Supporting Information For:

Probing the Influence of Local Coordination Environment on the Properties of Fe-type Nitrile Hydratase Model Complexes

Henry L. Jackson, Steven C. Shoner, Durrell Rittenberg, Jerry A. Cowen, Scott Lovell, David Barnhart, and Julie A. Kovacs*

Contribution from the Department of Chemistry, University of Washington, Seattle, WA 98195.

Supplementary Figures

Figure S-1 Electronic spectrum of [Fe(III)(DITIm)$_2$]Cl (**2**) in aprotic (MeCN, 298 K) vs. protic (H_2O, 298 K) solvents.

Figure S-2 Cyclic voltammogram of [Fe(III)(DITpy)$_2$]Cl (**1**) in MeCN at 298 K (0.1 M $(Bu_4N)PF_6$, glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.

Figure S-3 Cyclic voltammogram of [Fe(III)(DITIm)$_2$]Cl (**2**) in MeCN at 298 K (0.1 M $(Bu_4N)PF_6$; glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.

Figure S-4 Cyclic voltammogram of [Fe(III)(DITpy)$_2$]Cl (**1**) in H_2O at 298 K (0.1 M KCl, glassy carbon electrode, 50 mV/sec scan rate.) Peak potentials vs. SCE indicated.

Figure S-5 Cyclic voltammogram of [Fe(III)(ADIT)$_2$]Cl (**3**) in H_2O at 298 K (0.1 M KCl, glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.

Figure S-6 X-band EPR spectrum of [Fe(III)(DITIm)$_2$]Cl (**2**) in MeOH/EtOH (9:1) glass at 135 K. Microwave frequency, 9.419 GHz; microwave power, 2 mW; modulation frequency, 100 kHz; modulation amplitude, 2G.

Figure S-7 $1/\chi_m$ (molar susceptibility) vs. temperature plot for [Fe(III)(DITpy)$_2$]Cl (**1**) over the temperature range T = 5-300 K

Figure S-8 $1/\chi_m$ (molar susceptibility) vs. temperature plot for [Fe(III)(DITIm)$_2$]Cl (**2**) over the temperature range T = 5-300 K

Figure S-9 $1/\chi_m$ (molar susceptibility) vs. temperature plot for [Fe(III)(AMIT)$_2$]Cl (**4**) over the temperature range T = 5-300 K

Supplementary Tables

Crystal Data for [Fe(III)(DITpy)$_2$]Cl (**1**)

Positional and Equivalent Isotropic Thermal Parameters for [Fe(III)(DITpy)$_2$]Cl (**1**)

Bond Distances (Å) and Angles (deg) for [Fe(III)(DITpy)$_2$]Cl (**1**)

Anisotropic Thermal Parameters for [Fe(III)(DITpy)$_2$]Cl (**1**)

Hydrogen atoms for [Fe(III)(DITpy)$_2$]Cl (**1**)

Crystal Data for [Fe(III)(DITIm)$_2$]Cl (**2**)

Positional and Equivalent Isotropic Thermal Parameters for [Fe(III)(DITIm)$_2$]Cl (**2**)

Bond Distances (Å) and Angles (deg) for [Fe(III)(DITIm)$_2$]Cl (**2**)

Anisotropic Thermal Parameters for [Fe(III)(DITIm)$_2$]Cl (**2**)

Hydrogen atoms for [Fe(III)(DITIm)$_2$]Cl (**2**)

Crystal Data for [Fe(III)(AMIT)$_2$]Cl (**4**)

Positional and Equivalent Isotropic Thermal Parameters for [Fe(III)(AMIT)$_2$]Cl (**4**)

Bond Distances (Å) and Angles (deg) for [Fe(III)(AMIT)$_2$]Cl (**4**)

Anisotropic Thermal Parameters for [Fe(III)(AMIT)$_2$]Cl (**4**)

Hydrogen atoms for [Fe(III)(AMIT)$_2$]Cl (**4**)

Torsion Angles (deg) for [Fe(III)(AMIT)$_2$]Cl (**4**)

References for structure determination of [Fe(III)(AMIT)$_2$]Cl (**4**)

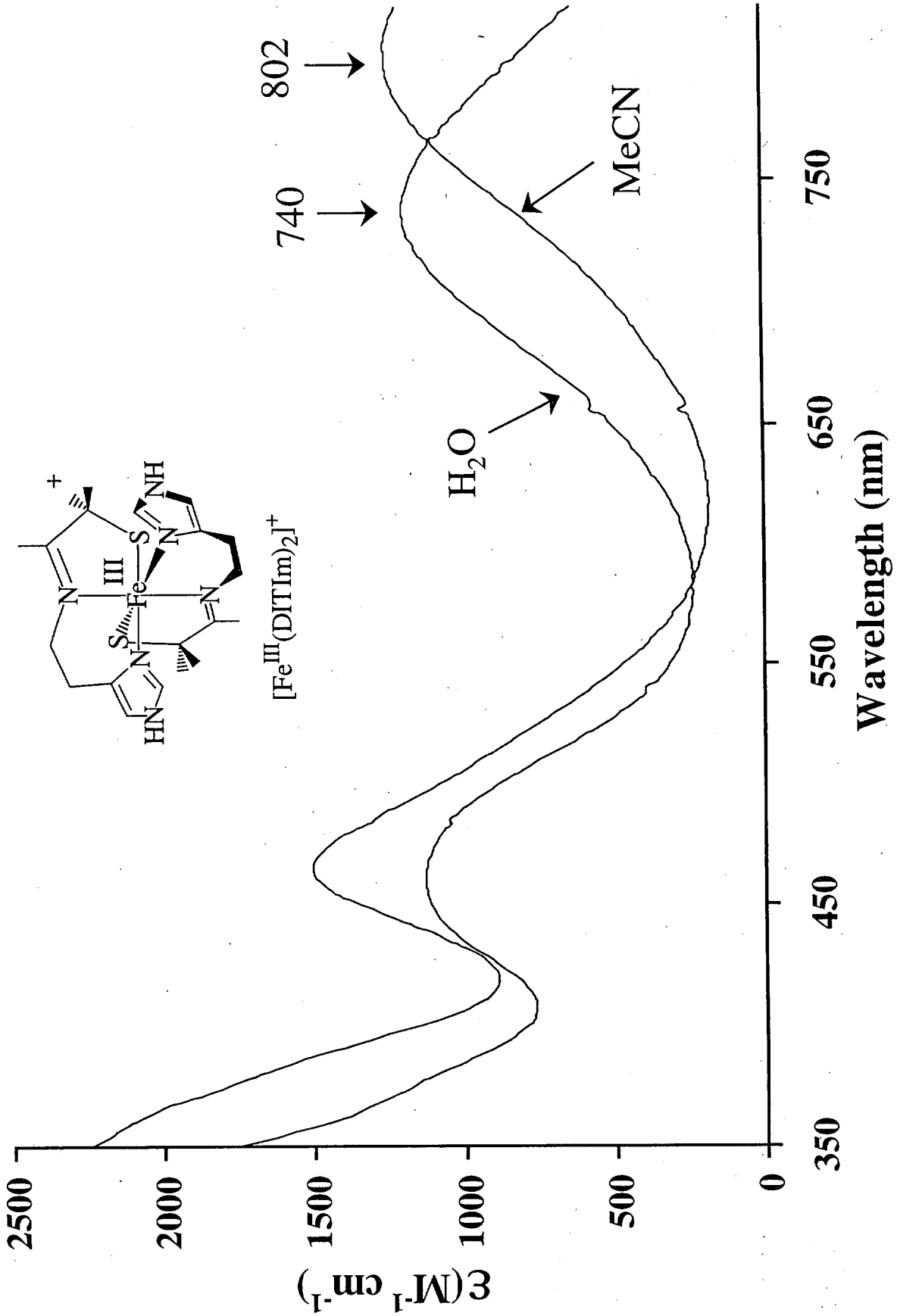
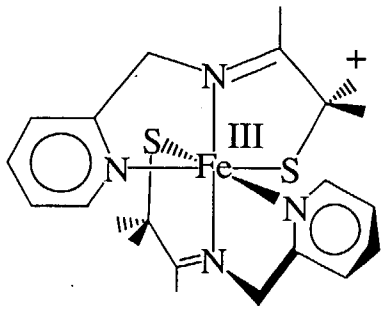


Figure S-1. Electronic spectrum of $[Fe(III)(DITIm)_2]Cl$ (**2**) in aprotic (MeCN, 298 K) *vs* protic (H_2O, 298 K) solvents.



