

## Supporting Information

### Proton-Assisted Air Oxidation Mechanisms of Iron(II) bis-Thiosemicarbazone Complexes at Physiological pH: a Kinetic-Mechanistic Study

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**Table S1.-** Values obtained for the observed pseudo first order rate constants as a function of the Fe<sup>II</sup> bis-thiosemicarbazone complexes studied, dioxygen concentration, temperature and pressure.

TSC	T /°C	P /atm	pH	[O <sub>2</sub> ] /mM	k <sub>obs</sub> /s <sup>-1</sup>	
Dp44mT	10	250	5.0	2.6×10 <sup>-1</sup>	2.3×10 <sup>-3</sup>	
		500		2.6×10 <sup>-1</sup>	2.0×10 <sup>-3</sup>	
		750		2.6×10 <sup>-1</sup>	1.8×10 <sup>-3</sup>	
		1000		2.6×10 <sup>-1</sup>	1.7×10 <sup>-3</sup>	
		1250		2.6×10 <sup>-1</sup>	1.6×10 <sup>-3</sup>	
		1500		2.6×10 <sup>-1</sup>	1.5×10 <sup>-3</sup>	
	15	1	6.3	2.4×10 <sup>-1</sup>	1.3×10 <sup>-3</sup>	
			6.7	2.4×10 <sup>-1</sup>	7.2×10 <sup>-4</sup>	
			7.1	2.4×10 <sup>-1</sup>	3.1×10 <sup>-4</sup>	
			7.3	2.4×10 <sup>-1</sup>	2.4×10 <sup>-4</sup>	
			7.7	2.4×10 <sup>-1</sup>	1.3×10 <sup>-4</sup>	
			6.3	1.9×10 <sup>-1</sup>	4.5×10 <sup>-3</sup>	
				1.1×10 <sup>-2</sup>	2.9×10 <sup>-3</sup>	
				9.4×10 <sup>-2</sup>	2.7×10 <sup>-3</sup>	
	25	1			7.5×10 <sup>-2</sup>	1.8×10 <sup>-3</sup>
					3.8×10 <sup>-2</sup>	8.4×10 <sup>-4</sup>
			6.7	1.9×10 <sup>-1</sup>	2.4×10 <sup>-3</sup>	
			6.9	1.9×10 <sup>-1</sup>	1.6×10 <sup>-3</sup>	
				1.5×10 <sup>-1</sup>	1.3×10 <sup>-3</sup>	
				1.2×10 <sup>-1</sup>	1.2×10 <sup>-3</sup>	
			9.4×10 <sup>-2</sup>	9.8×10 <sup>-4</sup>		
			7.5×10 <sup>-2</sup>	6.8×10 <sup>-4</sup>		
			5.6×10 <sup>-2</sup>	5.2×10 <sup>-4</sup>		
7.1			1.9×10 <sup>-1</sup>	9.8×10 <sup>-4</sup>		
			1.5×10 <sup>-1</sup>	7.9×10 <sup>-4</sup>		
			1.2×10 <sup>-1</sup>	6.5×10 <sup>-4</sup>		
			9.4×10 <sup>-2</sup>	5.4×10 <sup>-4</sup>		
			5.6×10 <sup>-2</sup>	3.4×10 <sup>-4</sup>		
			3.8×10 <sup>-2</sup>	1.9×10 <sup>-4</sup>		
			1	7.3	1.9×10 <sup>-1</sup>	6.6×10 <sup>-4</sup>
					1.5×10 <sup>-1</sup>	5.6×10 <sup>-4</sup>
					1.1×10 <sup>-1</sup>	3.6×10 <sup>-4</sup>
					9.4×10 <sup>-2</sup>	3.0×10 <sup>-4</sup>
					7.5×10 <sup>-2</sup>	2.7×10 <sup>-4</sup>
			5.6×10 <sup>-2</sup>	1.9×10 <sup>-4</sup>		
		7.7	1.9×10 <sup>-1</sup>	4.0×10 <sup>-4</sup>		
			1.5×10 <sup>-1</sup>	3.1×10 <sup>-4</sup>		
			1.1×10 <sup>-1</sup>	2.1×10 <sup>-4</sup>		
			9.4×10 <sup>-2</sup>	1.7×10 <sup>-4</sup>		
			5.6×10 <sup>-2</sup>	1.0×10 <sup>-4</sup>		
35	1	6.3	1.7×10 <sup>-1</sup>	1.3×10 <sup>-2</sup>		
		6.7	1.7×10 <sup>-1</sup>	7.0×10 <sup>-3</sup>		
		7.1	1.7×10 <sup>-1</sup>	2.9×10 <sup>-3</sup>		
		7.3	1.7×10 <sup>-1</sup>	2.0×10 <sup>-3</sup>		
		7.7	1.7×10 <sup>-1</sup>	9.8×10 <sup>-4</sup>		
DpT	10	250	5.0	2.6×10 <sup>-1</sup>	8.5×10 <sup>-4</sup>	
		500		2.6×10 <sup>-1</sup>	9.0×10 <sup>-4</sup>	
		750		2.6×10 <sup>-1</sup>	1.2×10 <sup>-3</sup>	
		1000		2.6×10 <sup>-1</sup>	1.3×10 <sup>-3</sup>	
		1150		2.6×10 <sup>-1</sup>	1.3×10 <sup>-3</sup>	
	10	250	8.0	2.6×10 <sup>-1</sup>	1.1×10 <sup>-4</sup>	
					2.6×10 <sup>-1</sup>	1.1×10 <sup>-4</sup>
					2.6×10 <sup>-1</sup>	1.2×10 <sup>-4</sup>
					2.6×10 <sup>-1</sup>	1.2×10 <sup>-4</sup>
					2.6×10 <sup>-1</sup>	1.2×10 <sup>-4</sup>

		1250		$2.6 \times 10^{-1}$	$1.2 \times 10^{-4}$
		1500		$2.6 \times 10^{-1}$	$1.3 \times 10^{-4}$
	15	1	6.3	$2.4 \times 10^{-1}$	$5.8 \times 10^{-4}$
			6.7	$2.4 \times 10^{-1}$	$3.6 \times 10^{-4}$
			7.1	$2.4 \times 10^{-1}$	$2.3 \times 10^{-4}$
			7.3	$2.4 \times 10^{-1}$	$1.9 \times 10^{-4}$
			7.7	$2.4 \times 10^{-1}$	$1.2 \times 10^{-1}$
	25	1	7.1	$1.9 \times 10^{-1}$	$5.7 \times 10^{-4}$
				$1.5 \times 10^{-1}$	$4.7 \times 10^{-4}$
				$1.1 \times 10^{-1}$	$3.4 \times 10^{-4}$
				$7.5 \times 10^{-2}$	$2.0 \times 10^{-4}$
				$5.6 \times 10^{-2}$	$1.6 \times 10^{-4}$
	35	1	6.3	$1.7 \times 10^{-1}$	$2.9 \times 10^{-3}$
			6.7	$1.7 \times 10^{-1}$	$2.0 \times 10^{-3}$
			7.1	$1.7 \times 10^{-1}$	$1.3 \times 10^{-3}$
			7.3	$1.7 \times 10^{-1}$	$1.2 \times 10^{-3}$
			7.7	$1.7 \times 10^{-1}$	$7.9 \times 10^{-4}$
BpT	15	1	6.3	$2.4 \times 10^{-1}$	$1.6 \times 10^{-3}$
			6.7	$2.4 \times 10^{-1}$	$1.0 \times 10^{-3}$
			7.1	$2.4 \times 10^{-1}$	$7.2 \times 10^{-4}$
			7.3	$2.4 \times 10^{-1}$	$6.2 \times 10^{-4}$
			7.7	$2.4 \times 10^{-1}$	$4.3 \times 10^{-4}$
	20	400	7.1	$2.2 \times 10^{-1}$	$7.8 \times 10^{-4}$
		700		$2.2 \times 10^{-1}$	$7.4 \times 10^{-4}$
		850		$2.2 \times 10^{-1}$	$6.9 \times 10^{-4}$
		1000		$2.2 \times 10^{-1}$	$6.7 \times 10^{-4}$
		1300		$2.2 \times 10^{-1}$	$6.4 \times 10^{-4}$
		1600		$2.2 \times 10^{-1}$	$6.0 \times 10^{-4}$
	25	1	7.1	$1.9 \times 10^{-1}$	$3.2 \times 10^{-3}$
				$1.9 \times 10^{-1}$	$1.6 \times 10^{-3}$
				$1.5 \times 10^{-1}$	$1.3 \times 10^{-3}$
				$1.3 \times 10^{-1}$	$8.4 \times 10^{-4}$
				$7.5 \times 10^{-2}$	$5.9 \times 10^{-4}$
				$5.6 \times 10^{-2}$	$5.1 \times 10^{-4}$
				$3.7 \times 10^{-2}$	$2.8 \times 10^{-4}$
	35		6.3	$1.7 \times 10^{-1}$	$6.3 \times 10^{-3}$
			6.7	$1.7 \times 10^{-1}$	$4.8 \times 10^{-3}$
			7.1	$1.7 \times 10^{-1}$	$2.9 \times 10^{-3}$
			7.3	$1.7 \times 10^{-1}$	$2.6 \times 10^{-3}$
			7.7	$1.7 \times 10^{-1}$	$2.2 \times 10^{-3}$

**Table S2.-** Summary of the kinetic parameters derived from Equation 1 for the systems studied. (15 mM MOPS buffer, 100 mM NaClO<sub>4</sub>).

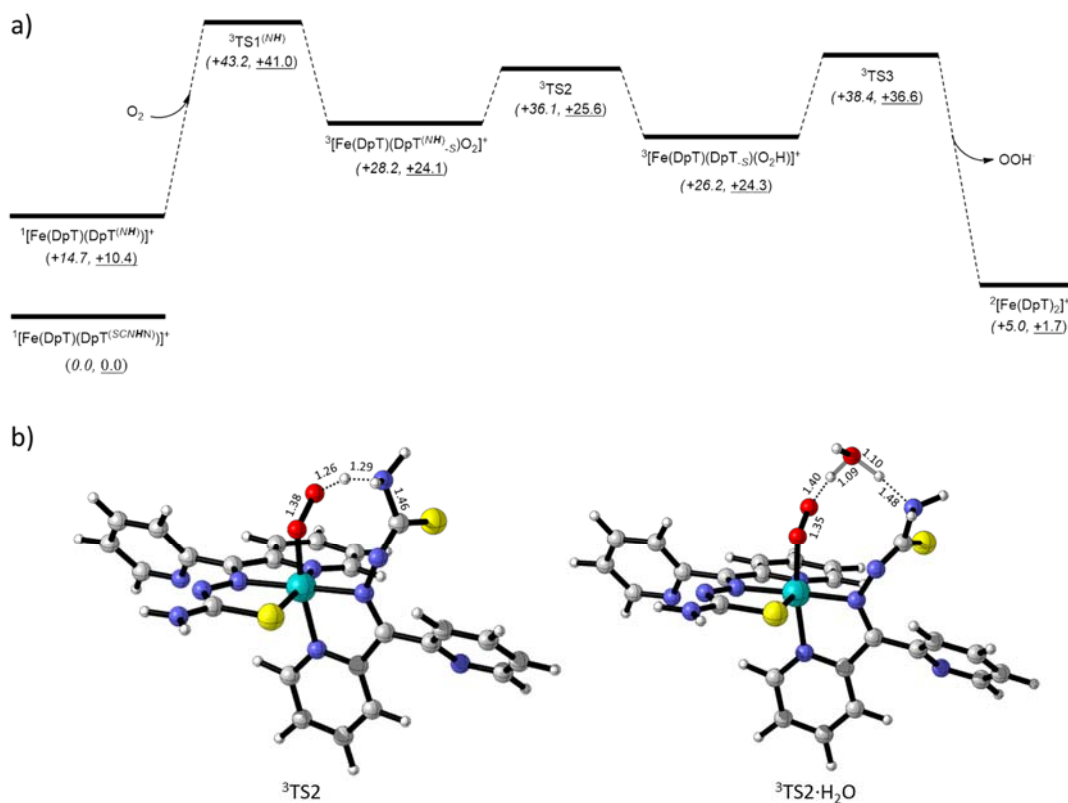
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TSC	pH	T (K)	$k_{ox} / s^{-1} M^{-1}$	
<b>HDp44mT</b>	6.3	288	1.4	
		298	6.0	
		308	19	
	6.5	298	4.3	
		6.7	288	0.75
			298	3.3
	308		10	
	6.9	298	2.2	
		7.1	288	0.33
			298	1.3
	308		4.3	
	7.3	288	0.25	
		298	0.85	
		308	3.0	
	7.5	298	0.63	
		7.7	288	0.14
			298	0.53
	308		1.5	
<b>HDpT</b>	6.3	288	0.60	
		298	1.7	
		308	4.3	
	6.7	288	0.38	
		298	1.1	
		308	3.0	
	7.1	288	0.25	
		298	0.75	
		308	2.0	
	7.3	288	0.20	
		298	0.63	
		308	1.8	
	7.7	288	0.15	
		298	0.45	
		308	1.3	
<b>HBpT</b>	6.3	288	1.6	
		298	4.3	
		308	9.3	
	6.7	288	1.1	
		298	3.0	
		308	7.0	
	7.1	288	0.75	
		298	2.0	
		308	4.3	
	7.3	288	0.65	
		298	1.8	
		308	3.8	
	7.7	288	0.45	
		298	1.2	
		308	3.3	

**Table S3.** Relative free energies (kcal mol<sup>-1</sup>) of the species discussed in the main text (See also Table S4).

<b>Neutral Structures</b>	<b>DpT</b>	<b>BpT</b>	<b>Dp44mT</b>
<sup>1</sup> [Fe(TSC) <sub>2</sub> ]	0.0	0.0	0.0
<sup>3</sup> [Fe(TSC) <sub>2</sub> ]	20.6	19.8	20.0
<sup>3</sup> TS1	31.9	31.3	32.2
<sup>1</sup> [Fe(TSC)(TSC <sub>s</sub> )O <sub>2</sub> ]	20.4	20.3	19.2
<sup>3</sup> [Fe(TSC)(TSC <sub>s</sub> )O <sub>2</sub> ]	20.5	19.5	20.3
<b>Protonated structures</b>	<b>DpT</b>	<b>BpT</b>	<b>Dp44mT</b>
<sup>1</sup> [Fe(TSC)(TSC <sup>(SCNHN)</sup> )] <sup>+</sup>	0.0	0.0	0.0
<sup>3</sup> [Fe(TSC)(TSC <sup>(SCNHN)</sup> )] <sup>+</sup>	17.1	18.7	16.2
<sup>1</sup> [Fe(TSC)(TSC <sup>(SH)</sup> )] <sup>+</sup>	13.4	12.6	10.9
<sup>1</sup> [Fe(TSC)(TSC <sup>(NH)</sup> )] <sup>+</sup>	14.7	14.5	11.4
<sup>3</sup> [Fe(TSC)(TSC <sup>(NH)</sup> )] <sup>+</sup>	30.7	30.3	28.9
<sup>3</sup> TS1 <sup>(SCNHN)</sup>	31.8	29.9	29.1
<sup>3</sup> TS1 <sup>(NH)</sup>	43.2	43.3	40.3
<sup>3</sup> [Fe(TSC)(TSC <sup>(SCNHN)</sup> <sub>s</sub> )(O <sub>2</sub> )] <sup>+</sup>	18.4	16.3	16.4
<sup>3</sup> [Fe(TSC)(TSC <sup>(NH)</sup> <sub>s</sub> )(O <sub>2</sub> )] <sup>+</sup>	28.2	25.9	24.7
<sup>3</sup> TS2	36.1	34.8	35.5
<sup>3</sup> [Fe(TSC)(TSC <sub>s</sub> )(O <sub>2</sub> H)] <sup>+</sup>	26.2	23.7	19.6
<sup>3</sup> TS3	38.4	36.7	35.5
<sup>2</sup> [Fe(TSC) <sub>2</sub> ] <sup>+</sup> + OOH·	5.0	4.1	3.6
<sup>1</sup> [Fe(TSC)(TSC <sup>(SCNHN)</sup> )] <sup>+</sup> ·H <sub>2</sub> O	0.0		
<sup>1</sup> [Fe(TSC)(TSC <sup>(NH)</sup> <sub>s</sub> )] <sup>+</sup> ·H <sub>2</sub> O	10.4		
<sup>3</sup> TS1 <sup>(NH)</sup> ·H <sub>2</sub> O	41.0		
<sup>3</sup> [Fe(TSC)(TSC <sup>(NH)</sup> <sub>s</sub> )(O <sub>2</sub> )] <sup>+</sup> ·H <sub>2</sub> O	24.1		
<sup>3</sup> TS2·H <sub>2</sub> O	25.6		
<sup>3</sup> [Fe(TSC)(TSC <sub>s</sub> )(O <sub>2</sub> H)] <sup>+</sup> ·H <sub>2</sub> O	24.3		
<sup>3</sup> TS3·H <sub>2</sub> O	36.6		
<sup>2</sup> [Fe(TSC) <sub>2</sub> ] <sup>+</sup> + H <sub>2</sub> O·OOH·	1.7		



**Figure S1.** a) Computed free energy profiles (kcal/mol) for the conversion of  $^1[\text{Fe}(\text{DpT})_2]$  and  $\text{O}_2$  into  $^2[\text{Fe}(\text{DpT})_2]^+$  and  $\text{OOH}\cdot$  both in the absence (italic) and presence (underlined) of one explicit  $\text{H}_2\text{O}$  molecule; b) Graphical representations of  $^3\text{TS2}$  and  $^3\text{TS2}\cdot\text{H}_2\text{O}$ .

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**Table S4.** Functional testing of the DpT structures discussed in the main text. Relative free energies (kcal mol<sup>-1</sup>) were obtained by performing single point calculations with the corresponding functional, together with the cc-pVTZ basis set, and including the solvent effects via the SMD approach. In all cases the BP86 free energy correction obtained at the optimization level was used. The data for BP86-D3BJ are those reported in the main text.

<i>Neutral Structures</i>	<b>BP86-D3BJ</b>	<b>B97D</b>	<b>B3LYP-D3BJ</b>	<b>M06-D3</b>	<b>PBE0-D3BJ</b>
<sup>1</sup> [Fe(DpT) <sub>2</sub> ]	0.0	0.0	0.0	0.0	0.0
<sup>3</sup> [Fe(DpT) <sub>2</sub> ]	20.6	10.5	8.1	1.7	5.8
<sup>3</sup> TS1	31.9	33.4	34.7	36.1	38.3
<sup>1</sup> [Fe(DpT)(DpT <sub>-s</sub> )O <sub>2</sub> ]	20.4	23.2	35.5	35.9	44.4
<sup>3</sup> [Fe(DpT)(DpT <sub>-s</sub> )O <sub>2</sub> ]	20.5	20.7	21.8	22.4	26.3
<i>Protonated structures</i>	<b>BP86-D3BJ</b>	<b>B97D</b>	<b>B3LYP-D3BJ</b>	<b>M06-D3</b>	<b>PBE0-D3BJ</b>
<sup>1</sup> [Fe(DpT)(DpT <sup>(SCNHN)</sup> )] <sup>+</sup>	0.0	0.0	0.0	0.0	0.0
<sup>3</sup> [Fe(DpT)(DpT <sup>(SCNHN)</sup> )] <sup>+</sup>	17.1	8.7	8.1	3.1	5.2
<sup>1</sup> [Fe(DpT)(DpT <sup>(SH)</sup> )] <sup>+</sup>	13.4	14.3	14.7	16.2	15.8
<sup>1</sup> [Fe(DpT)(DpT <sup>(NH)</sup> )] <sup>+</sup>	14.7	16.2	16.7	17.4	17.0
<sup>3</sup> [Fe(DpT)(DpT <sup>(NH)</sup> )] <sup>+</sup>	30.7	32.1	31.4	33.4	29.4
<sup>3</sup> TS1 <sup>(SCNHN)</sup>	31.8	35.6	36.4	38.4	39.4
<sup>3</sup> TS1 <sup>(NH)</sup>	43.2	40.3	40.3	42.2	45.3
<sup>3</sup> [Fe(DpT)(DpT <sup>(SCNHN)</sup> <sub>-s</sub> )(O <sub>2</sub> )] <sup>+</sup>	18.4	18.8	20.0	20.6	24.7
<sup>3</sup> [Fe(DpT)(DpT <sup>(NH)</sup> <sub>-s</sub> )(O <sub>2</sub> )] <sup>+</sup>	28.2	29.2	31.4	32.4	36.3
<sup>3</sup> TS2	36.1	39.8	45.0	47.3	50.3
<sup>3</sup> [Fe(DpT)(DpT <sub>-s</sub> )(O <sub>2</sub> H)] <sup>+</sup>	26.2	27.7	28.3	29.1	35.0
<sup>3</sup> TS3	38.4	45.5	42.1	45.5	46.7
<sup>2</sup> [Fe(DpT) <sub>2</sub> ] <sup>+</sup> + OOH·	5.0	8.7	4.3	6.1	5.5

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**Table S5.** Cartesian coordinates of the BP86-optimised structures

