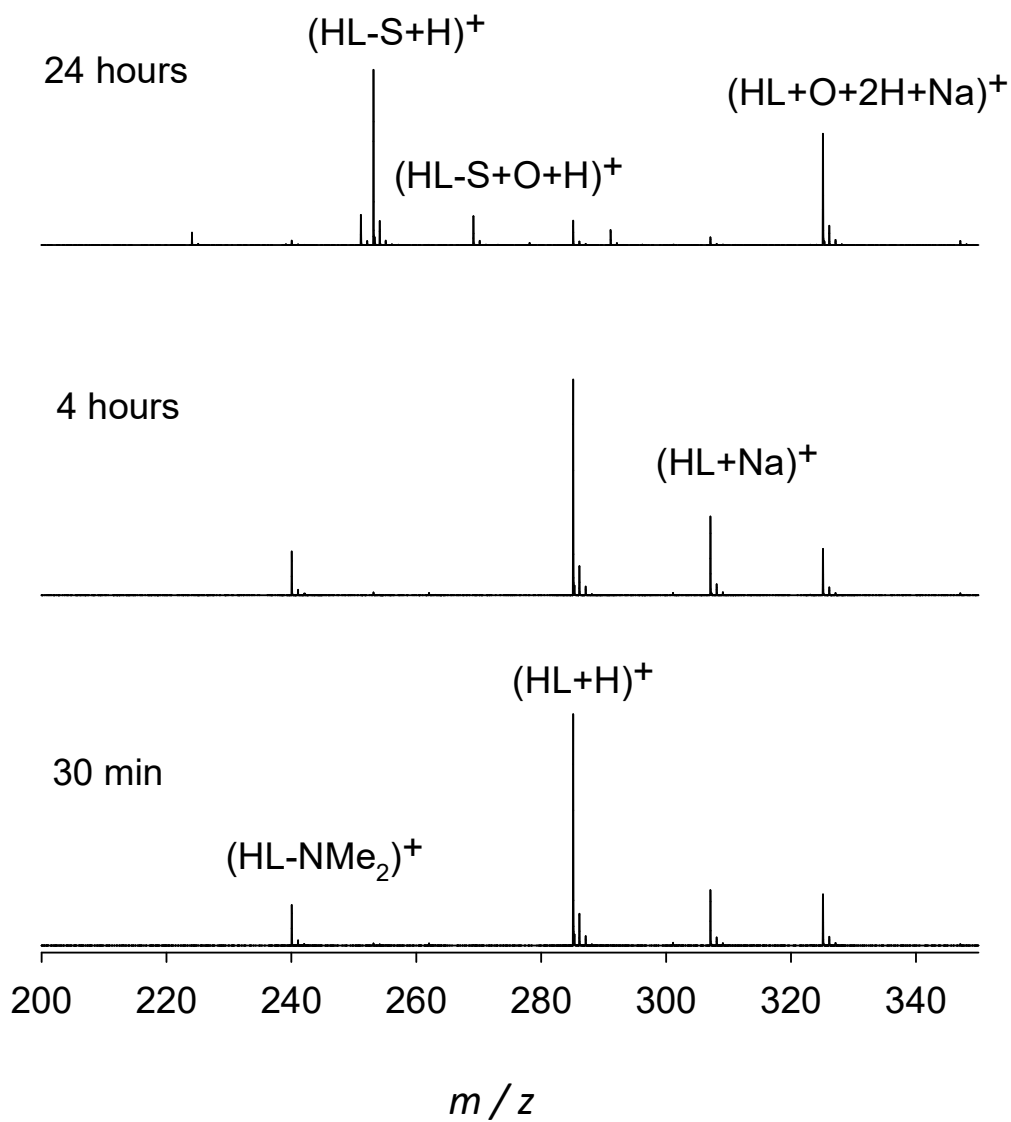
**Figure S11.** Time-resolved  $^1\text{H}$  NMR spectra of ligand HDpT after addition of 0.25 M  $\text{H}_2\text{O}_2$  to a  $3 \times 10^{-3}$  M  $\text{CD}_3\text{CN}$  solution. The signal intensity has been set independently between sections.



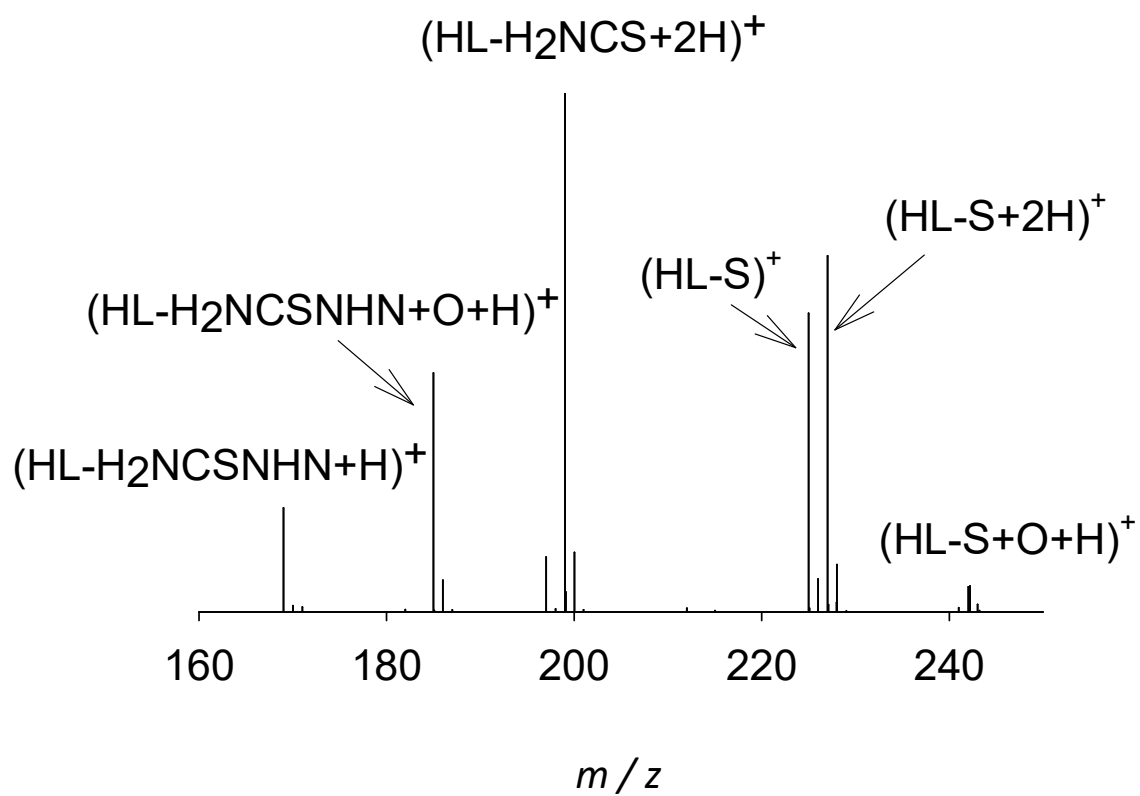
**Figure S12.** Time-resolved  $^1\text{H}$  NMR spectra of ligand HB44mpT after addition of 0.10 M  $\text{H}_2\text{O}_2$  to a  $3 \times 10^{-3}$  M  $\text{CD}_3\text{CN}$  solution. The signal intensity has been set independently between sections.



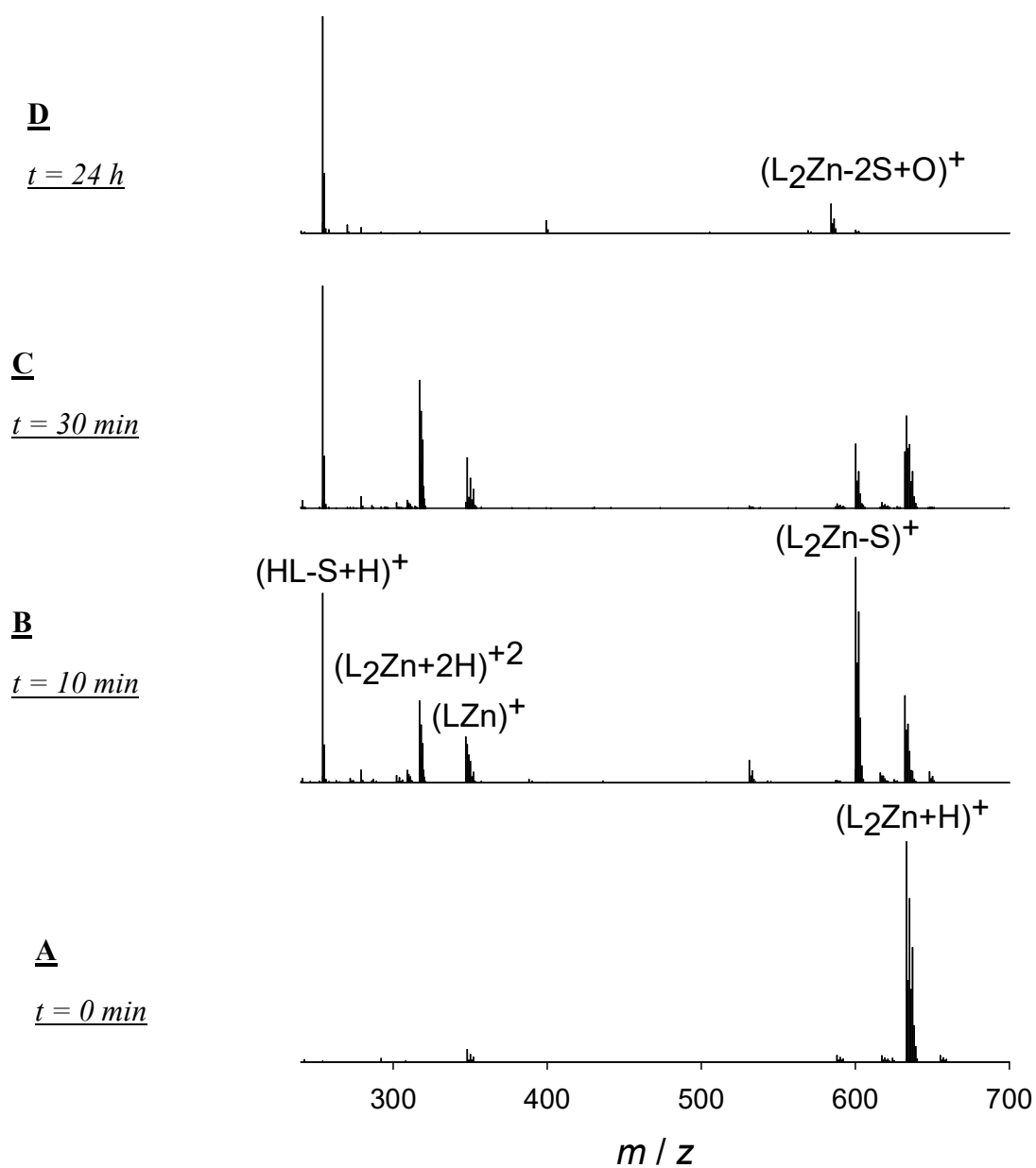
**Figure S13.** ESI-MS spectra recorded in the positive scan mode during the reaction of ligand HDp44mT ( $3 \times 10^{-3}$  M) with an excess of H<sub>2</sub>O<sub>2</sub> (0.25 M) in CD<sub>3</sub>CN solution at 25 °C.



**Figure S14.** ESI-MS spectra recorded in the positive scan mode during the reaction of ligand HBp44mT ( $3 \times 10^{-3}$  M) with an excess of  $\text{H}_2\text{O}_2$  (0.25 M) in  $\text{CD}_3\text{CN}$  solution at 25 °C.



**Figure S15.** ESI-MS spectrum recorded in the positive scan mode after 24 hours of reaction of ligand HDpT ( $3 \times 10^{-3}$  M) with an excess of  $\text{H}_2\text{O}_2$  (0.25M) in  $\text{CD}_3\text{CN}$  solution at 25 °C.



**Figure S16.** ESI-MS spectra recorded during the reaction of complex  $[Zn(Dp44mT)_2]$  ( $2 \times 10^{-3}$  M) with an excess of  $H_2O_2$  (0.25 M) in  $CH_3CN$  solution at 25 °C. The bottom spectrum (A) corresponds to the starting complex in the absence of  $H_2O_2$ .

**Table S1.** m/z values and assignment of the signals observed in the ESI-MS spectra during the reaction of the different complexes and ligands with H<sub>2</sub>O<sub>2</sub> in acetonitrile solution.

Starting complex or ligand	m/z value	Assignment
[Fe <sup>II</sup> (Dp44mT) <sub>2</sub> ]	624.12	(L <sub>2</sub> Fe) <sup>+</sup>
	640.12	(L <sub>2</sub> Fe + O) <sup>+</sup>
	641.13	(L <sub>2</sub> Fe + OH) <sup>+</sup>
	657.11	(L <sub>2</sub> Fe + O <sub>2</sub> H) <sup>+</sup>
	673.11	(L <sub>2</sub> Fe + O <sub>3</sub> H) <sup>+</sup>
	696.14	(L <sub>2</sub> Fe + O <sub>3</sub> HNa) <sup>+</sup>
	689.11	(L <sub>2</sub> Fe + O <sub>4</sub> H) <sup>+</sup>
	711.10	(L <sub>2</sub> Fe + O <sub>4</sub> Na) <sup>+</sup>
[Fe <sup>II</sup> (Bp44mT) <sub>2</sub> ]	622.14	(L <sub>2</sub> Fe) <sup>+</sup>
	638.14	(L <sub>2</sub> Fe + O) <sup>+</sup>
	639.13	(L <sub>2</sub> Fe + OH) <sup>+</sup>
	655.14	(L <sub>2</sub> Fe + O <sub>2</sub> H) <sup>+</sup>
	671.14	(L <sub>2</sub> Fe + O <sub>3</sub> H) <sup>+</sup>
	694.15	(L <sub>2</sub> Fe + O <sub>3</sub> HNa) <sup>+</sup>
	687.13	(L <sub>2</sub> Fe + O <sub>4</sub> H) <sup>+</sup>
	709.09	(L <sub>2</sub> Fe + O <sub>4</sub> Na) <sup>+</sup>
[Fe <sup>II</sup> (DpT) <sub>2</sub> ]	566.05	(L <sub>2</sub> Fe - 2 H) <sup>-</sup>
	583.05	(L <sub>2</sub> Fe - H + O) <sup>-</sup>
	599.05	(L <sub>2</sub> Fe - H + O <sub>2</sub> ) <sup>-</sup>
	615.06	(L <sub>2</sub> Fe - H + O <sub>3</sub> ) <sup>-</sup>
	631.05	(L <sub>2</sub> Fe - H + O <sub>4</sub> ) <sup>-</sup>
	647.04	(L <sub>2</sub> Fe - H + O <sub>5</sub> ) <sup>-</sup>
HDp44mT	286.11	(HL + H) <sup>+</sup>
	308.10	(HL + Na) <sup>+</sup>
	241.05	(HL - NMe <sub>2</sub> ) <sup>+</sup>
	225.07	(HL - NMe <sub>2</sub> - S + O) <sup>+</sup>
	270.13	(HL - S + O + H) <sup>+</sup>
	292.11	(HL - S + O + Na) <sup>+</sup>
HBp44mT	285.12	(HL + H) <sup>+</sup>
	307.10	(HL + Na) <sup>+</sup>
	240.05	(HL - NMe <sub>2</sub> ) <sup>+</sup>
	253.14	(HL - S + H) <sup>+</sup>
	269.15	(HL - S + O + H) <sup>+</sup>
	325.11	(HL + O + 2 H + Na) <sup>+</sup>
HDpT	225.01	(HL - S) <sup>+</sup>
	227.02	(HL - S + 2 H) <sup>+</sup>
	242.21	(HL - S + O + H) <sup>+</sup>
	199.03	(HL - H <sub>2</sub> NCS + 2 H) <sup>+</sup>
	169.02	(HL - H <sub>2</sub> NCSNHN + H) <sup>+</sup>
	185.01	(HL - H <sub>2</sub> NCSNHN + O + H) <sup>+</sup>
[Zn <sup>II</sup> (Dp44mT) <sub>2</sub> ]	633.17	(L <sub>2</sub> Zn + H) <sup>+</sup>
	317.09	(L <sub>2</sub> Zn + 2 H) <sup>+2</sup>
	347.05	(LZn) <sup>+</sup>
	600.20	(L <sub>2</sub> Zn - S) <sup>+</sup>
	584.23	(L <sub>2</sub> Zn - 2 S + O) <sup>+</sup>
	254.16	(HL - S + H) <sup>+</sup>

**Table S2.** The effect of temperature, concentrations and reaction time on the catalytic activity of the  $[\text{Fe}^{\text{II}}(\text{Bp44mT})_2]$  complex in the oxidation of styrene into benzaldehyde with  $\text{H}_2\text{O}_2$  in  $\text{CD}_3\text{CN}$  solution.