$[Fe^{III}(DITpy)_2]^+$

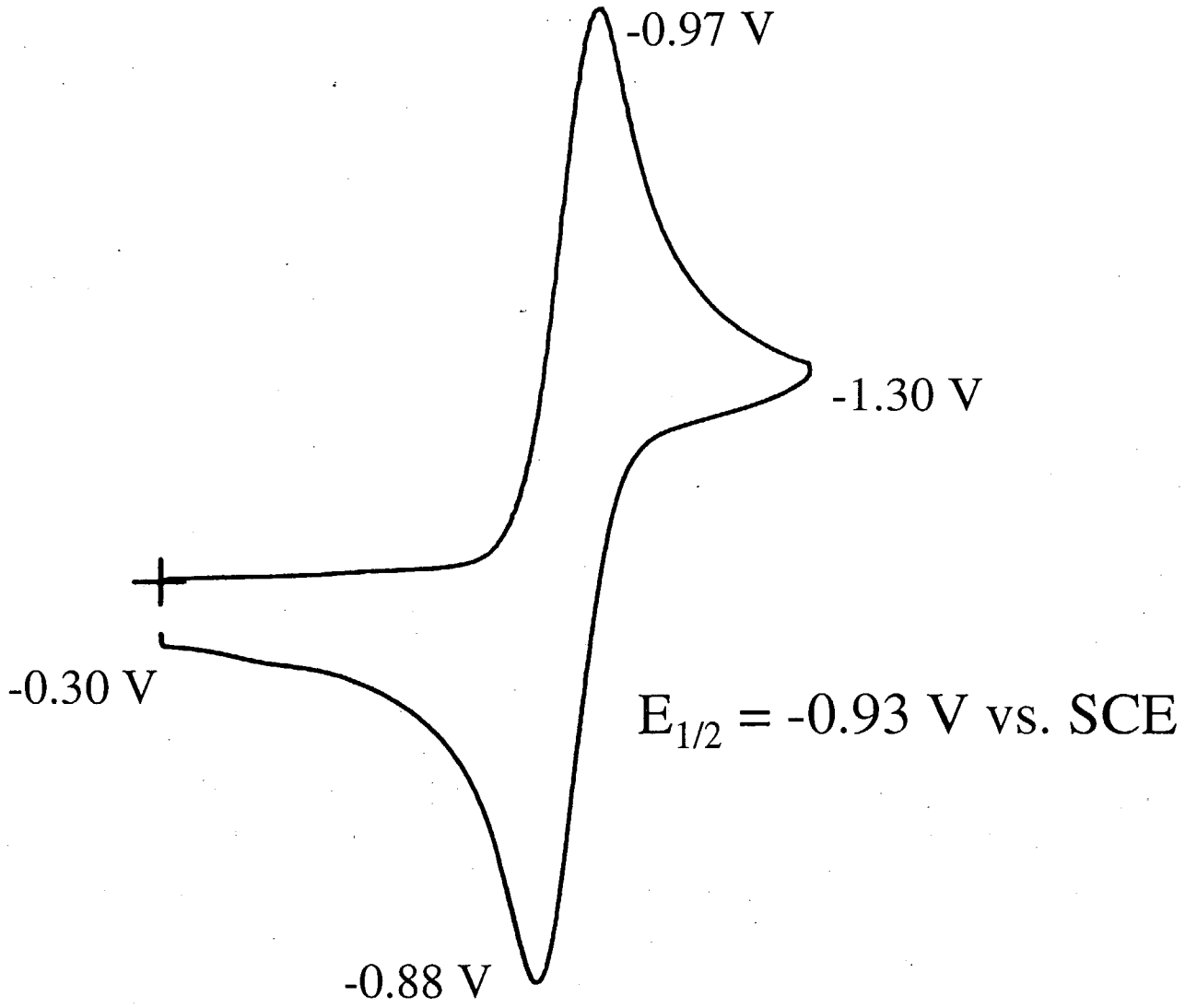
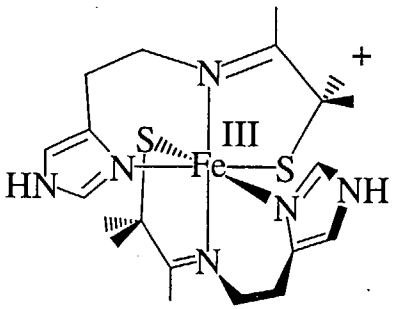


Figure S-2. Cyclic voltammogram of [Fe(III)$(DITpy)_2$]Cl (**1**) in MeCN solution at 298 K (0.1 M $(Bu_4N)PF_6$, glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.



$[Fe^{III}(DITIm)_2]^+$

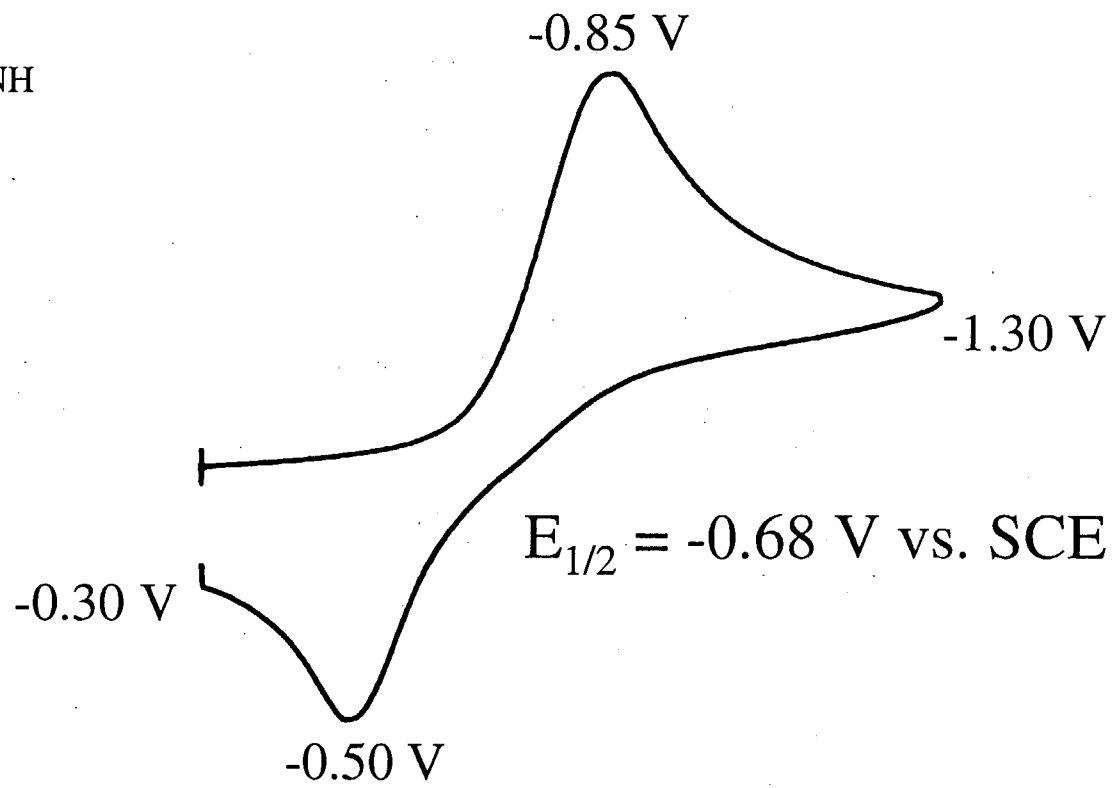
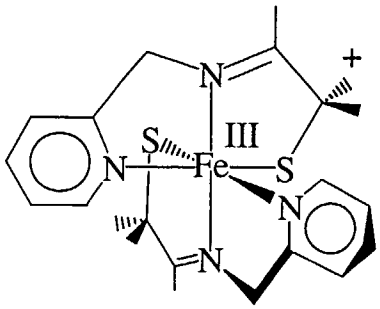