Neutral Structures	DpT ligand structure	BpT ligand structure	Dp44mT ligand structure
<sup>1</sup> [Fe(TSC) <sub>2</sub> ]	Fe -0.000001 0.643660 0.000005 C -2.608525 -0.255530 -0.417180 C -1.809991 -1.020611 -1.359031 C -2.311914 -1.963484 -2.281620 H -3.381225 -2.182314 -2.293120 C -1.434553 -2.606747 -3.159568 H -1.814954 -3.339192 -3.877636 C -0.064815 -2.294541 -3.109209 H 0.657734 -2.769115 -3.777968 C 0.375693 -1.345162 -2.180981 H 1.430081 -1.065242 -2.117754 C -4.073530 -0.452824 -0.252913 C -4.979802 0.622777 -0.371482 H -4.610372 1.626671 -0.594434 C -6.348304 0.378774 -0.204589 H -7.070383 1.196521 -0.294713 C -6.774373 -0.929726 0.073201 H -7.832668 -1.168452 0.212563 C -5.804154 -1.937463 0.159917 H -6.100545 -2.972492 0.369795 C -1.709865 2.169588 1.928888 N -0.463345 -0.717773 -1.322670 N -4.477647 -1.726235 0.008042 N -1.881160 0.620120 0.299163 N -2.535649 1.365067 1.240914 N -2.289248 2.985079 2.854525 H -3.256949 2.797473 3.117334 S 0.018607 2.262136 1.662604 H -1.697257 3.439562 3.546404 C 2.608531 -0.255516 0.417177 C 1.810003 -1.020603 1.359029 C 2.311934 -1.963470 2.281620 H 3.381247 -2.182294 2.293117 C 1.434582 -2.606735 3.159573 H 1.814990 -3.339175 3.877643 C 0.064841 -2.294538 3.109218 H -0.657702 -2.769112 3.777982 C -0.375676 -1.345165 2.180989 H -1.430066 -1.065251 2.117765 C 4.073532 -0.452811 0.252898 C 4.979810 0.622788 0.371446 H 4.610386 1.626687 0.594388 C 6.348310 0.378779 0.204545 H 7.070391 1.196525 0.294653 C 6.774373 -0.929725 -0.073230 H 7.832666 -1.168457 -0.212597 C 5.804149 -1.937462 -0.159922 H 6.100537 -2.972495 -0.369786 C 1.709844 2.169612 -1.928875 N 0.463355 -0.717774 1.322673 N 4.477645 -1.726227 -0.008039 N 1.881157 0.620138 -0.299157 N 2.535636 1.365092 -1.240906 N 2.289216 2.985102 -2.854515 H 3.256925 2.797526 -3.117315 S -0.018629 2.262145 -1.662585 H 1.697223 3.439608 -3.546377	C -4.672494 -1.653041 0.144150 C -4.107717 -0.401547 -0.195575 C -4.969492 0.701164 -0.402063 C -6.357490 0.554236 -0.267779 C -6.909083 -0.693321 0.075671 C -6.063007 -1.795728 0.280719 C -2.636756 -0.263267 -0.352195 N -1.873381 0.584386 0.358696 N -2.493431 1.337456 1.320209 C -1.640082 2.131527 1.982820 S 0.081289 2.212474 1.663109 Fe -0.000006 0.593953 0.000101 N -0.515571 -0.768677 -1.299620 C -1.870059 -1.041722 -1.310063 C -2.409356 -1.980068 -2.216457 C -1.561731 -2.655099 -3.100226 C -0.183718 -2.378137 -3.071533 C 0.294087 -1.428380 -2.161720 N 0.515600 -0.769043 1.299431 C 1.870097 -1.042045 1.309798 C 2.409429 -1.980599 2.215956 C 1.561828 -2.655894 3.099546 C 0.183801 -2.378992 3.070909 C -0.294037 -1.429013 2.161344 C 2.636766 -0.263317 0.352128 N 1.873366 0.584525 -0.358512 N 2.493386 1.337880 -1.319820 C 1.640020 2.132145 -1.982178 S -0.081351 2.212987 -1.662414 C 4.107722 -0.401570 0.195412 C 4.969521 0.701085 0.402109 C 6.357511 0.554171 0.267720 C 6.909075 -0.693314 -0.076037 C 6.062976 -1.795664 -0.281291 C 4.672472 -1.652993 -0.144622 N 2.182324 2.955025 -2.926617 N -2.182398 2.954089 2.927528 H 3.486247 -2.165453 2.217951 H 1.971123 -3.385104 3.804909 H -0.516560 -2.880314 3.743756 H -1.356077 -1.175156 2.116047 H 4.545448 1.672056 0.674914 H 7.011940 1.415964 0.435377 H 7.993102 -0.804766 -0.181860 H 6.483410 -2.769755 -0.552062 H 3.138277 2.764593 -3.227962 H 1.561485 3.388490 -3.606735 H -3.486165 -2.164972 -2.218490 H -1.970999 -3.384149 -3.805771 H 0.516659 -2.879244 -3.744524 H 1.356119 -1.174493 -2.116363 H -4.545392 1.672194 -0.674619 H -7.011901 1.416075 -0.435270 H -7.993116 -0.804786 0.181412 H -6.483468 -2.769874 0.551250 H -3.138341 2.763521 3.228825 H -1.561558 3.387331 3.607788 H 4.015448 -2.512691 -0.313505 H -4.015487 -2.512783 0.312869	N 4.578133 -0.543104 -1.948545 C 4.056600 -0.705153 -0.701865 C 4.866409 -0.915362 0.436467 C 6.257007 -0.955047 0.284266 C 6.803361 -0.784970 -0.997921 C 5.924240 -0.586681 -2.070918 C 2.574045 -0.676976 -0.594885 N 1.895675 0.130227 0.246037 N 2.621332 1.005427 0.997182 C 1.860809 1.766702 1.809116 S 0.104579 1.659623 1.843797 Fe 0.000003 0.000066 0.240136 N 0.361070 -1.351474 -1.124268 C 1.705943 -1.530444 -1.385048 C 2.132939 -2.503619 -2.315422 C 1.185656 -3.275673 -2.994067 C -0.180796 -3.071980 -2.731414 C -0.546459 -2.105636 -1.788309 N -0.361174 1.351463 -1.124375 C -1.706061 1.530354 -1.385126 C -2.133133 2.503410 -2.315587 C 1.185907 3.275437 -2.994341 C 0.180563 3.071839 -2.731702 C 0.546300 2.105615 -1.788502 C -2.574096 0.676937 -0.594839 N -1.895660 -0.130136 0.246152 N -2.621248 -1.005308 0.997406 C -1.860663 -1.766475 1.809385 S -0.104438 -1.659304 1.843937 C -4.056653 0.705020 -0.701792 C -4.866452 0.915265 0.436540 C -6.257055 0.954873 0.284361 C -6.803423 0.784705 -0.997807 C -5.924311 0.586404 -2.070808 N -4.578200 0.542895 -1.948456 N -2.524530 -2.622582 2.649695 N 2.524741 2.622754 2.649422 H -3.200990 2.635976 -2.497353 H -1.509424 4.029709 -3.717717 H 0.956817 3.650476 -3.238883 H 1.595651 1.923465 -1.542949 H -4.404915 1.053045 1.417344 H -6.903733 1.123555 1.151283 H -7.883968 0.807778 -1.166190 H -6.315327 -0.452713 -3.086982 C -3.960578 -2.864040 2.443398 C -1.796610 -3.681566 3.353849 H 3.200782 -2.636252 -2.497208 H 1.509115 -4.030040 -3.717370 H -0.957094 -3.650637 -3.238506 H -1.595795 -1.923421 -1.542739 H 4.404884 -1.053064 1.417287 H 6.903691 -1.123712 1.151187 H 7.883902 -0.808099 -1.166320 H 6.315244 -0.453061 -3.087107 C 3.960800 2.864128 2.443133 C 1.796901 3.681746 3.353652 H -2.426616 -4.055296 4.174543 H -1.549284 -4.527861 2.683861 H -0.863340 -3.285583 3.780541 H -4.366133 -3.342395 3.347091 H -4.482487 -1.914093 2.271580 H -4.140974 -3.529358 1.577709 H 2.427000 4.055457 4.174283 H 1.549518 4.528064 2.683713 H 0.863667 3.285783 3.780442 H 4.366421 3.342252 3.346918 H 4.482623 1.914173 2.271097 H 4.141220 3.529626 1.577585
<sup>3</sup> [Fe(TSC) <sub>2</sub> ]	Fe -0.060643 0.578771 0.043447 C -2.732174 -0.254757 -0.298104 C -2.019611 -1.116275 -1.218076 C -2.622923 -2.035594 -2.109479 H -3.709393 -2.142521 -2.122718 C -1.815235 -2.796887 -2.955118 H -2.268122 -3.512843 -3.647550 C -0.415812 -2.631740 -2.911646 H 0.249254 -3.213940 -3.554547 C 0.118144 -1.694726 -2.023836 H 1.196926 -1.522159 -1.959049 C -4.212705 -0.300921 -0.147238 C -5.006100 0.841493 -0.384168 H -4.534006 1.785667 -0.667547	C -4.829225 -1.481475 0.162185 C -4.166601 -0.269623 -0.148014 C -4.942153 0.902081 -0.322486 C -6.337438 0.859234 -0.192725 C -6.985500 -0.350689 0.116025 C -6.226685 -1.519792 0.291805 C -2.690756 -0.236789 -0.296937 N -1.878775 0.582723 0.418488 N -2.427357 1.363078 1.400040 C -1.526882 2.101965 2.038848 S 0.211390 2.044064 1.689717 Fe 0.000009 0.537508 0.000212 N -0.590677 -0.909881 -1.193573 C -1.968588 -1.093285 -1.201681	N -4.832063 -0.736072 1.659234 C -4.140351 -0.603763 0.490516 C -4.795967 -0.552643 -0.765332 C -6.190380 -0.635746 -0.812838 C -6.907108 -0.769381 0.389283 C -6.178335 -0.821510 1.584788 C -2.664436 -0.547650 0.578882 N -1.898827 0.325920 -0.140228 N -2.517546 1.309565 -0.854136 C -1.679398 2.071178 -1.555748 S 0.089124 1.849181 -1.479571 Fe -0.001413 0.034397 -0.129754 N -0.503417 -1.299322 1.224880 C -1.875239 -1.430691 1.401275



	<p>C -6.396515 0.738196 -0.259192  H -7.034849 1.607897 -0.444081  C -6.953300 -0.499421 0.099937  H -8.033871 -0.628480 0.210213  C -6.087118 -1.580593 0.313110  H -6.487906 -2.561954 0.594667  C -1.688480 2.141628 2.009173  N -0.652618 -0.950716 -1.198026  N -4.741656 -1.505480 0.197473  N -1.937235 0.584871 0.395143  N -2.553055 1.396808 1.315494  N -2.205723 3.025409 2.905117  H -3.196313 2.953409 3.138752  S 0.063620 2.062811 1.810011  H -1.589501 3.440858 3.600259  C 2.677881 -0.255065 0.304894  C 2.059644 -1.204904 1.215879  C 2.785319 -2.172657 1.952203  H 3.871732 -2.237809 1.849829  C 2.091706 -3.033885 2.806762  H 2.635129 -3.788439 3.383722  C 0.693159 -2.921178 2.916343  H 0.115143 -3.578288 3.571464  C 0.044586 -1.940712 2.153739  H -1.043263 -1.815842 2.200716  C 4.156050 -0.262499 0.064307  C 5.031329 0.344598 0.985232  H 4.631450 0.844543 1.872532  C 6.411489 0.295240 0.740426  H 7.115549 0.760210 1.437651  C 6.867005 -0.361895 -0.411444  H 7.933381 -0.428439 -0.645653  C 5.918965 -0.944546 -1.265477  H 6.243872 -1.471385 -2.170760  C 1.631034 2.312529 -1.801766  N 0.699759 -1.105149 1.324647  N 4.585052 -0.911025 -1.049638  N 1.862839 0.618074 -0.299235  N 2.476905 1.541314 -1.101286  N 2.207973 3.307849 -2.535452  H 3.219191 3.278468 -2.671066  S -0.113894 2.150521 -1.821794  H 1.652989 3.763432 -3.256360</p>	<p>C -2.538884 -2.061902 -2.070619  C -1.716007 -2.839620 -2.878564  C -0.311695 -2.657342 -2.827261  C 0.201890 -1.683395 -1.972518  N 0.590441 -0.911460 1.191863  C 1.968463 -1.094520 1.200438  C 2.538605 -2.063364 2.069269  C 1.715598 -2.841697 2.876448  C 0.311218 -2.659816 2.824577  C -0.202245 -1.685552 1.970157  C 2.690735 -0.237347 0.296528  N 1.878793 0.582985 -0.418153  N 2.427426 1.364181 -1.398997  C 1.527174 2.104105 -2.036854  S -0.211104 2.046242 -1.687756  C 4.166580 -0.270032 0.147778  C 4.942058 0.901705 0.322473  C 6.337359 0.858974 0.192882  C 6.985561 -0.350864 -0.115921  C 6.226842 -1.519997 -0.291927  C 4.829364 -1.481791 -0.162497  N 1.969818 3.003524 -2.974676  N -1.969274 3.000429 2.977605  H 3.624092 -2.184533 2.093318  H 2.153104 -3.586236 3.548244  H -0.367396 -3.248584 3.446358  H 1.300811 -1.491653 1.903820  H 4.444976 1.843737 0.572245  H 6.921998 1.773526 0.337408  H 8.075153 -0.380743 -0.218465  H 6.721544 -2.465267 -0.538485  H 2.923519 2.864159 -3.313004  H 1.300811 3.304612 -3.682242  H -3.624339 -2.183455 -2.094129  H -2.153602 -3.584001 -3.550474  H 0.366798 -3.245542 -3.449713  H 1.276069 -1.489228 -1.906521  H -4.445154 1.844175 -0.572203  H -6.922166 1.773756 -0.337070  H -8.075078 -0.380660 0.218701  H -6.721292 -2.465126 0.538304  H -2.923033 2.861243 3.315814  H -1.300120 3.301268 3.685130  H 4.242375 -2.392972 -0.317450  H -4.242136 -2.392634 0.316894</p>	<p>C -2.365339 -2.397384 2.321092  C -1.474413 -3.181387 3.046312  C -0.080266 -3.009133 2.867113  C 0.355234 -2.055612 1.949322  N 0.553474 1.149308 1.406156  C 1.927679 1.236588 1.557699  C 2.465847 2.043414 2.593569  C 1.610308 2.717834 3.460576  C 0.210918 2.588023 3.305297  C -0.270032 1.791075 2.266818  C 2.681979 0.475606 0.588330  N 1.892843 -0.256196 -0.241158  N 2.483267 -1.122245 -1.111296  C 1.613944 -1.759783 -1.901326  S -0.146644 -1.529354 -1.752700  C 4.162316 0.481023 0.508169  C 4.820108 0.668194 -0.730818  C 2.618177 0.679166 -0.765209  C 6.929225 0.501949 0.433813  C 6.195686 0.329049 1.615328  N 4.845603 0.311104 1.675411  N 2.111332 -2.595423 -2.872362  N -2.208801 3.023344 -2.403340  H 3.549162 2.105917 2.705290  H 2.023104 3.341775 4.259041  H -0.491369 3.104318 3.964150  H -1.341547 -0.629612 1.089217  H 4.236141 0.811266 -1.642897  H 6.745420 0.831204 -1.712432  H 8.022745 0.501260 0.455933  H 6.716004 0.190692 2.571283  C 3.522728 -3.002194 -2.788431  C 1.223003 -3.155819 -3.537507  H -3.443747 -2.486878 2.459964  H -1.853595 -3.923755 3.755270  H 0.649785 -3.607875 3.416990  H 1.419207 -1.885563 1.761613  H -4.210314 -0.463932 -1.682673  H -6.711726 -0.607212 -1.775048  H -7.998641 -0.837209 0.401642  H -6.700976 -0.931001 2.543465  C -3.643329 3.324144 -2.284228  C -1.378936 4.170105 -2.795601  H 1.729035 -3.930508 -4.439457  H 0.977776 -4.416201 -2.884714  H 0.288780 -3.063858 -3.845060  H 3.809803 -3.461959 -3.745383  H 4.157769 -2.126486 -2.601645  H 3.686459 -3.735516 -1.975552  H -1.885157 4.705290 -3.612388  H -1.221123 4.873680 -1.954309  H -0.399202 3.831117 -3.162578  H -3.947051 3.917657 -3.159472  H -4.222098 2.391363 -2.263328  H -3.870354 3.900080 -1.365995</p>
<sup>3</sup> TS1	<p>N 4.643991 -1.660201 0.266470  C 4.142680 -0.401996 0.160344  C 4.946452 0.726660 -0.100277  C 6.325860 0.548694 -0.262577  C 6.856171 -0.746751 -0.161843  C 5.978422 -1.806922 0.104272  C 2.672721 -0.256083 0.350770  N 1.858951 0.262639 -0.576047  N 2.380420 0.606098 -1.784262  C 1.460954 1.127998 -2.613677  S -0.239211 1.332527 -2.198234  Fe -0.000089 0.439318 -0.121700  N 0.621357 -0.446828 1.536094  C 1.977308 -0.684516 1.555747  C 2.586539 -1.294617 2.672983  C 1.790118 -1.713671 3.742372  C 0.398822 -1.516993 3.684350  C -0.142233 -0.870744 2.568389  N -0.480565 -1.344324 -0.780052  C -1.826781 -1.628996 -0.711084  C -2.314957 -2.906121 -1.070923  C -1.424995 -3.883266 -1.516522  C -0.054149 -3.575638 -1.592206  C 0.376012 -2.303075 -1.210097  C -2.646361 -0.532218 -0.255176  N -1.964547 0.565412 0.101174  N -2.708235 1.680498 0.293392  C -2.157892 2.628264 1.081095  S -0.785226 2.397507 2.109574  C -4.135209 -0.618521 -0.197141  C -4.888281 -0.787028 -1.375422</p>	<p>C -4.900378 -0.293317 0.993420  C -4.153878 -0.625850 -0.161345  C -4.842126 -1.041062 -1.324649  C -6.244607 -1.115104 -1.334121  C -6.976335 -0.783402 -0.182246  C -6.299763 -0.374149 0.981423  C -2.669277 -0.562621 -0.152122  N -1.972241 0.547028 0.142213  N -2.692705 1.688773 0.260882  C -2.113730 2.678226 0.969774  N -2.735568 3.891038 0.863428  C -1.843354 -1.696510 -0.510375  N -0.497598 -1.418378 -0.608746  C 0.360688 -2.410466 -0.952905  C -0.066100 -3.714742 -1.210821  C -1.434804 -4.018596 -1.094753  C -2.325885 -3.005329 -0.741109  Fe -0.008867 0.408924 -0.108586  N 0.679690 -0.346110 1.587464  C 2.041106 -0.551528 1.583796  C 2.697956 -1.045478 2.731687  C 1.944713 -1.387075 3.858477  C 0.547681 -1.230988 3.825712  C -0.042399 -0.697786 2.675048  C 2.693905 -0.217517 0.323863  N 1.838060 0.217059 -0.609552  N 2.313782 0.472967 -1.859507  C 1.362798 0.917732 -2.694584  N 1.735938 1.165239 -3.974157  C 4.154866 -0.365820 0.100913  C 4.785212 -1.617362 0.288836</p>	<p>N 4.635475 -1.467013 -0.406375  C 3.985847 -1.068112 0.719881  C 4.639848 -0.864862 1.950709  C 6.026301 -1.067671 2.023057  C 6.075605 -1.472412 0.867122  C 5.968683 -1.656441 -0.312160  C 2.508110 -0.892137 0.603542  N 1.945942 0.080139 -0.130822  N 2.783462 1.048406 -0.562470  C 2.358423 1.762072 -1.634284  N 3.019791 2.948035 -1.846105  C 1.570264 -1.740889 1.294484  N 0.249556 -1.376383 1.139898  C -0.711660 -2.092271 1.774026  C -0.416847 -3.190839 2.584137  C 0.926052 -3.583609 2.738323  C 1.923237 -2.856675 2.089165  Fe -0.033556 0.115918 -0.096538  N -0.578939 -1.234592 -1.441156  C -1.942826 -1.410513 -1.516022  C -2.500108 -2.328605 -2.433467  C -1.651577 -3.101235 -3.230305  C -0.258633 -2.951572 -3.102705  C 0.234132 -2.001904 -2.202423  C -2.701106 -0.581259 -0.591944  N -1.927927 0.182663 0.195462  N -2.519973 0.926288 1.159921  C -1.644360 1.645560 1.892061  N -2.149351 2.382025 2.923794  C -4.186579 -0.596126 -0.510507  N -4.772329 -1.809257 -0.329354</p>

	<p>C -6.284053 -0.889686 -1.278071  C -6.875344 -0.826408 -0.009234  C -6.041423 -0.665828 1.108797  N -4.697103 -0.563544 1.040117  N -2.802066 3.832680 1.050453  N 1.880103 1.476160 -3.851927  H -1.791571 -4.873813 -1.800625  H 0.680698 -4.306049 -1.939134  H 1.432980 -2.035134 -1.248806  H -4.384066 -0.831313 -2.345359  H -6.894627 -1.015305 -2.177597  H -7.958785 -0.902589 0.119879  H -6.472772 -0.620520 2.115948  H -2.615921 4.498938 1.796842  H -3.717030 3.874169 0.598978  H 3.666820 -1.448928 2.679394  H 2.248546 -2.195143 4.611096  H -0.261002 -1.842997 4.492124  H -1.211970 -0.665473 2.488092  H 4.492118 1.718620 -0.165773  H 6.975260 1.407011 -0.461003  H 7.926774 -0.935506 -0.282608  H 6.360338 -2.831207 0.191777  H 2.875818 1.450008 -0.4069361  H 1.253699 1.958935 -4.491255  O 1.247700 2.576435 0.237410  O 1.467942 3.424566 -0.693969</p>	<p>C 6.167434 -1.754614 0.082169  C 6.936492 -0.645813 -0.307444  C 6.317707 0.603886 -0.491182  C 4.937227 0.745009 -0.292100  S -0.325300 1.139489 -2.239624  S -0.727652 2.497951 1.993442  O 1.226923 2.593823 0.034231  O 1.367662 3.389016 -0.958292  H -3.394516 -3.205126 -0.636586  H -1.799291 -5.033837 -1.275729  H 0.669282 -4.472622 -1.491317  H 1.416581 -2.143381 -1.021674  H -4.274699 -1.294977 -2.226201  H -6.764072 -1.431364 -2.244514  H -8.069472 -0.843874 -0.189034  H -6.864533 -0.120281 1.884419  H -2.522967 4.605451 1.556321  H -3.657195 3.918322 0.424665  H 3.783771 -1.162544 2.723673  H 2.441137 -1.775468 4.752557  H -0.079786 -1.501169 4.678676  H -1.118745 -0.523737 2.610812  H 4.458143 1.718322 -0.432649  H 6.913000 1.473119 -0.789310  H 8.014234 -0.753646 -0.466999  H 6.641200 -2.731445 0.223536  H 2.728429 1.160545 -4.208290  H 1.093826 1.632268 -4.609900  H 4.187566 -2.486371 0.582667  H -4.377204 0.016379 1.903161</p>	<p>C -6.122575 -1.840622 -0.264841  C -6.938446 -0.706511 -0.377962  C -6.322636 0.540148 -0.570131  C -4.925395 0.599456 -0.635708  S 0.088049 1.625457 1.587691  S 1.111098 1.194775 -2.701704  O -1.089903 2.043425 -1.280209  O -1.334733 3.176332 -0.732949  H 2.976470 -3.131199 2.185191  H 1.187790 -4.445944 3.358236  H -1.232238 -3.724503 3.078290  H -1.742629 -1.765421 1.629038  H 4.068496 -0.549965 2.829092  H 6.560668 -0.911797 2.965400  H 7.787438 1.646028 0.872271  H 6.471932 -1.979245 -1.231481  C 2.990382 3.604605 -3.155599  C 4.169137 3.307223 -1.003256  H -3.584246 -2.436785 -2.493061  H -2.071331 -3.819393 -3.940934  H 0.439074 -3.547617 -3.696145  H 1.305484 -1.823561 -2.085461  H -4.406369 1.548761 -0.788788  H -6.920301 1.451396 -0.671294  H -8.026381 -0.802350 -0.318296  H -6.570178 -2.830636 -0.115029  C -3.598072 2.616533 3.027656  C -1.303177 3.332496 3.651950  H 3.184746 4.679502 -3.019196  H 3.762240 3.189600 -3.833165  H 2.004062 3.468495 -3.619416  H 4.350513 4.387803 -1.105813  H 3.956949 3.075317 0.048085  H 5.083762 2.765038 -1.309892  H -3.848813 2.809775 4.081452  H -3.900064 3.492528 2.423829  H -4.146963 1.735141 2.675686  H -1.790185 3.567826 4.609762  H -0.317424 2.890343 3.857790  H -1.163135 4.272140 3.084967</p>
<sup>1</sup> [Fe(TSC)(TSC <sub>3</sub> O <sub>2</sub> ) <sub>2</sub> ]	<p>N 4.919994 0.318491 1.362491  C 4.396638 0.238718 0.111708  C 5.182298 0.067921 -1.045645  C 6.572286 -0.029936 -0.903755  C 7.126653 0.040195 0.383043  C 6.263048 0.215779 1.473998  C 2.915194 0.356962 0.014602  N 2.137487 -0.565186 -0.557904  N 2.709303 -1.700263 -1.033265  C 1.806217 -2.572375 -1.508259  S 0.065274 -2.284398 -1.493037  Fe 0.237828 -0.177248 -0.618147  N 0.806796 1.394924 0.401652  C 2.172068 1.482797 0.559357  C 2.745284 2.594989 1.208422  C 1.911573 3.597491 1.712834  C 0.520420 3.480477 1.559016  C 0.002897 2.363079 0.894181  N -0.240739 -0.976624 1.185132  C -1.581923 -0.978836 1.468381  C -2.056409 -1.531884 2.677113  C -1.146231 -2.066206 3.593261  C 0.225493 -2.044543 3.293909  C 0.634847 -1.491588 2.077003  C -2.422298 -0.415019 0.408650  N -1.731522 0.045664 -0.639354  N -2.313940 0.529014 -1.753336  C -3.154670 1.582028 -1.732852  S -3.429197 2.706741 -0.434973  C -3.910120 -0.532797 0.444928  C -4.603875 -1.073119 -0.659860  C -5.989960 -1.247200 -0.567852  C -6.644274 -0.872234 0.615811  C -5.869992 -0.358189 1.665247  N -4.531056 -0.189676 1.602327  N -3.819010 1.769660 -2.925542  N 2.268945 -3.738223 -2.001442  H -3.127023 -1.517752 2.884356  H -1.504920 -2.496223 4.532889  H 0.971850 -2.449715 3.981469  H 1.690690 -1.463164 1.798453  H -4.063888 -1.351788 -1.568223  H -6.548260 -1.674095 -1.406796  H -7.726047 -0.984312 0.731309  H -6.343472 -0.067376 2.610771  H -4.156131 2.713826 -3.105986</p>	<p>C -4.629143 0.019171 1.565595  C -3.945353 -0.531087 0.457909  C -4.688754 -1.158022 -0.567828  C -6.086730 -1.232889 -0.481890  C -6.761308 -0.680628 0.621405  C -6.028927 -0.055242 1.644132  C -2.458470 -0.484954 0.394160  N -1.770537 0.002915 -0.632930  N -2.393729 0.401389 -1.772680  C -2.982443 1.594723 -1.861510  N -3.652068 1.801960 -3.060161  C -1.622584 -1.093639 1.433771  N -0.281407 -1.083882 1.155967  C 0.584546 -1.651169 2.024146  C 0.161925 -2.263736 3.208603  C -1.211299 -2.295259 3.498427  C -2.112327 -1.709028 2.603720  Fe 0.208185 -0.163434 -0.593014  O 0.260966 0.877062 -2.006246  O 1.295519 1.626207 -2.322336  N 2.114857 -0.553098 -0.556531  N 2.688063 -1.652051 -1.113350  C 1.787898 -2.488216 -1.647479  N 2.247398 -3.619284 -2.220925  C 2.898464 0.326864 0.073283  C 2.150882 1.404963 0.705595  N 0.784488 1.317971 0.559447  C -0.020499 2.230522 1.144345  C 0.496535 3.295773 1.892046  C 1.888191 3.419418 2.027900  C 2.723390 2.470594 1.428931  C 4.377691 0.225042 0.133528  C 5.041853 0.181098 1.380852  C 6.442156 0.096106 1.433300  C 7.192438 0.062773 0.246301  C 6.537755 0.111892 -0.997534  C 5.139484 0.188162 -1.057231  S 0.046100 -2.198291 -1.616550  S -3.032817 2.862975 -0.660873  H -3.186551 -1.731105 2.796693  H -1.578206 -2.777240 4.409023  H 0.900720 -2.711435 3.877724  H 1.642195 -1.616793 1.752432  H -4.170599 -1.591083 -1.427577  H -6.650215 -1.727961 -1.279395  H -7.852760 -0.738790 0.683429</p>	<p>N 4.331722 0.176902 2.190483  C 3.708007 0.650079 1.080485  C 4.356932 1.492231 0.149542  C 5.697448 1.833756 0.362084  C 6.356142 1.328656 1.494182  C 5.626007 0.518025 2.374071  C 2.257085 0.345153 0.915680  N 1.682676 0.042490 -0.261464  N 2.359187 -0.168645 -1.394192  C 3.411326 -1.025866 -1.492020  N 4.173363 -0.828324 -2.626801  C 1.299431 0.557821 1.999995  N -0.016741 0.467291 1.622905  C -0.994296 0.652942 2.538846  C -0.721417 0.948986 3.876731  C 0.620753 1.058741 4.277551  C 1.635704 0.863461 3.338408  Fe -0.301413 0.080310 -0.344989  O -0.201932 -0.425970 -2.026854  O -1.138818 -1.131219 -2.624104  N -2.226116 0.269312 -0.330231  N -2.891729 1.423512 -0.550015  C -2.076371 2.482093 -0.734161  N -2.645173 3.700946 -0.913471  C -2.927466 -0.835474 -0.047503  C -2.097238 -1.988318 0.253082  N -0.741968 -1.742858 0.217285  C 0.135844 -2.731164 0.501413  C -0.291789 -4.022907 0.827093  C -1.670088 -4.297126 0.853922  C -2.579971 -3.277222 0.563404  C -4.415609 -0.876028 -0.018909  N -4.980155 -1.282907 1.147504  C -6.330275 -1.333099 1.192213  C -7.162213 -0.999870 0.113884  C -6.564589 -0.587575 -1.087001  C -5.167259 -0.519423 -1.165696  S -0.310251 2.339129 -0.698134  S 3.725076 -2.352515 -0.409148  H 2.687625 0.920113 3.620187  H 8.874319 1.293304 5.315585  H -1.546666 1.091426 4.578561  H -2.022511 0.569109 2.179473  H 3.814773 1.873063 -0.720115  H 6.216158 2.491521 -0.342359  H 7.404312 1.564016 1.699199</p>