Entry	[complex] (M)	[ $\text{H}_2\text{O}_2$ ] (M)	[styrene] (M)	T ( $^{\circ}\text{C}$ )	Conversion (%)			Selectivity (%)			TON (5 days) <sup>a</sup>
					1 day	5 days	8 days	1 day	5 days	8 days	
1	$2.1 \times 10^{-3}$	0.32	0.32	35	4	5	6	38	51	52	8
2	$2.1 \times 10^{-3}$	0.32	0.32	50	5	11	16	72	62	58	17
3	$2.1 \times 10^{-3}$	0.32	0.32	65	23	27		19	38		41
4	$2.1 \times 10^{-3}$	0.64	0.32	50	7	10	12	54	57	54	15
5	$4.2 \times 10^{-3}$	0.32	0.32	50	16	35	37	79	55	49	27
6	$2.1 \times 10^{-3}$	0.32	0.64	50	8	16	16	60	62	52	49
7	$4.2 \times 10^{-3}$	0.64	0.32	50	17	38	42	58	58	62	29

<sup>a</sup> mmols of styrene converted by mmol of catalyst.

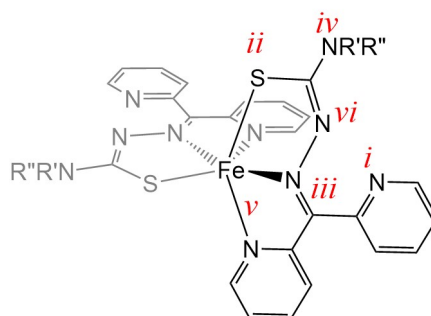


## Computational methods

DFT calculations were carried out with Gaussian 16 Rev. B.01.<sup>1</sup> Geometry optimizations employed the BP86 functional<sup>2,3</sup> and were performed by including the effect of the water solvent via the SMD approach.<sup>4</sup> SDD effective core potentials<sup>5</sup> and associated basis sets were used to represent Fe and S centres, with added d-orbital polarisation ( $\zeta = 0.503$ )<sup>6</sup> on the latter. Pople style 6-31G(d,p) basis sets<sup>7,8</sup> were used for all other atoms. The nature of the minima was confirmed through analytical frequency calculations, which showed zero imaginary frequencies. These calculations were also employed to obtain the thermal and entropic contributions to the Gibbs energy, evaluated at 298.15 K and 1 atm. The final Gibbs free energies also include dispersion corrections, obtained via single-point calculations using Grimme's D3 correction for dispersion effects (with the Becke–Johnson damping function).<sup>9,10</sup>

## Computational Results

The different possible reacting sites of the TSC ligands within the  $[\text{Fe}^{\text{II}}(\text{Dp44mT})_2]$  complex for the addition of up to five oxygen atoms were identified, and are indicated in Scheme S1.



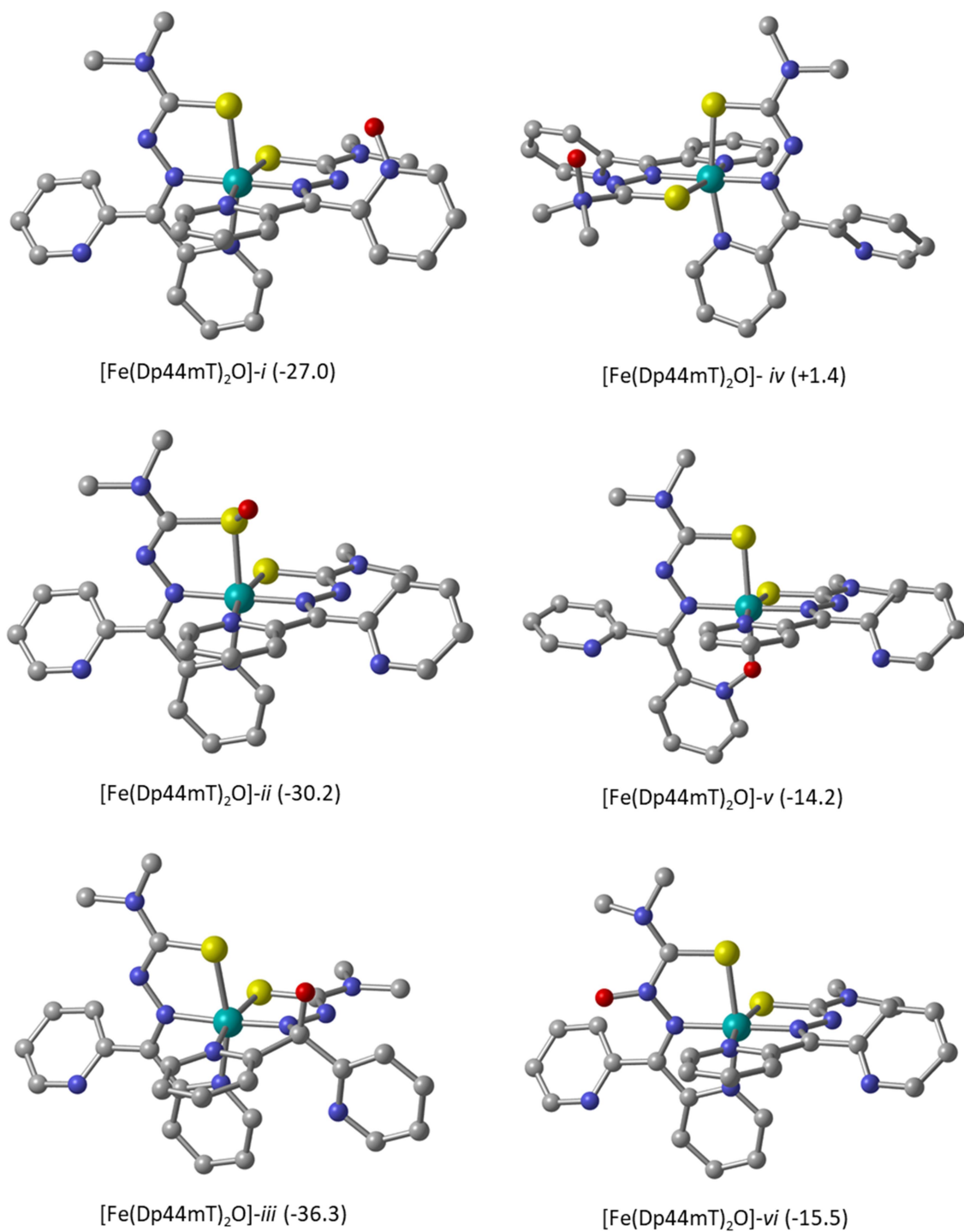
**Scheme S1.**

**Table S3.** Reaction free energies ( $\text{kcal mol}^{-1}$ ) associated to the incorporation of one oxygen atom into  $[\text{Fe}^{\text{II}}(\text{Dp44mT})_2]$ , see Scheme S1 for site labelling.

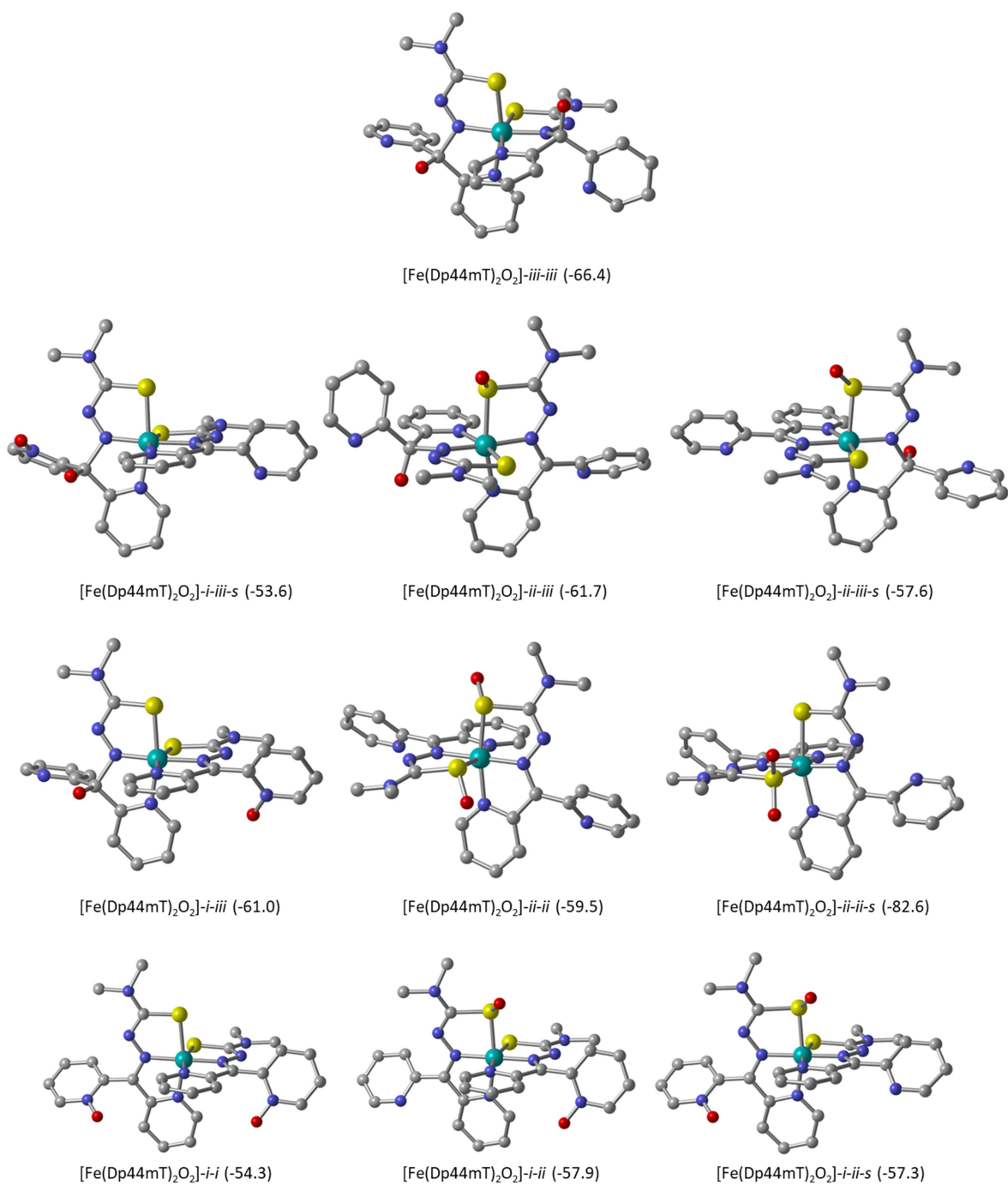
O binding position	$[\text{Fe}(\text{Dp44mT})_2\text{O}]$
<i>i</i> (uncoordinated pyridine)	-27.0
<i>ii</i> (coordinated S)	-30.2
<i>iii</i> ( $\text{py}_2\text{C}=\text{N}$ double bond)	-36.3
<i>iv</i> ( $\text{NMe}_2$ group)	+1.4
<i>v</i> ( $\text{N}_{\text{py}}\text{-Fe}$ bond)	-15.5
<i>vi</i> (central N in $\text{C}=\text{N}-\text{N}$ )	-14.2

The structures resulting from these additions are shown in Figure S17, whereas their relative free energy ( $\Delta G_r$ ) values, obtained considering that they result from an oxygen atom transfer (OAT) from  $\text{H}_2\text{O}_2$ , are included in Table S3. No attempt has been made to study the mechanistic details of such transformations and the values of  $\Delta G_r$  simply indicate the relative thermodynamic stability of the different isomers. The results indicate that the most favoured site of attack is the  $\text{py}_2\text{C}=\text{N}$  group (Scheme S1, site *iii*), which *a priori* could lead to an oxaziridine group.<sup>11</sup> Optimizations, nevertheless, lead to a structure with a quaternary C centre bound to a formally anionic oxygen that could easily protonate to produce the  $\{[\text{Fe}^{\text{II}}(\text{Dp44mT})_2\text{O}]^0 + \text{H}^+\}^+$  species at 640 m/z, found as a minor component in the reaction medium after 30 minutes and that prevails after 24 hours. The  $\Delta G_r$  values also indicate that the species resulting from attacks at the S atom or at the uncoordinated pyridine are quite stable. For the addition to the S atom (site *ii*), the optimized structure corresponds to a complex with a coordinated S=O group. This type of coordination has already been observed for some thiosemicarbazones and iron complexes containing coordinated thiolates.<sup>12,13,14</sup> Attack to the uncoordinated pyridine (site *i*) results in the formation of a complex containing a pyridine-N-oxide group, a process that has also been observed for the reaction of different substituted pyridines with  $\text{H}_2\text{O}_2$  and other oxidants.<sup>15,16</sup>

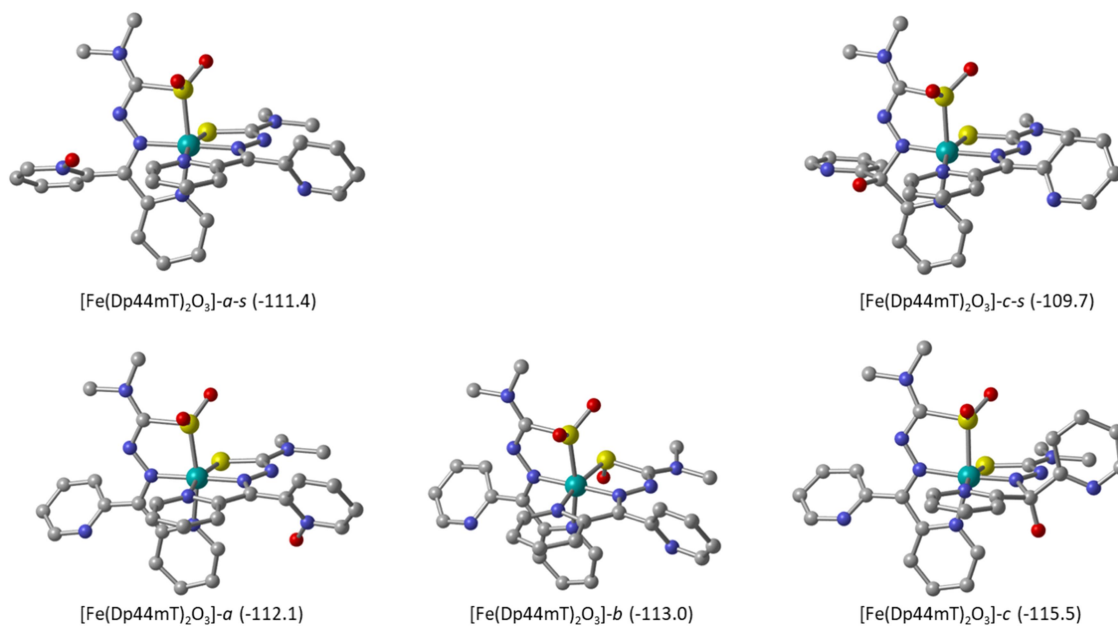
Calculations were also carried out to analyse the possible structures of the  $[\text{Fe}(\text{Dp44mT})_2\text{O}_n]$  ( $n = 2-5$ ) species found in the MS spectra (Figures S18-S21); the three most favoured binding sites (*i*, *ii* and *iii*) were considered. Calculations show that further O additions to  $[\text{Fe}(\text{Dp44mT})_2\text{O}]$  are always exergonic if  $\text{H}_2\text{O}_2$  is considered as the O donor, and the results show that for the structures with two and four added O atoms, ie. the species with one and two  $\text{SO}_2$  moieties  $[\text{Fe}(\text{Dp44mT})_2\text{O}_2]$  and  $[\text{Fe}(\text{Dp44mT})_2\text{O}_4]$ , respectively, are significantly more stable than any of their isomers (Figure S22). Specifically, such additional stabilisation amounts 16.2 kcal mol<sup>-1</sup> for the  $[\text{Fe}(\text{Dp44mT})_2\text{O}_2]$  complex with one  $\text{SO}_2$  moiety, and 24.9 kcal mol<sup>-1</sup> for the corresponding  $[\text{Fe}(\text{Dp44mT})_2\text{O}_4]$  complex. Formation of species containing coordinated sulfones upon addition of two oxygen atoms to metal-thiosemicarbazone complexes has already been observed in some cases.<sup>12,17</sup> Even so, the MS spectra indicate that species with 3 or 5 oxygen atoms accumulate during the reaction. These species probably contain one or two sulfone groups and one additional oxygen atom resulting from attack to either sites *i* or *ii*, as both possibilities lead to a similar stabilisation (Figures S19 and S21).