Figure S-3. Cyclic voltammogram of [Fe(III)$(DITIm)_2$]Cl (**2**) in MeCN solution at 298 K (0.1 M $(Bu_4N)PF_6$, glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.



$[Fe^{III}(DITpy)_2]^+$

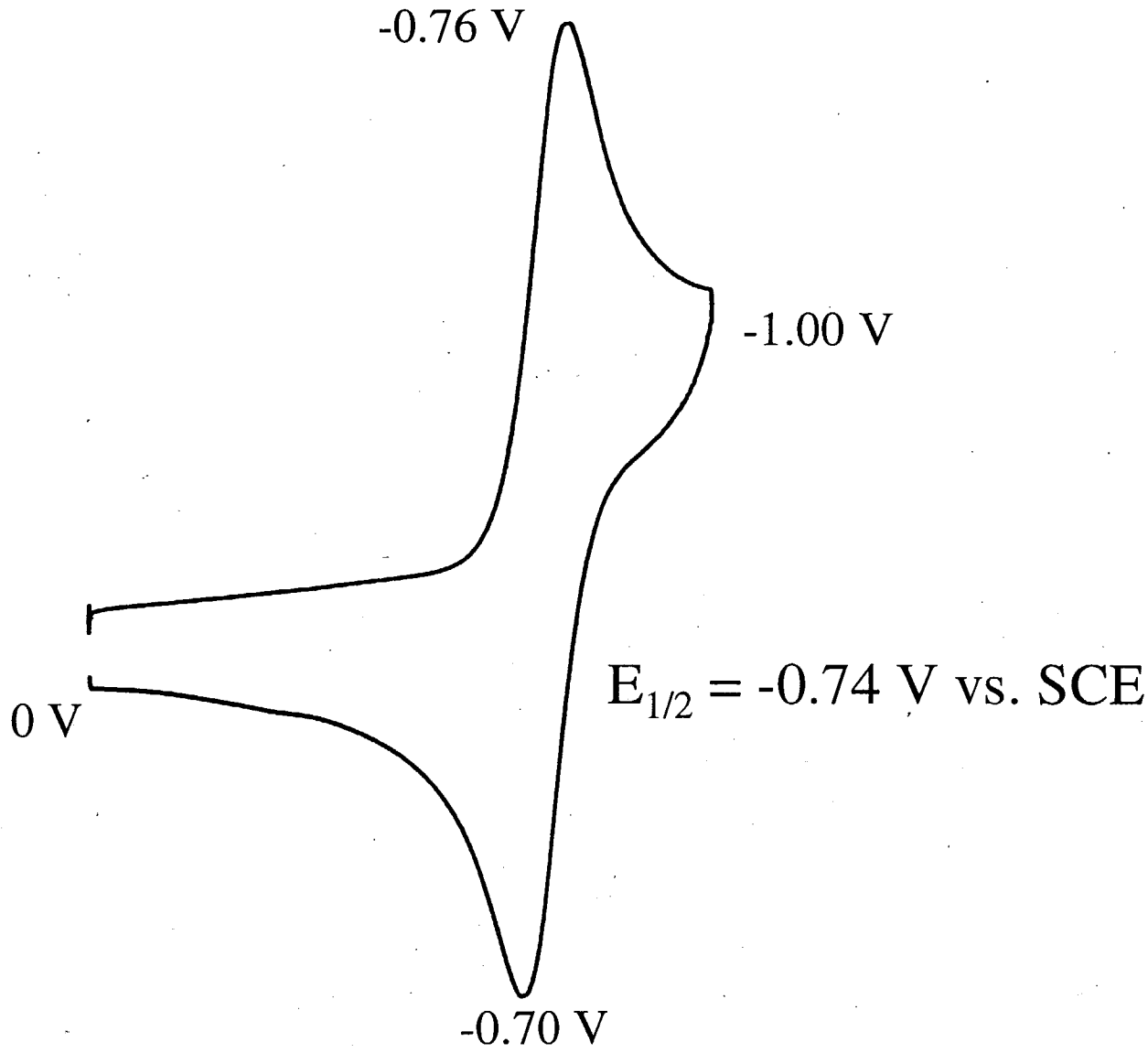


Figure S-4. Cyclic voltammogram of [Fe(III)(DITpy)$_2$]Cl (**1**) in H_2O solution at 298 K (0.1 M KCl, glassy carbon electrode, 50 mV/sec scan rate.) Peak potentials vs. SCE indicated.