	<p>H -3.452176 1.263435 -3.734193  H 3.828928 2.651619 1.321499  H 2.344356 4.464538 2.219931  H -0.164471 4.245792 1.932546  H -1.074415 2.251472 0.711409  H 4.709410 0.023091 -2.029713  H 7.210456 -0.156541 -1.783610  H 8.206078 -0.034085 0.542967  H 6.663528 0.278525 2.492758  H 3.269304 -3.935153 -1.981579  H 1.632272 -4.446939 -2.357486  O 0.311248 0.728203 -2.124336  O 1.346051 1.457083 -2.477859</p>	<p>H -6.545682 0.379655 2.505663  H -3.765988 2.782492 -3.312946  H -3.356356 1.198842 -3.831584  H 3.809421 2.540813 1.516688  H 2.321155 4.249492 2.593420  H -0.190201 4.019218 2.338682  H -1.095782 2.126618 0.952807  H 4.631258 0.233164 -2.024692  H 7.118402 0.092997 -1.925359  H 8.284548 0.000381 0.288932  H 6.945697 0.054008 2.404276  H 3.246774 -3.821365 -2.212622  H 1.608521 -4.299646 -2.624677  H 4.458435 0.197340 2.306952  H -4.063689 0.517752 2.359188</p>	<p>H 6.100150 0.119974 3.279509  C 4.989060 -1.909648 -3.185926  C 3.769955 0.195836 -3.599534  H -3.656028 -3.457229 0.584350  H -2.032871 -5.300306 1.095705  H 4.505888 -4.796170 1.039363  H 1.203250 -2.479162 0.433064  H -4.660375 -0.206642 -2.072952  H -7.174858 -0.324956 -1.956640  H -8.249094 -1.065801 0.216517  H -6.764467 -1.658857 2.144923  C -4.095626 3.851048 -1.103661  C -1.833893 4.871381 -1.261714  H -4.442810 4.725415 -0.530679  H -4.324069 4.014753 -2.172161  H -4.613210 2.950381 -0.755693  H -2.445932 5.771923 -1.111220  H -0.946506 4.939696 -0.614183  H -1.508030 4.834979 -2.317347  H 4.612081 0.376677 -4.284499  H 2.894048 -0.126748 -4.195542  H 3.518435 1.135598 -3.089736  H 5.786956 -1.470249 -3.804463  H 5.436605 -2.496112 -2.372980  H 4.384632 -2.589060 -3.819369</p>
<sup>3</sup> [Fe(TSC)(TSC <sub>3</sub> )O <sub>2</sub> ]	<p>N 4.904161 0.234035 1.400041  C 4.395648 0.243048 0.140836  C 5.195330 0.166774 -1.016760  C 6.584687 0.071348 -0.865943  C 7.124008 0.049811 0.428848  C 6.246766 0.135441 1.519678  C 2.912715 0.349078 0.040058  N 2.153653 -0.538093 -0.603869  N 2.737861 -1.616497 -1.185886  C 1.843067 -2.432158 -1.764173  S 0.096399 -2.131485 -1.774595  Fe 0.240549 -0.193900 -0.621655  N 0.787775 1.345593 0.475874  C 2.150159 1.428941 0.656746  C 2.711878 2.505159 1.370888  C 1.868994 3.482614 1.910458  C 0.482530 3.380531 1.718069  C -0.021648 2.299007 0.985829  N -0.187731 -1.111439 1.091138  C -1.523792 -1.111064 1.412595  C -1.968323 -1.734880 2.597398  C -1.041450 -2.347104 3.445157  C 0.320402 -2.333038 3.103184  C 0.705553 -1.703964 1.916458  C -2.385252 -0.474071 0.415381  N -1.708056 0.048681 -0.613998  N -2.295909 0.596965 -1.693441  C -3.138088 1.645859 -1.617341  S -3.431489 2.693839 -0.261282  C -3.871504 -0.593696 0.469046  C -4.585224 -1.052412 -0.659786  C -5.969862 -1.230599 -0.556977  C -6.603291 -0.941727 0.661744  C -5.810031 -0.506563 1.732371  N -4.471936 -0.335263 1.658999  N -3.795605 1.897979 -2.802851  N 2.309619 -3.542972 -2.365973  H -3.031702 -1.712601 2.838897  H -1.379701 -2.831922 4.365425  H 1.078854 -2.800536 3.735546  H 1.752515 -1.674860 1.607892  H -4.061618 -1.265779 -1.594980  H -6.543181 -1.594954 -1.415101  H -7.683258 -1.060364 0.787056  H -6.266555 -0.285493 2.704693  H -4.134294 2.850347 -2.929852  H -3.416411 1.444916 -3.636978  H 3.793893 2.559430 1.499811  H 2.293384 4.320425 2.471137  H -0.208707 4.127501 2.116158  H -1.096373 2.198990 0.780694  H 4.734789 0.189300 -2.007440  H 7.233878 0.016592 -1.745120  H 8.202299 -0.026476 0.595407  H 6.635657 0.125279 2.544774  H 3.309259 -3.745034 -2.354180  H 1.675605 -4.209781 -2.799592  O 0.446723 0.894197 -2.142104  O 0.483576 2.204285 -2.184136</p>	<p>C -4.595342 -0.163538 1.596079  C -3.875553 -0.576018 0.451635  C -4.578718 -1.165653 -0.623915  C -5.968813 -1.341579 -0.550813  C -6.776625 -0.932093 0.592980  C -5.985144 -0.345391 1.666450  C -2.393232 -0.466875 0.393701  N -1.707088 0.069073 -0.624063  N -2.290380 0.642622 -1.694000  C -3.168980 1.660486 -1.592025  N -3.864726 1.892410 -2.760320  C -1.541632 -1.119869 1.386564  N -0.198186 -1.093147 1.099921  C 0.684084 -1.685282 1.936437  C 0.280097 -2.339078 3.103696  C -1.090847 -2.393515 3.404184  C -2.006478 -1.786771 2.540578  Fe 0.243608 -0.199002 -0.623185  O 0.483256 0.842462 -2.169412  O 0.759746 2.125256 -2.232633  N 2.153105 -0.556519 -0.580363  N 2.731848 -1.656720 -1.129254  C 1.835607 -2.477491 -1.694681  N 2.295814 -3.609678 -2.263269  C 2.916697 0.342761 0.042530  C 2.150893 1.444133 0.620655  N 0.787739 1.356462 0.447849  C -0.019933 2.321460 0.937985  C 0.487262 3.423522 1.637002  C 1.874857 3.533957 1.816712  C 2.715170 2.542198 1.299667  C 4.394070 0.241825 0.156049  C 5.004830 0.213985 1.430919  C 6.400705 0.118410 1.544393  C 7.199672 0.059396 0.390732  C 6.598713 0.094494 -0.880170  C 5.204541 0.180405 -1.000631  S 0.091284 -2.159184 -1.736185  S -3.440628 2.716348 -0.237169  H -3.077665 -1.827872 2.745514  H -1.444631 -2.910239 4.300952  H 1.030259 -2.802226 3.748932  H 1.737537 -1.635409 1.653182  H -4.033755 -1.492200 -1.514743  H -6.498884 -1.807682 -1.387784  H -7.760988 -1.072591 0.647697  H -6.528132 -0.021577 2.560339  H -4.220711 2.838468 -2.887146  H -3.500901 1.437246 -3.600289  H 3.799335 2.608595 1.410914  H 2.301816 4.389127 2.348521  H -0.202861 4.180314 2.018323  H -1.095948 2.217385 0.739991  H 4.739780 0.212193 -1.990193  H 7.218073 0.056018 -1.781998  H 8.288410 -0.011472 0.480643  H 6.861839 0.087757 2.536667  H 3.291867 -3.825751 -2.229885  H 1.657573 -4.283280 -2.679548  H 4.382846 0.252101 2.331088  H -4.065465 0.314004 2.425864</p>	<p>N 4.300629 0.163227 2.225046  C 3.682581 0.633469 1.110168  C 4.339069 1.470308 0.179168  C 5.680111 1.806708 0.395001  C 6.332729 1.303823 1.531775  C 5.595361 0.500635 2.412326  C 2.232261 0.336435 0.939953  N 1.651788 0.050892 -0.243349  N 2.303055 -0.182069 -1.382263  C 3.398042 -0.992555 -1.483058  N 4.133817 -0.764143 -2.623933  C 1.270783 0.551280 2.016938  N -0.048879 0.492699 1.631705  C -1.031868 0.695443 2.539481  C -0.763287 0.977306 3.880230  C 0.578264 1.049202 4.293421  C 1.596813 0.834947 3.363270  Fe -0.314375 0.137530 -0.301376  O -0.388899 -0.390608 -2.105100  O -0.589604 -1.599825 -2.579181  N -2.243334 0.290696 -0.298549  N -2.918237 1.435255 -0.538872  C -2.106692 2.490597 -0.758437  N -2.676223 3.702561 -0.967499  C -2.921938 -0.830203 -0.035722  C -2.307483 -1.977981 0.244780  N -0.718088 -1.720653 0.198921  C 0.169416 -2.713927 0.425192  C -0.242790 -4.017599 0.723207  C -1.618272 -4.299272 0.773573  C -2.539811 -3.277285 0.527773  C -4.410282 -0.897365 -0.006960  N -4.963452 -1.309370 1.162789  C -6.312492 -1.379269 1.213994  C -7.153702 -1.060562 0.138433  C -6.567468 -0.642087 -1.065829  C -5.171376 -0.554109 -1.141970  S -0.332171 2.347062 -0.759046  S 3.768041 -2.306729 -0.405634  H 2.647224 0.859495 3.655022  H 0.828101 1.268473 5.335687  H -1.591290 1.136795 4.574887  H -2.057810 0.635581 2.170378  H 3.801801 1.852355 -0.693237  H 6.203976 2.459840 -0.310013  H 7.381046 1.535836 1.739816  H 6.063933 0.105661 3.322074  C 5.065670 -1.758285 -3.157118  C 3.707209 0.263239 -3.582583  H -3.614000 -3.467333 0.556200  H -1.971240 -5.310489 0.995994  H 0.507862 -4.791700 0.900421  H 1.234399 -2.454507 0.348762  H -4.673585 -0.233910 -2.060825  H -7.185446 -0.389644 -1.933019  H -8.239061 -1.142145 0.245883  H -6.737531 -1.709302 2.169341  C -4.128555 3.851922 -1.145799  C -1.870672 4.873813 -1.329235  H -4.476729 4.713401 -0.553843  H -4.359365 4.037456 -2.209975</p>

			H -4.641591 2.942638 -0.814353 H -2.486280 5.772271 -1.180634 H -0.979186 4.949623 -0.688762 H -1.551997 4.832333 -2.386615 H 4.546809 0.474256 -4.261874 H 2.842746 -0.073941 -4.186124 H 3.429667 1.189616 -3.061412 H 5.881658 -1.238813 -3.684055 H 5.478924 -2.354973 -2.333409 H 4.565583 -2.441943 -3.871186
<b>Protonated structures</b>			
<sup>1</sup> [Fe(TSC)(TSC <sup>(SC<sup>NH</sup>N))]<sup>+</sup></sup>	N 4.609905 -1.608592 0.028869 C 4.126309 -0.349500 0.200396 C 4.958659 0.788017 0.254754 C 6.342528 0.620434 0.122288 C 6.852915 -0.674073 -0.060685 C 5.949028 -1.744831 -0.097081 C 2.650690 -0.229780 0.356693 N 1.877593 0.538144 -0.424942 N 2.478335 1.220682 -1.441220 C 1.610339 1.948689 -2.162563 S -0.113005 2.019378 -1.847046 Fe 0.001927 0.553245 -0.053616 N 0.548653 -0.690427 1.361624 C 1.904886 -0.939131 1.383448 C 2.466673 -1.784956 2.362024 C 1.635034 -2.393372 3.307266 C 0.253072 -2.144227 3.265381 C -0.246963 -1.284807 2.281027 N -0.518263 -0.934463 -1.209589 C -1.870188 -1.211454 -1.194734 C -2.416222 -2.237153 -1.988445 C -1.568659 -3.000995 -2.798207 C -0.193066 -2.718960 -2.801643 C 0.290857 -1.679955 -1.998417 C -2.639889 -0.327072 -0.328143 N -1.856046 0.562959 0.284577 N -2.400535 1.459747 1.172946 C -1.572059 2.342126 1.806065 S 0.110331 2.321542 1.452268 C -4.117008 -0.412035 -0.167082 C -4.941390 0.694636 -0.458968 C -6.327896 0.561371 -0.293024 C -6.839342 -0.667349 0.144186 C -5.939405 -1.714998 0.397122 N -4.601286 -1.610886 0.254239 N -2.134308 3.201559 2.668169 N 2.131536 2.692401 -3.170716 H -3.490679 -2.427071 -1.956407 H -1.977003 -3.802463 -3.420012 H 0.506038 -3.287816 -3.419718 H 1.352982 -1.425487 -1.981569 H -4.507449 1.629591 -0.826691 H -6.993022 1.401136 -0.515177 H -7.913084 -0.820212 0.283978 H -6.309390 -2.690469 0.733967 H -3.409869 1.431566 1.364009 H -3.131839 3.173095 2.884979 H 3.544043 -1.959316 2.363262 H 2.060676 -3.053393 4.068630 H -0.435162 -2.598431 3.982425 H -1.314893 -1.060789 2.219757 H 4.523840 1.779304 0.404865 H 7.010881 1.486094 0.166032 H 7.926228 -0.854447 -0.169348 H 6.313876 -2.769775 -0.235666 H 3.108618 2.555961 -3.428630 H 1.512678 3.134430 -3.846167 H -1.547287 3.857787 3.180313	C 4.712067 -1.620864 -0.041514 C 4.124828 -0.362496 0.223772 C 4.963215 0.764784 0.384922 C 6.355280 0.633944 0.279785 C 6.931032 -0.620554 0.010022 C 6.106601 -1.746411 -0.150522 C 2.649988 -0.239779 0.357519 N 1.883992 0.539573 -0.419478 N 2.495852 1.232371 -1.425439 C 1.636514 1.969327 -2.144864 N 2.167557 2.722841 -3.143855 C 1.889784 -0.956103 1.369980 N 0.534043 -0.702291 1.341751 C -0.269266 -1.309602 2.245844 C 0.220659 -2.186857 3.219947 C 1.601274 -2.442048 3.267894 C 2.441425 -1.820498 2.338484 Fe 0.003559 0.561565 -0.061969 S -0.089132 2.050907 -1.838318 N -1.857221 0.564395 0.269595 N -2.406261 1.442368 1.174727 C -1.584784 2.323029 1.816250 N -2.153247 3.172598 2.685046 C -2.643019 -0.318505 -0.352067 N -1.869168 -1.179325 -1.240279 N -0.515393 -0.907674 -1.241408 C 0.294854 -1.641660 -2.039777 C -0.188401 -2.660910 -2.868638 C -1.565844 -2.933355 -2.883944 C -2.414687 -2.181941 -2.063602 C -4.112193 -0.418219 -0.171332 C -4.687819 -1.627411 0.286688 C -6.075650 -1.725301 0.461614 C -6.904225 -0.623989 0.184616 C -6.340851 0.578495 -0.274060 C -4.953413 0.684672 -0.456538 S 0.099568 2.314636 1.465954 H 3.520199 -1.991770 2.352348 H 2.019259 -3.115004 4.022150 H -0.474189 -2.649042 3.925435 H -1.336123 -1.081070 2.181300 H 4.519213 1.741222 0.600509 H 6.993226 1.513941 0.411778 H 8.018237 -0.719345 -0.072798 H 6.547173 -2.725986 -0.362677 H 3.138710 2.561152 -3.410264 H 1.550253 3.146789 -3.832459 H -3.492709 -2.358479 -2.054539 H -1.974688 -3.716255 -3.528697 H 0.512320 -3.220728 -3.493127 H 1.358290 -1.393720 -2.009553 H -4.522297 1.615067 -0.841088 H -6.982127 1.435532 -0.502274 H -7.986883 -0.704195 0.323972 H -6.510001 -2.663941 0.819728 H -3.151126 3.137220 2.898766 H -1.570393 3.826548 3.204595 H 4.071474 -2.499256 -0.172188 H -4.042395 -2.481810 0.513254 H -3.419387 1.413943 1.347102	N 4.545669 -0.733058 -1.890310 C 4.046267 -0.832255 -0.628914 C 4.860740 -0.975028 0.514051 C 2.625322 -1.000486 0.348277 C 6.780379 -0.892560 -0.945326 C 5.888414 -0.768447 -2.022589 C 2.563092 -0.791431 -0.511968 N 1.881938 0.096831 0.218945 N 2.558293 1.075738 0.906312 C 1.834217 2.034873 1.573085 N 2.512276 3.034977 2.167089 C 3.986491 3.043875 2.187783 C 1.672625 -1.721678 -1.193679 N 0.335209 -1.494925 -0.940046 C -0.584059 -2.313263 -1.504220 C 2.562981 -3.381540 -2.335664 C 1.129844 -3.623774 -2.592349 C 2.090271 -2.787715 -2.012948 Fe -0.001709 0.021454 0.247428 S 0.114865 1.872775 1.627961 N -1.905784 -0.084697 0.266159 N -2.638621 -0.846294 1.120387 C -1.888984 -1.503323 2.027860 N -2.556529 -2.247386 2.961123 C -1.830188 -3.197284 3.807976 C -2.568314 0.613023 -0.672816 C -1.693485 1.353442 -1.563994 N -0.351294 1.196702 -1.287205 C 0.560701 1.854068 -2.040032 C 0.198682 2.700281 -3.093662 C -1.166210 2.879390 -3.377010 C -2.117873 2.203873 -2.607305 C -4.051201 0.627031 -0.795582 N -4.566800 0.259224 -2.003311 C -5.900989 0.277710 -2.143564 C -6.790341 0.647771 -1.125521 C -6.257645 1.031081 0.115493 C -4.867949 1.021015 0.285604 S -0.130686 -1.406535 2.058958 C 1.779069 4.055598 2.930853 C -3.991542 -2.519386 2.783902 H 3.156067 -2.943524 -2.190770 H 1.438609 -4.454995 -2.232383 H -1.014346 -4.009743 -2.764947 H -1.630180 -2.097975 -1.274397 H 4.411957 1.084210 1.506211 H 6.910405 -1.113871 1.215821 H 7.858984 -0.910127 -1.124507 H 6.269358 -0.689917 -3.047631 H -3.185712 2.318590 -2.802729 H -1.485392 3.539928 -4.188439 H 0.977447 3.205679 -3.670013 H 1.610889 1.692689 -1.783593 H -4.414297 1.318408 1.234420 H -6.913042 1.337592 0.936768 H -7.869145 0.639303 -1.305615 H -6.282347 -0.024611 -3.126446 H 4.319500 3.932254 2.737609 H 4.381942 2.148077 2.696648 H 4.392374 3.100064 1.163045 H 2.453222 4.903397 3.107791 H 0.907909 4.406233 2.355719 H 1.433416 3.657831 3.901057 H -2.474574 -3.475154 4.654742 H -1.555532 -4.114490 3.252679 H -0.913198 -2.735579 4.202907 H -4.414514 -2.807885 3.757539 H -4.502149 -1.621125 2.416108 H -4.157958 -3.344545 2.065979 H 3.577992 1.129131 0.802173
<sup>3</sup> [Fe(TSC)(TSC <sup>(SC<sup>NH</sup>N))]<sup>+</sup></sup>	C -4.989453 -1.105263 -0.095372 C -4.249004 0.094058 -0.049908 N -4.816518 1.318981 -0.207703 C -6.150487 1.359250 -0.423285 C -6.966950 0.221599 -0.489239	C -4.932575 1.462798 0.104991 C -4.265868 0.217268 0.165902 C -5.027856 -0.972650 0.101763 C -6.423024 -0.914478 -0.021731 C -7.077939 0.328509 -0.089314	N -4.789755 0.114701 -0.323347 C -4.074108 0.798622 0.618675 C -4.712257 1.341378 1.759257 C -6.099550 1.211150 1.890407 C -6.828589 0.538673 0.897294