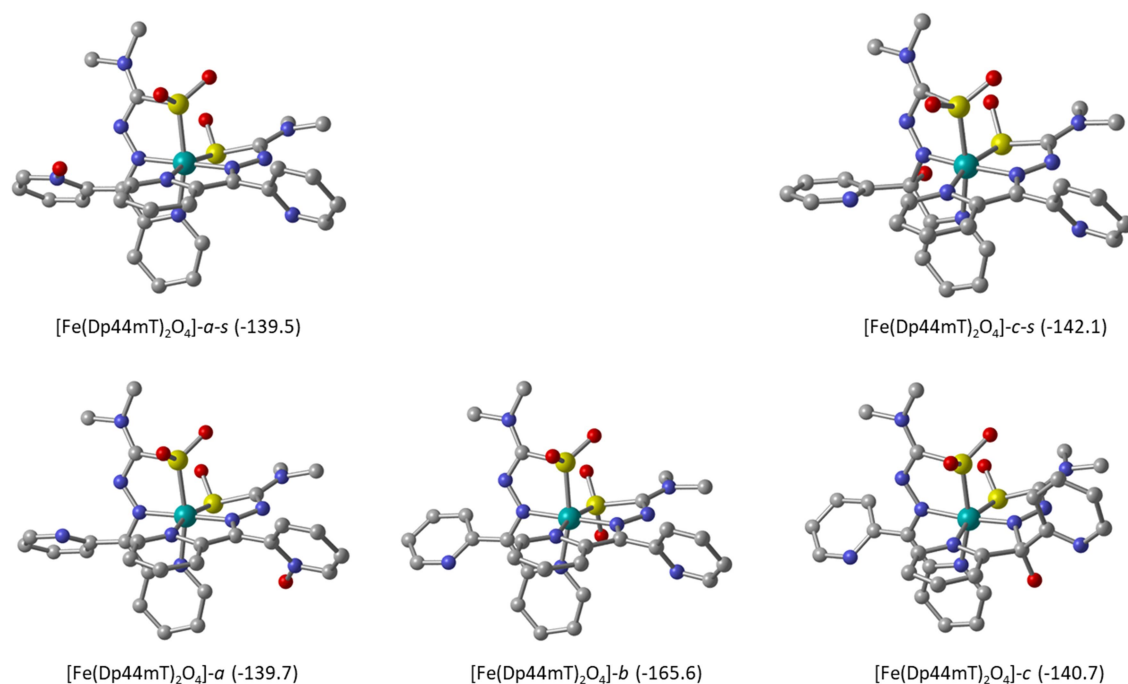
**Figure S17.** Optimized structures of selected [Fe(Dp44mT)<sub>2</sub>O] isomers. For simplicity, H atoms were not drawn. The numbers in parenthesis indicate the corresponding values of  $\Delta G_r$  (in kcal mol<sup>-1</sup>) for their formation via oxygen atom transfer from H<sub>2</sub>O<sub>2</sub> to [Fe(Dp44mT)<sub>2</sub>].



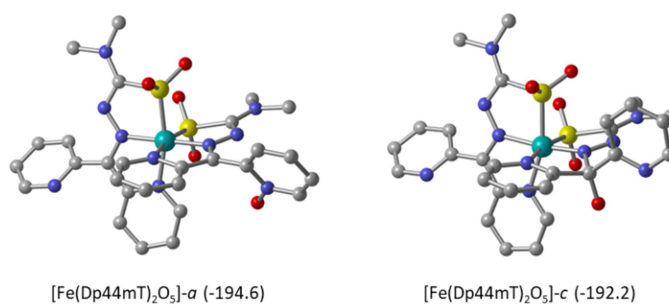
**Figure S18.** Optimized structures of selected [Fe(Dp44mT)<sub>2</sub>O<sub>2</sub>] species. For simplicity, H atoms were not drawn. The numbers in parenthesis indicate the corresponding values of  $\Delta G_r$  (in kcal mol<sup>-1</sup>) for their formation via oxygen atom transfers from two H<sub>2</sub>O<sub>2</sub> molecules. The suffix –s indicates that both O atoms were incorporated into the same Dp44mT ligand.



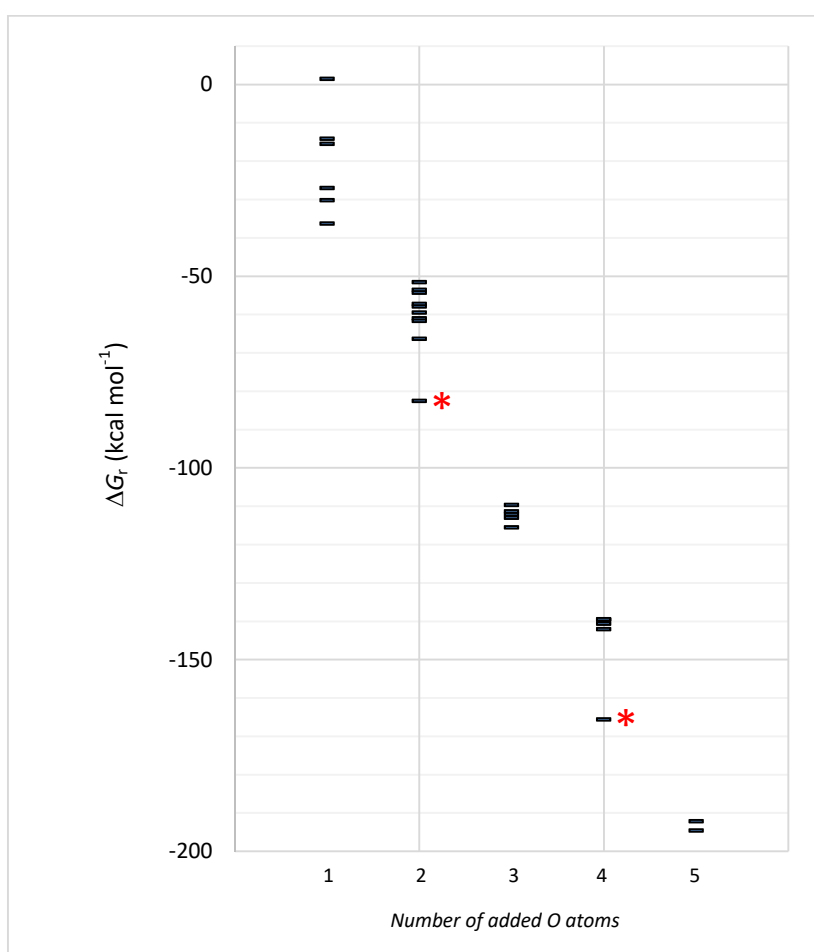
**Figure S19.** Optimized structures of selected [Fe(Dp44mT)<sub>2</sub>O<sub>3</sub>] species. For simplicity, H atoms were not drawn. The numbers in parenthesis indicate the corresponding values of  $\Delta G_r$  (in kcal mol<sup>-1</sup>) for their formation via oxygen atom transfers from three H<sub>2</sub>O<sub>2</sub> molecules. The suffix –s indicates that all O atoms were incorporated into the same Dp44mT ligand.



**Figure S20.** Optimized structures of selected [Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>] species. For simplicity H, atoms were not drawn. The numbers in parenthesis indicate the corresponding values of  $\Delta G_r$  (in kcal mol<sup>-1</sup>) for their formation via oxygen atom transfers from four H<sub>2</sub>O<sub>2</sub> molecules.



**Figure S21.** Optimized structures of selected  $[\text{Fe}(\text{Dp44mT})_2\text{O}_5]$  species. For simplicity, H atoms were not drawn. The numbers in parenthesis indicate the corresponding values of  $\Delta G_r$  (in  $\text{kcal mol}^{-1}$ ) for their formation via oxygen atom transfers from five  $\text{H}_2\text{O}_2$  molecules.



**Figure S22.** Representation of the relative reaction free energy  $\Delta G_r$  (in  $\text{kcal mol}^{-1}$ ) of all the computed  $[\text{Fe}(\text{Dp44mT})_2\text{O}_n]$  ( $n=1-5$ ) species assuming that their formation takes place via consecutive oxygen atom transfers from  $n$   $\text{H}_2\text{O}_2$  molecules. The symbols corresponding to the structures featuring one and two  $\text{SO}_2$  moieties, significantly stabilized with respect to their other possible conformers, are highlighted with red asterisks.

**Table S4.** For all the optimized species, summary of computed SCF energies, thermal correction to Gibbs free energy at the same level of theory ( $E \rightarrow G_{\text{corr.}}$ ), and Grimme's D3(BJ) dispersion correction ( $D3(\text{BJ})_{\text{corr.}}$ ). All the values are given in Hartrees.

Species	SCF Energy	$E \rightarrow G_{\text{corr.}}$	$D3(\text{BJ})_{\text{corr.}}$
H <sub>2</sub> O	-76.4254856	0.002872	-0.00045908
H <sub>2</sub> O <sub>2</sub>	-151.55824	0.002912	-0.00110592
[Fe(Dp44mT) <sub>2</sub> ]	-1776.00037	0.444664	-0.1905853
[Fe(Dp44mT) <sub>2</sub> O]-i	-1851.17636	0.447685	-0.1940197
[Fe(Dp44mT) <sub>2</sub> O]-ii	-1851.17879	0.447044	-0.19605358
[Fe(Dp44mT) <sub>2</sub> O]-iii	-1851.18877	0.44684	-0.19554579
[Fe(Dp44mT) <sub>2</sub> O]-iv	-1851.13208	0.449575	-0.19498803
[Fe(Dp44mT) <sub>2</sub> O]-v	-1851.15908	0.44629	-0.18955005
[Fe(Dp44mT) <sub>2</sub> O]-vi	-1851.1566	0.448074	-0.1957753
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-i-i	-1926.351995	0.44966	-0.19725904
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-i-ii	-1926.354772	0.44891	-0.19944368
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-i-ii-s	-1926.354299	0.449372	-0.1994189
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-i-iii	-1926.361065	0.45083	-0.19990965
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-ii-ii	-1926.356833	0.450819	-0.20184103
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-ii-ii-s	-1926.394014	0.450397	-0.2010862
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-i-iii-s	-1926.349784	0.45024	-0.19882617
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-ii-iii	-1926.359064	0.449563	-0.20178035
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-ii-iii-s	-1926.351626	0.44813	-0.20129701
[Fe(Dp44mT) <sub>2</sub> O <sub>2</sub> ]-iii-iii	-1926.368689	0.451098	-0.20128002
[Fe(Dp44mT) <sub>2</sub> O <sub>3</sub> ]-a	-2001.57306	0.453572	-0.20551247
[Fe(Dp44mT) <sub>2</sub> O <sub>3</sub> ]-a-s	-2001.572056	0.453401	-0.20517738
[Fe(Dp44mT) <sub>2</sub> O <sub>3</sub> ]-b	-2001.57273	0.453179	-0.20683136
[Fe(Dp44mT) <sub>2</sub> O <sub>3</sub> ]-c	-2001.576718	0.454018	-0.2076991
[Fe(Dp44mT) <sub>2</sub> O <sub>3</sub> ]-c-s	-2001.5663	0.452091	-0.2070409
[Fe(Dp44mT) <sub>2</sub> O <sub>4</sub> ]-a	-2076.748744	0.457344	-0.2110165
[Fe(Dp44mT) <sub>2</sub> O <sub>4</sub> ]-a-s	-2076.748714	0.457918	-0.21122105
[Fe(Dp44mT) <sub>2</sub> O <sub>4</sub> ]-b	-2076.787919	0.457209	-0.21284939
[Fe(Dp44mT) <sub>2</sub> O <sub>4</sub> ]-c	-2076.744997	0.454745	-0.21366436
[Fe(Dp44mT) <sub>2</sub> O <sub>4</sub> ]-c-s	-2076.748183	0.454605	-0.21258533
[Fe(Dp44mT) <sub>2</sub> O <sub>5</sub> ]-a	-2151.966603	0.460732	-0.2173338
[Fe(Dp44mT) <sub>2</sub> O <sub>5</sub> ]-c	-2151.958129	0.458358	-0.21959724

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## DFT optimized structures

H<sub>2</sub>O

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H -0.000000 -0.761005 -0.489401

H<sub>2</sub>O<sub>2</sub>

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O 0.728107 -0.108126 0.065953  
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H 1.006567 0.625709 -0.527627

[Fe(Dp44mT)<sub>2</sub>]

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[Fe(Dp44mT)<sub>2</sub>O]-i

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[Fe(Dp44mT)<sub>2</sub>O]-ii

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[Fe(Dp44mT)<sub>2</sub>O]-iii

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H -4.066682 0.763685 4.457729  
H -3.881713 2.509509 4.084346  
H -4.152888 1.331077 2.753012  
H -2.086630 1.597719 5.659808  
H -0.730770 0.656468 4.956067  
H -0.807755 2.432197 4.715919  
H 2.980766 5.503161 -1.310988  
H 1.990479 4.633922 -2.528086  
H 1.353538 4.897937 -0.870930  
H 4.814075 4.232010 -0.770269  
H 4.710394 2.438296 -0.693782  
H 4.575397 3.280969 -2.272332  
O -2.844110 1.856921 -1.389230

[Fe(Dp44mT)<sub>2</sub>O]-iv

N 4.473112 -2.097620 -0.961073  
C 3.965519 -1.211650 -0.062499  
C 4.788240 -0.476496 0.822546  
C 6.175467 -0.656106 0.762699  
C 6.706078 -1.559121 -0.172667  
C 5.812954 -2.253612 -1.002470  
C 2.486638 -1.083728 -0.034884  
N 1.826193 0.088659 0.007304  
N 2.576785 1.239278 -0.072267  
C 1.838024 2.330135 -0.001287

N 2.625814 3.612076 0.071875  
C 1.923542 4.755113 -0.625257  
C 1.580620 -2.226194 -0.024681  
N 0.248081 -1.870684 0.055935  
C -0.691439 -2.844121 0.090846  
C -0.369802 -4.206121 0.056197  
C 0.982600 -4.580181 -0.012055  
C 1.963595 -3.583841 -0.051064  
Fe -0.060633 0.060053 0.124773  
S 0.113427 2.371862 0.138017  
N -1.962499 0.035089 0.281726  
N -2.648086 -0.051083 1.449846  
C -1.855407 -0.068738 2.542095  
N -2.466762 -0.128626 3.759239  
C -1.694241 -0.264249 4.993225  
C -2.678751 0.071811 -0.861988  
C -1.843091 0.100319 -2.052282  
N -0.488779 0.100039 -1.782459  
C 0.392096 0.138958 -2.810144  
C -0.010419 0.188903 -4.148797  
C -1.386269 0.206398 -4.437810  
C -2.305777 0.163386 -3.386007  
C -4.163757 0.087616 -0.912986  
N -4.743191 -0.771054 -1.794820  
C -6.090289 -0.769109 -1.885347  
C -6.923140 0.066126 -1.126447  
C -6.319915 0.959343 -0.225699  
C -4.924650 0.972591 -0.113745  
S -0.096054 -0.004271 2.434101  
C 4.007199 3.474737 -0.535843  
C -3.911831 -0.353633 3.882837  
H 3.023752 -3.834334 -0.118724  
H 1.270547 -5.635559 -0.033626  
H -1.171271 -4.949129 0.088261  
H -1.729328 -2.508379 0.157216  
H 4.340384 0.211020 1.543769  
H 6.832156 -0.103297 1.442358  
H 7.783776 -1.729052 -0.254832  
H 6.188373 -2.972799 -1.741742  
H -3.380565 0.161440 -3.575278  
H -1.738903 0.253248 -5.472688  
H 0.744831 0.216894 -4.938826  
H 1.450175 0.134971 -2.536231  
H -4.422294 1.656539 0.574305  
H -6.927618 1.641681 0.377774  
H -8.009934 0.019876 -1.244274  
H -6.522208 -1.477187 -2.604457  
H 2.534767 5.646347 -0.429943  
H 1.843915 4.558895 -1.706227  
H 0.931387 4.871093 -0.172594  
H 4.501162 4.440202 -0.360982  
H 4.526618 2.673074 -0.002317