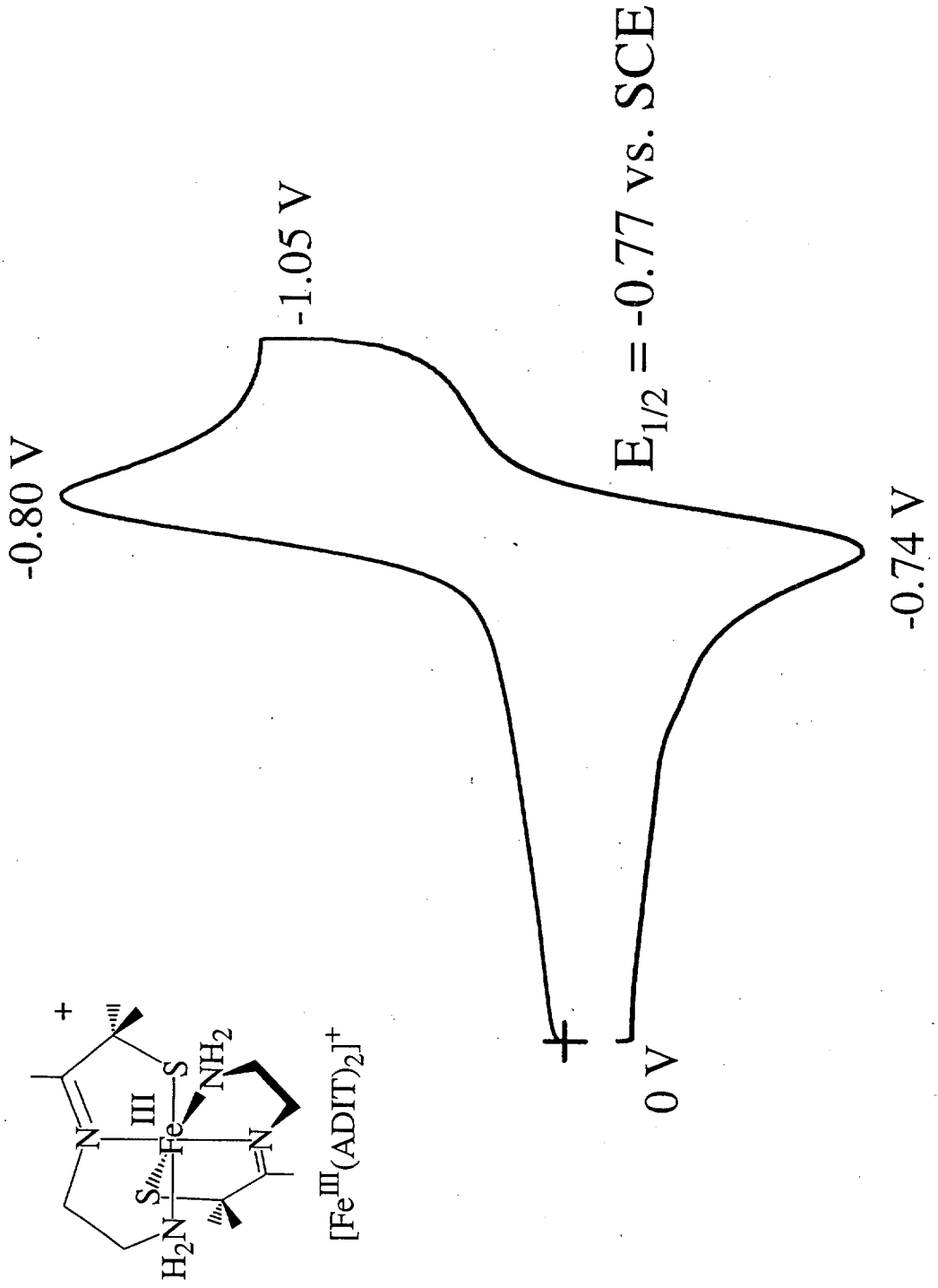


Figure S-5. Cyclic voltammogram of $[Fe(III)(ADIT)_2]Cl$ (**3**) in H_2O solution at 298 K (0.1 M KCl, glassy carbon electrode, 100 mV/sec scan rate.) Peak potentials vs. SCE indicated.

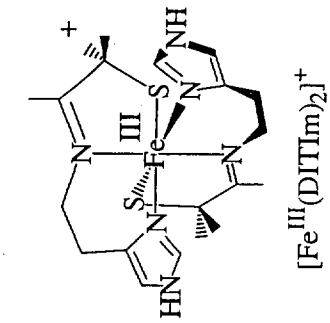


Figure S-6. X-band EPR spectrum of [Fe(III)(DITIm)$_2$]Cl (**2**) in MeOH/EtOH (9:1) glass at 135 K. Microwave frequency, 9.419 GHz; microwave power, 2 mW; modulation frequency, 100 kHz; modulation amplitude, 2G.

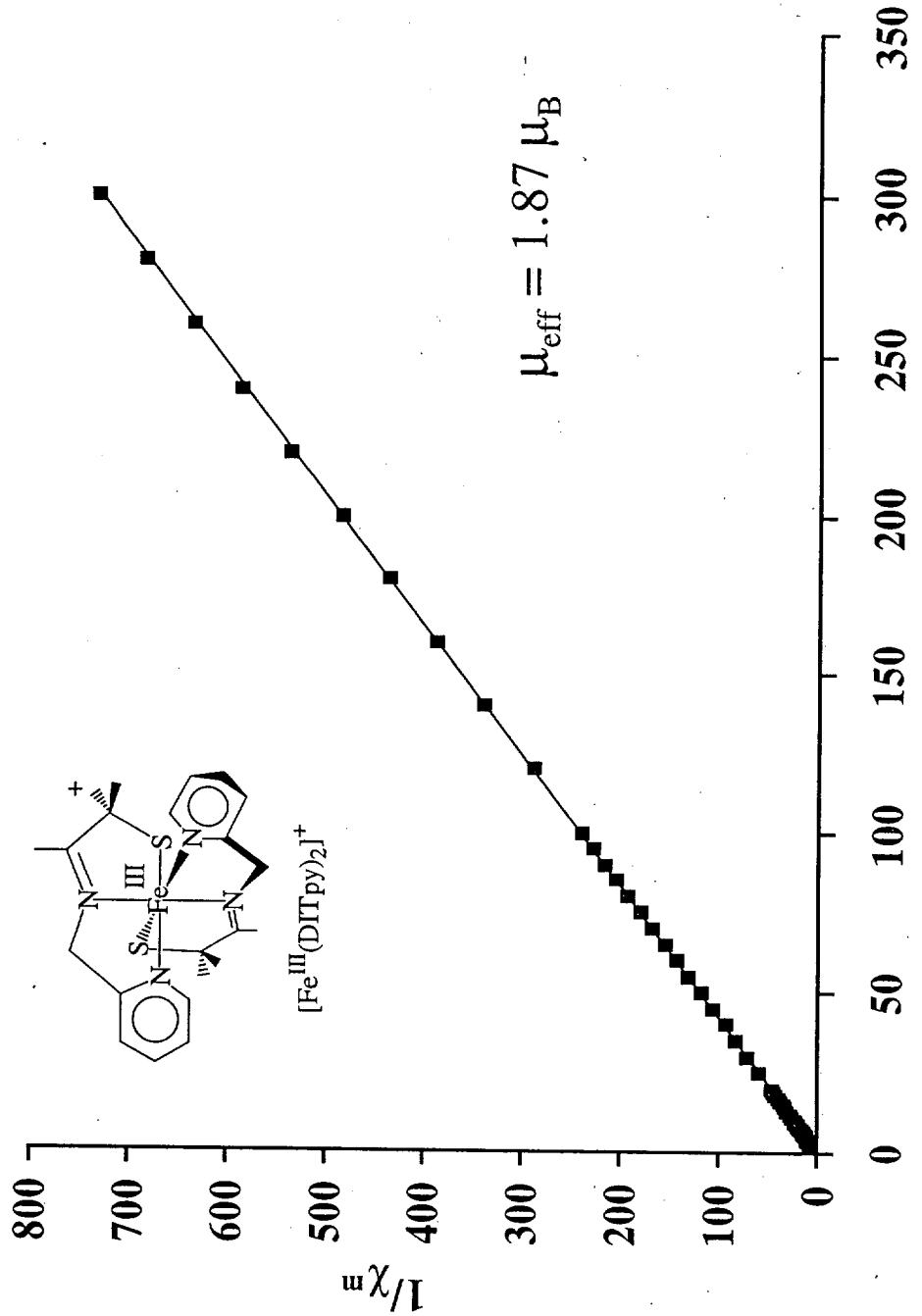


Figure S-7. $1/\chi_m$ (molar susceptibility) vs. temperature plot for [Fe(III)(DITpy)$_2$]Cl (1) over the temperature range T = 5-300 K.