	<p>C -6.370418 -1.037065 -0.317158  C -2.782271 0.087267 0.205216  C -2.175362 0.816597 1.299476  N -0.804762 0.688413 1.363646  C -0.120403 1.315289 2.349937  C -0.754984 2.087042 3.325031  C -2.157513 2.212129 3.281570  C -2.873076 1.574092 2.267412  Fe -0.046980 -0.495972 -0.059582  S 0.299072 -1.759481 -1.929122  C -1.422138 -1.876614 -2.329085  N -1.784078 -2.580669 -3.424211  H -1.092623 -3.092224 -3.966440  N 1.875422 -0.469268 0.350183  N 2.455903 -1.524268 0.999589  C 1.692564 -2.457545 1.645345  S -0.020116 -2.415556 1.625607  C 2.694923 0.464083 -0.166433  C 1.975672 1.631691 -0.711125  N 0.653017 1.416832 -0.966201  C -0.109704 2.435115 -1.413043  C 0.398479 3.719947 -1.639189  C 1.750042 3.960696 -1.344199  C 2.547981 2.913558 -0.868749  C 4.169396 0.342593 -0.230836  N 4.778867 -0.467535 0.687031  C 6.117198 -0.620314 0.646024  C 6.928854 0.016256 -0.301205  C 6.308693 0.810626 -1.277175  C 4.918995 0.973885 -1.251215  N 2.387203 -3.404794 2.302053  H 1.886927 -4.134854 2.804537  H 3.408306 -3.412799 2.310098  N -1.896416 -0.590253 -0.547194  N -2.387397 -1.286428 -1.618562  H -2.771171 -2.690138 -3.654216  H 3.588449 3.097034 -0.593089  H 2.179256 4.959131 -1.469200  H -0.255728 4.509972 -2.016782  H -1.164606 2.201653 -1.593308  H 4.421138 1.556969 -2.028232  H 6.898437 1.291118 -2.063420  H 8.011539 -0.131999 -0.286590  H 6.545537 -1.286075 1.402665  H -3.959468 1.657249 2.204803  H -2.685385 2.802733 4.035945  H -0.160814 2.574475 4.101790  H 0.964910 1.181871 2.345243  H -4.488260 -2.065703 0.047494  H -6.970712 -1.951516 -0.351687  H -8.041373 0.323848 -0.666586  H -6.583405 2.358595 -0.551303  H 3.512344 -1.394411 1.146449</p>	<p>C -6.329788 1.515418 -0.025241  C -2.789329 0.168521 0.319493  N -1.964282 -0.444993 -0.549306  N -2.536032 -1.012511 -1.659168  C -1.634275 -1.571449 -2.467345  N -2.078924 -2.180314 -3.590282  C -2.094364 0.777852 1.436997  N -0.725781 0.624736 1.395939  C 0.035055 1.161794 2.377637  C -0.515279 1.864192 3.452256  C -1.914993 2.006797 3.519966  C -2.710111 1.459859 2.511056  Fe -0.090856 -0.473376 -0.161653  S 0.109163 -1.565806 -2.144685  N 1.855832 -0.577763 0.191959  N 2.383964 -1.638784 0.884506  C 1.590941 -2.601470 1.450444  N 2.248353 -3.604664 2.059267  C 2.706063 0.352318 -0.244570  C 2.075786 1.473882 -0.945560  N 0.710249 1.451531 -0.961932  C 0.048598 2.443339 -1.590012  C 0.703208 3.503809 -2.231889  C 2.108011 3.524512 -2.229059  C 2.807276 2.499068 -1.582600  C 4.180854 0.279648 -0.054197  C 4.837883 1.259730 0.725893  C 6.226987 1.198692 0.908603  C 6.974065 0.166708 0.314400  C 6.329168 -0.806252 -0.467273  C 4.938935 -0.754197 -0.654411  S -0.115417 -2.514901 1.389083  H -3.798099 1.550708 2.540936  H -2.379400 2.538574 4.355469  H 0.140873 2.281387 4.220115  H 1.114857 1.013306 2.286775  H -4.522112 -1.940939 0.157623  H -7.001523 -1.843072 -0.063747  H -8.167303 0.370093 -0.189769  H -6.832101 2.486533 -0.080634  H -3.067249 -2.127621 -3.834867  H -1.421899 -2.539688 -4.278040  H 3.899639 2.483315 -1.572361  H 2.654121 4.329841 -2.728840  H 0.121436 4.289797 -2.720318  H -1.044857 2.380239 -1.571458  H 4.440639 -1.502546 -1.279871  H 6.907951 -1.605403 -0.940641  H 8.058235 0.123232 0.458374  H 6.726298 1.958992 1.517320  H 3.268385 -3.655429 2.074472  H 1.715956 -4.347162 2.508005  H -4.351185 2.389720 0.145148  H 4.254394 2.061336 1.189635  H 3.407026 -1.682097 0.985239</p>	<p>C -6.124034 -0.009809 -0.181112  C -2.606943 0.869911 0.435893  N -1.878681 -0.050825 -0.226802  N -2.562760 -1.027258 -0.899355  C -1.896295 -1.945130 -1.679314  N -2.671033 -2.870131 -2.288807  C -4.110628 -2.995644 -1.996396  C -1.796593 1.960978 1.007589  N -0.462773 1.692412 1.100889  C 0.374997 2.643459 1.560245  C -0.063359 3.911718 1.959865  C -1.429872 4.210244 1.835626  C -2.306545 3.233794 1.349602  Fe 0.069681 -0.158029 -0.036658  S -0.183553 -1.890118 -1.849871  N 1.952765 -0.331212 0.234265  N 2.539382 -1.124957 1.175680  C 1.652864 -1.785564 1.934807  N 2.140664 -2.665615 2.854284  C 1.284157 -3.226470 3.903103  C 2.774088 0.398528 -0.546984  C 2.081260 1.233781 -1.501927  N 0.707727 1.153432 -1.423689  C -0.075314 1.885645 -2.271165  C 0.501751 2.722152 -3.241509  C 1.905283 2.796359 -3.347356  C 2.700217 2.048644 -2.478302  C 4.259130 0.356431 -0.440739  N 4.871370 1.542997 -0.186401  C 2.622079 1.535870 -0.097846  C 7.009382 0.388102 -0.257500  C 6.366356 -0.829694 -0.528305  C 4.969187 -0.848908 -0.620163  S -0.101268 -1.547605 1.765163  C -2.088328 -3.818965 -3.247843  C 3.879161 -2.704580 3.119960  H -3.363317 3.468019 1.206945  H -1.811242 5.200540 2.101349  H 6.163228 2.085536 -2.338574  H 1.434841 2.369724 1.604183  H -4.130074 1.826395 2.545236  H -6.603586 1.620562 2.770823  H -7.912492 0.416592 0.966340  H -6.637298 -0.577644 -0.964273  H 3.789454 2.085536 -2.537610  H 2.371384 3.432251 -4.105720  H -0.153103 3.295775 -3.901959  H -1.531706 -3.321602 -2.157336  H 4.430885 -1.775589 -0.834490  H 6.942825 -1.749214 -0.669528  H 8.098108 0.452053 -0.174304  H 6.690455 2.504554 0.111408  H -4.433490 -4.005320 -2.282023  H -4.298744 -2.867647 -0.919433  H -4.704235 -2.259825 -2.566509  H -2.891289 -4.181629 -3.904212  H -1.321706 -3.321602 -3.859684  H -1.628650 -4.679683 -2.730787  H 1.748039 -4.152644 4.272857  H 1.164868 -2.524674 4.750045  H 0.290968 -3.468972 3.499026  H 3.824278 -3.656514 3.616924  H 4.144933 -2.634753 2.177694  H 3.895378 -1.870783 3.777703  H -3.614043 -0.821187 -0.954982</p>
<sup>1</sup> [Fe(TSC)(TSC <sup>SH</sup> <sub>s</sub> ) <sup>+</sup>	<p>N 4.593248 -1.619249 0.153911  C 4.117175 -0.348523 0.228966  C 4.952676 0.786813 0.189219  C 6.335460 0.603125 0.064964  C 6.839019 -0.703948 -0.019366  C 5.930922 -1.770761 0.030427  C 2.642029 -0.206645 0.379390  N 1.873661 0.487641 -0.468683  N 2.464102 1.050086 -1.560917  C 1.595785 1.729887 -2.326818  S -0.115375 1.919898 -1.950898  Fe -0.005817 0.565570 -0.083602  N 0.536005 -0.576860 1.426869  C 1.893990 -0.819524 1.467707  C 2.457673 -1.579778 2.512155  C 1.627137 -2.114108 3.502487  C 0.243943 -1.879644 3.437462  C -0.259695 -1.105053 2.386753  N -0.519058 -0.982045 -1.138022  C -1.872204 -1.253637 -1.118644  C -2.412272 -2.318934 -1.865407</p>	<p>C -4.667329 -1.658029 0.338803  C -4.115106 -0.443844 -0.132267  C -4.979492 0.632775 -0.439167  C -6.364867 0.494765 -0.274758  C -6.906410 -0.713094 0.199836  C -6.054726 -1.787269 0.506639  C -2.648076 -0.319998 -0.312941  N -1.883666 0.614595 0.259871  N -2.510315 1.500449 1.117314  C -1.715520 2.396020 1.643394  N -2.146715 3.367482 2.462882  C -1.870461 -1.227381 -1.148334  N -0.516322 -0.958761 -1.158853  C 0.299834 -1.741233 -1.905556  C -0.179125 -2.807523 -2.673631  C -1.557549 -3.076997 -2.685079  C -2.409721 -2.276880 -1.918348  Fe -0.004624 0.580600 -0.093699  S 0.105609 2.369838 1.289581  N 1.878944 0.490426 -0.466780  N 2.476626 1.047180 -1.560627</p>	<p>C 4.864550 0.290301 0.997172  C 4.033869 -0.809454 0.700508  N 4.513641 -2.057231 0.457612  C 5.854813 -2.325078 0.501654  C 6.759940 -1.188330 0.786225  C 6.250619 0.093740 1.041426  C 2.552781 -0.661434 0.660696  C 1.653358 -1.434030 1.501211  N 0.319253 -1.131636 1.314421  C -0.609629 -1.777366 2.060146  C -0.267455 -2.735256 3.019750  C 1.088572 -3.040959 3.226441  C 2.056222 -2.382964 2.462576  Fe 0.002229 0.235635 -0.028292  N -1.907088 0.244259 0.125217  N -2.607694 0.988095 1.018927  C -1.826358 1.768037 1.793897  N -2.439040 2.489430 2.774409  C -3.907191 2.564975 2.837871  N -0.383423 -1.136087 -1.390203  C -1.733070 -1.377028 -1.551446</p>

	<p>C -1.560879 -3.127391 -2.623726  C -0.183461 -2.852006 -2.625634  C 0.296508 -1.773209 -1.876042  C -2.644128 -0.329311 -0.300310  N -1.880730 0.604707 0.271936  N -2.509955 1.500020 1.116286  C -1.713373 2.395997 1.641148  S 0.109312 2.355395 1.299444  C -4.119550 -0.429127 -0.130823  C -4.960372 0.659964 -0.437754  C -6.343474 0.506146 -0.279154  C -6.838910 -0.723237 0.179866  C -5.924105 -1.749495 0.456722  N -4.586587 -1.627058 0.308514  N -2.144226 3.371065 2.454211  N 2.093086 2.320641 -3.437035  H -3.487424 -2.502572 -1.834775  H -1.965780 -3.958896 -3.207138  H 0.520259 -3.455880 -3.203922  H 1.359443 -1.524275 -1.863833  H -4.535092 1.598957 -0.800440  H -7.021610 1.331967 -0.514919  H -7.910875 -0.889552 0.319243  H -6.277796 -2.723039 0.816367  H 0.069689 3.447644 0.462884  H -3.136986 3.433249 2.686411  H 3.535656 -1.747375 2.531803  H 2.055381 -2.706022 4.316390  H -0.443463 -2.281307 4.185888  H -1.328130 -0.891002 2.304450  H 4.522268 1.788844 0.262306  H 7.007716 1.466387 0.038321  H 7.911029 -0.896882 -0.118754  H 6.290789 -2.804762 -0.031849  H 3.066231 2.160992 -3.696106  H 1.471531 2.760911 -4.110657  H -1.490781 3.994884 2.924223</p>	<p>C 1.617201 1.733199 -2.328055  N 2.123303 2.325343 -3.436119  C 2.641560 -0.207669 0.384230  C 1.879789 -0.808495 1.471900  N 0.522135 -0.564090 1.419815  C -0.281035 -1.089644 2.374955  C 0.213175 -1.861765 3.432211  C 1.595680 -2.095795 3.510483  C 2.434096 -1.564307 2.525047  C 4.112626 -0.368387 0.249284  C 4.678682 -1.659560 0.140269  C 6.069093 -1.819120 0.026219  C 6.910740 -0.694702 0.026818  C 6.356405 0.592719 0.141039  C 4.968228 0.757814 0.249475  S -0.094469 1.941149 -1.958052  H -3.487941 -2.450127 -1.910273  H -1.962936 -3.895314 -3.286520  H 0.525706 -3.404416 -3.257813  H 1.363134 -1.494375 -1.885626  H -4.563066 1.570414 -0.817892  H -7.024249 1.332952 -0.521889  H -7.988560 -0.816364 0.328984  H -6.468422 -2.729391 0.880151  H 0.054332 3.461235 0.452393  H -3.136841 3.416219 2.708656  H 3.513793 -1.724891 2.559845  H 2.017171 -2.683554 4.330902  H -0.480778 -2.260516 4.176171  H -1.348593 -0.874671 2.283801  H 4.542617 1.761051 0.345352  H 7.008084 1.472531 0.148589  H 7.994903 -0.820066 -0.059523  H 6.492437 -2.824585 -0.065493  H 3.088154 2.133228 -3.704359  H 1.501008 2.743663 -4.123062  H -1.491073 3.975249 2.950462  H 4.024753 -2.537829 0.133269  H -4.005750 -2.493809 0.588274</p>	<p>C -2.184930 -2.307093 -2.510982  C -1.254982 -3.006573 -3.286469  C 0.116536 -2.767322 -3.097471  C 0.508162 -1.823061 -2.142437  C -2.588907 -0.582592 -0.683841  C -4.073426 -0.690550 -0.687651  C -4.882095 0.446592 -0.896681  C -6.273800 0.293973 -0.909310  C -6.815780 -0.984987 -0.709719  C -5.934377 -2.056616 -0.510727  N -4.587928 -1.934619 -0.497960  S -0.072163 1.869911 1.585874  N 1.904316 0.196014 -0.135006  N 2.666996 0.949703 -0.997083  C 1.985915 1.799934 -1.739856  N 2.602001 2.702504 -2.525080  C 1.942271 3.491651 -3.572524  C -1.714358 3.532664 3.505002  S 0.125975 1.758558 -1.689973  C 4.073469 2.774678 -2.508019  H 3.118882 -2.593682 2.594157  H 1.387062 -3.779341 3.975765  H -1.059042 -3.222495 3.594439  H -1.651964 -1.505420 1.881594  H 4.427411 1.271853 1.197314  H 6.919999 0.927082 1.275997  H 7.834727 -1.389600 0.809186  H 6.219585 -3.234607 0.299269  H -3.256397 -2.474593 -2.630959  H -1.597730 -3.730082 -4.031767  H 0.878579 -3.292510 -3.678380  H 1.563622 -1.598031 -1.968774  H -4.422266 1.425516 -1.053094  H -6.923506 1.158616 -1.077029  H -7.896551 -1.153086 -0.710169  H -6.323529 -3.069801 -0.353472  H -4.201752 2.765434 3.878750  H -4.292948 3.379054 2.196593  H -4.345782 1.615619 2.508460  H -2.281518 3.780560 4.413852  H -0.716716 3.174466 3.800188  H -1.599160 4.450599 2.898610  H 4.371367 3.751502 -2.914229  H 4.441312 2.673089 -1.477930  H 4.510589 1.974001 -3.129341  H 2.077282 4.566527 -3.369880  H 2.400155 3.251214 -4.546936  H 0.869611 3.265008 -3.625054  H 0.014147 2.995966 -1.097411</p>
<sup>1</sup> [Fe(TSC)(TSC <sup>(NH)<sub>s</sub>)]<sup>+</sup></sup>	<p>N 4.596406 -1.510438 0.587680  C 4.125655 -0.266103 0.304964  C 4.968758 0.805092 -0.058198  C 6.349312 0.584354 -0.133547  C 6.846069 -0.696930 0.151586  C 5.932502 -1.699661 0.504984  C 2.653805 -0.079297 0.420985  N 1.878275 0.383449 -0.571167  N 2.473743 0.660232 -1.767056  C 1.603770 1.107663 -2.687395  S -0.110223 1.334727 -2.386697  Fe -0.002043 0.516710 -0.223012  N 0.552863 -0.166449 1.526255  C 1.910540 -0.389153 1.631340  C 2.475255 -0.837050 2.843695  C 1.646789 -1.073569 3.945019  C 0.264292 -0.854905 3.821980  C -0.239857 -0.399549 2.598977  N -0.494582 -1.271077 -0.835260  C -1.845783 -1.545433 -0.752996  C -2.366273 -2.776124 -1.197055  C -1.498268 -3.745495 -1.711595  C -0.124479 -3.464178 -1.774744  C 0.334930 -2.218129 -1.330887  C -2.632039 -0.440965 -0.218232  N -1.868605 0.616939 0.085344  N -2.501436 1.721827 0.635475  C -1.636352 2.675495 0.891099  S 0.054638 2.695860 0.625708  C -4.106003 -0.497408 -0.038814  C -4.947735 0.490016 -0.592095  C -6.330780 0.379155 -0.401383  C -6.828048 -0.708607 0.331994  C -5.913846 -1.644026 0.838019  N -4.576345 -1.560449 0.667364  N -2.286419 3.879698 1.473420  N 2.115718 1.428877 -3.901501</p>	<p>C -4.682262 1.539869 0.529036  C -4.126892 0.257767 0.311848  C -4.991429 -0.821323 0.015095  C -6.376833 -0.618693 -0.064752  C -6.920088 0.661407 0.145797  C -6.069606 1.739272 0.442381  C -2.658168 0.058058 0.418642  N -1.879105 -0.381358 -0.580796  N -2.472158 -0.629659 -1.786717  C -1.600228 -1.054488 -2.713632  N -2.109323 -1.356569 -3.936231  C -1.914493 0.331276 1.638288  N -0.556092 0.109700 1.532519  C 0.231362 0.315162 2.614574  C -0.277087 0.743258 3.846075  C -1.659395 0.963420 3.968665  C -2.483372 0.753152 2.858341  Fe 0.003302 -0.520631 -0.234189  S 0.115274 -1.285483 -2.417399  N 1.873965 -0.614118 0.075546  N 2.512099 -1.728508 0.601116  C 1.653654 -2.694304 0.828065  N 2.311298 -3.907010 1.386027  C 2.634180 0.453659 -0.203686  C 1.836888 1.561652 -0.718267  N 0.485326 1.284816 -0.798046  C -0.348709 2.241835 -1.267027  C 0.104242 3.499033 -1.685724  C 1.478033 3.781470 -1.629827  C 2.351180 2.801572 -1.144224  C 4.103800 0.519422 -0.028584  C 4.677794 1.552598 0.750063  C 6.069088 1.624297 0.918861  C 6.904707 0.674005 0.308622  C 6.342698 -0.352001 -0.471774  C 4.953322 -0.432932 -0.639775  S -0.036810 -2.725910 0.553402</p>	<p>N -4.478309 -1.048295 -1.852207  C -3.997353 -0.024089 -1.097840  C -4.830377 0.935662 -0.485830  C -6.216755 0.828767 -0.653745  C -6.726227 -0.230543 -1.419859  C -5.819288 -1.132490 -1.994786  C -2.519089 0.038705 -0.960061  N -1.867614 0.077459 0.210236  N -2.632313 0.029908 1.365039  C -1.872167 0.046645 2.433112  N -2.642316 -0.066426 3.716692  C -3.410766 -1.301802 3.864585  C -1.606578 0.057479 -2.095024  N -0.275680 0.120723 -1.731683  C 0.665651 0.157783 -2.702747  C 0.343110 0.140677 -4.065392  C -1.007746 0.091271 -4.444728  C -1.991136 0.053779 -3.449941  Fe 0.026182 0.156176 0.199712  S -0.162837 0.130194 2.523213  N 1.935999 0.268898 0.153883  N 2.651720 1.421588 0.067994  C 1.882830 2.528820 0.091238  N 2.527996 3.732642 0.058855  C 1.780877 4.978987 -0.126191  C 2.617695 -0.889758 0.149086  C 1.760631 -2.060590 0.190009  N 0.412323 -1.767231 0.216901  C -0.484285 -2.780020 0.268343  C -0.099963 -4.124905 0.300585  C 1.270550 -4.436214 0.288801  C 2.206456 -3.398843 0.237022  C 4.102330 -0.974276 0.093973  N 4.232422 -1.695880 -0.933898  C 5.970348 -1.796880 -0.999545  C 6.846078 -1.207084 -0.077897  C 6.297137 -0.469594 0.983041</p>