H 3.940496 3.253960 -1.612543  
H -2.323615 0.060319 5.836015  
H -1.383481 -1.312861 5.166533  
H -0.795240 0.370078 4.957246  
H -4.312450 0.298407 4.676639  
H -4.405111 -0.124913 2.931239  
H -4.117657 -1.406538 4.154577  
O 2.727299 3.847430 1.424415

[Fe(Dp44mT)<sub>2</sub>O]-v

Fe 0.162195 -0.025832 0.205352  
C 5.052378 -0.767281 0.379041  
C 4.222382 -0.647707 -0.760671  
N 4.732135 -0.561766 -2.019521  
C 6.074709 -0.581141 -2.160097  
C 6.971990 -0.685451 -1.087097  
C 6.441684 -0.786055 0.209829  
C 2.740741 -0.642651 -0.648685  
C 1.879763 -1.466341 -1.489634  
N 0.531295 -1.314167 -1.237092  
C -0.361548 -2.041914 -1.944900  
C 0.020258 -2.959978 -2.930994  
C 1.390256 -3.135209 -3.189337  
C 2.324137 -2.386577 -2.465188  
S 0.215758 1.611062 1.838496  
C 1.977535 1.720654 1.829898  
N 2.616899 2.584267 2.672429  
C 4.061230 2.825770 2.576648  
N -1.733397 -0.209901 0.197781  
N -2.367165 -1.240501 0.843984  
C -2.593925 0.615411 -0.432210  
C -2.214564 1.807727 -1.156278  
N -0.892513 2.137980 -1.463227  
C -0.576111 3.286248 -2.153594  
C -1.546810 4.164349 -2.596836  
C -2.901499 3.875893 -2.321902  
C -3.209145 2.720722 -1.616212  
C -4.069760 0.301786 -0.370340  
N -4.577689 -0.346266 -1.446351  
C -5.899908 -0.629674 -1.436778  
C -6.763471 -0.280205 -0.388170  
C -6.228110 0.400822 0.717095  
C -4.858554 0.697597 0.728744  
C -1.556922 -2.027076 1.574314  
S 0.164065 -1.709702 1.718205  
N -2.136449 -3.090420 2.215763  
C -1.378210 -3.874188 3.188422  
C -3.598279 -3.209895 2.259617  
N 2.055347 0.114163 0.231484  
N 2.754297 0.970086 1.018144  
C 1.874780 3.530429 3.503519  
H -4.250182 2.486585 -1.388173

H -3.698239 4.547962 -2.651191  
H -1.239876 5.060471 -3.141300  
H 0.495352 3.416117 -2.312962  
H -4.400588 1.226776 1.569988  
H -6.866726 0.697075 1.555824  
H -7.826898 -0.532421 -0.441249  
H -6.283611 -1.158997 -2.318381  
H 3.394604 -2.489547 -2.651551  
H 1.729422 -3.848754 -3.946833  
H -0.745313 -3.519947 -3.474850  
H -1.414899 -1.876579 -1.702118  
H 4.606170 -0.847564 1.373012  
H 7.101558 -0.884244 1.078210  
H 8.051418 -0.693149 -1.265907  
H 6.448686 -0.506568 -3.189576  
H -3.855903 -4.248022 2.518796  
H -4.042027 -2.533870 3.016467  
H -4.025434 -2.963397 1.278111  
H -1.895350 -4.832315 3.348688  
H -0.365440 -4.079158 2.806555  
H -1.286782 -3.353231 4.162664  
H 2.518420 3.837057 4.342584  
H 1.583804 4.433975 2.932753  
H 0.965542 3.058397 3.905288  
H 4.485871 2.884317 3.592699  
H 4.537986 2.009897 2.021820  
H 4.260746 3.782637 2.057039  
O 0.149244 1.364456 -1.165720

[Fe(Dp44mT)<sub>2</sub>O]-vi

N 4.597521 -1.270273 -1.774572  
C 3.994724 -0.871962 -0.622620  
C 4.725173 -0.681579 0.578741  
C 6.107682 -0.891991 0.575361  
C 6.735164 -1.282427 -0.619699  
C 5.933308 -1.462539 -1.756708  
C 2.521764 -0.721130 -0.640345  
N 1.819820 0.202038 0.066420  
N 2.451016 1.371462 0.463581  
C 1.713386 2.184282 1.323655  
N 2.337947 3.258824 1.884548  
C 3.732982 3.195673 2.360157  
C 1.635857 -1.705503 -1.254754  
N 0.294874 -1.506357 -0.983329  
C -0.621853 -2.358721 -1.498751  
C -0.274276 -3.453551 -2.296780  
C 1.086392 -3.679387 -2.568555  
C 2.043083 -2.805972 -2.044697  
Fe -0.069955 0.014076 0.185424  
S 0.033547 1.849248 1.574758  
N -1.958117 -0.152402 0.274423  
N -2.634840 -0.936306 1.154575

C -1.836251 -1.573783 2.036038  
N -2.440960 -2.362222 2.971125  
C -1.658791 -3.188606 3.889323  
C -2.684031 0.530843 -0.637097  
C -1.860134 1.279519 -1.572065  
N -0.503273 1.156101 -1.342105  
C 0.365463 1.820263 -2.142298  
C -0.052002 2.639782 -3.196091  
C -1.430552 2.785466 -3.431769  
C -2.337687 2.103564 -2.616275  
C -4.169117 0.528047 -0.687986  
N -4.728052 0.324262 -1.911407  
C -6.075290 0.338685 -2.000178  
C -6.928161 0.552406 -0.907475  
C -6.346434 0.774084 0.351787  
C -4.951505 0.762006 0.467072  
S -0.081107 -1.404587 2.015365  
C 1.525227 4.269628 2.568502  
C -3.875935 -2.663366 2.907531  
H 3.106649 -2.935895 -2.251364  
H 1.399804 -4.528755 -3.183662  
H -1.057845 -4.109078 -2.686081  
H -1.664762 -2.150015 -1.246996  
H 4.203496 -0.406282 1.499319  
H 6.688397 -0.753594 1.493510  
H 7.814844 -1.452787 -0.669859  
H 6.383451 -1.775532 -2.707935  
H -3.413919 2.182536 -2.779801  
H -1.794258 3.423484 -4.243188  
H 0.694737 3.149378 -3.810811  
H 1.427584 1.684743 -1.921186  
H -4.465361 0.935349 1.430037  
H -6.970572 0.960970 1.231897  
H -8.013806 0.550716 -1.043493  
H -6.490339 0.167805 -3.001987  
H 4.184217 4.196306 2.265702  
H 3.747013 2.897739 3.426051  
H 4.298902 2.479209 1.752326  
H 2.136454 5.179389 2.674985  
H 0.627240 4.505492 1.978178  
H 1.214574 3.933556 3.576955  
H -2.294848 -3.451461 4.748371  
H -1.313449 -4.122777 3.405048  
H -0.780476 -2.634187 4.253992  
H -4.291546 -2.654348 3.928600  
H -4.385950 -1.912472 2.293361  
H -4.043951 -3.665250 2.467911  
O 3.609105 1.710868 -0.018730

[Fe(Dp44mT)<sub>2</sub>O]-i-i

N -4.630476 -1.689036 -0.370629  
C -4.069316 -0.449329 -0.694894

C -4.909300 0.633253 -0.990289  
C -6.302984 0.497099 -0.989277  
C -6.844118 -0.765273 -0.687652  
C -6.005855 -1.832465 -0.390178  
C -2.593813 -0.380214 -0.699930  
N -1.889011 0.379231 0.161555  
N -2.589541 1.072458 1.096143  
C -1.801747 1.769682 1.942936  
N -2.423214 2.455162 2.946382  
C -3.885318 2.580297 2.981676  
C -1.766221 -1.104146 -1.642622  
N -0.414282 -0.886026 -1.479210  
C 0.455841 -1.508513 -2.309627  
C 0.039868 -2.365432 -3.334508  
C -1.337840 -2.588225 -3.514207  
C -2.246520 -1.954145 -2.662859  
Fe 0.002412 0.346555 -0.011714  
S 0.130505 2.104015 -1.509803  
N 0.350276 -1.156247 1.201002  
C 1.693104 -1.408981 1.387956  
C 2.123896 -2.414108 2.281837  
C 1.175455 -3.179028 2.965643  
C -0.192237 -2.936601 2.740812  
C -0.559490 -1.918139 1.854674  
C 2.564219 -0.554860 0.605339  
N 1.895947 0.339225 -0.152967  
N 2.633195 1.153300 -0.952095  
C 1.883211 2.012794 -1.674935  
N 2.542666 2.824048 -2.552769  
C 1.846719 3.895991 -3.262839  
C 4.037541 -0.617994 0.664527  
N 4.636133 -1.822674 0.278304  
C 6.011450 -1.949806 0.360591  
C 6.817044 -0.898243 0.777273  
C 6.240311 0.331855 1.141843  
C 4.847186 0.449744 1.081092  
S -0.046873 1.806545 1.782890  
C -1.677184 3.355286 3.824433  
C 4.009446 2.877494 -2.573209  
H -3.322905 -2.102797 -2.778254  
H -1.697215 -3.248787 -4.309348  
H 0.786678 -2.841078 -3.975874  
H 1.515118 -1.301180 -2.137582  
H -4.436636 1.589517 -1.231717  
H -6.948327 1.346518 -1.226994  
H -7.924350 -0.936898 -0.678986  
H -6.346296 -2.837694 -0.136954  
H 3.192965 -2.583981 2.427027  
H 1.496783 -3.960412 3.661309  
H -0.968703 -3.519062 3.244030  
H -1.610264 -1.697570 1.647656  
H 4.348517 1.379712 1.367607

H 6.858615 1.169460 1.474560  
H 7.898925 -1.055613 0.811824  
H 6.379545 -2.929484 0.051969  
H -4.210984 2.639442 4.032293  
H -4.218426 3.496118 2.456180  
H -4.344880 1.707919 2.501234  
H -2.262446 3.513122 4.743173  
H -0.706462 2.911226 4.093272  
H -1.497175 4.337951 3.346039  
H 1.718101 4.793145 -2.626077  
H 2.440336 4.174172 -4.147026  
H 0.854164 3.554143 -3.594143  
H 4.389610 3.660821 -1.889329  
H 4.421636 1.908254 -2.266668  
H 4.340418 3.113433 -3.596898  
O -3.880715 -2.691805 -0.052341  
O 3.924580 -2.809923 -0.155010

[Fe(Dp44mT)<sub>2</sub>O]-i-ii

N -4.519448 -0.523427 -1.549037  
C -3.963905 0.383094 -0.641355  
C -4.802898 1.168014 0.158509  
C -6.197584 1.075722 0.058411  
C -6.734900 0.173525 -0.875847  
C -5.894323 -0.604523 -1.663300  
C -2.486148 0.436051 -0.607967  
N -1.757815 -0.059859 0.405562  
N -2.429138 -0.639778 1.436265  
C -1.611506 -1.145185 2.383066  
N -2.194654 -1.791370 3.432430  
C -3.652456 -1.787524 3.605896  
C -1.689545 1.016188 -1.669392  
N -0.329869 0.950407 -1.447575  
C 0.511895 1.456379 -2.379197  
C 0.058458 2.052084 -3.561464  
C -1.327045 2.126486 -3.795256  
C -2.207114 1.603578 -2.843747  
Fe 0.127973 0.072397 0.238492  
S 0.249966 2.043235 1.347748  
O -0.587621 3.244262 0.739395  
N 0.429896 -1.648676 -0.660800  
C 1.764122 -1.979356 -0.792734  
C 2.147966 -3.237488 -1.307982  
C 1.166870 -4.138200 -1.729984  
C -0.187776 -3.770077 -1.635723  
C -0.511841 -2.523726 -1.091360  
C 2.670372 -0.930130 -0.346040  
N 2.017657 0.155330 0.108864  
N 2.777887 1.247951 0.447217  
C 2.052857 2.283058 0.867018  
N 2.630731 3.498389 0.992097  
C 2.022549 4.580153 1.777042

C 4.150532 -1.047438 -0.408786  
N 4.664971 -1.546452 -1.564760  
C 6.004643 -1.687592 -1.648868  
C 6.891615 -1.353553 -0.614566  
C 6.354406 -0.849294 0.580929  
C 4.967691 -0.691506 0.689155  
S 0.148740 -1.004657 2.288608  
C -1.408592 -2.236148 4.582892  
C 4.044741 3.679110 0.634693  
H -3.289332 1.648369 -2.992291  
H -1.714507 2.586730 -4.709392  
H 0.783158 2.447168 -4.278311  
H 1.579141 1.382463 -2.152977  
H -4.331421 1.863229 0.859102  
H -6.845974 1.694836 0.683460  
H -7.815266 0.061540 -1.005278  
H -6.234318 -1.330473 -2.403449  
H 3.209428 -3.478723 -1.387661  
H 1.454001 -5.113604 -2.134607  
H -0.987494 -4.434208 -1.974972  
H -1.552180 -2.194653 -1.006591  
H 4.515649 -0.304459 1.605205  
H 7.005839 -0.586535 1.420840  
H 7.969427 -1.490761 -0.743626  
H 6.384775 -2.088471 -2.597324  
H -3.957111 -2.737486 4.073321  
H -3.971059 -0.953064 4.259746  
H -4.142009 -1.682048 2.630130  
H -1.980355 -3.008443 5.119166  
H -0.452458 -2.668774 4.250949  
H -1.198235 -1.402260 5.280496  
H 2.376822 4.547133 2.824853  
H 2.322329 5.543544 1.335083  
H 0.926455 4.498361 1.742692  
H 4.702206 3.437124 1.490555  
H 4.302051 3.021400 -0.206764  
H 4.202077 4.731303 0.350895  
O -3.762160 -1.281343 -2.272125

[Fe(Dp44mT)<sub>2</sub>O]-i-ii-s

C 4.759468 -0.995560 0.847010  
C 4.017081 -0.778182 -0.322406  
N 4.680778 -0.579197 -1.536721  
C 6.062378 -0.639563 -1.565674  
C 6.805009 -0.858996 -0.412519  
C 6.158329 -1.037348 0.823570  
C 2.540355 -0.752458 -0.365170  
N 1.799976 0.142512 0.309269  
N 2.479551 1.125296 0.984977  
C 1.670696 1.997780 1.585480  
N 2.179911 3.145457 2.083078  
C 3.614321 3.432117 1.938954

C 1.741902 -1.711897 -1.104508  
N 0.384701 -1.499555 -0.995962  
C -0.460274 -2.325912 -1.660084  
C -0.009885 -3.389223 -2.447841  
C 1.374703 -3.627616 -2.542961  
C 2.257022 -2.784546 -1.864194  
Fe -0.086330 -0.038701 0.243131  
S -0.186606 -1.579060 1.967209  
C -1.934893 -1.804611 1.828395  
N -2.573132 -2.733438 2.598022  
C -1.878905 -3.434653 3.677482  
N -2.691835 -1.092250 0.970715  
N -1.975232 -0.237505 0.191467  
C -2.649978 0.508910 -0.706708  
C -1.775039 1.345719 -1.516199  
N -0.435281 1.216381 -1.206956  
C 0.475450 1.944953 -1.894723  
C 0.118339 2.845906 -2.903090  
C -1.243576 3.001443 -3.215208  
C -2.193231 2.247397 -2.520039  
C -4.126742 0.486147 -0.866298  
N -4.590767 0.412906 -2.143624  
C -5.927428 0.409008 -2.331252  
C -6.863156 0.477368 -1.288531  
C -6.380208 0.563119 0.027566  
C -4.997531 0.566554 0.245854  
O 4.021963 -0.334821 -2.620168  
C -4.038091 -2.827110 2.602200  
S -0.157162 1.604560 1.801409  
O -0.987674 2.900371 1.422902  
C 1.447409 3.980526 3.043464  
H -3.257007 2.329112 -2.749377  
H -1.562210 3.701512 -3.993746  
H 0.897238 3.409209 -3.423936  
H 1.520747 1.797655 -1.611951  
H -4.587757 0.633088 1.256049  
H -7.071529 0.631957 0.874024  
H -7.935718 0.468406 -1.504680  
H -6.263656 0.345347 -3.374331  
H 3.336725 -2.946000 -1.908846  
H 1.757310 -4.461312 -3.139589  
H -0.735988 -4.018916 -2.969157  
H -1.527006 -2.117757 -1.541527  
H 4.206290 -1.142257 1.778853  
H 6.728072 -1.213629 1.739354  
H 7.895203 -0.887919 -0.496051  
H 6.487935 -0.483311 -2.558095  
H -4.324539 -3.869265 2.814100  
H -4.476919 -2.174029 3.380906  
H -4.433402 -2.527298 1.623658  
H -2.430798 -4.358993 3.906623  
H -0.856313 -3.698870 3.368145