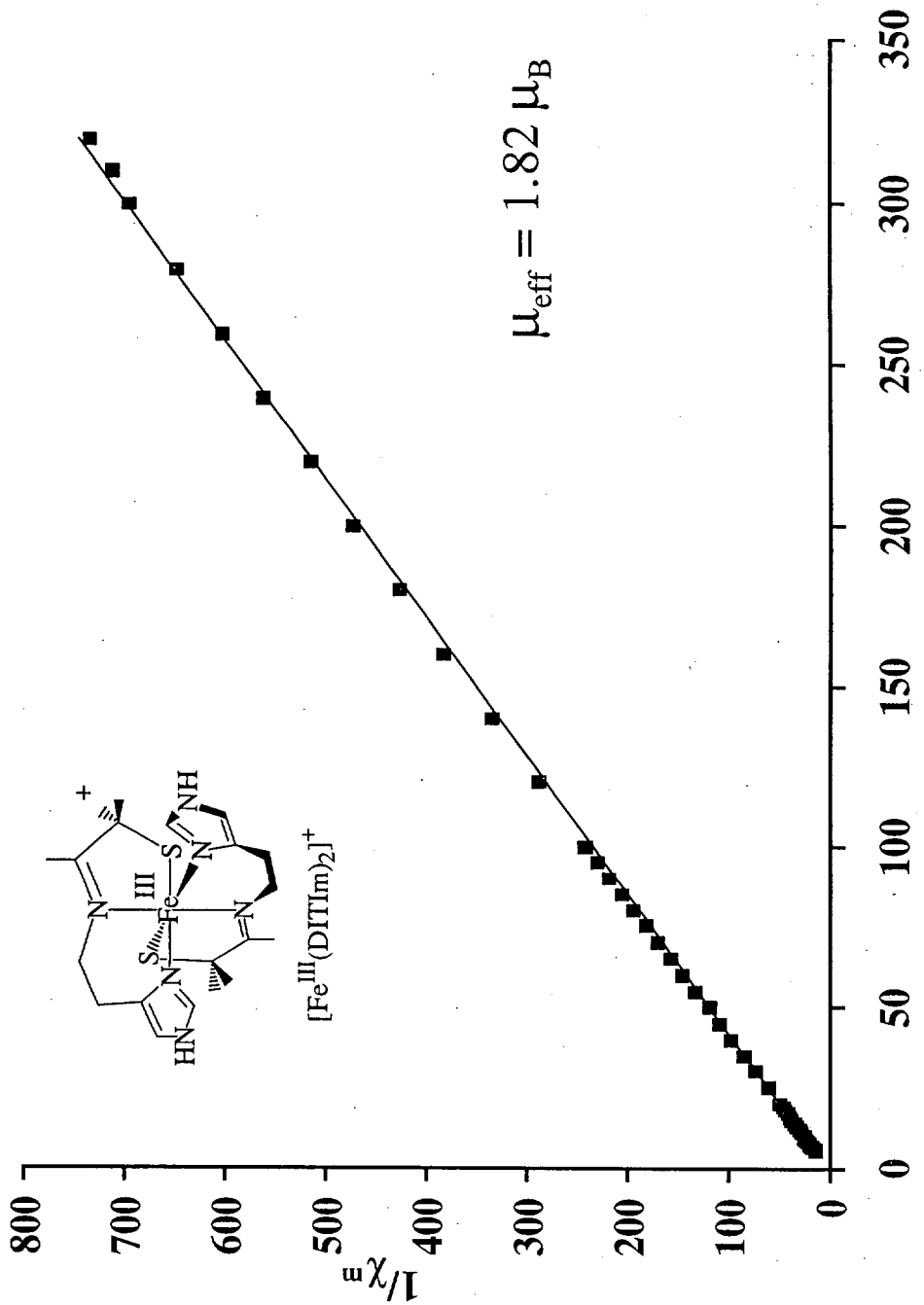


Figure S-8. $1/\chi_m$ (molar susceptibility) vs. temperature plot for $[Fe(III)(DITIm)_2]Cl$ (**2**) over the temperature range T = 5-300 K.

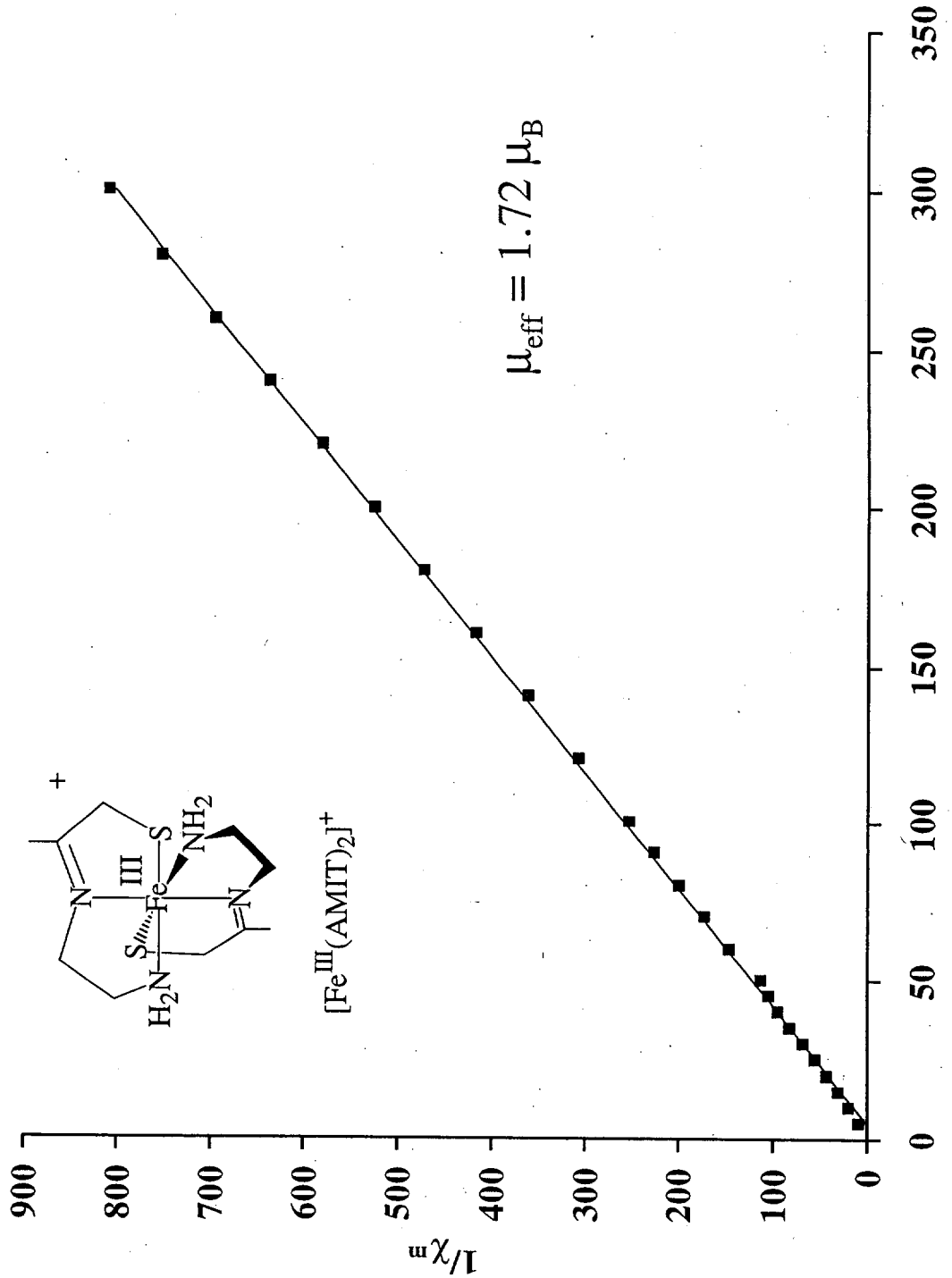


Figure S-9. $1/\chi_m$ (molar susceptibility) vs. temperature plot for [Fe(III)(AMIT)$_2$]Cl (**4**) over the temperature range T = 5-300 K.

Table 1. Crystal data and structure refinement for 1.