	<p>H -3.439840 -2.959484 -1.128198  H -1.889914 -4.705258 -2.059877  H 0.592139 -4.189224 -2.168760  H 1.395117 -1.959700 -1.375946  H -4.522289 1.316409 -1.166402  H -7.008399 1.127339 -0.824145  H -7.900124 -0.836651 0.506528  H -6.268610 -2.508188 1.412309  H -3.308129 3.725608 1.549666  H -1.919448 4.088262 2.419664  H 3.552939 -0.998610 2.904321  H 2.074982 -1.422071 4.889276  H -0.421466 -1.028675 4.654904  H -1.307687 -0.211314 2.463172  H 4.543941 1.789893 -0.267808  H 7.025667 1.400780 -0.405378  H 7.916386 -0.917365 0.105061  H 6.286483 -2.712042 0.734271  H 3.088954 1.202135 -4.103879  H 1.496864 1.648649 -4.678306  H -2.125697 4.716238 0.883590</p>	<p>H -3.563096 0.906586 2.921793  H -2.090781 1.290767 4.919035  H 0.405568 0.894458 4.685956  H 1.299223 0.126358 2.479653  H -4.574544 -1.820460 -0.142880  H -7.035287 -1.464068 -0.289943  H -8.001879 0.816761 0.080448  H -6.484113 2.739534 0.604915  H -3.077155 -1.107921 -4.139550  H -1.483121 -1.529611 -4.719089  H 3.427300 2.982212 -1.096447  H 1.865799 4.747992 -1.963418  H -0.617123 4.230553 -2.058567  H -1.408517 1.981949 -1.311610  H 4.520714 -1.226139 -1.255928  H 6.989478 -1.091146 -0.955355  H 7.989978 0.732404 0.439684  H 6.498848 2.423026 1.531793  H 3.334241 -3.754417 1.447556  H 1.959300 -4.125548 2.335754  H -4.021042 2.382918 0.755347  H 4.028985 2.287431 1.237402  H 2.139562 -4.736668 0.789895</p>	<p>C 4.905024 -0.348820 1.071445  S 0.123384 2.460833 0.184927  C -3.538917 1.200745 3.887475  C 3.959365 3.789094 -0.273219  H -3.051816 0.011590 -3.704208  H -1.292675 0.085683 -5.500498  H 1.146432 0.172448 -4.805819  H 1.704589 0.207816 -2.369109  H -4.394054 1.750809 0.096520  H -6.886908 1.563303 -0.196580  H -7.801342 -0.355773 -1.576839  H -6.182938 -1.969814 -2.602331  H 3.278099 -3.606230 0.224701  H 1.606675 -5.476596 0.322434  H -0.866141 -4.903268 0.338002  H -1.538559 -2.493243 0.283029  H 4.438717 0.212383 1.885138  H 4.624106 0.000304 1.732198  H 7.927392 -1.328181 -0.189539  H 6.364483 -2.381553 -1.839539  H -3.840557 -1.318570 4.875038  H -4.198345 -1.321102 3.101574  H -2.710056 -2.136367 3.727710  H -3.981849 1.146826 4.890891  H -2.922006 2.103659 3.785750  H -4.313922 1.164390 3.112153  H 2.399706 5.815892 0.230292  H 1.529416 5.154068 -1.189780  H 0.849918 4.958120 0.458963  H 4.363730 4.748216 0.082595  H 4.493805 2.965001 0.215427  H 4.119440 3.719030 -1.365626  H -1.944031 0.025422 4.480555</p>
$^3[\text{Fe}(\text{TSC})(\text{TSC}^{\text{NH}})_2]^+$	<p>N 4.689381 -1.494583 0.181432  C 4.168208 -0.240525 0.211454  C 4.956525 0.924207 0.123449  C 6.344663 0.787590 -0.004927  C 6.895881 -0.501913 -0.046661  C 6.030779 -1.600889 0.052466  C 2.687104 -0.154744 0.352814  N 1.895608 0.454776 -0.536783  N 2.460672 1.013955 -1.641332  C 1.549520 1.542168 -2.471137  S -0.193259 1.508588 -2.165511  Fe 0.005127 0.503373 -0.156794  N 0.599230 -0.570974 1.416776  C 1.961323 -0.752528 1.464628  C 2.550328 -1.451288 2.539481  C 1.732567 -1.974518 3.544968  C 0.340208 -1.794087 3.470013  C -0.187360 -1.083133 2.387430  N -0.584171 -1.201104 -0.927221  C -1.963286 -1.403204 -0.886498  C -2.512204 -2.545964 -1.537235  C -1.675958 -3.457316 -2.167361  C -0.274634 -3.243658 -2.167122  C 0.220194 -2.101099 -1.543187  C -2.697954 -0.372367 -0.216827  N -1.873163 0.633524 0.247820  N -2.395814 1.639266 0.988510  C -1.489444 2.497903 1.391618  S 0.230156 2.424707 1.086866  C -4.166215 -0.357141 -0.073942  C -4.916735 0.825870 -0.289909  C -6.307808 0.786643 -0.154325  C -6.925253 -0.426495 0.192913  C -6.107893 -1.550991 0.375913  N -4.763280 -1.540250 0.258215  N -2.030653 3.630457 2.173133  N 1.997042 2.126725 -3.601641  H -3.593375 -2.690665 -1.514518  H -2.100645 -4.334473 -2.664843  H 0.415860 -3.941962 -2.645579  H 1.290700 -1.879870 -1.530344  H -4.410733 1.750408 -0.575555  H -6.902987 1.689102 -0.326717  H -8.009431 -0.504129 0.313954  H -6.553802 -2.517608 0.642076  H -3.050825 3.506032 2.302608  H -1.597553 3.699415 3.111905  H 3.633295 -1.580146 2.570416  H 2.177714 -2.517887 4.383331  H -0.331847 -2.188317 4.236047  H -1.260790 -0.903998 2.284943  H 4.487099 1.910538 0.161355  H 6.984015 1.673395 -0.069321</p>	<p>C -4.845800 1.468872 0.465072  C -4.239284 0.217856 0.205517  C -5.055780 -0.873355 -0.173895  C -6.443674 -0.712927 -0.290205  C -7.037955 0.535901 -0.034188  C -6.235749 1.625374 0.342555  C -2.770356 0.060681 0.358905  N -1.950572 -0.365312 -0.619430  N -2.516379 -0.637044 -1.838858  C -1.619064 -1.051117 -2.735170  N -2.062800 -1.373616 -3.971961  C -2.077845 0.353931 1.600524  N -0.712987 0.172215 1.540659  C 0.039926 0.413550 2.639615  C -0.514890 0.832772 3.851009  C -1.910715 1.001690 3.932040  C -2.697646 0.760968 2.804034  Fe -0.071709 -0.483416 -0.249378  S 0.114208 -1.214233 -2.389527  N 1.872047 -0.603753 0.056776  N 2.517223 -1.741314 0.498301  C 1.713781 -2.726658 0.830843  N 2.524414 -3.921518 1.245806  C 2.667781 0.449085 -0.178356  C 1.973427 1.653297 -0.635611  N 0.607510 1.566755 -0.638099  C -0.118067 2.618804 -1.067148  C 0.467529 3.812741 -1.509541  C 1.869767 3.905859 -1.523087  C 2.633415 2.817720 -1.087654  C 4.145458 0.430396 -0.016287  C 4.762553 1.340103 0.872958  C 6.157931 1.346084 1.026851  C 6.953003 0.457510 0.284376  C 6.347106 -0.441095 -0.612032  C 4.953138 -0.460648 -0.760141  S 0.018521 -2.872163 0.869814  H -3.782996 0.877506 2.841016  H -2.378826 1.315435 4.869637  H 0.134328 1.013183 4.711307  H 1.116754 0.257346 2.528839  H -4.599292 -1.848107 -0.367885  H -7.064462 -1.567692 -0.577973  H -8.121900 0.657926 -0.127679  H -6.689493 2.601952 0.540100  H -3.040557 -1.212265 -4.211881  H -1.407229 -1.600498 -4.715778  H 3.724863 2.857048 -1.105745  H 2.364341 4.816072 -1.874724  H -0.164175 4.643892 -1.833603  H -1.206121 2.494360 -1.045715  H 4.485772 -1.157322 -1.461952  H 6.963091 -1.129028 -1.200148</p>	<p>C 4.790771 -0.536850 1.776549  C 4.069989 -0.846922 0.607169  N 4.661044 -1.238773 -0.551178  C 6.009660 -1.311493 -0.555086  C 6.815363 -1.008275 0.553336  C 6.189832 -0.615303 1.744765  C 2.576992 -0.777421 0.610320  C 1.768637 -1.727538 1.365243  N 0.146241 -1.546586 1.253086  C -0.413921 -2.379355 1.911606  C 0.048793 -3.432803 2.711946  C 1.435982 -3.627504 2.829263  C 2.308443 -2.771204 2.150250  Fe -0.067801 0.198192 0.003159  N 1.892838 0.153928 -0.061184  N 2.663622 1.107632 -0.693152  C 1.991756 1.884838 -1.517623  N 9.298419 2.930745 -2.078844  C 2.600417 4.313135 -1.573904  N -1.975404 0.276537 0.144286  N -2.660262 1.046803 1.040771  C -1.852518 1.780255 1.820472  N -3.425414 2.526063 2.805200  C -2.890659 2.652163 2.867674  C -2.701122 -0.521342 -0.661131  C -1.902269 -1.329957 -1.556832  N -0.543623 -1.143540 -1.420309  C 0.306936 -1.846228 -2.204734  C -0.139682 -2.754126 -3.167482  C -1.526962 -2.937895 -3.331928  C -2.414112 -2.222876 -2.526335  C -4.189616 -0.587797 -0.626083  C -4.975772 0.547050 -0.911260  C -6.370822 0.427299 -0.879461  C -6.935238 -0.818159 -0.563446  C -6.072999 -1.891293 -0.299142  N -4.723966 -1.800754 -0.324064  S -0.079305 1.767957 1.629105  S 0.352728 1.879903 -1.986819  C 3.021334 2.888003 -3.582001  H 1.669651 3.544349 3.541254  H 3.390989 -2.902235 2.220894  H 1.833574 -4.441863 3.441949  H -0.664675 -4.086724 3.219920  H -1.485710 -2.193903 1.782157  H 4.260719 -0.235607 2.685020  H 7.794446 -0.372565 2.634808  H 6.9703788 -1.085898 0.479088  H 6.468483 -1.632009 -1.497942  H -3.493637 -2.345917 -2.630630  H -1.909182 -3.632762 -4.085441  H 0.585754 -3.297715 -3.777778  H 1.373082 -1.659445 -2.048013</p>

	<p>H 7.973602 -0.657842 -0.149040  H 6.428009 -2.622499 0.025425  H 2.991376 2.097628 -3.826250  H 1.347039 2.496825 -4.290973  H -1.879695 4.537974 1.695575</p>	<p>H 8.041465 0.466180 0.401066  H 6.621847 2.047941 1.727215  H 3.535410 -3.708300 1.170105  H 2.317354 -4.190916 2.223288  H -4.222868 2.322344 0.752165  H 4.144084 2.032947 1.452880  H 2.312217 -4.738091 0.646421</p>	<p>H -4.496355 1.498137 -1.157015  H -7.005281 1.291229 -1.100918  H -8.019103 -0.959805 -0.525037  H -6.479831 -2.878733 -0.050183  H 3.386387 4.994204 -1.927438  H 1.621442 4.607910 -1.973608  H 2.579944 4.281176 -0.476203  H 3.804007 3.595756 -3.887020  H 3.284287 1.865093 -3.883696  H 2.049195 3.180133 -4.000306  H -4.167626 2.969956 3.883453  H -4.260186 3.403773 2.146234  H -4.361080 1.686328 2.644494  H -2.150365 3.698660 4.518708  H -0.635021 3.212627 3.706460  H -1.654835 4.506990 2.996330  H 3.859210 2.673560 -1.699668</p>
<sup>3</sup> TS1(SCMHN)	<p>C 4.835994 0.160869 -1.222954  C 4.148168 -0.339139 -0.099890  N 4.722896 -1.154826 0.821637  C 6.016527 -1.492244 0.623372  C 6.781935 -1.048996 -0.464655  C 6.176823 -0.201373 -1.404911  C 2.720297 0.012292 0.147223  C 2.250693 0.604080 1.394033  N 0.888640 0.787220 1.444850  C 0.320288 1.247914 2.582317  C 1.077409 1.585935 3.708627  C 2.475815 1.460257 3.647613  C 3.069764 0.964719 2.482558  Fe -0.014639 0.308200 -0.234863  S -0.611926 -0.388218 -2.341645  C 0.989085 -1.030699 -2.696980  N 1.195237 -1.678536 -3.863320  H 0.454873 -1.755068 -4.556309  N -2.006563 0.585198 0.095521  N -2.759691 1.657435 -0.272185  C -2.259223 2.938103 -0.299152  S -0.654857 3.302941 0.109919  C -2.681791 -0.547943 0.357022  C -1.808432 -1.624196 0.821532  N -0.476489 -1.435998 0.547110  C 0.416123 -2.375301 0.949374  C 0.036548 -3.517961 1.656804  C -1.313024 -3.689102 1.997580  C -2.240404 -2.731524 1.579970  C -4.135495 -0.749331 0.140504  N -4.931139 0.360826 0.150195  C -6.253871 0.230031 -0.068283  C -6.865280 -1.006143 -0.311367  C -6.051429 -2.146501 -0.372559  C -4.674060 -2.023587 -0.152918  N -3.165385 3.862987 -0.676861  H -2.908913 4.847844 -0.662759  H -4.134155 3.610573 -0.878886  O 1.013373 1.972086 -1.634567  O 2.185035 2.396233 -1.357099  N 1.737078 -0.268153 -0.714254  N 2.036383 -0.925756 -1.862835  H 2.130677 -2.008671 -4.098578  H -3.290775 -2.819666 1.861928  H -1.639182 -4.548958 2.588746  H 0.801005 -4.241312 1.950021  H 1.463537 -2.197940 0.706029  H -4.026975 -2.898240 -0.240688  H -6.479490 -3.126006 -0.604203  H -7.944364 -1.062924 -0.474965  H -6.834766 1.157868 -0.054704  H 4.150923 0.835230 2.409561  H 3.096968 1.737271 4.504186  H 0.573012 1.948858 4.607370  H -0.766905 1.350799 2.571238  H 4.327030 0.824466 -1.926179  H 6.739270 0.175351 -2.264799  H 7.825842 -1.359183 -0.565946  H 6.459233 -2.152920 1.378218  H -3.816490 1.473593 -0.160065</p>	<p>C -4.809526 -1.567559 -0.718836  C -4.143292 -0.695072 0.173517  C -4.897229 0.071177 1.094549  C -6.294994 -0.038718 1.118155  C -6.951961 -0.902373 0.224758  C -6.208587 -1.663852 -0.692922  C -2.659300 -0.601341 0.148852  C -1.808287 -1.756297 0.384359  N -0.469012 -1.541350 0.156466  C 0.394127 -2.570271 0.345481  C -0.027837 -3.834401 0.769186  C -1.390746 -4.056733 1.018602  C -2.289407 -3.004974 0.824008  Fe 0.008406 0.301103 -0.333654  N 1.823048 -0.163321 -0.680456  N 2.266286 -0.652632 -1.869235  C 1.316253 -0.668819 -2.816338  N 1.659566 -1.161619 -4.027418  N 0.707183 0.589835 1.483339  C 2.071999 0.435394 1.563771  C 2.755031 0.686047 2.770873  C 2.024019 1.039616 3.910017  C 0.624908 1.135815 3.827889  C 0.005762 0.912243 2.593333  C 2.699263 0.005449 0.317066  C 4.150858 -0.287427 0.200291  C 4.950231 0.367496 -0.764409  C 6.319118 0.080891 -0.859372  C 6.907084 -0.865471 -0.001165  C 6.119891 -1.521350 0.959442  C 4.749770 -1.233378 1.064397  S -0.334731 -0.104179 -2.561744  N -1.978788 0.509411 -0.132093  N -2.724490 1.579542 -0.555980  C -2.297002 2.878772 -0.423342  N -3.159764 3.805008 -0.882638  O 1.182863 2.203673 -1.416518  O 2.301496 2.593369 -0.952067  S -0.790826 3.248008 0.264451  H 1.005135 -1.123097 -4.805107  H -2.915174 4.789611 -0.801358  H -4.074617 3.555646 -1.263096  H 2.630179 -1.412276 -4.213354  H -3.358217 -3.131074 1.009257  H -1.747070 -5.032495 1.359525  H 0.715666 -4.624225 0.901065  H 1.448352 -2.373248 0.150332  H -4.228108 -2.159772 -1.432413  H -6.716919 -2.335751 -1.391340  H -8.043313 -0.983375 0.245075  H -6.870890 0.548506 1.839980  H 3.842939 0.597803 2.804709  H 2.541214 1.233264 4.854077  H 0.014919 1.392471 4.697347  H -1.075909 1.002054 2.471668  H 4.496018 1.109030 -1.427288  H 6.929763 0.600048 -1.605105  H 7.975771 -1.089290 -0.080815  H 6.569306 -2.262369 1.628224  H -3.704614 1.388063 -0.802957  H -4.384804 0.735230 1.798022  H 4.136773 -1.754307 1.807056</p>	<p>C -4.903513 0.449321 1.010055  C -4.266172 0.160991 -0.212865  N -4.927090 -0.316388 -1.299536  C -6.257347 -0.519195 -1.172083  C -6.977718 -0.265539 0.003670  C -6.283174 0.232303 1.116715  C -2.800919 0.375014 -0.387320  C -2.239751 1.190114 -1.455700  N -0.864979 1.199837 -1.487000  C -0.226135 1.841710 -2.491468  C -0.915777 2.542184 -3.486220  C -2.319378 2.595335 -3.427005  C -2.988966 1.913599 -2.406603  Fe -0.057472 0.205300 0.014335  S 0.400906 -1.068858 1.860727  C -1.274231 -1.596147 2.066177  N -1.589609 -2.530100 3.006251  C -0.616716 -2.910498 4.035420  N 1.959286 0.284170 -0.238459  N 2.828634 1.096153 0.425320  C 2.464820 2.371499 0.821177  S 0.963289 3.031096 0.365550  C 2.487621 -0.805717 -0.824777  C 1.490965 -1.589800 -1.549531  N 0.190548 -1.318568 -1.201454  C -0.809923 -1.995703 -1.819896  C -0.571445 -2.938850 -2.821412  C -0.749161 -3.175993 -3.231200  C 1.786197 -2.493738 -2.591395  C 3.899853 -1.239381 -0.705371  N 4.821518 -0.273247 -0.423941  C 6.115845 -0.611793 -0.270569  C 6.573247 -1.930009 -0.390313  C 5.625542 -2.938205 -0.637428  C 4.279684 -2.598783 -0.790353  N 3.391539 3.028040 1.564686  C 3.216751 4.463929 1.826251  C 4.704248 2.433735 1.873685  O -0.880162 1.583739 1.799226  O -1.986789 2.210411 1.658113  N -1.875720 -0.242695 0.358970  N -2.280652 -1.117499 1.308400  C -3.001728 -2.802083 3.318173  H 2.819854 -2.632450 -2.912361  H 0.969160 -3.874314 -4.043156  H -1.418319 -3.454217 -3.280624  H -1.828337 -1.762998 -1.509216  H 3.532600 -3.380613 -0.938515  H 5.936205 -3.986538 -0.695939  H 7.634747 -2.157788 -0.264596  H 6.801288 0.209182 -0.036013  H -4.078553 1.916091 -2.345178  H -2.886753 3.155454 -4.175851  H -0.355778 3.042441 -4.279976  H 0.864834 1.793733 -2.476819  H -4.324617 0.842318 1.849287  H -6.806503 0.452089 2.052427  H -8.054974 -0.451065 0.040296  H -6.769129 -0.905847 -2.061450  H -3.059614 -3.758362 3.857192  H -3.429649 -2.006342 3.955008  H -3.587742 -2.870711 2.392991  H -0.932850 -3.865724 4.478493  H 0.380936 -3.045088 3.592005  H -0.554486 -2.149079 4.835433  H 3.961078 4.773329 2.571536  H 3.357929 5.056780 0.905225  H 2.206655 4.656444 2.218087  H 5.147957 2.992960 2.707799</p>



			H 4.589206 1.385318 2.187375 H 5.389829 2.488794 1.009413 H 3.853220 0.831692 0.223734
<sup>3</sup> TS1 <sup>(NH)</sup>	N -4.632574 -0.274786 1.088185 C -4.102021 -0.656276 -0.103891 C -4.883835 -1.081541 -1.196251 C -6.279411 -1.102310 -1.057395 C -6.839657 -0.712146 0.166177 C -5.976584 -0.313126 1.199610 C -2.618101 -0.624941 -0.209829 N -1.888601 0.477939 -0.019295 N -2.596285 1.656864 0.033576 C -2.140281 2.621825 0.804647 N -2.991482 3.851005 0.552554 C -1.829835 -1.791953 -0.566148 N -0.488213 -1.527923 -0.740029 C 0.339979 -2.526759 -1.128584 C -0.119011 -3.830144 -1.342825 C -1.478122 -4.121032 -1.136384 C -2.340341 -3.093762 -0.743405 Fe 0.021915 0.274050 -0.280812 N 0.575851 -0.362395 1.507947 C 1.933501 -0.570433 1.612914 C 2.505584 -1.020836 2.818985 C 1.673058 -1.296551 3.909279 C 0.286156 -1.117461 3.778487 C -0.220958 -0.643114 2.563326 C 2.676945 -0.268509 0.398131 N 1.904717 0.119267 -0.619613 N 2.498332 0.370947 -1.821932 C 1.622665 0.803083 -2.740169 N 2.098690 1.067676 -3.975690 C 4.160659 -0.387580 0.304622 N 4.674060 -1.633834 0.470060 C 6.018903 -1.757295 0.396804 C 6.891777 -0.684062 0.168620 C 6.346677 0.598850 0.009001 C 4.956003 0.752484 0.075487 S -0.105063 1.019227 -2.427634 S -0.936752 2.768501 1.985999 O 1.417622 2.898881 -0.129812 O 1.399446 3.593575 -1.167194 H -3.402445 -3.282870 -0.572031 H -1.860156 -5.135394 -1.279988 H 0.589463 -4.599505 -1.659107 H 1.390946 -2.265682 -1.266165 H -4.405666 -1.375219 -2.135183 H -6.913044 -1.417298 -1.892040 H -7.921614 -0.716719 0.325392 H -6.384153 -0.009959 2.171130 H -3.376507 4.219881 1.438742 H -3.774027 3.628013 -0.087934 H 3.586210 -1.159479 2.885351 H 2.102428 -1.651787 4.850454 H -0.399809 -1.330450 4.601888 H -1.289927 -0.470806 2.421515 H 4.487258 1.733480 -0.039155 H 6.992314 1.465709 -0.162394 H 7.971349 -0.853785 0.123357 H 6.413346 -2.771945 4.288000 H 3.099795 0.999083 -4.156883 H 1.493314 1.452506 -4.696735 H -2.420323 4.601820 0.127522	C 4.970252 0.683608 -0.273610 C 4.166261 -0.388974 0.177666 C 4.776497 -1.631117 0.468368 C 6.161128 -1.796637 0.305086 C 6.952148 -0.725723 -0.142238 C 6.353051 0.514117 -0.428731 C 2.702851 -0.214737 0.356002 N 1.873579 0.180016 -0.616971 N 2.379663 0.379782 -1.865471 C 1.455366 0.814026 -2.733832 S -0.238061 1.092095 -2.312513 Fe 0.015341 0.380713 -0.175400 N 0.655437 -0.276368 1.573011 C 2.017059 -0.476289 1.617160 C 2.644466 -0.890799 2.810257 C 1.863120 -1.151260 3.940592 C 0.468753 -0.995981 3.865019 C -0.093923 -0.548504 2.664923 N -1.943280 0.510711 0.086497 N -2.716293 1.626668 0.313974 C -2.162993 2.576936 1.038365 S -0.706962 2.709192 1.882600 C -2.636577 -0.595883 -0.193197 C -1.810225 -1.729662 -0.565574 N -0.464540 -1.453913 -0.647961 C 0.387276 -2.442124 -1.012119 C -0.053760 -3.735789 -1.309202 C -1.425492 -4.027712 -1.232144 C -2.311525 -3.013894 -0.859833 C -4.123679 -0.686993 -0.164000 C -4.764485 -1.406346 0.867994 C -6.164811 -1.514553 0.886337 C -6.932051 -0.916398 -0.126596 C -6.296380 -0.207117 -1.161103 C -4.898896 -0.090523 -1.182992 N -3.114260 3.749089 1.105352 N 1.852108 1.022005 -4.009201 O 1.318973 2.658501 -0.079612 O 1.400532 3.407229 -1.096322 H -3.386507 -3.195305 -0.792931 H -1.798428 -5.029420 -1.462471 H 0.677984 -4.493515 -1.599433 H 1.446199 -2.185003 -1.067340 H -4.403803 0.458161 -1.990093 H -6.889948 0.255759 -1.955979 H -8.023138 -1.004389 -0.112526 H -6.654089 -2.068948 1.693501 H -3.436602 3.975282 2.087777 H -3.989487 3.537777 0.593520 H 3.729927 -1.006222 2.838167 H 2.337734 -1.476300 4.870927 H -0.178936 -1.203314 4.720247 H -1.169497 -0.386789 2.564090 H 4.507152 1.650118 -0.491770 H 6.965615 1.353965 -0.772286 H 8.031935 -0.855668 -0.267589 H 6.619566 -2.765962 0.525781 H 2.840917 0.945334 -4.245914 H 1.215192 1.427888 -4.690390 H 4.162073 -2.471158 0.808081 H -4.165022 -1.874066 1.655710 H -2.680847 4.590864 0.687195	C -4.962694 0.564682 -0.688816 C -4.150024 -0.585817 -0.757197 N -4.657338 -1.845456 -0.828246 C -6.002857 -1.970737 -0.831570 C -6.890081 -0.886985 -0.768274 C -6.354420 0.408181 -0.697576 C -2.665834 -0.485369 -0.763754 N -1.962385 0.170733 0.170444 N -2.632107 0.770085 1.184560 C -1.821456 1.403967 2.054310 S -0.059184 1.457418 1.847856 Fe -0.053767 1.828775 0.023827 N -0.478655 -0.979357 -1.561013 C -1.831736 -1.137545 -1.763720 C -2.311711 -1.860540 -2.876145 C -1.399297 -2.461337 -3.748304 C -0.021612 -2.336521 -3.499438 C 0.395927 -1.581259 -2.399021 N 1.904622 0.053760 0.037975 N 2.792407 1.066087 -0.245382 C 2.500996 1.830307 -1.278787 S 1.304677 1.748732 -2.467314 C 2.439339 -1.017689 0.626568 C 1.461860 -1.939633 1.173802 N 0.159532 -1.501756 1.075171 C -0.829949 -2.253738 1.613870 C -0.577209 -3.472657 2.251023 C 0.742810 -3.947139 2.325445 C 1.771107 -3.173900 1.780648 C 3.908468 -1.241091 0.738613 N 4.592547 -1.345081 -0.431642 C 5.922090 -1.558378 -0.344929 C 6.621546 -1.673836 0.867368 C 5.902949 -1.567484 2.065413 C 4.517883 -1.353567 2.003206 N 3.531412 2.952733 -1.328485 C 4.380408 2.894279 -2.570524 C 2.906631 4.308747 -1.133422 N -2.398346 1.996734 3.134904 C -1.623549 2.867417 4.024491 C -3.858849 2.162223 3.196214 O -1.105825 2.386962 -1.004558 O -1.253610 3.408867 -0.280506 H 2.810518 -3.507415 1.819255 H 0.966871 -4.905091 2.802643 H -1.413420 -4.035567 2.672691 H -1.845431 -1.862952 1.532416 H 3.918127 -1.263812 2.913505 H 6.406972 -1.650004 3.033079 H 7.701690 -1.844981 0.864067 H 6.455375 -1.646004 -1.298712 H -3.387454 -1.953114 -3.033566 H -1.759413 -3.026461 -4.612936 H 0.918127 -6.802330 -4.148257 H 1.455194 -1.434947 -2.177430 H -4.506147 1.555768 -0.637666 H -7.009104 1.284117 -0.654208 H -7.970327 -1.058043 -0.776474 H -6.386455 -2.996664 -0.887215 H 3.718276 5.046810 -1.077092 H 2.251094 4.515958 -1.989277 H 2.330176 4.293587 -0.198548 H 5.150543 3.673535 -2.490956 H 4.840492 1.898638 -2.626926 H 3.735044 3.073616 -3.440553 H -4.158097 2.231985 4.252369 H -4.172693 3.084074 2.672703 H -4.356175 1.302913 2.730753 H -2.161777 2.955102 4.979499 H -0.631308 2.434872 4.218091 H -1.497679 3.878293 3.593535 H 4.150328 2.768065 -0.517438
<sup>3</sup> [Fe(TSC)(TSC <sup>(SCNH<sub>2</sub>)<sub>s</sub>)(O<sub>2</sub>)]<sup>+</sup></sup>	N -4.497982 -0.410026 1.599588 C -3.875466 -0.650328 0.418493 C -4.549424 -1.116344 -0.729418 C -5.934418 -1.314874 -0.655810 C -6.595413 -1.039548 0.549406 C -5.833363 -0.598689 1.642423 C -2.389783 -0.501913 0.391988 N -1.691682 0.054000 -0.589645 N -2.341363 0.701974 -1.625593 C -3.127753 1.855588 -1.487872 N -3.574255 2.300002 -2.680228	C 5.216148 0.134052 -1.034522 C 4.419276 0.207674 0.131021 C 5.041213 0.169010 1.400525 C 6.435935 0.048311 1.499435 C 7.222026 -0.021530 0.337609 C 6.609566 0.026579 -0.927446 C 2.944196 0.332916 0.035226 C 2.200276 1.432985 0.640440 N 0.835022 1.358024 0.483779 C 0.043069 2.320858 1.001983 C 0.568592 3.409499 1.708270	C -5.168037 -0.614004 -1.112308 C -4.418823 -0.914108 0.042555 N -4.981532 -1.303815 1.215309 C -6.329319 -1.394669 1.250205 C -7.159781 -1.119915 0.154074 C -6.563431 -0.724367 -1.052724 C -2.932026 -0.833561 0.035025 C -2.076699 -1.946448 0.418054 N -0.277633 -1.671119 0.387649 C 0.165961 -2.622424 0.736798 C -0.235133 -3.904079 1.126555