H -1.824369 -2.818183 4.595993  
H 1.696234 3.688777 4.081375  
H 1.745418 5.030092 2.892065  
H 0.365200 3.889845 2.871117  
H 4.195061 2.958095 2.752123  
H 3.974828 3.046419 0.975409  
H 3.759639 4.522178 1.985082

[Fe(Dp44mT)<sub>2</sub>O]-i-iii

N 4.654726 -0.657043 0.680544  
C 4.097774 0.501034 0.122118  
C 4.933635 1.446172 -0.488917  
C 6.316975 1.245981 -0.584555  
C 6.849463 0.061259 -0.048354  
C 6.016680 -0.864696 0.568387  
C 2.636768 0.663303 0.252055  
C 2.014000 1.706717 1.040686  
N 0.636354 1.663459 1.033004  
C -0.067294 2.556717 1.767570  
C 0.563582 3.556983 2.518961  
C 1.967537 3.628481 2.520305  
C 2.699585 2.689741 1.786982  
Fe -0.122861 0.229910 -0.089786  
S -0.222875 1.639337 -1.902754  
C -1.955177 1.821751 -1.824138  
N -2.655077 2.535879 -2.732737  
C -1.965223 3.206082 -3.835299  
O 3.925211 -1.521718 1.298314  
N -0.410897 -0.862046 1.523406  
C -1.697702 -0.911389 1.968179  
C -2.047724 -1.690083 3.085170  
C -1.061554 -2.419112 3.757951  
C 0.267210 -2.340194 3.303428  
C 0.556033 -1.553394 2.185425  
C -2.690516 0.080805 1.329583  
O -2.803456 1.155809 2.084187  
C -4.006309 -0.611229 0.871262  
N -5.156144 0.060419 1.102108  
C -6.310481 -0.520176 0.705525  
C -6.384504 -1.770444 0.072502  
C -5.186113 -2.463013 -0.162673  
C -3.981006 -1.874880 0.244997  
N -1.905082 0.535676 0.012996  
N -2.661628 1.204458 -0.815175  
N 1.759867 -0.154182 -0.353920  
N 2.271582 -1.120528 -1.145353  
C 1.324722 -1.900886 -1.707799  
S -0.396380 -1.663223 -1.395493  
N 1.739497 -2.891635 -2.543421  
C 3.164352 -3.216213 -2.687780  
C 0.796661 -3.862333 -3.098963  
C -4.099265 2.776449 -2.608656

H -3.090949 -1.710152 3.414386  
H -1.320277 -3.037555 4.623380  
H 1.075736 -2.882185 3.801915  
H 1.576344 -1.465465 1.794527  
H -3.027479 -2.390675 0.084615  
H -5.191134 -3.444398 -0.649314  
H -7.352716 -2.187009 -0.222355  
H -7.228678 0.048182 0.907882  
H 3.792469 2.702443 1.783730  
H 2.487345 4.399995 3.096873  
H -0.044905 4.258042 3.096829  
H -1.156101 2.398171 1.778130  
H 4.464680 2.342805 -0.905048  
H 6.957495 1.985578 -1.071381  
H 7.919819 -0.158295 -0.098277  
H 6.356026 -1.798641 1.018895  
H -4.282626 3.854999 -2.458187  
H -4.602517 2.456439 -3.536565  
H -4.496387 2.213383 -1.756524  
H -2.717761 3.570931 -4.548031  
H -1.370452 4.063415 -3.469310  
H -1.288871 2.503021 -4.350414  
H 1.251343 -4.321293 -3.989763  
H 0.559777 -4.661154 -2.370067  
H -0.139096 -3.362986 -3.394462  
H 3.354729 -3.519560 -3.729701  
H 3.771620 -2.337221 -2.441084  
H 3.445959 -4.050813 -2.018159

[Fe(Dp44mT)<sub>2</sub>O]-ii-ii

N -4.646484 -0.705046 1.898929  
C -4.097088 -0.637041 0.656830  
C -4.883656 -0.596973 -0.517031  
C -6.278504 -0.619834 -0.397762  
C -6.851750 -0.678410 0.882662  
C -5.992808 -0.722262 1.991203  
C -2.611843 -0.640207 0.598290  
C -1.783314 -1.560557 1.365686  
N -0.428594 -1.374454 1.177042  
C 0.443533 -2.160317 1.854407  
C 0.029225 -3.165532 2.732339  
C -1.349556 -3.380342 2.913210  
C -2.259952 -2.574907 2.225125  
Fe -0.000014 -0.000062 -0.151634  
S -0.034056 -1.530536 -1.827125  
O -0.927720 -2.815341 -1.595419  
N 0.428454 1.374453 1.176964  
C 1.783157 1.560617 1.365665  
C 2.259717 2.575078 2.225017  
C 1.349260 3.380571 2.912952  
C -0.029505 3.165699 2.732028  
C -0.443734 2.160370 1.854192



C 2.611749 0.640213 0.598392  
N 1.885447 -0.207961 -0.149077  
N 2.564379 -1.181761 -0.840601  
C 1.767306 -1.993966 -1.529807  
N 2.260648 -3.139079 -2.050095  
C 1.577002 -3.876597 -3.120408  
C 4.096991 0.637095 0.657006  
C 4.883630 0.596975 -0.516806  
C 6.278469 0.619843 -0.397457  
C 6.851643 0.678457 0.882998  
C 5.992636 0.722330 1.991487  
N 4.646318 0.705119 1.899135  
N -1.885481 0.207892 -0.149205  
N -2.564314 1.181698 -0.840803  
C -1.767144 1.993871 -1.529952  
S 0.034129 1.530231 -1.827298  
N -2.260355 3.139077 -2.050164  
C -3.663832 3.505798 -1.813924  
C -1.576646 3.876624 -3.120412  
C 3.664318 -3.505337 -1.814149  
H 3.336175 2.704914 2.349588  
H 1.708610 4.167023 3.583651  
H -0.778124 3.764795 3.257503  
H -1.504394 1.969702 1.670890  
H 4.403283 0.555163 -1.497029  
H 6.908587 0.597121 -1.292576  
H 7.936637 0.695428 1.022967  
H 6.401907 0.773061 3.008665  
H -3.336421 -2.704702 2.349644  
H -1.708968 -4.166703 3.583982  
H 0.777797 -3.764583 3.257931  
H 1.504208 -1.969711 1.671124  
H -4.403252 -0.555215 -1.497227  
H -6.908572 -0.597140 -1.292917  
H -7.936752 -0.695379 1.022569  
H -6.402140 -0.772961 3.008357  
H 3.755577 -4.600567 -1.880156  
H 4.324943 -3.044446 -2.571988  
H 3.974697 -3.162575 -0.817643  
H 1.816638 -4.946370 -3.015050  
H 0.488907 -3.746966 -3.033045  
H 1.925473 -3.532411 -4.112586  
H -1.925339 3.532705 -4.112607  
H -1.815995 4.946436 -3.014813  
H -0.488577 3.746680 -3.033253  
H -4.324637 3.046090 -2.572326  
H -3.974458 3.162118 -0.817819  
H -3.754550 4.601152 -1.878761  
O 0.927970 2.814933 -1.595756

[Fe(Dp44mT)<sub>2</sub>O]-ii-ii-s

C -4.859935 0.260293 -1.717710

C -4.072936 -0.485236 -0.815635  
N -4.607471 -1.374367 0.063073  
C -5.947614 -1.522257 0.061235  
C -6.812205 -0.818576 -0.794532  
C -6.252652 0.089398 -1.704261  
C -2.588099 -0.350498 -0.805106  
N -1.890904 0.078146 0.260504  
N -2.583125 0.475495 1.355318  
C -1.787584 0.831531 2.388036  
N -2.399669 1.281216 3.519516  
C -3.857413 1.211372 3.677901  
S -0.027614 0.725895 2.311423  
Fe 0.010692 0.113529 0.091280  
S 0.108749 2.203625 -0.636402  
O -0.376580 3.364074 0.244371  
N 0.334888 -1.750744 0.631315  
C 1.667458 -2.101731 0.659343  
C 2.067508 -3.400770 1.044455  
C 1.097063 -4.346158 1.384326  
C -0.260624 -3.981032 1.338555  
C -0.596533 -2.677620 0.960326  
C 2.564008 -1.013377 0.303944  
N 1.916920 0.120098 -0.013714  
N 2.704247 1.182585 -0.391478  
C 2.040035 2.297746 -0.655967  
N 2.688351 3.431330 -0.976039  
C 2.000229 4.646318 -1.426968  
C 4.046404 -1.155034 0.315477  
N 4.545463 -2.209397 -0.380744  
C 5.884267 -2.386876 -0.375772  
C 6.778807 -1.551534 0.309647  
C 6.253949 -0.471787 1.037985  
C 4.868710 -0.266435 1.042859  
N -0.401386 -0.534931 -1.717257  
C -1.752105 -0.712192 -1.935071  
C -2.220744 -1.227456 -3.163650  
C -1.305463 -1.549081 -4.170900  
C 0.067381 -1.359083 -3.936842  
C 0.473723 -0.853759 -2.695885  
C -1.637568 1.572322 4.732968  
O -0.248967 2.413717 -2.116571  
C 4.152931 3.445473 -1.113284  
H -3.293947 -1.371592 -3.311800  
H -1.658947 -1.947263 -5.126948  
H 0.818298 -1.597586 -4.694511  
H 1.530602 -0.690162 -2.468689  
H -4.384909 0.964654 -2.407474  
H -6.886838 0.659909 -2.390637  
H -7.892486 -0.985385 -0.746070  
H -6.351643 -2.247185 0.779709  
H 3.129866 -3.651117 1.056725  
H 1.393906 -5.356216 1.682650

H -1.053865 -4.687874 1.596126  
H -1.639058 -2.350662 0.919425  
H 4.423071 0.559814 1.602401  
H 6.913175 0.198808 1.598733  
H 7.854606 -1.748092 0.276519  
H 6.255614 -3.244037 -0.951821  
H -4.144965 0.315403 4.260522  
H -4.201038 2.108112 4.218747  
H -4.335249 1.167140 2.692203  
H -2.236650 2.240932 5.369653  
H -1.410685 0.650398 5.302880  
H -0.690896 2.074103 4.479931  
H 2.498377 5.517777 -0.971043  
H 2.064383 4.739206 -2.526446  
H 0.949417 4.627623 -1.112491  
H 4.529033 4.422965 -0.772318  
H 4.591657 2.643086 -0.507084  
H 4.440201 3.301048 -2.171214

[Fe(Dp44mT)<sub>2</sub>O]-i-iii-s

N 4.873280 0.648879 -0.867050  
C 4.351981 -0.409629 -0.192532  
C 5.150086 -1.325491 0.523384  
C 6.539939 -1.133763 0.553608  
C 7.084959 -0.039407 -0.132102  
C 6.210709 0.815307 -0.824996  
C 2.871680 -0.581695 -0.267599  
C 2.240387 -1.718297 -0.908506  
N 0.861954 -1.690406 -0.875433  
C 0.155899 -2.677497 -1.475900  
C 0.784238 -3.755364 -2.113154  
C 2.188638 -3.809031 -2.140530  
C 2.922402 -2.778666 -1.544888  
Fe 0.107729 -0.140950 0.074626  
S 0.114113 -1.294812 2.068416  
C -1.615754 -1.510274 2.087447  
N -2.277048 -2.112708 3.099036  
C -1.557806 -2.595082 4.277415  
N -0.281540 0.721172 -1.654653  
C -1.587849 0.702694 -2.041287  
C -1.991462 1.297120 -3.252092  
C -1.044164 1.917552 -4.070758  
C 0.305418 1.913159 -3.670185  
C 0.645620 1.303917 -2.461512  
C -2.528232 -0.222077 -1.233650  
O -2.627403 -1.353391 -1.897071  
C -3.827168 0.504941 -0.787309  
N -4.983889 -0.228267 -0.494258  
C -6.155577 0.462075 -0.204955  
C -6.210267 1.845545 -0.123377  
C -5.048336 2.600703 -0.352876  
C -3.880522 1.903922 -0.688616

N -1.665032 -0.497338 0.087691  
N -2.372479 -1.041762 1.036077  
N 1.997316 0.308654 0.227108  
N 2.498900 1.378336 0.888918  
C 1.546705 2.205813 1.364163  
S -0.176913 1.901501 1.127797  
N 1.955118 3.307331 2.053302  
C 3.370655 3.693125 2.105621  
C 1.000066 4.309786 2.524299  
C -3.712909 -2.422513 3.023798  
H -3.047925 1.263108 -3.533862  
H -1.347050 2.396365 -5.007379  
H 1.086837 2.375340 -4.279574  
H 1.679197 1.278179 -2.106165  
H -2.959443 2.457340 -0.895268  
H -5.052630 3.691589 -0.282526  
H -7.165890 2.316754 0.125343  
H -7.002404 -0.201319 -0.021221  
H 4.015088 -2.779162 -1.565982  
H 2.706895 -4.638935 -2.630860  
H 0.173069 -4.530413 -2.583708  
H -0.935144 -2.541235 -1.473213  
H 4.685141 -2.165093 1.049143  
H 7.182304 -1.827015 1.106328  
H 8.162250 0.151803 -0.136982  
H 6.604838 1.676511 -1.379833  
H -3.853257 -3.508684 3.161983  
H -4.247861 -1.891761 3.830308  
H -4.109184 -2.119585 2.045899  
H -2.286823 -2.786624 5.077718  
H -1.013782 -3.532080 4.054703  
H -0.832575 -1.838802 4.620445  
H 1.476780 4.896275 3.324297  
H 0.698527 4.998598 1.711712  
H 0.099172 3.823125 2.929274  
H 3.606776 4.054745 3.119819  
H 3.998660 2.827649 1.864252  
H 3.578178 4.505232 1.383322  
O -5.022346 -1.513194 -0.469214

[Fe(Dp44mT)<sub>2</sub>O]-ii-iii

N 4.978381 -1.318886 -0.534239  
C 4.280881 -0.351227 0.114959  
C 4.899394 0.781250 0.687205  
C 6.288553 0.919521 0.572933  
C 7.016064 -0.068961 -0.108620  
C 6.315638 -1.163333 -0.638224  
C 2.811960 -0.575010 0.222426  
C 2.237147 -1.809299 0.737711  
N 0.861730 -1.798825 0.786752  
C 0.197082 -2.895286 1.224354  
C 0.872988 -4.035964 1.674686

C 2.278536 -4.047854 1.667404  
C 2.967366 -2.930511 1.186349  
Fe 0.017993 -0.122615 0.169237  
S 0.050417 0.766222 2.275315  
C -1.677941 0.651045 2.484944  
N -2.312490 1.135852 3.574064  
C -1.556188 1.795845 4.638451  
N -0.377996 -1.008241 -1.553755  
C -1.668394 -1.419674 -1.710501  
C -2.082800 -2.065121 -2.888855  
C -1.163167 -2.290865 -3.918109  
C 0.168711 -1.874699 -3.739851  
C 0.522069 -1.240919 -2.547125  
C -2.586653 -1.331570 -0.473215  
O -2.654863 -2.501938 0.130465  
C -3.931604 -0.617558 -0.791211  
N -5.030602 -1.100146 -0.170379  
C -6.210141 -0.490327 -0.420469  
C -6.360469 0.606671 -1.283039  
C -5.215711 1.099759 -1.928307  
C -3.984753 0.476925 -1.679181  
N -1.749700 -0.372786 0.492975  
N -2.446167 0.048430 1.512840  
N 1.886117 0.324707 -0.133597  
N 2.339940 1.506037 -0.659851  
C 1.373981 2.382616 -0.914470  
S -0.429927 1.851387 -0.891490  
O -1.261724 2.936364 -0.108456  
N 1.688314 3.649273 -1.261010  
C 3.099400 4.056464 -1.330512  
C 0.729188 4.556785 -1.905377  
C -3.748739 0.933295 3.808952  
H -3.125412 -2.383550 -2.981050  
H -1.474945 -2.782842 -4.844842  
H 0.927850 -2.033451 -4.510561  
H 1.543589 -0.896941 -2.365038  
H -3.074750 0.828718 -2.177368  
H -5.280982 1.949445 -2.616579  
H -7.345794 1.054732 -1.445183  
H -7.085318 -0.905206 0.098120  
H 4.057623 -2.915087 1.134350  
H 2.832288 -4.922216 2.023093  
H 0.296788 -4.897033 2.024853  
H -0.900483 -2.838836 1.147631  
H 4.299123 1.527392 1.213829  
H 6.795004 1.784615 1.012987  
H 8.101801 0.000463 -0.224449  
H 6.850126 -1.958493 -1.173233  
H -3.891086 0.317624 4.714541  
H -4.233830 1.911715 3.964705  
H -4.197722 0.428780 2.945973  
H -2.264770 2.303262 5.308037