Identification code	hj961
Empirical formula	$C_{44}H_{72}Cl_2Fe_2N_8O_6S_4$ ⇒ $[Fe(III)(DIT_{PY})_2]Cl \cdot 3H_2O$ (1)
Formula weight	1119.98
Temperature	183 K
Wavelength	0.71073 Å
Crystal system	Orthorhombic
Space group	$Pca2_1$
Unit cell dimensions	a = 19.800(4) Å α = 90° b = 18.450(4) Å β = 90° c = 14.800(3) Å γ = 90°
Volume	5406(1) Å^3
Z	8
Density (calculated)	1.361 Mg/m^3
Absorption coefficient	0.851 mm^{-1}
F(000)	2400
Crystal size	.35 x .35 x .35 mm
θ range for data collection	1.51 to 24.97°
Index ranges	$0 \le h \le 22$, $-21 \le k \le 0$, $0 \le \ell \le 17$
Reflections collected	5247
Independent reflections	4886 (R_{int} = 0.1397)
Absorption correction	Semi-empirical from ψ-scans
Max. and min. transmission	0.999 and 0.754
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4876 / 0 / 564
Goodness-of-fit on F^2	1.034
Final R indices [$I>2\sigma(I)$]	R1 = 0.0584, wR2 = 0.1589
R indices (all data)	R1 = 0.0978, wR2 = 0.1940
Absolute structure parameter	0.10(4)
Largest diff. peak and hole	1.083 and -0.859 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
FeA	933(1)	567(1)	7500	21(1)
S(1A)	1730(1)	1196(1)	8178(2)	29(1)
N(1A)	66(4)	47(4)	7202(5)	24(2)
N(2A)	316(4)	1244(4)	8061(6)	29(2)
C(1A)	1(5)	-599(5)	6777(7)	32(2)
C(2A)	-612(6)	-912(5)	6626(7)	38(3)
C(3A)	-1203(6)	-574(5)	6917(9)	44(3)
C(4A)	-1116(5)	76(6)	7349(8)	41(3)
C(5A)	-509(5)	380(5)	7497(7)	31(2)
C(6A)	-399(5)	1091(5)	7962(8)	33(2)
C(7A)	496(5)	1846(4)	8442(7)	27(2)
C(8A)	1237(5)	1989(5)	8536(7)	31(2)
C(9A)	4(6)	2385(6)	8803(10)	51(3)
C(10A)	1423(6)	2165(7)	9513(8)	48(3)
C(11A)	1422(7)	2638(5)	7911(10)	50(3)
S(2A)	900(1)	1126(1)	6196(2)	31(1)
N(3A)	969(4)	-173(4)	8516(6)	28(2)
N(4A)	1543(4)	-101(4)	6949(6)	27(2)
C(12A)	638(6)	-141(6)	9321(7)	34(2)
C(13A)	677(6)	-681(6)	9943(7)	42(3)
C(14A)	1070(6)	-1303(6)	9764(8)	42(3)
C(15A)	1407(6)	-1326(5)	8951(7)	36(2)
C(16A)	1356(5)	-746(5)	8355(6)	24(2)
C(17A)	1728(5)	-747(4)	7483(6)	28(2)
C(18A)	1808(5)	1(5)	6148(6)	26(2)
C(19A)	1609(5)	665(6)	5637(7)	31(2)
C(20A)	2300(6)	-524(6)	5753(7)	40(3)
C(21A)	1389(7)	470(8)	4669(7)	58(4)
C(22A)	2223(5)	1192(6)	5626(9)	47(3)
FeB	953(1)	4382(1)	2356(1)	23(1)
S(1B)	984(1)	3876(1)	1026(2)	34(1)
N(1B)	930(4)	5084(4)	3437(5)	21(2)
N(2B)	1561(4)	5098(4)	1893(5)	29(2)
C(1B)	547(5)	5024(5)	4184(6)	29(2)
C(2B)	543(6)	5551(6)	4837(6)	38(3)
C(3B)	935(6)	6160(6)	4740(7)	40(3)
C(4B)	1326(5)	6231(5)	3957(6)	29(2)
C(5B)	1309(5)	5676(5)	3329(6)	26(2)
C(6B)	1737(5)	5716(5)	2477(7)	28(2)
C(7B)	1853(5)	5039(5)	1111(7)	32(2)
C(8B)	1683(6)	4384(6)	539(7)	40(3)
C(9B)	2351(6)	5581(6)	765(8)	44(3)
C(10B)	2318(5)	3892(6)	512(9)	53(3)
C(11B)	1496(7)	4614(8)	-429(8)	59(4)
S(2B)	1766(1)	3775(1)	3044(2)	34(1)
N(3B)	63(4)	4877(4)	2082(5)	25(2)
N(4B)	363(4)	3635(4)	2815(5)	29(2)
C(12B)	-44(5)	5557(5)	1755(7)	33(2)

C(13B)	-661(6)	5873(6)	1701(8)	45(3)
C(14B)	-1202(6)	5487(6)	1975(9)	49(3)
C(15B)	-1120(6)	4793(6)	2272(8)	43(3)
C(16B)	-485(5)	4500(5)	2329(7)	27(2)

C(17B)	-362(5)	3730(5)	2626(7)	34(2)
C(18B)	567(5)	3038(5)	3165(7)	32(2)
C(19B)	1303(6)	2944(5)	3355(8)	43(3)
C(20B)	90(7)	2426(6)	3406(10)	56(3)
C(21B)	1575(7)	2307(6)	2787(13)	71(5)
C(22B)	1402(9)	2809(7)	4373(10)	74(5)
Cl(1)	-931(1)	2152(2)	11068(2)	48(1)
Cl(2)	-3371(2)	2324(2)	11775(2)	51(1)
O(1S)	2667(4)	7614(4)	94(6)	48(2)
O(2S)	3055(4)	7008(4)	2286(6)	54(2)
O(3S)	1934(4)	8584(4)	3579(6)	49(2)
O(4S)	3153(5)	6659(5)	4067(6)	64(2)
O(5S)	130(7)	7379(6)	1158(10)	107(4)
O(6S)	4366(7)	6341(7)	4948(10)	106(4)

Table 3. Selected bond lengths [Å] and angles [°] for 1.

FeA-N(4A)	1.909(8)	FeA-N(2A)	1.934(8)
FeA-N(1A)	2.014(8)	FeA-N(3A)	2.032(8)
FeA-S(2A)	2.189(3)	FeA-S(1A)	2.202(3)
N(4A)-FeA-N(2A)	179.8(4)	N(4A)-FeA-N(1A)	98.0(3)
N(2A)-FeA-N(1A)	82.2(3)	N(4A)-FeA-N(3A)	82.0(3)
N(2A)-FeA-N(3A)	97.9(3)	N(1A)-FeA-N(3A)	82.7(3)
N(4A)-FeA-S(2A)	86.9(2)	N(2A)-FeA-S(2A)	93.2(3)
N(1A)-FeA-S(2A)	90.4(2)	N(3A)-FeA-S(2A)	165.9(2)
N(4A)-FeA-S(1A)	94.6(2)	N(2A)-FeA-S(1A)	85.2(2)
N(1A)-FeA-S(1A)	164.1(2)	N(3A)-FeA-S(1A)	89.5(2)
S(2A)-FeA-S(1A)	100.06(11)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for 1.