	<p>C -1.526943 -1.146848 1.393685  N -0.189171 -1.123664 1.084245  C 0.697008 -1.731714 1.901913  C 0.297802 -2.391259 3.070747  C -1.064151 -2.425841 3.397617  C -1.987085 -1.802125 2.549448  Fe 0.259187 -0.176300 -0.614723  O 0.424565 0.947650 -2.118519  O 0.363996 2.256818 -2.110618  N 2.162211 -0.529342 -0.615263  N 2.738032 -1.599615 -1.218648  C 1.841361 -2.396340 -1.815028  N 2.292506 -3.495996 -2.444532  C 2.931651 0.342498 0.036834  C 2.183611 1.418686 0.673171  N 0.819540 1.339976 0.508411  C 0.019845 2.285009 1.047863  C 0.537027 3.357452 1.783830  C 1.926631 3.458903 1.951308  C 2.759370 2.485886 1.388494  C 4.413426 0.217323 0.135767  N 4.910738 0.150353 1.397257  C 6.251096 0.034396 1.522100  C 7.135954 -0.008241 0.434732  C 6.606686 0.072795 -0.861701  C 5.218652 0.182729 -1.018823  S 0.095737 -2.080168 -1.810487  S -3.504067 2.610278 -0.019773  H -3.054155 -1.799405 2.774000  H -1.409403 -2.935874 4.301012  H 1.052918 -2.868163 3.700059  H 1.747862 -1.688991 1.609118  H -4.002728 -1.327810 -1.651523  H -6.483817 -1.683641 -1.527143  H -7.675831 -1.174484 0.650623  H -6.314255 -0.392082 2.605634  H -3.353884 1.819273 -3.554416  H -1.772683 0.667634 -2.479947  H 3.843444 2.539315 1.497635  H 2.360739 4.291080 2.512576  H -0.147948 4.096951 2.205632  H -1.057051 2.180353 0.872412  H 4.765263 0.249614 -2.010893  H 7.261924 0.051474 -1.737796  H 8.212385 -0.098985 0.605657  H 6.632020 -0.026222 2.548334  H 3.290048 -3.709844 -2.440986  H 1.650414 -4.144592 -2.894613  H -4.077288 3.183852 -2.721474</p>	<p>C 1.959353 3.510049 1.863906  C 2.784169 2.518546 1.321288  Fe 0.259750 -0.176536 -0.605887  S 0.080052 -2.104271 -1.760922  C 1.822347 -2.441272 -1.747246  N 2.261933 -3.563540 -2.347043  N -1.696304 0.054184 -0.585489  N -2.356793 0.690376 -1.624388  C -3.129223 1.849326 -1.495856  S -3.452041 2.653288 -0.038353  C -2.397620 -0.506077 0.391955  C -1.535843 -1.145165 1.398424  N -0.193991 -1.093577 1.114164  C 0.688609 -1.682661 1.949234  C 0.280904 -2.348739 3.111694  C -1.086730 -2.422665 3.406622  C -2.005869 -1.822910 2.537044  C -3.874097 -0.648323 0.423138  C -4.622583 -0.262029 1.558596  C -6.010116 -0.462850 1.587890  C -6.663107 -1.049509 0.490509  C -5.922307 -1.439309 -0.638887  C -4.535026 -1.238986 -0.678682  N -3.609228 2.267810 -2.685967  O 0.425220 0.913299 -2.131562  O 0.313150 2.220770 -2.151476  N 2.160939 -0.546095 -0.594902  N 2.724920 -1.640801 -1.168447  H -3.078081 -1.883472 2.730436  H -1.439080 -2.947734 4.298530  H 1.033628 -2.806550 3.757803  H 1.743690 -1.619929 1.675571  H -3.961336 -1.555958 -1.554387  H -6.423785 -1.908139 -1.491284  H -7.745998 -1.206927 0.516292  H -6.581177 -0.155643 2.469536  H -3.423421 1.760319 -3.552772  H -1.815317 0.622145 -2.493595  H 3.870434 2.576463 1.413663  H 2.400893 4.356000 2.398173  H -0.111002 4.163004 2.113777  H -1.035277 2.217919 0.831893  H 4.742004 0.175094 -2.019079  H 7.219412 -0.019976 -1.835233  H 8.310140 -0.111550 0.416524  H 6.906246 0.006792 2.486901  H 3.255994 -3.791671 -2.330753  H 1.612407 -4.217513 -2.77832  H -4.101454 3.157088 -2.734774  H -4.121065 0.216588 2.404538  H 4.429065 0.215433 2.306847</p>	<p>C -1.606435 -4.209217 1.144369  C -2.535131 -3.227563 0.787458  Fe -0.334779 0.135240 -0.278152  S -0.358126 2.284276 -0.931166  C -2.135104 2.430372 -0.925617  N -2.701346 3.620925 -1.225580  C -1.891312 4.767647 -1.657524  N 1.632712 0.096224 -0.224438  N 2.340248 -0.218945 -1.360636  C 3.375681 -1.191234 -1.433866  S 3.744822 -2.271352 -0.179163  C 2.241620 0.478499 0.892061  C 1.290541 0.767986 1.975914  N -0.030972 0.657137 1.618338  C -0.997598 0.931873 2.521418  C -0.699806 1.331853 3.828707  C 0.644198 1.459035 4.206681  C 1.648520 1.177982 3.273358  C 3.697857 0.780903 1.020474  N 4.323433 0.352063 2.145364  C 5.625563 0.676009 2.289824  C 6.351813 1.432094 1.357073  C 5.685628 1.894399 0.213110  C 4.335577 1.564751 0.036002  N 3.997742 -1.186256 -2.636731  C 4.903401 -2.289306 -2.989618  C 3.715585 -0.186137 -3.681837  O -0.358666 -0.548211 -2.041310  O -0.526394 -1.806179 -2.382052  N -2.256788 0.272654 -0.295709  N -2.936777 1.390814 -0.622374  C -4.158699 3.766198 -1.367924  H 2.704663 1.254641 3.533977  H 0.911649 1.775047 5.218758  H -1.515820 1.542020 4.524036  H -2.030704 0.831125 2.182104  H 3.784826 1.914209 -0.841245  H 6.203894 2.507766 -0.530099  H 7.606672 1.659519 1.534082  H 6.109325 0.314694 3.204845  H -3.606316 -3.434033 0.795303  H -1.950246 -5.206476 1.433479  H 0.521400 -4.643952 1.398481  H 1.225984 -2.347759 0.681131  H -1.950246 -0.311485 -2.033025  H -7.172909 -0.506756 -1.935096  H -8.244967 -1.217932 0.248270  H -6.762369 -1.705701 2.208212  H -4.477486 4.685466 -0.851910  H -4.428590 3.845340 -2.435646  H -4.665906 2.900337 -0.928225  H -2.517770 5.668768 -1.602872  H -1.023425 4.904892 -0.994504  H -1.536458 4.644386 -2.696265  H 5.141541 -2.210069 -4.058681  H 5.835352 -2.231907 -2.402613  H 4.425337 -3.261666 -2.792475  H 4.615635 -0.069590 -4.301359  H 2.877597 -0.503454 -4.328353  H 3.475484 0.783828 -3.223967  H 1.692992 -0.232358 -2.160343</p>
$^3[\text{Fe}(\text{TSC})(\text{TSC}^{\text{NH}})_2(\text{O}_2)]^+$	<p>N -4.439947 -0.504770 1.625425  C -3.894977 -0.688833 0.396120  C -4.661198 -0.951485 -0.756888  C -6.055684 -1.012810 -0.632409  C -6.633670 -0.806406 0.628413  C -5.785547 -0.562311 1.718988  C -2.404969 -0.633262 0.331187  N -1.720435 0.062115 -0.566696  N -2.348685 0.702181 -1.608577  C -2.914106 1.869888 -1.410966  N -3.454464 2.353054 -2.743257  C -1.548079 -1.432728 1.216158  N -0.212590 -1.372318 0.904307  C 0.674449 -2.101612 1.616488  C 0.277034 -2.931587 2.670340  C -1.084915 -3.008018 2.995992  C -2.007363 -2.254772 2.261021  Fe 0.230303 -0.131593 -0.595737  O 0.409874 1.258861 -1.856440  O 0.460499 2.541654 -1.606801  N 2.141411 -0.451081 -0.658714  N 2.733442 -1.382238 -1.448685  C 1.846692 -2.071505 -2.180548  N 2.319155 -3.030857 -2.997825  C 2.900029 0.311819 0.128947</p>	<p>C 5.177177 0.320963 -1.038946  C 4.399557 0.205770 0.135965  C 5.044943 0.005068 1.377741  C 6.444164 -0.087098 1.439274  C 7.211199 0.031895 0.268545  C 6.574804 0.238148 -0.968415  C 2.920578 0.314650 0.078582  C 2.174114 1.319835 0.828440  N 0.806873 1.244046 0.690633  C 0.012567 2.107610 1.358409  C 0.537568 3.098689 2.196285  C 1.930465 3.206900 2.328205  C 2.757491 2.315096 1.636634  Fe 0.233788 -0.136069 -0.593583  S 0.059862 -1.899944 -1.988640  C 1.799950 -2.244573 -2.001768  N 2.242629 -3.291027 -2.725785  N -1.723594 0.066696 -0.551100  N -2.373016 0.658808 -1.610927  C -2.960472 1.819666 -1.442668  S -3.213897 2.882955 -0.142623  C -2.398845 -0.595888 0.377329  C -1.531729 -1.338075 1.300272  N -0.194127 -1.260877 1.005190  C 0.697119 -1.927074 1.771499</p>	<p>C -5.146791 -0.659759 -1.089811  C -1.391316 -0.896194 0.075638  N -4.948684 -1.210645 1.273562  C -6.296972 -1.286860 1.323491  C -7.133144 -1.068259 0.219042  C -6.542715 -0.751501 -1.013534  C -2.903875 -0.820420 0.057324  C -2.050208 -1.911520 0.501205  N -0.701632 -1.635043 0.468589  C 0.189242 -2.562764 0.880697  C -0.213293 -3.823033 1.335781  C -1.583297 -4.131918 1.350852  C -2.509767 -3.173431 0.929524  Fe -0.297398 -1.46782 -0.266398  S -0.332399 2.276366 -0.990607  C -2.107395 2.398854 -1.042428  N -2.680814 3.568497 -1.411059  C -1.869468 4.698777 -1.879455  N 1.663846 0.171561 -0.168762  C 2.399734 0.056426 -1.324813  C 3.121577 -1.021269 -1.541836  S 3.472699 -2.426376 -0.661461  C 2.223638 0.542890 0.973859  C 1.248585 0.821863 2.034450  N -0.059723 0.724111 1.632122</p>

	<p>C 2.135565 1.223278 0.970081  N 0.771205 1.144090 0.806915  C -0.041855 1.929076 1.545902  C 0.460404 2.840889 2.481387  C 1.850192 2.948339 2.645396  C 2.696809 2.136574 1.883465  C 4.387533 0.233726 0.166519  N 4.935342 -0.022730 1.381886  C 6.283670 -0.089594 1.445486  C 7.127704 0.099510 0.341377  C 6.546705 0.374011 -0.905468  C 5.150472 0.438757 -0.999640  O 0.097952 -1.783983 -2.124220  S -3.163216 2.892126 -0.079601  H -3.073300 -2.283795 2.489661  H -1.428699 -3.649527 3.812077  H 1.031595 -3.504798 3.214204  H 1.723862 -2.021794 1.325467  H -4.176261 -1.110910 -1.722826  H -6.677746 -1.223947 -1.507442  H -7.717251 -0.841267 0.771651  H -6.201905 -0.407008 2.721094  H -2.951457 3.205679 -3.043448  H -3.340544 1.629237 -3.475111  H 3.781019 2.191609 1.991542  H 2.273058 3.659508 3.360693  H -0.234503 3.456359 3.057786  H -1.115986 1.833948 1.360138  H 4.657364 0.653288 -1.951015  H 7.168451 0.536671 -1.791059  H 8.212861 0.036623 0.462322  H 6.705452 -0.303652 2.434546  H 3.321267 -3.218533 -3.032820  H 1.691765 -3.594194 -3.567605  H -4.456094 2.595689 -2.661206</p>	<p>C 0.301187 -2.706195 2.864651  C -1.064197 -2.805389 3.168635  C -1.991186 -2.118780 2.375927  C -3.881242 -0.686975 0.440733  C -4.571299 -0.282448 1.605898  C -5.968657 -0.393855 1.670374  C -6.686626 -0.912070 0.579373  C -6.003226 -1.322523 -0.578773  C -4.607178 -1.209807 -0.652935  N -3.531242 2.250086 -2.781046  O 0.404495 1.143730 -1.961041  O 0.368859 2.445103 -1.819813  N 2.138790 -0.494780 -0.639340  N 2.704543 -1.515000 -1.336158  H -3.062087 -2.186088 2.577239  H -1.406432 -3.414380 4.009868  H 1.060034 -3.226661 3.453683  H 1.749951 -1.832587 1.497769  H -4.077039 -1.536895 -1.552238  H -6.557397 -1.736725 -1.426953  H -7.776454 -1.000068 0.632361  H -6.495481 -0.073122 2.574576  H -3.055387 3.106734 -3.112395  H -3.409551 1.509208 -3.494263  H 3.844819 2.379533 1.713019  H 2.371467 3.981445 2.962128  H -0.142745 3.775366 2.719029  H -1.065429 2.008105 1.194203  H 4.684498 0.489321 -2.000790  H 7.169000 0.336920 -1.882387  H 8.302674 -0.035236 0.318880  H 6.933386 -0.251266 2.404610  H 3.235326 -3.525217 -2.724447  H 1.593115 -3.905572 -3.211062  H 4.447960 -0.091276 2.290228  H -4.013082 0.130184 2.452065  H -4.537253 2.470337 -2.690777</p>	<p>C -1.050966 1.005479 2.506498  C -0.788727 1.397998 3.823681  C 0.543974 1.507197 4.246731  C 1.573787 1.220226 3.343659  C 3.686249 0.777578 1.161884  N 4.256363 0.169239 2.232576  C 5.571748 0.395317 2.440305  C 6.360973 1.219592 1.624345  C 5.753188 1.857083 0.533065  C 4.390707 1.632734 0.291368  N 3.744294 -0.857371 -2.933895  C 5.243830 -0.756377 -2.882570  C 3.283174 -1.921038 -3.893561  O -0.270676 -0.611126 -1.988190  O -0.124877 -1.879671 -2.283626  N -2.227436 0.267956 -0.327038  N -2.908727 1.365121 -0.717380  C -4.130518 3.670352 -1.645597  H 2.621557 1.291700 3.637978  H 0.781313 1.816376 5.268355  H 1.246884 -2.167354 4.493480  H -2.074476 0.917466 2.136134  H 3.880491 2.116601 -0.545079  H 6.326161 2.523645 -0.118530  H 7.421565 1.362929 1.849077  H 6.011687 -0.110636 3.307448  H -3.580355 -3.383058 0.934191  H -1.928491 -5.113366 1.688428  H 0.541523 -4.543571 1.659747  H 1.246884 -2.287995 0.816033  H -4.646249 -0.418802 -2.030834  H -7.157124 -0.580715 -1.902743  H -2.818551 -1.148363 0.326921  H -6.725452 -1.536992 2.301209  H -4.490086 4.629696 -1.242500  H -4.342614 3.637657 -2.729169  H -4.648605 2.842738 -1.148242  H -2.504242 5.595770 -1.890401  H -1.023620 4.878887 -1.198587  H -1.482237 4.524457 -2.899404  H 5.599958 -0.523994 -3.895558  H 5.512532 0.047438 -2.184017  H 5.645793 -1.719077 -2.540860  H 3.678171 -1.670217 -4.887563  H 3.673199 -2.888575 -3.552130  H 2.184577 -1.926367 -3.900322  H 3.378372 0.050652 -3.274041</p>
<sup>3</sup> TS2	<p>N -4.661059 -0.654868 1.371499  C -4.051207 -0.612586 0.159100  C -4.753602 -0.523676 -1.059071  C -6.153344 -0.466973 -1.018531  C -6.796739 -0.492250 0.226940  C -6.009126 -0.591810 1.384288  C -2.563418 -0.660181 0.178298  N -1.799423 0.145298 -0.542087  N -2.235370 0.998392 -1.501209  C -2.335964 2.294746 -1.217360  N -1.881905 3.082447 -2.357196  C -1.782089 -1.593033 1.001692  N -0.424006 -1.486089 0.829794  C 0.410953 -2.288690 1.524890  C -0.067161 -3.248313 2.423657  C -1.452513 -3.384449 2.596151  C -2.319133 -2.551415 1.879266  Fe 0.169387 -0.135207 -0.518911  O 0.354294 1.158889 -1.875395  O 0.398235 2.490049 -1.527220  N 2.097473 -0.467940 -0.635549  N 2.668631 -1.282815 -1.551574  C 1.767287 -1.904446 -2.322769  N 2.212557 -2.727123 -3.287136  C 2.867383 0.213723 0.211866  C 2.116758 1.024978 1.161034  N 0.748414 0.954208 1.020326  C -0.055249 1.592766 1.899325  C 0.463395 2.382281 2.931615  C 1.855534 2.511216 3.053814  C 2.691370 1.824787 2.166543  C 4.356150 0.139916 0.208990  N 4.925747 -0.241374 1.380625  C 6.274722 -0.309825 1.411087  C 7.097294 -0.004402 0.316683  C 6.492305 0.395483 -0.883953  C 5.094105 0.465232 -0.945134  S 0.013474 -1.716492 -2.109638  S -2.736363 3.087754 0.232718</p>	<p>C 5.082182 0.364981 -1.009252  C 4.361123 0.093879 0.176149  C 5.062224 -0.253357 1.353674  C 6.463179 -0.335607 1.340009  C 7.174752 -0.060604 0.160635  C 6.482014 0.293824 -1.010744  C 2.880522 0.185293 0.195313  C 2.153402 1.081111 1.088041  N 0.782357 1.025882 0.970336  C 0.001732 1.742964 1.807846  C 0.547649 2.598890 2.771321  C 1.943224 2.712013 2.865706  C 2.754862 1.945496 2.022005  Fe 0.162977 -0.147762 -0.487324  S -0.046132 -1.825855 -1.969927  C 1.700012 -2.083741 -2.169331  N 2.114939 -2.992061 -3.069809  N -1.810820 0.162560 -0.521060  N -2.243904 0.958721 -1.532493  C -2.300860 2.272344 -1.332221  S -2.653385 3.174828 0.067442  C -2.581737 -0.603770 0.234199  C -1.806161 -1.488543 1.113965  N -0.446376 -1.394331 0.953553  C 0.376473 -2.153475 1.708790  C -0.116475 -3.052645 2.661018  C -1.504399 -3.179271 2.820030  C -2.358594 -2.393764 2.037094  C -4.064140 -0.587433 0.192851  C -4.808395 -0.372422 1.376092  C -6.210463 -0.355391 1.330306  C -6.880283 -0.559337 0.112047  C -6.143673 -0.777767 -1.065320  C -4.741951 -0.788465 -1.031047  N -1.840335 2.974540 -2.525534  O 0.365683 1.050873 -1.925015  O 0.433843 2.402110 -1.665184  N 2.081302 -0.538361 -0.591067  N 2.622574 -1.433545 -1.450798</p>	<p>C -4.956258 1.801448 0.149738  C -4.302717 0.713176 -0.457537  N -4.953043 -0.300408 -1.083571  C -6.301147 -0.237622 -1.101819  C -7.046343 0.797357 -0.514098  C -6.358685 1.838107 0.123629  C -2.812743 0.638981 -0.452174  C -1.974226 1.596347 -1.150412  N -0.619582 1.386335 -1.013213  C 0.253935 2.166288 -1.687343  C -0.173719 3.227975 -2.492029  C -1.550717 3.473391 -2.619718  C -2.460673 2.647337 -1.953027  Fe -0.177356 -0.168851 0.129499  S -0.232582 -2.166723 1.155613  C -1.981882 -2.126341 1.503463  N -2.519205 -3.035058 2.347456  N 1.814366 -0.126102 0.206223  N 2.337806 0.331316 1.366205  C 2.606309 1.630771 1.491666  S 3.139145 2.710569 0.286789  C 2.490216 -0.756018 -0.741841  C 1.626671 -1.300839 -1.795756  C 0.284901 -1.108285 -1.578165  N -0.616036 -1.565954 -2.474995  C -0.224242 -2.244556 -3.633963  C 1.142177 -2.469088 -3.859767  C 2.077078 -1.996337 -2.932327  C 3.972513 -0.903847 -0.729583  N 4.615178 -0.577937 -1.880227  C 5.960121 -0.696569 -1.885883  C 6.709252 -1.141901 -0.785908  C 6.029121 -1.489885 0.389748  C 4.633609 -1.365009 0.425601  N 2.229936 2.111145 2.836015  O -0.243347 0.656491 1.811198  O -0.095984 2.029151 1.887887  N -2.131914 -0.314023 0.186784  N -2.795105 -1.221721 0.926195</p>