H -0.970679 1.062646 5.223708  
H -0.863012 2.540057 4.211366  
H 0.971576 5.588893 -1.607491  
H 0.804049 4.478869 -3.006364  
H -0.293542 4.325506 -1.577450  
H 3.156909 5.144750 -1.176453  
H 3.674792 3.537535 -0.552506  
H 3.530789 3.809595 -2.318514

[Fe(Dp44mT)<sub>2</sub>O]-*ii-iii-s*

C -3.989256 -0.009581 -1.677934  
C -3.962410 -0.863334 -0.555422  
N -5.082448 -1.245202 0.094206  
C -6.263240 -0.772838 -0.364842  
C -6.390003 0.086224 -1.466886  
C -5.220114 0.476196 -2.138753  
C -2.615185 -1.422840 -0.009453  
N -1.776422 -0.202969 0.562007  
N -2.500848 0.569780 1.349022  
C -1.779701 1.528992 1.993078  
N -2.424725 2.505188 2.646967  
C -3.895131 2.540779 2.709819  
S 0.045805 1.295084 1.992153  
Fe -0.016724 -0.074857 0.187039  
S -0.424350 1.630424 -1.305389  
O 0.818092 2.665583 1.983460  
N 0.838672 -1.481306 1.278825  
C 2.215726 -1.492155 1.222682  
C 2.951707 -2.402429 2.011954  
C 2.273585 -3.304424 2.838015  
C 0.868873 -3.299130 2.856098  
C 0.183804 -2.371160 2.061244  
C 2.783959 -0.489862 0.332524  
N 1.853064 0.256418 -0.287119  
N 2.273822 1.194945 -1.164442  
C 1.272424 1.918173 -1.703410  
N 1.601349 2.899213 -2.586448  
C 0.573692 3.669184 -3.287423  
C 4.249208 -0.313619 0.144261  
N 4.959292 -1.445742 -0.103896  
C 6.295162 -1.328179 -0.260975  
C 6.986169 -0.110181 -0.178038  
C 6.248188 1.053867 0.091172  
C 4.860837 0.955691 0.253146  
N -0.432881 -1.463489 -1.174148  
C -1.712009 -1.925501 -1.154672  
C -2.138771 -2.922513 -2.047877  
C -1.236697 -3.447143 -2.979819  
C 0.083292 -2.962991 -2.991734  
C 0.447428 -1.975103 -2.073572  
C -1.735459 3.477348 3.504864  
O -2.684950 -2.296007 0.979145

C 2.975040 3.065252 -3.077132  
H -3.173917 -3.273552 -2.000150  
H -1.554753 -4.218619 -3.688069  
H 0.826699 -3.341756 -3.698433  
H 1.461713 -1.569078 -2.045060  
H -3.056193 0.267299 -2.181940  
H -5.266975 1.142115 -3.007252  
H -7.376529 0.433889 -1.789020  
H -7.157686 -1.102169 0.181322  
H 4.041493 -2.397402 1.953247  
H 2.837768 -4.010423 3.455456  
H 0.300789 -4.001420 3.472348  
H -0.914837 -2.344292 1.980313  
H 4.253971 1.838999 0.465947  
H 6.746249 2.024961 0.178876  
H 8.071143 -0.079122 -0.315736  
H 6.837051 -2.260655 -0.464806  
H -4.235287 2.130803 3.677602  
H -4.220123 3.589923 2.631348  
H -4.320241 1.947007 1.891925  
H -2.181721 4.470959 3.339666  
H -1.880585 3.195745 4.563993  
H -0.663995 3.506196 3.263007  
H 1.034761 4.589410 -3.676209  
H 0.146844 3.100362 -4.135542  
H -0.240234 3.945049 -2.598747  
H 3.230429 4.137855 -3.079034  
H 3.669043 2.520123 -2.427460  
H 3.062701 2.679157 -4.109987

[Fe(Dp44mT)<sub>2</sub>O]-*iii-iii*

C -1.770859 -2.135624 2.879903  
C -1.496029 -1.197729 1.869040  
N -0.233747 -1.043356 1.383732  
C 0.784685 -1.777229 1.907972  
C 0.570809 -2.722820 2.912924  
C -0.734221 -2.916483 3.400335  
C -2.546732 -0.157600 1.429928  
C -3.869066 -0.811373 0.941456  
C -3.856710 -2.000049 0.183351  
C -5.071702 -2.549932 -0.249266  
C -6.264821 -1.894753 0.092569  
C -6.177139 -0.718787 0.853932  
N -5.014056 -0.176817 1.276662  
Fe -0.025855 0.262358 -0.091027  
S -0.262443 1.983947 -1.592155  
C -2.003153 2.041911 -1.464986  
N -2.650845 1.251254 -0.533617  
N -1.837736 0.527445 0.172496  
N -2.767876 2.829251 -2.249458  
C -2.147242 3.677525 -3.267918  
C -4.214791 2.990288 -2.046483

N 1.711094 -0.067250 -0.590812  
C 2.807221 1.078721 -0.217296  
C 2.165136 1.697605 1.036338  
N 0.828543 1.508377 1.191784  
C 0.162552 2.137158 2.196910  
C 0.821672 2.997304 3.080084  
C 2.202072 3.213305 2.925916  
C 2.877081 2.553022 1.893442  
N 2.162134 -0.908864 -1.466064  
C 1.174373 -1.682575 -2.044333  
N 1.550611 -2.639661 -2.912745  
C 2.953377 -2.868910 -3.288139  
S -0.492870 -1.384889 -1.637811  
O 2.838401 1.921102 -1.222248  
C 4.121964 0.337170 0.109432  
N 4.098943 -0.558614 1.124109  
C 5.250076 -1.202939 1.413483  
C 6.454914 -0.984087 0.724856  
C 6.465537 -0.049268 -0.322366  
C 5.275306 0.623555 -0.636163  
C 0.542436 -3.489282 -3.550934  
H 3.951803 2.688394 1.739389  
H 2.742734 3.880449 3.604988  
H 0.253142 3.484020 3.877656  
H -0.906406 1.885616 2.290095  
H 5.204196 1.364322 -1.437979  
H 7.385382 0.151049 -0.882552  
H 7.357861 -1.533976 1.007591  
H 5.206747 -1.926899 2.237495  
H -2.796486 -2.236675 3.246842  
H -0.934788 -3.659712 4.178402  
H 1.418397 -3.293374 3.302370  
H 1.785683 -1.575207 1.510872  
H -2.907879 -2.490777 -0.059670  
H -5.086880 -3.473838 -0.837398  
H -7.239625 -2.283754 -0.217597  
H -7.090783 -0.181315 1.142277  
H 3.242994 -3.895165 -3.005083  
H 3.058175 -2.756027 -4.380437  
H 3.598279 -2.146387 -2.775796  
H 1.057357 -4.259553 -4.140575  
H -0.089340 -3.977875 -2.788813  
H -0.104926 -2.893364 -4.219219  
H -2.934006 4.055188 -3.935776  
H -1.625544 4.535281 -2.804546  
H -1.417547 3.096135 -3.856225  
H -4.737154 2.788654 -2.996503  
H -4.561766 2.294787 -1.274055  
H -4.429279 4.027730 -1.734919  
O -2.642531 0.797014 2.334597

[Fe(Dp44mT)<sub>2</sub>O]-*α*

C 4.932837 -0.434555 1.083365  
C 4.102674 -1.246782 0.279544  
N 4.588125 -2.264228 -0.478553  
C 5.921176 -2.479672 -0.459568  
C 6.822986 -1.719528 0.299913  
C 6.311816 -0.678348 1.091372  
C 2.625232 -1.062077 0.248728  
C 1.690949 -2.147495 0.502919  
N 0.369532 -1.757710 0.470634  
C -0.598898 -2.679343 0.694980  
C -0.303397 -4.017778 0.976246  
C 1.041863 -4.423856 1.032628  
C 2.046582 -3.482807 0.794994  
Fe 0.108059 0.151338 0.077167  
S 0.280674 2.288292 -0.485483  
O -0.175091 3.390511 0.481544  
N -0.295706 -0.346040 -1.782777  
C 0.584459 -0.605464 -2.774551  
C 0.183001 -1.007441 -4.054032  
C -1.190588 -1.154526 -4.314794  
C -2.111364 -0.894003 -3.295217  
C -1.646472 -0.481469 -2.027312  
C -2.483641 -0.186935 -0.879821  
C -3.957033 -0.248895 -0.907705  
C -4.748017 0.576079 -1.721021  
C -6.145683 0.485409 -1.719283  
C -6.743166 -0.460971 -0.869456  
C -5.954067 -1.284190 -0.075600  
N -4.574022 -1.210191 -0.095605  
N 2.016950 0.109266 0.000705  
N 2.840284 1.171716 -0.289698  
C 2.213834 2.322613 -0.482471  
N 2.899261 3.455042 -0.718717  
C 2.252812 4.723134 -1.074648  
N -1.789463 0.161429 0.218870  
N -2.496055 0.498048 1.318112  
C -1.713248 0.751202 2.393056  
N -2.336566 1.135873 3.540529  
C -3.799773 1.113195 3.659424  
S 0.041739 0.591010 2.339466  
C 4.364260 3.435080 -0.849184  
C -1.592391 1.307579 4.787733  
O -0.057928 2.624583 -1.946844  
H -3.185423 -1.007264 -3.463459  
H -1.540172 -1.472869 -5.301742  
H 0.937677 -1.201150 -4.820671  
H 1.641435 -0.479067 -2.524958  
H -4.233231 1.309913 -2.348383  
H -6.750112 1.140995 -2.351092  
H -7.829528 -0.575301 -0.814112  
H -6.341791 -2.049719 0.598309  
H 3.101295 -3.763160 0.814768

H 1.303488 -5.462180 1.258306  
H -1.121074 -4.722279 1.151762  
H -1.635354 -2.323360 0.644774  
H 4.497831 0.363320 1.690450  
H 6.976590 -0.067175 1.710434  
H 7.893613 -1.943490 0.274082  
H 6.281638 -3.305049 -1.086706  
H -4.138402 0.180242 4.148825  
H -4.119664 1.969986 4.274127  
H -4.253514 1.181999 2.663799  
H -2.187593 1.937729 5.465725  
H -1.400139 0.336438 5.283551  
H -0.628378 1.802650 4.593279  
H 2.780985 5.539682 -0.555102  
H 2.320089 4.897376 -2.163979  
H 1.202014 4.716635 -0.759421  
H 4.771220 4.356440 -0.402969  
H 4.772047 2.557087 -0.333151  
H 4.651989 3.397568 -1.916090  
O -3.883545 -2.027720 0.624503

[Fe(Dp44mT)<sub>2</sub>O]-*α-s*

N -4.696963 -1.386552 0.262397  
C -4.106171 -0.777928 -0.799822  
C -4.832433 -0.336458 -1.925289  
C -6.223203 -0.521215 -1.950125  
C -6.841147 -1.140155 -0.854575  
C -6.034319 -1.553112 0.219399  
C -2.625406 -0.617248 -0.734221  
N -2.003523 0.118646 0.201413  
N -2.769483 0.799745 1.087911  
C -2.046066 1.473997 2.008477  
S -0.282355 1.409938 2.063782  
Fe -0.094241 0.164596 0.137119  
N 1.804359 0.196736 0.112923  
N 2.603395 1.186615 -0.395695  
C 1.939851 2.175850 -0.978842  
N 2.584668 3.258263 -1.443497  
C 4.051276 3.342353 -1.356190  
N 0.232444 -1.456361 1.213767  
C 1.565755 -1.794187 1.310107  
C 1.974582 -2.975681 1.967048  
C 1.011247 -3.802737 2.549525  
C -0.345746 -3.440925 2.461125  
C -0.690771 -2.267904 1.781819  
C 2.450699 -0.832032 0.683937  
C 3.922047 -0.947340 0.701319  
C 4.681249 -0.944836 1.880378  
C 6.076239 -1.066303 1.852159  
C 6.701061 -1.192571 0.599885  
C 5.941038 -1.207902 -0.563226  
N 4.563191 -1.105354 -0.534269

S 0.027763 1.946726 -1.172187  
O -0.119708 1.694413 -2.681272  
N -0.381797 -1.008286 -1.414292  
C 0.563076 -1.585496 -2.190131  
C 0.239084 -2.444675 -3.248624  
C -1.113596 -2.722793 -3.507709  
C -2.097054 -2.138761 -2.702572  
C -1.713998 -1.274096 -1.654021  
O -0.625599 3.266394 -0.738950  
C 1.932152 4.285683 -2.263449  
N -2.735969 2.217896 2.918744  
C -2.060175 2.886717 4.029258  
C -4.198795 2.142218 3.013817  
H -3.156977 -2.345498 -2.870710  
H -1.399988 -3.392146 -4.324837  
H 1.039976 -2.883374 -3.849843  
H 1.605928 -1.350079 -1.945481  
H -4.312916 0.148503 -2.757404  
H -6.811079 -0.182947 -2.809650  
H -7.922385 -1.305644 -0.827718  
H -6.484674 -2.048664 1.089208  
H 3.037097 -3.228033 2.010415  
H 1.311759 -4.719744 3.065331  
H -1.132238 -4.056050 2.906335  
H -1.734152 -1.957025 1.680604  
H 4.145761 -0.827376 2.827106  
H 6.658160 -1.053205 2.776968  
H 7.787136 -1.284947 0.509351  
H 6.350819 -1.314075 -1.568770  
H -4.502441 1.453779 3.825513  
H -4.594325 3.146173 3.238078  
H -4.613597 1.783661 2.064549  
H -2.694452 3.716900 4.376710  
H -1.887995 2.194777 4.876607  
H -1.091227 3.291479 3.699760  
H 2.305046 5.273979 -1.948534  
H 2.180711 4.137994 -3.330263  
H 0.844603 4.249394 -2.121309  
H 4.337048 4.404311 -1.309973  
H 4.401140 2.821008 -0.455180  
H 4.519188 2.881707 -2.245426  
O 3.896895 -1.163957 -1.636605

[Fe(Dp44mT)<sub>2</sub>O]-b

C 0.451727 1.257369 -2.608220  
N -0.420313 0.835181 -1.664834  
C -1.771890 0.905028 -1.925109  
C -2.251741 1.408838 -3.152893  
C -1.339622 1.845086 -4.118306  
C 0.037192 1.767212 -3.843665  
Fe 0.000523 0.073973 0.111958  
N 1.903127 0.159029 0.022437