FeA-N(4A)	1.909(8)	FeA-N(2A)	1.934(8)
FeA-N(1A)	2.014(8)	FeA-N(3A)	2.032(8)
FeA-S(2A)	2.189(3)	FeA-S(1A)	2.202(3)
S(1A)-C(8A)	1.837(9)	N(1A)-C(1A)	1.354(12)
N(1A)-C(5A)	1.365(13)	N(2A)-C(7A)	1.296(11)
N(2A)-C(6A)	1.452(12)	C(1A)-C(2A)	1.362(14)
C(2A)-C(3A)	1.40(2)	C(3A)-C(4A)	1.37(2)
C(4A)-C(5A)	1.344(14)	C(5A)-C(6A)	1.498(13)
C(7A)-C(9A)	1.491(14)	C(7A)-C(8A)	1.497(14)
C(8A)-C(10A)	1.53(2)	C(8A)-C(11A)	1.557(14)
S(2A)-C(19A)	1.838(10)	N(3A)-C(16A)	1.329(12)
N(3A)-C(12A)	1.361(13)	N(4A)-C(18A)	1.310(13)
N(4A)-C(17A)	1.475(11)	C(12A)-C(13A)	1.36(2)
C(13A)-C(14A)	1.41(2)	C(14A)-C(15A)	1.38(2)
C(15A)-C(16A)	1.391(13)	C(16A)-C(17A)	1.486(13)
C(18A)-C(19A)	1.494(13)	C(18A)-C(20A)	1.492(14)
C(19A)-C(21A)	1.54(2)	C(19A)-C(22A)	1.557(14)
FeB-N(2B)	1.914(8)	FeB-N(4B)	1.930(8)
FeB-N(3B)	2.026(8)	FeB-N(1B)	2.059(7)
FeB-S(1B)	2.179(3)	FeB-S(2B)	2.209(3)
S(1B)-C(8B)	1.820(12)	N(1B)-C(5B)	1.334(12)
N(1B)-C(1B)	1.346(12)	N(2B)-C(7B)	1.298(13)
N(2B)-C(6B)	1.473(11)	C(1B)-C(2B)	1.371(13)
C(2B)-C(3B)	1.37(2)	C(3B)-C(4B)	1.40(2)
C(4B)-C(5B)	1.384(12)	C(5B)-C(6B)	1.522(13)
C(7B)-C(9B)	1.493(14)	C(7B)-C(8B)	1.515(14)
C(8B)-C(11B)	1.54(2)	C(8B)-C(10B)	1.55(2)
S(2B)-C(19B)	1.844(11)	N(3B)-C(16B)	1.339(12)
N(3B)-C(12B)	1.361(12)	N(4B)-C(18B)	1.282(12)
N(4B)-C(17B)	1.474(12)	C(12B)-C(13B)	1.36(2)
C(13B)-C(14B)	1.35(2)	C(14B)-C(15B)	1.36(2)
C(15B)-C(16B)	1.37(2)	C(16B)-C(17B)	1.507(13)
C(18B)-C(19B)	1.49(2)	C(18B)-C(20B)	1.514(14)
C(19B)-C(22B)	1.54(2)	C(19B)-C(21B)	1.54(2)

N(4A)-FeA-N(2A)	179.8(4)	N(4A)-FeA-N(1A)	98.0(3)
N(2A)-FeA-N(1A)	82.2(3)	N(4A)-FeA-N(3A)	82.0(3)
N(2A)-FeA-N(3A)	97.9(3)	N(1A)-FeA-N(3A)	82.7(3)

N(4A)-FeA-S(2A)	86.9(2)	N(2A)-FeA-S(2A)	93.2(3)
N(1A)-FeA-S(2A)	90.4(2)	N(3A)-FeA-S(2A)	165.9(2)
N(4A)-FeA-S(1A)	94.6(2)	N(2A)-FeA-S(1A)	85.2(2)
N(1A)-FeA-S(1A)	164.1(2)	N(3A)-FeA-S(1A)	89.5(2)
S(2A)-FeA-S(1A)	100.06(11)	C(8A)-S(1A)-FeA	99.8(3)
C(1A)-N(1A)-C(5A)	117.7(8)	C(1A)-N(1A)-FeA	127.0(7)
C(5A)-N(1A)-FeA	115.2(6)	C(7A)-N(2A)-C(6A)	118.6(8)
C(7A)-N(2A)-FeA	124.6(7)	C(6A)-N(2A)-FeA	116.5(6)
C(2A)-C(1A)-N(1A)	122.3(10)	C(1A)-C(2A)-C(3A)	120.5(10)
C(4A)-C(3A)-C(2A)	115.4(10)	C(5A)-C(4A)-C(3A)	123.7(11)
C(4A)-C(5A)-N(1A)	120.4(9)	C(4A)-C(5A)-C(6A)	124.8(9)
N(1A)-C(5A)-C(6A)	114.8(8)	N(2A)-C(6A)-C(5A)	111.0(7)
N(2A)-C(7A)-C(9A)	123.2(9)	N(2A)-C(7A)-C(8A)	117.4(8)
C(9A)-C(7A)-C(8A)	119.4(8)	C(7A)-C(8A)-C(10A)	111.2(9)
C(7A)-C(8A)-C(11A)	108.1(8)	C(10A)-C(8A)-C(11A)	110.0(9)
C(7A)-C(8A)-S(1A)	110.8(6)	C(10A)-C(8A)-S(1A)	108.3(7)
C(11A)-C(8A)-S(1A)	108.5(7)	C(19A)-S(2A)-FeA	99.0(3)
C(16A)-N(3A)-C(12A)	118.0(8)	C(16A)-N(3A)-FeA	114.9(6)
C(12A)-N(3A)-FeA	127.0(7)	C(18A)-N(4A)-C(17A)	120.0(8)
C(18A)-N(4A)-FeA	123.2(6)	C(17A)-N(4A)-FeA	116.8(6)
C(13A)-C(12A)-N(3A)	122.3(10)	C(12A)-C(13A)-C(14A)	120.1(10)
C(15A)-C(14A)-C(13A)	117.1(9)	C(14A)-C(15A)-C(16A)	119.7(10)
N(3A)-C(16A)-C(15A)	122.7(9)	N(3A)-C(16A)-C(17A)	116.3(8)
C(15A)-C(16A)-C(17A)	121.0(9)	N(4A)-C(17A)-C(16A)	109.9(8)
N(4A)-C(18A)-C(19A)	118.0(8)	N(4A)-C(18A)-C(20A)	121.5(9)
C(19A)-C(18A)-C(20A)	120.4(8)	C(18A)-C(19A)-C(21A)	110.8(9)
C(18A)-C(19A)-C(22A)	108.1(8)	C(21A)-C(19A)-C(22A)	110.9(10)
C(18A)-C(19A)-S(2A)	110.7(7)	C(21A)-C(19A)-S(2A)	108.1(8)
C(22A)-C(19A)-S(2A)	108.2(7)	N(2B)-FeB-N(4B)	178.1(3)
N(2B)-FeB-N(3B)	99.4(3)	N(4B)-FeB-N(3B)	82.3(3)
N(2B)-FeB-N(1B)	81.8(3)	N(4B)-FeB-N(1B)	99.3(3)
N(3B)-FeB-N(1B)	81.5(3)	N(2B)-FeB-S(1B)	87.4(2)
N(4B)-FeB-S(1B)	91.7(2)	N(3B)-FeB-S(1B)	92.1(2)
N(1B)-FeB-S(1B)	166.4(2)	N(2B)-FeB-S(2B)	93.3(3)
N(4B)-FeB-S(2B)	85.2(2)	N(3B)-FeB-S(2B)	162.6(2)
N(1B)-FeB-S(2B)	88.7(2)	S(1B)-FeB-S(2B)	100.32(11)
C(8B)-S(1B)-FeB	99.1(3)	C(5B)-N(1B)-C(1B)	118.8(8)
C(5B)-N(1B)-FeB	114.2(6)	C(1B)-N(1B)-FeB	126.9(6)
C(7B)-N(2B)-C(6B)	118.8(8)	C(7B)-N(2B)-FeB	122.8(7)
C(6B)-N(2B)-FeB	118.2(6)	N(1B)-C(1B)-C(2B)	121.6(9)