	<p>H -3.400968 -2.619016 1.999036  H -1.857538 -4.132822 3.282787  H 0.644083 -3.875000 2.966739  H 1.481020 -2.155223 1.349109  H -4.217268 -0.506878 -2.010450  H -6.729029 -0.406601 -1.946914  H -7.886340 -0.444849 0.306436  H -6.479538 -0.623619 2.373750  H -0.621798 2.942069 -2.115698  H -2.094799 2.630658 -3.259652  H 3.777225 1.883234 2.252982  H 2.289304 3.133359 3.841656  H -0.222591 2.887938 3.615226  H -1.131280 1.479916 1.748635  H 4.581818 0.772393 -1.860288  H 7.096595 0.650107 -1.759876  H 8.184563 -0.076007 0.410111  H 6.715670 -0.625739 2.363685  H 3.215845 -2.872874 -3.404122  H 1.567587 -3.231804 -3.891984  H -2.214330 4.055029 -2.340842</p>	<p>H -3.443004 -2.478412 2.129556  H -1.920325 -3.886033 3.543215  H 0.585228 -3.644359 3.253444  H 1.449027 -2.032766 1.538665  H -4.172500 -0.967313 -1.947283  H -6.661478 -0.944179 -2.015112  H -7.974356 -0.548358 0.079798  H -6.778208 -0.178612 2.249086  H -0.586591 2.831090 -2.280377  H -2.068197 2.467414 -3.394208  H 3.843392 2.004188 2.080386  H 2.398255 3.386803 3.596142  H -0.119822 3.169503 3.421341  H -1.077757 1.640012 1.675282  H 4.544432 0.643729 -1.919877  H 7.033414 0.515412 -1.929964  H 8.267759 -0.120486 0.153449  H 6.997143 -0.616336 2.253266  H 3.112324 -3.179535 -3.175460  H 1.450372 -3.523601 -3.628735  H -2.154648 3.952339 -2.572181  H 4.507746 -0.474594 2.271186  H -4.289014 -0.196574 2.323227</p>	<p>H 3.147186 -2.146567 -3.078930  H 1.478321 -3.009192 -4.749092  H -0.986948 -2.594554 -4.333486  H 1.466956 -1.383793 -2.249866  H 4.066996 -1.625519 1.322778  H 6.572885 -1.854533 1.266361  H 7.797853 -1.217507 -0.857378  H 6.460560 -0.420512 -2.821276  H 0.950864 2.149883 2.533705  C 2.397741 1.133762 3.955048  H -3.538279 2.794601 -2.054421  H -1.913487 4.293832 -3.245241  H 0.568603 3.843048 -3.006124  H 1.314781 1.939387 -1.550929  H -4.376391 2.591921 0.634868  H -6.899158 2.665262 0.593590  H -8.138847 0.782466 -0.561836  H -6.811422 -1.059912 -1.616881  C -3.980786 -3.135489 2.500726  C -1.732244 -4.161854 2.864935  C 2.712253 3.460274 3.228766  H -2.212027 -4.524441 3.784858  H -1.687632 -4.988350 2.132968  H -0.708948 -3.839200 3.107810  H -4.195809 -3.545379 3.498139  H -4.437280 -2.143201 2.403308  H -4.408244 -3.808101 1.735930  H 1.866456 1.532841 4.830796  H 1.967541 0.167680 3.668585  H 3.467988 1.014518 4.190816  H 2.214967 3.728749 4.172240  H 3.805144 3.452330 3.373461  H 2.450326 4.187451 2.450404</p>
<sup>3</sup> [Fe(TSC)(TSC.s)(O <sub>2</sub> H)] <sup>+</sup>	<p>N -4.453448 1.200199 -1.348435  C -4.030414 0.761259 -0.133918  C -4.904948 0.396688 0.909367  C -6.284928 0.489717 0.686055  C -6.738289 0.926476 -0.566882  C -5.788198 1.265898 -1.542747  C -2.554671 0.704950 0.041977  N -1.887190 -0.456686 0.333718  N -2.668912 -1.500228 0.520812  C -2.211841 -2.813793 0.555278  C -2.283146 -3.459557 1.720897  C -1.714634 1.866031 -1.114516  N -0.368783 1.636271 0.056066  C 0.493754 2.666486 -0.055266  C 0.069090 3.972343 -0.342033  C -1.301702 4.223550 -0.506450  C -2.204381 3.164017 -0.387501  Fe 0.092086 -0.254523 0.501918  O 0.230545 -1.994133 0.917034  O 1.346120 -2.727431 0.304350  N 1.971194 0.068353 0.727218  N 2.550869 0.384006 1.910481  C 1.663354 0.521120 2.911807  N 2.158951 0.840711 4.124314  C 2.727693 -0.041638 -0.365358  C 1.973441 -0.339584 -1.574446  N 0.617480 -0.469355 -1.379671  C -0.192446 -0.714151 -2.432318  C 0.307309 -0.867644 -3.730779  C 1.692095 -0.771544 -3.939870  C 2.534551 -0.505139 -2.855277  C 4.207614 0.135317 -0.356752  N 4.691918 1.118740 -1.157831  C 6.032417 1.292934 -1.170235  C 6.928675 0.519860 -0.418050  C 6.412424 -0.497613 0.397906  C 5.025913 -0.694449 0.434102  S -0.078624 0.313796 2.732906  S -2.030884 -3.553261 -0.973818  H -3.277618 3.321419 -0.503863  H -1.663686 5.233228 -0.717993  H 0.811974 4.769362 -0.423173  H 1.552099 2.443299 0.093161  H -4.508533 0.063223 1.871573  H -6.991229 0.225393 1.478608  H -7.806032 1.009403 -0.788270  H -6.110549 1.610390 -2.532217  H 1.251291 -3.581898 0.782402  H -2.380769 -2.940056 2.595678  H 3.614031 -0.413650 -2.986453  H 2.112848 -0.899903 -4.941193  H -0.384789 -1.066545 -4.552362  H -1.261056 -0.793241 -2.221701</p>	<p>C 5.035661 -0.672458 0.444997  C 4.205002 0.136787 -0.363703  C 4.791485 1.121516 -1.191356  C 6.183947 1.298596 -1.201227  C 7.003432 0.490169 -0.396380  C 6.426255 -0.496498 0.422914  C 2.732198 -0.048368 -0.361289  C 1.973216 -0.366945 -1.565597  N 0.616726 -0.491137 -1.370583  C -0.193204 -0.749790 -2.419746  C 0.305626 -0.921134 -3.716505  C 1.690522 -0.832849 -3.926200  C 2.533025 -0.554907 -2.844260  Fe 0.089680 -0.259458 0.506663  S -0.084953 0.325529 2.733419  C 1.657294 0.540459 2.910076  N 2.149247 0.873643 4.121720  N -1.890935 -0.452032 0.329660  N -2.672606 -1.494750 0.502089  C -2.221342 -2.809326 0.563324  S -2.028637 -3.586840 -0.945440  C -2.559683 0.713858 0.028542  C -1.706252 1.871111 -0.116899  N -0.361816 1.631118 0.049861  C 0.509090 2.655076 -0.056914  C 0.096698 3.966248 -0.335360  C -1.272526 4.230553 -0.488617  C -2.183667 3.177808 -0.371243  C -4.023784 0.779448 -0.151305  C -4.556244 1.278340 -1.365763  C -5.944169 1.339877 -1.554465  C -6.814876 0.928248 -0.531379  C -6.293261 0.445734 0.682713  C -4.908527 0.360284 0.872877  N -2.305280 -3.430675 1.742856  O 0.222593 -1.995742 0.934133  O 1.336280 -2.736946 0.322417  N 1.970306 0.064995 0.729583  N 2.545822 0.396117 1.912582  H -3.257007 3.352683 -0.463842  H -1.628002 5.245340 -0.686471  H 0.846562 4.756992 -0.413552  H 1.565311 2.421841 0.090450  H -4.506059 -0.006875 1.820560  H -6.968460 0.135252 1.486110  H -7.898061 0.984255 -0.678517  H -6.344073 1.709069 -2.503871  H 1.222589 -3.596217 0.787348  H -2.407577 -2.893499 2.606151  H 3.614270 -0.479541 -2.976397  H 2.112028 -0.977828 -4.924945  H -0.386895 -1.129922 -4.535277  H -1.261646 -0.826094 -2.207604</p>	<p>C -4.941139 0.486859 -0.853350  C -4.161167 -0.656665 -0.590457  N -4.693680 -1.877200 -0.325781  C -6.042470 -1.968619 -0.310926  C -6.901787 -0.888686 -0.558646  C -6.36518 0.364179 -0.840370  C -2.672620 -0.582683 -0.602520  C -1.845122 -1.389597 -1.484359  N -0.492452 -1.173617 -1.348408  C 0.380891 -1.893685 -2.085438  C -0.044321 -2.847105 -3.017492  C -1.402247 -3.052800 -3.193949  C -2.331568 -2.321071 -2.423477  Fe -0.068912 0.205718 -0.010820  S -0.053463 1.620110 1.806425  C -1.818668 1.710096 1.898454  N -2.409526 2.535095 2.803238  N 1.925716 0.150379 -0.113900  N 2.781789 0.852718 -0.833227  C 2.408516 1.688348 -1.885976  S 2.310585 0.856118 -3.382261  C 2.514213 -0.762809 0.722640  C 1.593087 -1.557082 1.499091  N 0.262652 -1.287590 1.274384  C -0.674790 -1.980748 1.952281  C -0.344345 -2.970095 2.889053  C 1.009053 -3.238818 3.147065  C 1.987610 -2.525231 2.451423  C 3.987943 -0.937628 0.806530  N 4.446787 -2.196227 0.575668  C 5.781625 -2.384895 0.652193  C 6.699150 -1.370187 0.965773  C 6.209987 -0.079573 1.213678  C 4.830540 0.146966 1.127440  N 2.504872 3.016524 -1.729097  O -0.063936 1.577544 -1.162436  O -1.126050 1.596054 -2.184860  N -1.975157 0.223541 0.203948  N -2.634025 0.985779 1.103220  H 3.048487 -2.703814 2.630102  H 1.298401 -3.991522 3.885249  H -1.144779 -3.503122 3.407508  H -1.717829 -1.734928 1.742304  H 4.407815 1.136890 1.316544  H 6.888778 0.739303 1.469917  H 7.768595 -1.593098 1.016266  H 6.132451 -3.403831 0.451371  H -0.817057 2.368748 -2.709306  C 2.461451 3.638531 -0.398376  H -3.407525 -2.468279 -2.528281  H -1.786979 -3.781643 -3.923450  H 0.698436 -3.405231 -3.592354  H 1.441523 -1.690007 -1.923923</p>

	<p>H 4.580844 -1.477936 1.052482  H 7.076340 -1.129343 0.995908  H 8.003732 0.712330 -0.476320  H 6.404188 2.094983 -1.818748  H 3.158915 1.008373 4.233959  H 1.542281 0.997194 4.918260  H -2.133490 -4.468227 1.756377</p>	<p>H 4.589280 -1.444366 1.078104  H 7.061949 -1.132741 1.046985  H 8.089446 0.627479 -0.407152  H 6.626588 2.070262 -1.839007  H 3.147262 1.052212 4.230492  H 1.529084 1.042211 4.910266  H -2.161584 -4.439074 1.800616  H 4.152996 1.756672 -1.813825  H -3.878987 1.588312 -2.167707</p>	<p>H -4.459199 1.443425 -1.070746  H -6.969935 1.231954 -1.048325  H -7.985786 -1.031996 -0.534129  H -6.451544 -2.961591 -0.090098  C -3.866203 2.475220 3.008387  C -1.627095 3.164820 3.872148  C 2.331942 3.918380 -2.871673  H -4.182749 3.404132 3.503849  H -4.379636 2.381201 2.043416  H -4.143715 1.616251 3.646213  H -2.201291 4.013658 4.269831  H -1.420758 2.455450 4.694938  H -0.671637 3.542087 3.478095  H 2.817059 4.876026 -2.632048  H 2.800060 3.484149 -3.767843  H 1.260890 4.096491 -3.073223  H 3.197560 4.456696 -0.362824  H 1.456052 4.049448 -0.204535  H 2.708797 2.897678 0.373361</p>
<sup>3</sup> TS3	<p>N -4.765110 -0.372208 1.112898  C -4.211096 -0.514379 -0.118490  C -4.963276 -0.702197 -1.292557  C -6.362861 -0.728775 -1.194681  C -6.950834 -0.576900 0.067836  C -6.112957 -0.406434 1.181683  C -2.719297 -0.488115 -0.179337  N -1.999107 0.604397 0.080428  N -2.685285 1.755918 0.275382  C -1.991086 2.698957 0.931860  N -2.591027 3.897032 1.101250  C -1.928716 -1.656518 -0.488240  N -0.570052 -1.437792 -0.497660  C 0.269943 -2.468383 -0.756883  C -0.200497 -3.756271 -1.024968  C -1.585669 -3.995070 -1.022187  C -2.455887 -2.939159 -0.748154  Fe -0.033102 0.409972 -0.144300  O 0.640120 2.644622 -0.618633  O 1.993073 3.013408 -0.566689  N 1.835425 0.161664 -0.629074  N 2.312114 0.310474 -1.889160  C 1.364221 0.621320 -2.783705  N 1.753853 0.804036 -4.061281  C 2.680990 -0.182818 0.343496  C 2.023073 -0.468025 1.612488  N 0.658934 -0.326196 1.580155  C -0.080259 -0.664326 2.659232  C 0.507370 -1.119378 3.843816  C 1.908363 -1.205167 3.915953  C 2.674794 -0.880240 2.793273  C 4.147858 -0.342812 0.136468  N 4.666686 -1.550493 0.478378  C 5.997354 -1.716393 0.311201  C 6.853130 -0.721406 -0.183004  C 6.302842 0.522096 -0.527653  C 4.924870 0.717729 -0.369685  S -0.351889 0.781174 -2.393907  S -0.400449 2.416373 1.603721  H -3.538190 -3.085440 -0.730069  H -1.979777 -4.994123 -1.227569  H 0.519046 -4.552403 -1.229129  H 1.339171 -2.254453 -0.750164  H -4.458884 -0.819023 -2.256272  H -6.977869 -0.866065 -2.089232  H -8.036870 -0.591917 0.195969  H -6.543437 -0.293922 2.183672  H 1.956419 3.979299 -0.761916  H -3.563619 4.017059 0.816153  H 3.762823 -0.958051 2.808368  H 2.398752 -1.529873 4.837966  H -0.128281 -1.381440 4.692902  H -1.162433 -0.546025 2.564282  H 4.454673 1.670871 -0.623092  H 6.934810 1.328760 -0.911489  H 7.923223 -0.920230 -0.290624  H 6.394667 -2.699814 0.588814  H 2.734421 0.678392 -4.312177  H 1.080598 1.019854 -4.793120  H -2.145978 4.622452 1.658265</p>	<p>C 4.916368 0.724742 -0.430613  C 4.153291 -0.332548 0.116363  C 4.798249 -1.540059 0.470708  C 6.180781 -1.685796 0.276418  C 6.933376 -0.629053 -0.261778  C 6.298062 0.575512 -0.612709  C 2.692475 -0.176049 0.328552  C 2.050958 -0.384381 1.622795  N 0.685625 -0.251333 1.603346  C -0.036590 -0.539748 2.707609  C 0.569111 -0.933347 3.905350  C 1.971691 -1.001216 3.964115  C 2.720747 -0.726479 2.816127  Fe -0.033911 0.390956 -0.146739  S -0.353378 2.492090 1.497893  C -1.945753 2.757959 0.820272  N -2.521169 3.977705 0.918856  N -2.660028 1.791250 0.226031  N -1.998670 0.614637 0.096200  C -2.740112 -0.480392 -0.104896  C -1.951676 -1.674914 -0.334076  N -0.592791 -1.465593 -0.377319  C 0.241171 -2.516236 -0.568439  C -0.234942 -3.819679 -0.725863  C -1.619928 -4.052710 -0.676910  C -2.482740 -2.974379 -0.476162  C -4.224625 -0.493073 -0.090917  C -4.942181 -0.066572 1.050196  C -6.343394 -0.101862 1.054542  C -7.044518 -0.553508 -0.078041  C -6.338430 -0.978103 -1.215446  C -4.934636 -0.954543 -1.222931  O 0.634187 2.591174 -0.760681  O 1.990231 2.953958 -0.781920  N 1.825376 0.106636 -0.647244  N 2.278662 0.175874 -1.924577  C 1.317480 0.437769 -2.818012  S -0.390701 0.635695 -2.408136  N 1.684009 0.552093 -4.112736  H -3.564003 -3.116688 -0.423811  H -2.019709 -5.064194 -0.789846  H 0.479641 -4.631615 -0.879298  H 1.310369 -2.303359 -0.597623  H -4.384385 -1.281506 -2.111287  H -6.878406 -1.328589 -2.100720  H -8.139023 -0.575951 -0.071881  H -6.889896 0.222204 1.945958  H 1.949719 3.908750 -1.024452  H -3.495700 4.097720 0.641020  H 3.811198 -0.781204 2.826777  H 2.477010 -1.272491 4.895333  H -0.053497 -1.158572 4.774420  H -1.120586 -0.431372 2.621314  H 4.423668 1.663216 -0.699128  H 6.880789 1.403389 -1.029080  H 8.012103 -0.743393 -0.409074  H 6.668228 -2.628013 0.546283  H 2.650032 0.359956 -4.377908  H 0.987847 0.664406 -4.846384  H -2.060215 4.722306 1.436307  H -4.399194 0.276406 1.935550  H 4.213104 -2.368759 0.881907</p>	<p>C -4.921011 0.868785 0.010315  C -4.194045 -0.120821 -0.681682  N -4.782266 -1.169126 -1.314019  C -6.130557 -1.244767 -1.256978  C -6.938548 -0.309242 -0.595239  C -6.317707 0.771717 0.048778  C -2.707951 -0.058430 -0.768128  C -1.980334 -0.138063 -2.027034  N -0.614612 -0.113352 -1.888647  C 0.176160 -0.285807 -2.970684  C -0.351719 -0.446425 -4.255420  C -1.747072 -0.406209 -4.423548  C -2.569411 -0.252451 -3.304263  Fe -0.003466 0.171137 -0.009072  S 0.756818 2.433913 -1.254980  C 2.276701 2.412778 -0.378495  N 2.993511 3.549228 -0.165067  N 2.808865 1.254760 0.065429  N 1.992311 0.185494 -0.050224  C 2.573432 -1.016777 0.008916  C 1.648959 -2.122642 0.002750  N 0.322084 -1.757070 -0.021085  C -0.632184 -2.719316 -0.041133  C -0.314610 -4.079298 -0.035136  C 1.036666 -4.468122 -0.011588  C 2.046729 -3.483810 0.004479  C 4.054229 -1.206070 0.059277  N 4.738466 -0.915564 -1.076548  C 6.075968 -1.098170 -1.046456  C 6.778549 -1.565530 0.075559  C 6.056751 -1.869016 1.237481  C 4.665052 -1.689907 1.230998  O -0.582549 2.329343 0.787948  O -1.885012 2.823299 0.587000  N -1.913548 0.009887 0.305342  N -2.469146 -0.044784 1.533585  C -1.581291 0.041054 2.541799  S 0.172718 0.081212 2.273874  N -2.064958 0.089553 3.809876  H 3.086018 -3.742518 0.018186  H 1.312486 -5.526197 -0.008801  H -1.123970 -4.812926 -0.050909  H -1.670786 -2.387830 -0.061438  H 4.059505 -1.916234 2.113609  H 6.563386 -2.238767 2.134151  H 7.864217 -1.689926 0.030947  H 6.612154 -0.860084 -1.972668  H -1.817599 3.739702 0.943429  C 4.348451 3.465667 0.402773  H -3.656086 -0.241206 -3.397934  H -2.189476 -0.501469 -5.419228  H 0.325232 -0.582711 -5.102081  H 1.253903 -0.276678 -2.790171  H -4.396899 1.694034 0.497859  H -6.909748 1.529326 0.571299  H -8.025745 -0.427964 -0.589474  H -6.583176 -2.101315 -1.770422  C -3.491991 -0.151772 4.079062  C -1.170813 -0.016797 4.968652  C 2.640426 4.815454 -0.812054  H 3.033861 5.642066 -0.202620  H 3.074592 4.882049 -1.827088  H 1.548220 4.912705 -0.886241  H 4.610668 4.448771 0.818702  H 4.379177 2.712783 1.200245  H 5.087066 3.195526 -0.373496  H -1.705610 0.357639 5.853185</p>

			H -0.868475 -1.063981 5.153279 H -0.269191 0.595529 4.818161 H -3.782911 0.429848 4.966739 H -4.094116 0.161091 3.218408 H -3.674586 -1.223237 4.279840
$^{2+}[\text{Fe}(\text{TSC})_2]^{+}$	C 4.951775 0.830439 0.376780 C 4.150513 -0.303175 0.137790 N 4.655276 -1.510563 -0.224595 C 5.997314 -1.599336 -0.360211 C 6.876679 -0.528531 -0.143623 C 6.340201 0.711008 0.235324 C 2.670393 -0.240174 0.295879 C 1.934879 -1.107752 1.203128 N 0.576034 -0.892166 1.220360 C -0.216189 -1.632904 2.026640 C 0.303755 -2.619905 2.869091 C 1.691365 -2.844025 2.874953 C 2.514126 -2.084305 2.039265 Fe 0.000000 0.558723 0.000334 S 0.193703 2.056010 1.673035 C -1.551625 2.182144 1.944290 N -2.001490 3.055024 2.866502 N -2.457402 1.444994 1.286480 N -1.888507 0.604625 0.383181 C -2.670181 -0.240629 -0.295504 C -1.934430 -1.108125 -1.202674 N -0.575647 -0.892195 -1.219936 C 0.216671 -1.632314 -2.026695 C -0.303075 -2.619279 -2.869297 C -1.690576 -2.844084 -2.874773 C -2.513462 -2.084841 -2.038773 C -4.150420 -0.303651 -0.137959 N -4.655326 -1.510779 0.224952 C -5.997455 -1.599485 0.359878 C -6.876722 -0.528877 0.142010 C -6.340045 0.710498 -0.237239 C -4.951535 0.829882 -0.377892 N 1.888439 0.604981 -0.382707 N 2.456960 1.445229 -1.286306 C 1.550927 2.182096 -1.944120 S -0.194314 2.056154 -1.672180 N 2.000326 3.053335 -2.867987 H -3.593171 -2.240311 -2.015319 H -2.127421 -3.604034 -3.528761 H 0.373256 -3.190557 -3.509399 H 1.286945 -1.414222 -1.996002 H -4.491837 1.776370 -0.673776 H -6.990535 1.570440 -0.423675 H -7.954371 -0.668895 0.265557 H -6.384051 -2.581031 0.658392 H -2.998306 3.094889 3.079688 H 3.593914 -2.239281 2.016078 H 2.128418 -3.603803 3.529004 H -0.372520 -3.191669 3.508817 H -1.286539 -1.415196 1.995835 H 4.492295 1.777032 0.672655 H 6.990765 1.571077 0.420921 H 7.954247 -0.668527 -0.267897 H 6.383789 -2.581059 -0.658307 H 2.997750 3.097789 3.077262 H 1.354826 3.614066 -3.420140 H -1.355622 3.610047 3.424015	C 4.962356 0.807246 0.397525 C 4.146881 -0.320953 0.150703 C 4.750780 -1.539852 -0.234578 C 6.144645 -1.624129 -0.377505 C 6.948844 -0.499488 -0.129790 C 6.354397 0.713846 0.260737 C 2.672745 -0.240658 0.306734 C 1.926601 -1.090470 1.225485 N 0.566968 -0.878588 1.227280 C -0.230893 -1.610351 2.035970 C 0.282438 -2.584922 2.896970 C 1.670800 -2.801756 2.923299 C 2.499506 -2.050105 2.085892 Fe -0.000002 0.567837 -0.000025 S 0.183203 2.067343 1.673546 C -1.563307 2.173733 1.949316 N -2.018838 3.039118 2.878014 N -0.566985 -0.878594 -1.227309 C -1.926622 -1.090454 -1.225518 C -2.499535 -2.050104 -2.085904 C -1.670834 -2.801801 -2.923273 C -0.282466 -2.584999 -2.896930 C 0.230872 -1.610407 -2.035958 C -2.672753 -0.240636 -0.306764 N -1.891762 0.604873 0.375826 N -2.463992 1.434845 1.288785 C -4.146889 -0.320918 -0.150722 C -4.962352 0.807291 -0.397533 C -6.354394 0.713907 -0.260735 C -6.948853 -0.499421 0.129788 C -6.144666 -1.624073 0.377491 C -4.750801 -1.539812 0.234557 S -0.183178 2.067320 -1.673614 C 1.563336 2.173710 -1.949359 N 2.464010 1.434844 -1.288798 N 1.891765 0.604862 -0.375853 N 2.018927 3.039494 -2.877673 H 3.582202 -2.191482 2.090270 H 2.104077 -3.547406 3.595876 H -0.398851 -3.149884 3.537419 H -1.301243 -1.394789 1.992621 H 4.502198 1.750840 0.704822 H 6.977394 1.591327 0.461337 H 8.035941 -0.567351 -0.239310 H 6.600439 -2.570704 -0.684852 H 3.013528 3.058040 -3.103259 H -3.582234 -2.191461 -2.090289 H -2.104117 -3.547463 -3.595832 H 0.398819 -3.150001 -3.537346 H 1.301225 -1.394860 -1.992608 H -4.502186 1.750882 -0.704826 H -6.977382 1.591398 -0.461327 H -8.035951 -0.567272 0.239314 H -6.600469 -2.570644 0.684836 H -3.013463 3.057822 3.103471 H -1.374891 3.581277 3.449938 H 1.374981 3.581453 -3.449790 H 4.124720 -2.415341 -0.434821 H -4.124750 -2.415308 0.434794	C -4.889935 0.429910 -0.925224 C -4.098927 -0.690066 -0.600323 N -4.622160 -1.902249 -0.281651 C -5.969650 -2.009261 -0.277939 C -6.838792 -0.952759 -0.585081 C -6.283973 0.291785 -0.919793 C -2.611505 -0.607498 -0.601702 C -1.772433 -1.467968 -1.417634 N -0.421368 -1.242872 -1.281068 C 0.462115 -1.973537 -1.996665 C 0.049671 -2.960449 -2.896157 C -1.327462 -3.193879 -3.060307 C -2.545062 -2.445018 -2.320105 Fe 0.000108 0.208867 0.000318 S 0.012484 1.701356 -1.682120 C 1.782703 1.879661 -1.709709 N 2.349490 2.820253 -2.505794 N 0.422327 -1.243398 1.280752 C 1.773473 -1.468278 1.416793 C 2.246530 -2.445739 2.318611 C 1.329277 -3.195074 3.058758 C -0.047950 -2.961718 2.895242 C -0.460830 -1.974462 1.996338 C 2.612123 -0.607196 0.601060 N 1.918029 0.255326 -0.154378 N 2.592627 1.099548 -0.968485 C 4.099530 -0.689646 0.599011 C 4.890561 0.430409 0.923677 C 6.284603 0.292428 0.917720 C 6.839434 -0.952048 0.582734 C 5.970289 -2.008622 0.275883 N 4.622786 -1.901739 0.280087 S -0.013433 1.699693 1.684398 C -1.783603 1.878210 1.710735 N -2.592985 1.098586 0.968507 N -1.917850 0.254621 0.154520 N -2.351382 2.818564 2.506615 H -3.319365 -2.605564 -2.423670 H -1.682120 -3.952538 -3.763738 H 0.798948 -3.523710 -3.457308 H 1.520468 -1.748972 -1.843074 H -4.417563 1.381415 -1.182336 H -6.924483 1.141621 -1.174862 H -7.921284 -1.107635 -0.565741 H -6.369622 -2.995304 -0.013566 C -3.808980 2.841266 2.713567 H 3.320891 -2.606224 2.421675 H 1.684273 -3.954048 3.761681 H -0.796947 -3.525305 3.456440 H -1.519256 -1.749905 1.843191 H 4.418189 1.381849 1.181025 H 6.925121 1.142313 1.172603 H 7.921934 -1.106811 0.562959 H 6.370254 -2.994611 0.011294 C 3.807014 2.845568 -2.712786 C 1.545246 3.584998 -3.465885 C -1.549217 3.579481 3.471299 H 4.108876 3.878880 -2.937982 H 4.319790 2.501080 -1.806980 H 4.093670 2.195945 -3.559664 H 2.110574 4.482856 -3.753693 H 1.326007 2.995336 -4.374730 H 0.597348 3.901359 -3.005301 H -2.111443 4.480584 3.755176 H -1.339244 2.988884 4.381758 H -0.596612 3.890388 3.016887 H -4.111690 3.873107 2.944273 H -4.321387 2.501543 1.805748 H -4.095064 2.186662 3.556787
$^{1+}[\text{Fe}(\text{TSC})(\text{TSC}^{\text{SCN}^{\text{Mn}}})]^{+} \cdot \text{H}_2\text{O}$	N -4.575142 -1.380361 1.190915 C -4.094235 -0.689851 0.122317 C -4.922391 0.006370 -0.783001 C -6.308326 0.002024 -0.566293 C -6.815788 -0.699792 0.535046 C -5.912765 -1.374427 1.371978 C -2.617645 -0.710522 -0.059937 N -1.848330 0.378789 -0.129061 N -2.407505 1.623222 0.024641 C -1.595641 2.725942 -0.014600 N -2.155847 3.922923 0.170381 C -1.834018 -1.931637 -0.197530		