N 2.682006 1.218295 0.425551  
C 2.009935 2.242912 0.928326  
N 2.639242 3.367545 1.304598  
C 4.090981 3.516757 1.122742  
C -2.603607 0.391293 -0.850198  
N -1.900203 -0.058374 0.194288  
N -2.607637 -0.555307 1.257341  
C -1.832481 -1.095851 2.194683  
S 0.038550 -0.835012 2.188783  
C -4.092109 0.312037 -0.937105  
C -4.873603 1.482660 -1.000382  
C -6.268181 1.358268 -1.099006  
C -6.829984 0.074735 -1.136036  
C -5.967831 -1.033527 -1.076498  
N -4.626272 -0.936222 -0.980027  
N -2.390694 -1.816208 3.189746  
C -1.654685 -2.177822 4.408118  
C -3.847190 -2.013727 3.225003  
S 0.082899 2.095579 0.991231  
O -0.396449 3.256633 0.109879  
N 0.318493 -1.676276 -0.713524  
C 1.650908 -1.963394 -0.916632  
C 2.048000 -3.198670 -1.474436  
C 1.075942 -4.134494 -1.835370  
C -0.281375 -3.824598 -1.636024  
C -0.614674 -2.588828 -1.074034  
C 2.550447 -0.904056 -0.482523  
C 4.031197 -1.006302 -0.591231  
N 4.509658 -1.401439 -1.800393  
C 5.846763 -1.528083 -1.935968  
C 6.762103 -1.281516 -0.901671  
C 6.259919 -0.884769 0.347990  
C 4.876295 -0.741985 0.509650  
O -0.312368 2.277448 2.466937  
C 1.969158 4.478228 1.990085  
H -3.328448 1.449329 -3.335656  
H -1.696774 2.237392 -5.075199  
H 0.785761 2.091262 -4.571477  
H 1.512144 1.181269 -2.352746  
H -4.394677 2.465862 -0.964723  
H -6.901326 2.250277 -1.143079  
H -7.911455 -0.072297 -1.212725  
H -6.373862 -2.052478 -1.112133  
H 3.109898 -3.398375 -1.627973  
H 1.371684 -5.095285 -2.267605  
H -1.076060 -4.525272 -1.905613  
H -1.657052 -2.312153 -0.894997  
H 4.449160 -0.436762 1.467784  
H 6.935660 -0.692458 1.187677  
H 7.835911 -1.402904 -1.072983  
H 6.199845 -1.843456 -2.926125  
H -4.062046 -2.952643 3.757983

H -4.343405 -1.178739 3.753702  
H -4.236788 -2.065565 2.199311  
H -1.775500 -1.398599 5.183753  
H -2.063423 -3.124869 4.793139  
H -0.589550 -2.321135 4.177405  
H 2.545756 4.731333 2.896749  
H 1.937929 5.365601 1.334104  
H 0.952818 4.190377 2.285891  
H 4.627611 3.225708 2.043803  
H 4.430209 2.885223 0.290924  
H 4.308039 4.574112 0.902657  
O 0.722535 -2.258768 2.293559

[Fe(Dp44mT)<sub>2</sub>O]-c

C -3.983556 1.084741 -1.136125  
C -3.959983 -0.300709 -0.872458  
N -5.078023 -1.017101 -0.626001  
C -6.256731 -0.354947 -0.630471  
C -6.382576 1.020908 -0.875096  
C -5.214235 1.755704 -1.134058  
C -2.617385 -1.084919 -0.865186  
N -1.750233 -0.566167 0.376849  
N -2.408977 -0.596129 1.497016  
C -1.605733 -0.435188 2.610182  
N -2.208141 -0.431672 3.816135  
C -3.639211 -0.719480 3.990636  
S 0.115108 -0.239292 2.416488  
Fe 0.019488 -0.203435 0.123609  
S -0.361016 2.003058 0.007022  
O -1.020682 2.691664 1.205003  
N 0.841748 -2.000277 0.056784  
C 2.216959 -2.007617 0.020484  
C 2.935015 -3.222063 0.039040  
C 2.233454 -4.430697 0.069470  
C 0.828564 -4.406740 0.066930  
C 0.165044 -3.173575 0.062386  
C 2.810596 -0.679247 -0.004670  
N 1.903896 0.304867 -0.015441  
N 2.395541 1.583542 -0.069351  
C 1.485456 2.539971 -0.007368  
N 1.830782 3.837932 0.004079  
C 0.857770 4.933470 -0.088419  
C 4.284425 -0.455541 -0.007357  
N 4.977171 -1.116939 -0.969187  
C 6.317668 -0.956472 -0.995440  
C 7.024069 -0.158161 -0.082972  
C 6.300113 0.509906 0.917169  
C 4.907536 0.363857 0.957980  
N -0.420784 -0.397189 -1.788207  
C -1.718721 -0.705635 -2.060335  
C -2.163748 -0.854471 -3.385402  
C -1.262206 -0.691257 -4.441758

C 0.080608 -0.393650 -4.147108  
C 0.461823 -0.255316 -2.811561  
C -1.419478 -0.254062 5.036561  
O -2.681837 -2.394787 -0.734512  
C 3.243250 4.227545 -0.136603  
H -3.213703 -1.101325 -3.568817  
H -1.596100 -0.794937 -5.478981  
H 0.826447 -0.264858 -4.936128  
H 1.490676 -0.012063 -2.534676  
H -3.048290 1.623213 -1.335983  
H -5.262237 2.831721 -1.334677  
H -7.367618 1.498007 -0.865560  
H -7.149917 -0.961609 -0.427717  
H 4.025946 -3.200364 0.013837  
H 2.777303 -5.380076 0.086315  
H 0.241829 -5.329529 0.068960  
H -0.931948 -3.083423 0.008862  
H 4.308806 0.865432 1.722589  
H 6.811460 1.133778 1.657274  
H 8.112206 -0.069316 -0.154239  
H 6.849441 -1.497201 -1.788405  
H -3.756967 -1.647921 4.576218  
H -4.110124 0.111567 4.541691  
H -4.117076 -0.836493 3.011719  
H -2.105912 -0.044413 5.868671  
H -0.839487 -1.166529 5.268032  
H -0.719764 0.590112 4.919584  
H 1.186638 5.744976 0.580577  
H 0.814486 5.321296 -1.122102  
H -0.136524 4.593060 0.224893  
H 3.403337 5.166378 0.415377  
H 3.889605 3.439046 0.269251  
H 3.491342 4.389222 -1.201623  
O -0.872429 2.524011 -1.343538

[Fe(Dp44mT)<sub>2</sub>O]-c-s

C -0.453377 -2.550010 1.398427  
N 0.432648 -1.775822 0.720849  
C 1.713329 -2.203780 0.566892  
C 2.138001 -3.434950 1.093994  
C 1.229120 -4.233508 1.796556  
C -0.092874 -3.781121 1.951472  
Fe 0.019020 -0.029951 -0.149159  
N -1.853702 0.117259 0.417917  
N -2.272641 0.719625 1.552518  
C -1.268937 1.218160 2.300857  
N -1.594238 1.853954 3.457408  
C -2.967178 1.844352 3.978783  
C 2.624117 -1.355954 -0.341939  
O 2.707398 -1.858730 -1.563024  
C 3.962085 -1.004622 0.370355

C 3.969798 -0.524715 1.696315  
C 5.194715 -0.223087 2.306237  
C 6.376405 -0.422053 1.574206  
C 6.267761 -0.912870 0.264285  
N 5.093076 -1.201083 -0.339874  
N 1.782956 -0.026912 -0.529154  
N 2.530910 0.946997 -1.030962  
C 1.848867 2.036289 -1.434719  
S -0.079141 1.862218 -1.320918  
N 2.479288 3.099845 -1.918864  
C 1.769892 4.307496 -2.363535  
C 3.943531 3.134232 -2.087712  
S 0.429754 1.062222 1.836441  
N -0.829324 -1.042279 -1.613376  
C -2.204669 -1.070431 -1.566264  
C -2.937981 -1.704220 -2.591487  
C -2.255605 -2.329015 -3.640676  
C -0.851516 -2.326716 -3.645986  
C -0.170531 -1.668973 -2.613545  
C -2.778223 -0.390920 -0.411550  
C -4.244658 -0.277818 -0.183111  
N -4.956920 -1.429579 -0.291831  
C -6.293169 -1.360261 -0.110652  
C -6.980358 -0.171285 0.175972  
C -6.238807 1.016990 0.275046  
C -4.850838 0.967239 0.096213  
C -0.565012 2.345993 4.373885  
H 3.175139 -3.750007 0.946459  
H 1.544087 -5.191933 2.220990  
H -0.840235 -4.368000 2.492192  
H -1.468149 -2.156387 1.495494  
H 3.027761 -0.392047 2.240955  
H 5.227979 0.154107 3.333997  
H 7.358619 -0.207062 2.006458  
H 7.171759 -1.086114 -0.335119  
H -4.028069 -1.713124 -2.539633  
H -2.816798 -2.820974 -4.441221  
H -0.280205 -2.821906 -4.435869  
H 0.927403 -1.660153 -2.529017  
H -4.240372 1.871046 0.163812  
H -6.734358 1.970539 0.484656  
H -8.065903 -0.179194 0.312290  
H -6.838332 -2.308489 -0.200505  
H 4.167216 3.367259 -3.141990  
H 4.355853 3.932594 -1.448376  
H 4.374087 2.164986 -1.812234  
H 2.288087 5.186149 -1.946502  
H 1.805054 4.364296 -3.464890  
H 0.730751 4.290806 -2.011198  
H -1.017818 3.105461 5.028966  
H -0.158781 1.531077 5.002976  
H 0.261246 2.810126 3.813274

H -3.217399 2.851068 4.351613  
H -3.664029 1.559619 3.182373  
H -3.054178 1.125172 4.814677  
O -0.629508 3.136204 -0.676772  
O -0.463195 1.719788 -2.797354

[Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>]-a

N -4.575433 -1.232549 0.477989  
C -3.968085 -0.785501 -0.702590  
C -4.762876 -0.478986 -1.816900  
C -6.158864 -0.578212 -1.768889  
C -6.748530 -0.996156 -0.563690  
C -5.953914 -1.312183 0.531411  
C -2.495690 -0.691331 -0.708530  
C -1.642674 -1.464677 -1.593829  
N -0.302537 -1.164022 -1.474998  
C 0.589580 -1.817256 -2.253485  
C 0.205794 -2.784666 -3.188693  
C -1.157663 -3.108157 -3.309349  
C -2.088960 -2.449341 -2.501869  
Fe 0.080922 0.103118 0.000312  
S 0.013263 1.326755 1.893845  
O 0.901299 2.628743 1.978493  
O -3.878255 -1.576995 1.507262  
N 1.991057 0.050183 -0.045947  
N 2.807009 1.001857 -0.602122  
C 2.163192 2.002604 -1.187160  
N 2.831682 3.057304 -1.682365  
C 4.301164 3.097195 -1.620462  
C 2.600410 -0.968243 0.577699  
C 1.679787 -1.869102 1.245049  
N 0.356484 -1.491986 1.142450  
C -0.595316 -2.249222 1.739692  
C -0.282681 -3.405422 2.464571  
C 1.061239 -3.808568 2.563496  
C 2.049716 -3.038852 1.944700  
C 4.079197 -1.164793 0.577470  
N 4.653922 -1.390054 -0.632857  
C 5.987321 -1.586953 -0.659587  
C 6.803351 -1.573690 0.484605  
C 6.200176 -1.348252 1.729634  
C 4.812920 -1.142570 1.780817  
S 0.251576 1.809071 -1.377673  
O 0.120887 1.483561 -2.874925  
O -0.413760 3.141492 -1.011391  
N -1.816501 0.151106 0.083364  
N -2.550221 0.987679 0.869054  
C -1.792430 1.776314 1.638212  
N -2.355844 2.809073 2.293950  
C -1.700601 3.485327 3.420526  
C -3.784842 3.105470 2.115303  
C 2.194069 4.091524 -2.505035



H 3.102327 -3.328284 1.993878  
H 1.333619 -4.714196 3.114002  
H -1.086628 -3.976359 2.936953  
H -1.633767 -1.915180 1.619318  
H 4.304039 -0.957909 2.731790  
H 6.796473 -1.329416 2.647545  
H 7.881078 -1.739727 0.394886  
H 6.426015 -1.769194 -1.649022  
H -3.154012 -2.688070 -2.558640  
H -1.489566 -3.869160 -4.022085  
H 0.966731 -3.271043 -3.804737  
H 1.639598 -1.543590 -2.117211  
H -4.253244 -0.141140 -2.724119  
H -6.767959 -0.326631 -2.640592  
H -7.833456 -1.086712 -0.458872  
H -6.335345 -1.655430 1.494198  
H 4.740757 2.602891 -2.506193  
H 4.621000 4.150215 -1.601922  
H 4.649371 2.584509 -0.713727  
H 2.607266 5.072085 -2.217432  
H 2.409099 3.918239 -3.575362  
H 1.109599 4.095020 -2.334748  
H -1.977705 4.551218 3.399793  
H -2.043083 3.050004 4.378264  
H -0.608423 3.395740 3.331490  
H -3.939803 4.183216 2.279067  
H -4.097486 2.831701 1.098806  
H -4.395331 2.540575 2.843981

[Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>]-*α-s*

C 4.707746 -0.784575 1.885650  
C 3.923193 -0.922545 0.731107  
N 4.539131 -1.220178 -0.492056  
C 5.916562 -1.322893 -0.538628  
C 6.700885 -1.174756 0.598631  
C 6.101953 -0.907951 1.841613  
C 2.452666 -0.808602 0.730830  
C 1.581902 -1.667581 1.509806  
N 0.246127 -1.335312 1.411458  
C -0.661510 -2.043790 2.124322  
C -0.299883 -3.109113 2.955290  
C 1.056718 -3.473361 3.041276  
C 2.003930 -2.751756 2.310797  
Fe -0.105868 0.100767 0.091132  
N -2.012708 0.065556 0.167383  
N -2.780152 0.952624 0.871610  
C -2.057201 1.860331 1.531869  
N -2.668322 2.933914 2.072529  
C -4.113735 3.126792 1.886015  
N -0.418958 -1.343372 -1.226136  
C -1.746869 -1.693935 -1.341240  
C -2.143237 -2.778657 -2.153091

C -1.173430 -3.492009 -2.863826  
C 0.177239 -3.122453 -2.739104  
C 0.514644 -2.051067 -1.902807  
C -2.646826 -0.865008 -0.556376  
C -4.127175 -1.044777 -0.549812  
N -4.687354 -1.387102 0.639767  
C -6.023259 -1.566004 0.668206  
C -6.856382 -1.420213 -0.454246  
C -6.268517 -1.074844 -1.678987  
C -4.879094 -0.885630 -1.731723  
O 3.850393 -1.406383 -1.565985  
S -0.226376 1.545186 1.815086  
O 0.592495 2.891487 1.710506  
N 1.793487 0.135354 0.038411  
N 2.568193 1.061446 -0.599265  
C 1.882221 1.969636 -1.283329  
S -0.011814 1.635168 -1.481979  
O -0.776090 2.951151 -1.293631  
N 2.499870 3.005566 -1.870622  
C 1.816675 3.925210 -2.787309  
C 3.962834 3.144028 -1.795339  
O -0.075074 1.126458 -2.931570  
C -2.039704 3.766849 3.105440  
H 3.064485 -3.012549 2.350061  
H 1.369927 -4.312141 3.670223  
H -1.072591 -3.640944 3.516599  
H -1.706406 -1.739499 2.013836  
H 4.192641 -0.558339 2.823936  
H 6.703059 -0.788363 2.746323  
H 7.785164 -1.275098 0.495978  
H 6.305476 -1.542025 -1.534191  
H -3.199925 -3.051265 -2.212198  
H -1.466288 -4.331021 -3.502401  
H 0.966980 -3.652706 -3.278248  
H 1.557622 -1.742029 -1.762399  
H -4.381670 -0.610117 -2.666639  
H -6.878118 -0.950670 -2.579823  
H -7.935252 -1.578431 -0.364085  
H -6.449728 -1.844853 1.640308  
H 4.440677 2.657544 -2.665259  
H 4.212958 4.216290 -1.802476  
H 4.332854 2.678610 -0.872500  
H 2.164177 4.950307 -2.578999  
H 2.064464 3.674513 -3.834824  
H 0.730721 3.874914 -2.633852  
H -2.376444 4.807275 2.971450  
H -2.344087 3.424696 4.112753  
H -0.945354 3.729178 3.006589  
H -4.333705 4.202920 1.960020  
H -4.415220 2.749762 0.899361  
H -4.685888 2.589323 2.664986

[Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>]-b

C -4.890437 0.087004 -0.913516  
C -4.071757 -1.005836 -0.556094  
N -4.572844 -2.230294 -0.250771  
C -5.914427 -2.382182 -0.281119  
C -6.807248 -1.353326 -0.616635  
C -6.278894 -0.094610 -0.944656  
C -2.586216 -0.891065 -0.532588  
C -1.716236 -1.782382 -1.289188  
N -0.380350 -1.462677 -1.202383  
C 0.522052 -2.198448 -1.889656  
C 0.151111 -3.280213 -2.694896  
C -1.210674 -3.612689 -2.797519  
C -2.152282 -2.858083 -2.092386  
Fe 0.000083 0.042664 0.018019  
S -0.042554 1.604550 1.575196  
O 0.646109 2.947733 1.306993  
N 0.410938 -1.335313 1.374288  
C -0.470126 -2.025732 2.131444  
C -0.075635 -3.057663 2.990109  
C 1.286586 -3.397769 3.061599  
C 2.207180 -2.691379 2.282305  
C 1.749667 -1.650068 1.446287  
C 2.595803 -0.824576 0.600999  
C 4.080875 -0.958844 0.550810  
C 4.866705 -0.724985 1.696985  
C 6.258871 -0.874092 1.601196  
C 6.813603 -1.256051 0.371995  
C 5.946921 -1.476394 -0.712327  
N 4.608009 -1.335490 -0.642915  
N -1.916087 0.046488 0.150572  
N -2.662373 0.934254 0.881570  
C -1.957638 1.849133 1.533879  
N -2.562424 2.838022 2.210269  
C -1.840616 3.754942 3.100532  
N 1.911751 0.063181 -0.130105  
N 2.645101 0.952032 -0.870692  
C 1.921406 1.802876 -1.586478  
N 2.501418 2.803659 -2.266387  
C 3.964503 2.961784 -2.250343  
S 0.023725 1.450843 -1.681126  
O -0.099906 0.827723 -3.079460  
C -4.030749 2.903850 2.282427  
C 1.777489 3.635311 -3.235050  
O 0.163425 1.117525 3.017436  
H 3.271827 -2.935542 2.308626  
H 1.626236 -4.206405 3.715722  
H -0.828799 -3.580403 3.585435  
H -1.519082 -1.731508 2.042227  
H 4.393563 -0.424575 2.636769  
H 6.895571 -0.691600 2.472813  
H 7.893079 -1.385594 0.249425

H 6.347357 -1.785158 -1.686333  
H -3.217091 -3.093335 -2.139911  
H -1.535005 -4.450237 -3.422506  
H 0.920767 -3.840465 -3.232277  
H 1.568740 -1.898967 -1.790009  
H -4.440692 1.050368 -1.166724  
H -6.937375 0.733893 -1.224870  
H -7.885441 -1.538970 -0.625401  
H -6.289312 -3.380914 -0.023861  
H 4.424219 2.385541 -3.073931  
H 4.201045 4.028659 -2.383089  
H 4.366312 2.605296 -1.292667  
H 2.117316 4.677877 -3.124546  
H 1.995806 3.299771 -4.265227  
H 0.697486 3.587506 -3.044460  
H -2.260114 4.766040 2.973024  
H -1.971538 3.448082 4.154120  
H -0.773500 3.773224 2.844514  
H -4.329500 3.960841 2.356030  
H -4.468715 2.451966 1.383408  
H -4.395437 2.363984 3.175623  
O -0.745828 2.770388 -1.557265

[Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>]-c

C 4.924258 0.783891 0.443472  
C 4.290492 -0.432241 0.111168  
N 4.966877 -1.512668 -0.355324  
C 6.301781 -1.390942 -0.517372  
C 7.018094 -0.221164 -0.221365  
C 6.311353 0.885330 0.275181  
C 2.822939 -0.620741 0.291541  
C 2.261040 -1.717946 1.066521  
N 0.888154 -1.694620 1.151730  
C 0.240151 -2.662157 1.842356  
C 0.933415 -3.683372 2.504661  
C 2.336870 -3.705893 2.450743  
C 3.007692 -2.719689 1.721012  
Fe 0.016123 -0.173789 0.219530  
S -0.408314 1.588874 -1.072424  
O -1.113774 2.783007 -0.423752  
N -0.425727 -1.452649 -1.241485  
C 0.443082 -1.897038 -2.185512  
C 0.065290 -2.812201 -3.170262  
C -1.256712 -3.290826 -3.179390  
C -2.146091 -2.836670 -2.199871  
C -1.705265 -1.912164 -1.238186  
C -2.594490 -1.507012 -0.042915  
N -1.751111 -0.333125 0.613941  
N -2.448996 0.360909 1.482622  
C -1.703035 1.252610 2.201649  
N -2.323320 2.157342 2.963403  
C -3.791745 2.212846 3.061847

N 1.895377 0.195892 -0.219965  
N 2.350856 1.247752 -0.964664  
C 1.419921 2.077363 -1.403152  
N 1.723950 3.181092 -2.102568  
C 0.715848 4.061027 -2.706251  
S 0.123098 0.979906 2.156141  
O 0.937721 2.318918 2.264790  
C 3.116830 3.479724 -2.471858  
O -2.636409 -2.453131 0.878045  
C -3.956398 -0.924929 -0.521396  
C -4.004887 0.052284 -1.537223  
C -5.251998 0.543490 -1.946560  
C -6.410326 0.035869 -1.335756  
C -6.258457 -0.940401 -0.339739  
N -5.063084 -1.420579 0.071419  
C -1.604114 3.077175 3.854387  
O -0.921556 1.272120 -2.483417  
H -3.181344 -3.188636 -2.165943  
H -1.586149 -4.005051 -3.940492  
H 0.798858 -3.139190 -3.912037  
H 1.458396 -1.494867 -2.140788  
H -3.076888 0.422030 -1.991908  
H -5.320348 1.305399 -2.730866  
H -7.407363 0.383582 -1.623890  
H -7.142747 -1.362915 0.156471  
H 4.095852 -2.718093 1.637015  
H 2.903863 -4.487426 2.965626  
H 0.370504 -4.445932 3.049965  
H -0.860241 -2.616682 1.793524  
H 4.338364 1.621581 0.829925  
H 6.831848 1.813931 0.530660  
H 8.101079 -0.184332 -0.372249  
H 6.820553 -2.277655 -0.902808  
H -4.101768 1.848532 4.056940  
H -4.109164 3.261967 2.950178  
H -4.245063 1.591311 2.281407  
H -2.040457 4.083078 3.746060  
H -1.736408 2.744464 4.899655  
H -0.537088 3.104524 3.594761  
H 1.048450 5.103764 -2.577171  
H 0.622801 3.849874 -3.786523  
H -0.255522 3.932957 -2.213092  
H 3.308728 4.550104 -2.292958  
H 3.800717 2.869308 -1.870278  
H 3.272883 3.262346 -3.543918

[Fe(Dp44mT)<sub>2</sub>O<sub>4</sub>]-c-s

N -4.609651 -1.435284 0.613830  
C -4.034938 -1.107070 -0.571620  
C -4.766011 -0.963464 -1.767406  
C -6.156121 -1.153777 -1.732249  
C -6.761084 -1.486034 -0.512374

C -5.945311 -1.617783 0.624587  
C -2.553711 -0.925378 -0.554045  
C -1.638847 -1.784782 -1.289052  
N -0.313505 -1.439671 -1.153118  
C 0.634019 -2.187442 -1.762772  
C 0.309381 -3.292030 -2.559951  
C -1.040460 -3.648050 -2.718059  
C -2.023690 -2.895441 -2.068369  
Fe 0.019914 0.086744 0.064806  
S -0.141470 1.696854 1.643007  
O 0.548935 3.042598 1.211282  
N 0.358726 -1.269519 1.503950  
C 1.673371 -1.479779 1.781323  
C 2.075951 -2.504979 2.655310  
C 1.109739 -3.312455 3.263400  
C -0.248724 -3.063286 2.997562  
C -0.583663 -2.036136 2.112870  
C 2.654936 -0.400272 1.297867  
N 1.808901 0.302639 0.097432  
N 2.526493 1.247940 -0.476400  
C 1.840494 2.085088 -1.285465  
N 2.451087 3.071767 -1.931857  
C 3.894698 3.329522 -1.790966  
C 3.926484 -0.976416 0.639279  
C 5.182864 -0.576331 1.119122  
C 6.334727 -1.109569 0.522378  
C 6.185162 -2.021292 -0.534599  
C 4.885556 -2.359367 -0.946751  
N 3.768954 -1.856391 -0.376886  
S 0.026128 1.518929 -1.620940  
O 0.186078 0.896255 -3.014747  
N -1.936490 0.023141 0.152647  
N -2.715071 0.923616 0.817221  
C -2.013214 1.884262 1.415092  
N -2.644943 2.954140 1.933318  
C -2.002303 3.887944 2.867336  
O -0.922408 2.717628 -1.606082  
C -4.105189 3.078405 1.805269  
C 1.735720 3.977760 -2.839676  
H -3.081418 -3.157660 -2.149076  
H -1.322954 -4.509247 -3.331008  
H 1.110388 -3.859113 -3.041524  
H 1.674253 -1.897251 -1.576015  
H -4.254129 -0.700607 -2.698133  
H -6.752596 -1.041966 -2.643314  
H -7.840895 -1.645094 -0.436665  
H -6.385658 -1.886364 1.593229  
H 3.142262 -2.649955 2.852901  
H 1.406319 -4.120933 3.939119  
H -1.042310 -3.655334 3.461182  
H -1.625968 -1.816223 1.866787  
H 5.216560 0.140103 1.945143

H 7.331375 -0.820106 0.872974  
H 7.052817 -2.465303 -1.032171  
H 4.732391 -3.068131 -1.770733  
H -4.614189 2.575229 2.647661  
H -4.365973 4.147637 1.815695  
H -4.434943 2.619951 0.863392  
H -2.414557 4.894186 2.693741  
H -2.214319 3.593611 3.911935  
H -0.918116 3.918162 2.695752  
H 2.009223 5.014196 -2.582289  
H 2.046784 3.776786 -3.879217  
H 0.651120 3.845855 -2.731255  
H 4.038045 4.322275 -1.332302  
H 4.351682 2.553897 -1.165905  
H 4.349926 3.329315 -2.795371  
O 2.837657 0.486829 2.246830

[Fe(Dp44mT)<sub>2</sub>O<sub>5</sub>]-a

N 4.571833 -1.225267 -0.453420  
C 3.970684 -0.789684 0.733983  
C 4.768209 -0.486950 1.846635  
C 6.164412 -0.580022 1.789802  
C 6.748754 -0.988854 0.579008  
C 5.950085 -1.301233 -0.514344  
C 2.497200 -0.704226 0.743942  
N 1.813326 0.144429 -0.035085  
N 2.555165 1.001685 -0.794709  
C 1.839579 1.791155 -1.587833  
S -0.044216 1.374403 -1.728849  
O -0.854855 2.674746 -1.727452  
C 1.652718 -1.493566 1.623571  
N 0.312240 -1.198327 1.515391  
C -0.571715 -1.854249 2.299711  
C -0.177819 -2.830455 3.221311  
C 1.186958 -3.151492 3.328546  
C 2.110658 -2.481010 2.522016  
Fe -0.092579 0.082493 0.061482  
N -2.012944 0.042441 0.135160  
N -2.804205 0.954325 0.785086  
C -2.143687 1.927633 1.397572  
N -2.793940 2.939374 1.993480  
C -4.265027 2.965269 2.023778  
N -0.395006 -1.512389 -1.063418  
C -1.719359 -1.869111 -1.175634  
C -2.102280 -3.004732 -1.920806  
C -1.118006 -3.781961 -2.538100  
C 0.231241 -3.412964 -2.404203  
C 0.552413 -2.271361 -1.660691  
C -2.636214 -0.953233 -0.508047  
C -4.116965 -1.108169 -0.571301  
C -4.949335 -0.061772 -1.023286  
C -6.331244 -0.281155 -1.086349

C -6.839694 -1.529934 -0.695017  
C -5.933970 -2.511924 -0.266473  
N -4.598135 -2.323551 -0.203985  
S -0.224269 1.743997 1.503904  
O -0.040620 1.366444 2.981260  
O 0.431551 3.084859 1.154674  
C -2.122108 3.931162 2.841641  
N 2.421804 2.760542 -2.306907  
C 1.712816 3.524700 -3.340157  
C 3.879975 2.954767 -2.252397  
O -0.089709 0.652655 -3.083300  
H 3.177528 -2.711720 2.573521  
H 1.526096 -3.918073 4.031693  
H -0.933123 -3.326528 3.836382  
H -1.622448 -1.577951 2.179621  
H 4.261820 -0.157839 2.758847  
H 6.777330 -0.331639 2.659675  
H 7.833408 -1.075278 0.468133  
H 6.328004 -1.636940 -1.481133  
H -3.159165 -3.268135 -1.991744  
H -1.400371 -4.665947 -3.118011  
H 1.032064 -3.992088 -2.871855  
H 1.592468 -1.946345 -1.536429  
H -4.514677 0.895065 -1.323215  
H -6.999937 0.510378 -1.439753  
H -7.912274 -1.743655 -0.725719  
H -6.293035 -3.501776 0.042462  
H 4.377309 2.348527 -3.031177  
H 4.096486 4.018843 -2.432622  
H 4.258243 2.657039 -1.265652  
H 2.016835 4.581403 -3.264865  
H 1.984012 3.149136 -4.343451  
H 0.627915 3.450638 -3.190146  
H -2.566128 4.919480 2.640077  
H -2.272159 3.687161 3.909021  
H -1.049496 3.965256 2.611735  
H -4.595747 4.015177 2.031541  
H -4.665035 2.453000 1.139539  
H -4.639231 2.463442 2.935020  
O 3.868068 -1.561513 -1.480598

[Fe(Dp44mT)<sub>2</sub>O<sub>5</sub>]-c

C 4.920898 0.804892 0.364100  
C 4.292907 -0.420796 0.059258  
N 4.971462 -1.509709 -0.381806  
C 6.306101 -1.387240 -0.546378  
C 7.018146 -0.208675 -0.275859  
C 6.307920 0.906739 0.194875  
C 2.825520 -0.608990 0.246882  
C 2.268080 -1.674059 1.070645  
N 0.897741 -1.644878 1.169536  
C 0.254649 -2.589883 1.891090

C	0.952276	-3.593293	2.576124	H	-4.246328	3.237507	2.566931
C	2.354687	-3.616747	2.514878	H	-4.316169	1.438682	2.445310
C	3.020669	-2.652802	1.750845	H	-2.164659	4.232343	3.487770
Fe	0.017331	-0.171087	0.177167	H	-1.743579	2.984201	4.704752
S	-0.416858	1.495686	-1.242867	H	-0.629947	3.309429	3.316779
O	-1.174237	2.694885	-0.667527	H	0.987974	4.965199	-2.882323
N	-0.420747	-1.526652	-1.219698	H	0.638236	3.644462	-4.044649
C	0.454245	-2.030354	-2.126653	H	-0.292770	3.773838	-2.506232
C	0.085946	-3.016606	-3.044137	H	3.233303	4.477922	-2.660261
C	-1.232404	-3.503887	-3.022491	H	3.775398	2.931254	-1.913842
C	-2.129441	-2.985914	-2.082253	H	3.331406	2.984709	-3.654441
C	-1.697509	-1.991678	-1.188791	O	0.814355	2.510747	1.838804
C	-2.593259	-1.501288	-0.033287				
N	-1.757631	-0.294193	0.556750				
N	-2.487016	0.470502	1.345672				
C	-1.787335	1.374158	2.068669				
N	-2.404288	2.254349	2.841985				
C	-3.872569	2.285898	2.980018				
N	1.897232	0.179326	-0.300280				
N	2.342803	1.196790	-1.096806				
C	1.406237	2.001539	-1.567771				
N	1.702881	3.086744	-2.297439				
C	0.690616	3.908230	-2.973232				
S	0.135292	1.147443	1.959858				
O	0.412500	0.443219	3.290772				
C	3.100777	3.384870	-2.650445				
O	-2.633074	-2.370849	0.964306				
C	-3.955158	-0.964565	-0.555200				
C	-4.008093	-0.089553	-1.659550				
C	-5.256843	0.368241	-2.101721				
C	-6.410976	-0.070485	-1.432920				
C	-6.254265	-0.947161	-0.348586				
N	-5.057474	-1.393169	0.094849				
C	-1.678332	3.254886	3.637302				
O	-0.891791	1.080713	-2.639350				
H	-3.162644	-3.340963	-2.027862				
H	-1.554025	-4.273836	-3.730690				
H	0.823811	-3.389726	-3.759306				
H	1.465995	-1.617483	-2.109393				
H	-3.083060	0.230525	-2.155281				
H	-5.328945	1.051582	-2.954888				
H	-7.409044	0.254632	-1.742922				
H	-7.135550	-1.313254	0.195322				
H	4.108102	-2.654342	1.658127				
H	2.925306	-4.382213	3.049496				
H	0.392942	-4.339014	3.147670				
H	-0.845134	-2.539485	1.857227				
H	4.331810	1.649141	0.731421				
H	6.825435	1.842353	0.429827				
H	8.101198	-0.171984	-0.426188				
H	6.828065	-2.280661	-0.911268				
H	-4.120348	2.237038	4.052849				