	<p>N -0.484193 -1.705778 -0.376907  C 0.338022 -2.768830 -0.542195  C -0.129407 -4.087957 -0.539338  C -1.502512 -4.325406 -0.363973  C -2.363299 -3.235880 -0.193536  Fe 0.011389 0.186033 -0.392348  S 0.088614 2.510079 -0.321194  N 1.885885 -0.047799 -0.668881  N 2.483204 -0.189386 -1.887081  C 1.615058 -0.086517 -2.907004  N 2.132766 -0.185632 -4.157997  C 2.662157 -0.130322 0.422535  C 1.915877 -0.028600 1.666259  N 0.556552 0.124901 1.490123  C -0.241306 0.247774 2.576510  C 0.258517 0.229323 3.883171  C 1.642981 0.086847 4.075461  C 2.476839 -0.041155 2.960354  C 4.139610 -0.303739 0.376805  N 4.642065 -1.361277 1.068223  C 5.983999 -1.526250 1.057148  C 6.872199 -0.678120 0.381675  C 6.342852 0.413901 -0.323510  C 4.955945 0.605785 -0.328373  S -0.101043 0.213287 -2.708115  H -3.436167 -3.380533 -0.052951  H -1.898087 -5.344856 -0.362724  H 0.580035 -4.907665 -0.677729  H 1.397784 -2.545007 -0.684618  H -4.491072 0.520307 -1.647615  H -6.975959 0.529299 -1.254237  H -7.888710 -0.733786 0.743514  H -6.279642 -1.938270 2.237652  H -3.159102 4.003643 0.346960  H -3.413756 1.702624 0.217805  H 3.555856 -0.157306 3.075203  H 2.068036 0.077024 5.083254  H -0.431489 0.330582 4.724498  H -1.310957 0.364811 2.384378  H 4.505105 1.446651 -0.861357  H 6.999256 1.108109 -0.857470  H 7.948692 -0.869156 0.413368  H 6.363242 -2.388132 1.619352  H 3.105176 -0.472548 -4.266287  H 1.511903 -0.279564 -4.958338  H -1.558040 4.787921 0.141868  H 0.182267 5.947145 0.720557  O -0.525569 6.157514 0.079767  H -0.073603 6.076906 -0.783524</p>		
$^1[\text{Fe}(\text{TSC})(\text{TSC}^{(NH)_s})]^+ \cdot \text{H}_2\text{O}$	<p>N -4.374959 -2.068527 0.617864  C -3.972483 -0.955295 -0.052016  C -4.876309 -0.006279 -0.574582  C -6.249361 -0.210930 -0.391252  C -6.676701 -1.350977 0.306029  C -5.704694 -2.241605 0.783856  C -2.505621 -0.794637 -0.227810  N -1.817347 0.303050 0.113068  N -2.520619 1.329510 0.725188  C -1.728217 2.337467 1.019828  N -2.429569 3.470910 1.638024  C -1.648851 -1.823323 -0.803030  N -0.320334 -1.454161 -0.879453  C 0.569392 -2.320957 -1.415984  C 0.194826 -3.579212 -1.903068  C -1.155225 -3.959182 -1.839901  C -2.085049 -3.071874 -1.286752  Fe 0.049933 0.342243 -0.204322  S -0.045177 2.483482 0.708864  N 1.934470 0.344962 -0.548434  N 2.518134 0.708973 -1.728215  C 1.624348 1.131683 -2.636668  N 2.120032 1.554807 -3.828400  C 2.734439 -0.105999 0.428300  C 2.013821 -0.497290 1.626469  N 0.644889 -0.352908 1.527577  C -0.128381 -0.654858 2.597426  C 0.406569 -1.107205 3.808589  C 1.799725 -1.250756 3.923016  C 2.609002 -0.942472 2.825320  C 4.215358 -0.208837 0.305575  N 4.740172 -1.455429 0.442722  C 6.083578 -1.573932 0.342253  C 6.949479 -0.496415 0.109456  C 6.396251 0.786626 -0.021733  C 5.007228 0.935099 0.077069  S -0.104624 1.210691 -2.347051</p>		

	<p>H -3.142243 -3.332841 -1.216353  H -1.481039 -4.932079 -2.218489  H 0.956711 -4.238206 -2.327068  H 1.608403 -1.986537 -1.456485  H -4.504387 0.864221 -1.120298  H -6.972912 0.505866 -0.791752  H -7.738507 -1.552216 0.474189  H -6.003858 -3.144206 1.330203  H -3.375493 3.180468 1.936959  H -1.920307 3.818214 2.466961  H 3.695011 -1.039484 2.881068  H 2.250318 -1.595422 4.858220  H -0.264292 -1.336993 4.640083  H -1.205790 -0.525874 2.469217  H 4.536896 1.917717 -0.014069  H 7.035525 1.658012 -0.194750  H 8.028302 -0.662376 0.038556  H 6.482899 -2.589294 0.453413  H 3.102419 1.379271 -4.038917  H 1.487713 1.725627 -4.607034  H -2.523840 4.319457 0.917880  H -1.792032 5.933022 -0.052023  O -2.649219 5.460541 -0.064774  H -2.670009 5.042895 -0.949854</p>		
<sup>3</sup> TS1 <sup>(<i>opt</i>)</sup> · H <sub>2</sub> O	<p>C 4.963130 0.700519 0.050049  C 4.198871 -0.478894 0.158081  N 4.743814 -1.722850 0.128960  C 6.085310 -1.803455 -0.018379  C 6.927116 -0.688529 -0.137709  C 6.351501 0.590500 -0.097424  C 2.720345 -0.411928 0.328101  N 1.905071 0.190027 -0.542404  N 2.436398 0.719351 -1.679673  C 1.515355 1.337680 -2.433490  S -0.195541 1.450605 -2.001350  Fe 0.031952 0.225330 -0.114832  N 0.656502 -0.829265 1.435630  C 2.020870 -1.011382 1.457866  C 2.636025 -1.715946 2.512355  C 1.840755 -2.275262 3.517775  C 0.445394 -2.122023 3.457734  C -0.105485 -1.384912 2.404119  N -1.898543 0.260745 0.153198  N -2.643236 1.374210 0.451706  C -2.112368 2.192036 1.340021  S -0.779832 2.024802 2.378992  C -2.574847 -0.803821 -0.281670  C -1.730877 -1.819462 -0.885214  N -0.407541 -1.452014 -1.000392  C 0.463658 -2.297732 -1.600275  C 0.068170 -3.542768 -2.099068  C -1.270924 -3.943239 -1.958700  C -2.177426 -3.074939 -1.344860  C -4.056302 -0.922842 -0.201156  N -4.605145 -0.837133 1.039894  C -5.946730 -0.952687 1.123940  C -6.788856 -1.148608 0.017177  C -6.210007 -1.235707 -1.255721  C -4.816322 -1.126449 -1.370023  N -2.831243 3.490637 1.334886  N 1.929366 1.885543 -3.595975  O 1.319398 2.546611 0.551271  O 1.248908 3.551933 -0.219043  H -3.226043 -3.352060 -1.214732  H -1.603228 -4.919124 -2.323022  H 0.811125 -4.183658 -2.579914  H 1.498924 -1.962480 -1.680010  H -4.322456 -1.184956 -2.344236  H -6.828015 -1.384756 -2.146279  H -7.870156 -1.231693 0.158425  H -6.369127 -0.887049 2.133462  H -2.834768 3.924280 2.270424  H -3.804867 3.377621 1.006597  H 3.721103 -1.827909 2.525092  H 2.305510 -2.829134 4.338478  H -0.213209 -2.552969 4.215702  H -1.181854 -1.215337 2.328750  H 4.473075 1.676544 0.091605  H 6.972453 1.488155 -0.176321  H 8.006239 -0.824275 -0.253338  H 6.502249 -2.817265 -0.043862  H 2.921171 1.881558 -3.832637  H 1.285361 2.411981 -4.181490  H -2.284391 4.144147 0.627452  O -1.383935 4.879453 -0.392178  H -0.545630 4.357398 -0.413218</p>		



${}^3[\text{Fe}(\text{TSC})(\text{TSC}^{(\text{NH})_s}(\text{O}_2))^+ \cdot \text{H}_2\text{O}$	H -1.789466 4.706245 -1.265938 C -5.186348 0.903585 0.471722 C -4.411791 0.012150 -0.294637 N -4.943756 -0.968892 -1.067557 C -6.290486 -1.080040 -1.074359 C -7.146951 -0.242430 -0.344907 C -6.581143 0.772958 0.440031 C -2.923661 0.101028 -0.309197 C -2.156144 0.298944 -1.530602 N -0.790600 0.301536 -1.357413 C 0.024295 0.452927 -2.423743 C -0.479743 0.626183 -3.717685 C -1.870410 0.651900 -3.908398 C -2.717812 0.489097 -2.807812 Fe -0.248628 0.119818 0.531734 S -0.120822 -0.319209 2.729245 C -1.878365 -0.396702 2.972285 N -2.349591 -0.618185 4.212256 N 1.710325 0.198352 0.383869 N 2.351594 1.324113 0.829037 C 2.913227 2.149905 -0.027752 S 3.174339 2.115390 -1.711268 C 2.359424 -0.916595 0.081647 C 1.467340 -2.062170 -0.142738 N 0.140569 -1.788529 0.075262 C -0.778288 -2.771253 -0.045238 C -0.421382 -4.080069 -0.386753 C 0.931258 -4.376657 -0.609403 C 1.885666 -3.360655 -0.485233 C 3.845918 -1.046089 0.061956 N 4.371743 -1.666208 -1.024697 C 5.712743 -1.818624 -1.058910 C 6.573889 -1.384924 -0.039904 C 6.014871 -0.761014 1.084724 C 4.625919 -0.582326 1.139923 N 3.337008 3.381494 0.698743 O -0.360844 1.979740 0.780431 O -0.381037 2.856089 -0.218603 N -2.169270 -0.030771 0.780991 N -2.764913 -0.251665 1.978600 O 1.188711 4.899969 0.657020 H 2.945061 -3.552892 -0.658364 H 1.243018 -5.390626 -0.874648 H -1.198698 -4.843519 -0.468676 H -1.818793 -2.498081 0.143091 H 4.155323 -0.102049 2.001021 H 6.646791 -0.421351 1.910886 H 7.652468 -1.542974 -0.127087 H 6.113639 -2.317725 -1.948682 H 4.137953 3.824975 0.226160 H 2.466705 4.083057 0.707889 H -3.802873 0.501580 -2.922426 H -2.292285 0.798297 -4.906761 H 0.215763 0.748533 -4.551479 H 1.100104 0.463250 -2.221923 H -4.703993 1.681707 1.068529 H -7.213393 1.453156 1.018724 H -8.230026 -0.384856 -0.397423 H -6.700650 -1.882004 -1.699234 H -3.355853 -0.690263 4.365229 H -1.720467 -0.766494 4.998455 H 0.515526 4.210896 0.371120 H 0.962088 5.077392 1.591889 H 3.592098 3.165959 1.676490		
${}^3\text{TS2} \cdot \text{H}_2\text{O}$	C -5.172540 0.899226 0.439341 C -4.404307 -0.026468 -0.291993 N -4.942519 -1.034861 -1.024213 C -6.289719 -1.138266 -1.026026 C -7.140494 -0.266805 -0.330263 C -6.568172 0.775771 0.413123 C -2.915657 0.054274 -0.313738 C -2.149485 0.186053 -1.546208 N -0.783652 0.210037 -1.375448 C 0.031099 0.299708 -2.449036 C -0.475256 0.396481 -3.750097 C -1.865936 0.401512 -3.940740 C -2.712292 0.296432 -2.832021 Fe -0.229662 0.127782 0.520693 S -0.101080 -0.259861 2.723980 C -1.859259 -0.265749 2.986515 N -2.319259 -0.401818 4.242050 N 1.732302 0.235639 0.375499 N 2.351628 1.379562 0.781248 C 2.848476 2.234423 -0.099960 S 3.042727 2.104630 -1.804651 C 2.395420 -0.883460 0.117875		

	<p>C 1.522247 -2.049165 -0.064696  N 0.191061 -1.787269 0.140365  C -0.715411 -2.785033 0.051483  C -0.340639 -4.099437 -0.245062  C 1.016706 -4.385161 -0.454885  C 1.957461 -3.353381 -0.363797  C 3.884137 -0.986444 0.103117  N 4.423479 -1.636714 -0.958723  C 5.767738 -1.761835 -0.987543  C 6.618954 -1.268750 0.012412  C 6.046090 -0.614083 1.112485  C 4.653751 -0.464043 1.161658  N 3.204750 3.482242 0.527840  O -0.340054 1.979170 0.815090  O -0.439738 2.812649 -0.246982  N -2.159984 -0.017064 0.780454  N -2.749440 -0.158381 1.992193  O 0.960482 4.746999 0.455304  H 3.019462 -3.537152 -0.529809  H 1.342437 -5.403422 -0.684447  H -1.107595 -4.875478 -0.302165  H -1.759860 -2.519203 0.228472  H 4.172101 0.041078 2.001925  H 6.670417 -0.227448 1.923676  H 7.700889 -1.405146 -0.069749  H 6.179700 -2.286536 -1.857310  H 3.958921 3.956185 0.018573  H 1.953631 4.269699 0.505470  H -3.797181 0.288989 -2.948380  H -2.288956 0.485671 -4.945754  H 0.218996 0.474935 -4.590254  H 1.106834 0.335053 -2.247389  H -4.685098 1.697304 1.004763  H -7.195901 1.482799 0.963844  H -8.224426 -0.404659 -0.376746  H -6.704938 -1.962899 -1.617052  H -3.324927 -0.429311 4.412933  H -1.683354 -0.501745 5.030547  H 0.275685 3.941981 0.175254  H 0.730814 5.004584 1.373264  H 3.465619 3.351100 1.515239</p>		
<sup>3</sup> [Fe(TSC)(TSC <sub>s</sub> )(O <sub>2</sub> H)] <sup>+</sup> ·H <sub>2</sub> O	<p>C -5.170646 0.897181 0.424891  C -4.405357 -0.032158 -0.304860  N -4.945607 -1.036843 -1.040350  C -6.292978 -1.134298 -1.046041  C -7.141592 -0.258854 -0.352254  C -6.566805 0.780811 0.393096  C -2.916409 0.039716 -0.319747  C -2.140896 0.147956 -1.550299  N -0.776112 0.183419 -1.372261  C 0.046137 0.254699 -2.440831  C -0.452310 0.322107 -3.747202  C -1.841115 0.314023 -3.946936  C -2.694775 0.227001 -2.841723  Fe -0.227444 0.135193 0.529681  S -0.113152 -0.223957 2.733214  C -1.873940 -0.213771 2.992410  N -2.334419 -0.321320 4.249175  N 1.737158 0.250215 0.395692  N 2.356270 1.388586 0.795888  C 2.871677 2.244398 -0.084673  S 3.040465 2.073865 -1.796804  C 2.395135 -0.872801 0.134514  C 1.520113 -2.037791 -0.034120  N 0.190311 -1.775327 0.182212  C -0.718081 -2.773406 0.113293  C -0.345828 -4.089663 -0.177047  C 1.008708 -4.376753 -0.401413  C 1.950464 -3.344658 -0.328520  C 3.883729 -0.978188 0.107645  N 4.411280 -1.637562 -0.954239  C 5.754834 -1.767039 -0.994556  C 6.616258 -1.270639 -0.005099  C 6.055147 -0.607295 1.095935  C 4.663975 -0.451023 1.155911  N 3.277963 3.456430 0.517101  O -0.322933 1.967199 0.832041  O -0.396180 2.770080 -0.297259  N -2.169370 -0.012331 0.780956  N -2.760164 -0.126198 1.992805  H 3.010536 -3.529438 -0.505063  H 1.331777 -5.396608 -0.627340  H -1.113642 -4.865787 -0.217929  H -1.760153 -2.507206 0.301699  H 4.191567 0.063142 1.995898  H 6.687824 -0.217718 1.899191</p>		

	H 7.697006 -1.410787 -0.096050 H 6.157231 -2.298126 -1.864888 H 0.097169 3.691738 0.049650 H 3.505251 3.357838 1.513693 H -3.778444 0.207843 -2.965975 H -2.258043 0.373521 -4.956173 H 0.247394 0.387915 -4.583886 H 1.120529 0.303326 -2.232857 H -4.681465 1.692490 0.992518 H -7.192827 1.490899 0.941718 H -8.225997 -0.391496 -0.402144 H -6.710253 -1.956634 -1.638702 H -3.340474 -0.341920 4.419884 H -1.699774 -0.399945 5.041355 H 4.021126 3.928553 -0.003664 O 0.843076 4.784989 0.475048 H 0.849480 5.419973 -0.269894 H 1.785202 4.405896 0.492948		
<sup>3</sup> TS3·H <sub>2</sub> O	C 4.880594 0.393821 -0.177233 C 4.064605 -0.725586 0.080183 N 4.541685 -1.994844 0.152890 C 5.868256 -2.164119 -0.042860 C 6.759638 -1.114404 -0.307781 C 6.252876 0.192164 -0.371797 C 2.601602 -0.562037 0.309192 C 1.917576 -1.089429 1.482963 N 0.561888 -0.880183 1.479701 C -0.207492 -1.422544 2.448286 C 0.341008 -2.166526 3.497596 C 1.736131 -2.329959 3.554864 C 2.533005 -1.789262 2.541654 Fe -0.074058 0.251667 -0.035437 S -0.343781 1.822281 2.122276 C -1.908204 2.334059 1.541388 N -2.449390 3.494255 1.979085 N -2.649589 1.608739 0.685476 N -2.026399 0.494623 0.233625 C -2.801036 -0.471951 -0.263216 C -2.070994 -1.587328 -0.817528 N -0.702951 -1.445418 -0.780437 C 0.085587 -2.437886 -1.257098 C -0.446972 -3.611312 -1.795959 C -1.843140 -3.771848 -1.841969 C -2.660794 -2.754846 -1.347383 C -4.294055 -0.425185 -0.221902 N -4.869715 -0.588894 0.996707 C -6.219100 -0.564618 1.041413 C -7.037966 -0.383141 -0.084353 C -6.428471 -0.224076 -1.335948 C -5.027471 -0.249315 -1.409847 O 0.714638 2.505987 -0.070296 O 2.058195 2.824028 -0.002002 N 1.779659 0.014488 -0.570073 N 2.270418 0.387499 -1.777623 C 1.347263 0.929267 -2.583758 S -0.357116 1.111790 -2.157578 N 1.756355 1.353887 -3.797161 H -3.749508 -2.844019 -1.362017 H -2.286023 -4.681200 -2.257368 H 0.232576 -4.380853 -2.169355 H 1.163988 -2.281915 -1.206706 H -4.506612 -0.132433 -2.364844 H -7.028238 -0.083408 -2.240320 H -8.126116 -0.372281 0.024952 H -6.667015 -0.700951 2.032767 H 2.047823 3.865947 -0.068509 H -3.422984 3.704602 1.755914 H 3.616142 -1.918776 2.543311 H 2.197997 -2.880639 4.379125 H -0.318861 -2.589117 4.259014 H -1.281337 -1.232373 2.379506 H 4.443337 1.394440 -0.214099 H 6.914154 1.041705 -0.567793 H 7.823627 -1.320495 -0.455026 H 6.232219 -3.196678 0.016105 H 2.723411 1.201762 -4.083103 H 1.091687 1.710957 -4.479564 H -1.989456 4.027971 2.713092 H 1.083305 5.612536 -0.348633 O 2.018681 5.397484 -0.159185 H 2.475215 5.614034 -0.997173		
	OOH- O 0.056310 -0.616698 0.000000 O 0.056310 0.726628 0.000000 H -0.900961 -0.879444 0.000000		

H<sub>2</sub>O·OOH·  
O 1.486604 -0.492840 -0.031981  
O 0.749227 0.631051 0.047324  
O -1.692675 -0.182934 -0.099745  
H -0.244913 0.302258 -0.009854  
H -2.222131 0.639674 -0.088095  
H -1.878203 -0.584150 0.773168

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