C(1B)-C(2B)-C(3B)	120.2(10)	C(2B)-C(3B)-C(4B)	118.5(9)
C(5B)-C(4B)-C(3B)	118.2(9)	N(1B)-C(5B)-C(4B)	122.7(9)

N(1B)-C(5B)-C(6B)	116.9(7)	C(4B)-C(5B)-C(6B)	120.5(8)
N(2B)-C(6B)-C(5B)	108.5(7)	N(2B)-C(7B)-C(9B)	123.0(9)
N(2B)-C(7B)-C(8B)	117.8(9)	C(9B)-C(7B)-C(8B)	119.3(9)
C(7B)-C(8B)-C(11B)	110.6(10)	C(7B)-C(8B)-C(10B)	107.6(9)
C(11B)-C(8B)-C(10B)	109.5(10)	C(7B)-C(8B)-S(1B)	111.0(7)
C(11B)-C(8B)-S(1B)	109.1(8)	C(10B)-C(8B)-S(1B)	109.0(8)
C(19B)-S(2B)-FeB	100.0(4)	C(16B)-N(3B)-C(12B)	116.7(8)
C(16B)-N(3B)-FeB	114.6(6)	C(12B)-N(3B)-FeB	128.4(7)
C(18B)-N(4B)-C(17B)	119.1(8)	C(18B)-N(4B)-FeB	124.4(7)
C(17B)-N(4B)-FeB	116.0(6)	C(13B)-C(12B)-N(3B)	123.8(10)
C(12B)-C(13B)-C(14B)	118.1(10)	C(13B)-C(14B)-C(15B)	119.8(11)
C(14B)-C(15B)-C(16B)	120.0(11)	N(3B)-C(16B)-C(15B)	121.4(9)
N(3B)-C(16B)-C(17B)	116.0(8)	C(15B)-C(16B)-C(17B)	122.5(9)
N(4B)-C(17B)-C(16B)	108.9(7)	N(4B)-C(18B)-C(19B)	118.8(8)
N(4B)-C(18B)-C(20B)	122.6(10)	C(19B)-C(18B)-C(20B)	118.5(9)
C(18B)-C(19B)-C(22B)	109.0(11)	C(18B)-C(19B)-C(21B)	109.0(9)
C(22B)-C(19B)-C(21B)	111.4(11)	C(18B)-C(19B)-S(2B)	110.0(7)
C(22B)-C(19B)-S(2B)	108.4(8)	C(21B)-C(19B)-S(2B)	108.9(9)

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:
$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
FeA	20(1)	19(1)	25(1)	1(1)	-1(1)	1(1)
S(1A)	24(1)	24(1)	39(1)	-3(1)	-4(1)	0(1)
N(1A)	28(4)	21(3)	25(4)	1(3)	-6(3)	-7(3)
N(2A)	24(4)	23(4)	41(5)	-4(3)	-2(4)	5(3)
C(1A)	27(5)	33(5)	36(5)	0(4)	-5(5)	-3(4)
C(2A)	47(7)	25(5)	43(6)	0(4)	-13(5)	-6(5)
C(3A)	35(6)	34(5)	63(8)	7(5)	-27(6)	-3(5)
C(4A)	17(5)	53(6)	54(7)	5(6)	-3(5)	-11(5)
C(5A)	26(6)	34(5)	33(5)	4(4)	-6(5)	5(4)
C(6A)	16(5)	32(5)	52(6)	-5(5)	4(5)	5(4)
C(7A)	23(5)	20(4)	36(5)	1(4)	-5(4)	7(4)
C(8A)	37(6)	17(4)	39(5)	-1(4)	-9(5)	6(4)
C(9A)	34(7)	52(7)	68(8)	-24(6)	1(6)	11(6)
C(10A)	30(6)	57(7)	58(8)	-16(6)	-8(6)	14(6)
C(11A)	51(8)	18(5)	80(9)	6(5)	-3(7)	2(5)
S(2A)	31(1)	29(1)	34(1)	9(1)	-3(1)	3(1)
N(3A)	22(4)	29(4)	33(4)	5(3)	5(4)	2(4)
N(4A)	28(5)	18(3)	35(4)	2(3)	-7(4)	-3(3)
C(12A)	33(6)	40(6)	29(5)	-9(4)	1(5)	-3(5)
C(13A)	37(7)	68(7)	20(5)	5(5)	0(5)	-16(6)
C(14A)	44(7)	38(6)	43(6)	21(5)	0(5)	-1(5)
C(15A)	37(6)	32(5)	39(6)	5(4)	-5(5)	-6(5)
C(16A)	20(5)	26(4)	27(5)	0(4)	-11(4)	-8(4)
C(17A)	43(6)	22(4)	19(5)	6(4)	5(5)	7(4)
C(18A)	26(5)	32(5)	20(4)	-1(4)	-1(4)	1(4)
C(19A)	21(5)	47(6)	25(5)	5(4)	-3(4)	2(4)
C(20A)	43(7)	43(6)	35(6)	-2(5)	5(5)	12(5)
C(21A)	67(9)	87(9)	20(5)	7(6)	0(6)	22(8)
C(22A)	35(6)	40(6)	67(8)	26(6)	9(6)	-7(5)
FeB	25(1)	21(1)	22(1)	-3(1)	-1(1)	1(1)
S(1B)	32(1)	38(1)	30(1)	-14(1)	-1(1)	-2(1)
N(1B)	21(4)	21(4)	22(4)	-1(3)	3(3)	7(3)
N(2B)	39(5)	22(4)	27(4)	-3(3)	-1(4)	6(4)
C(1B)	31(6)	32(5)	24(5)	3(4)	-7(4)	3(4)
C(2B)	50(7)	44(6)	20(5)	-5(4)	6(5)	10(5)
C(3B)	43(7)	48(6)	30(5)	-9(5)	0(5)	5(5)
C(4B)	34(6)	26(5)	29(5)	-4(4)	-6(4)	3(4)
C(5B)	27(5)	25(5)	25(5)	-7(4)	-3(4)	2(4)
C(6B)	21(5)	29(4)	34(5)	-7(4)	13(5)	-10(4)
C(7B)	30(6)	36(5)	30(5)	-1(4)	3(5)	2(4)
C(8B)	31(6)	62(7)	27(5)	-16(5)	7(5)	2(5)
C(9B)	37(7)	61(7)	35(6)	0(5)	7(5)	-20(5)
C(10B)	29(7)	57(7)	72(9)	-38(7)	4(6)	8(5)
C(11B)	46(8)	100(10)	32(6)	-22(6)	7(6)	-27(7)
S(2B)	29(1)	27(1)	46(2)	-3(1)	-11(1)	0(1)
N(3B)	33(5)	23(4)	20(4)	-11(3)	-2(3)	2(3)
N(4B)	27(5)	28(4)	31(4)	-3(3)	-1(4)	-1(3)
C(12B)	34(6)	34(5)	31(5)	-6(4)	-3(5)	-1(5)

C(13B)	58(8)	32(5)	46(7)	-3(5)	-20(6)	13(6)
C(14B)	37(7)	44(6)	66(8)	-4(6)	-18(6)	18(6)
C(15B)	37(7)	46(6)	46(7)	-12(5)	2(5)	-4(5)
C(16B)	12(5)	38(5)	32(5)	-13(5)	9(4)	-6(4)

C(17B)	21(5)	41(5)	39(6)	7(4)	5(4)	-9(4)
C(18B)	35(6)	16(4)	44(6)	2(4)	-7(5)	-5(4)
C(19B)	45(7)	23(5)	61(7)	-2(5)	-13(6)	1(5)
C(20B)	61(9)	43(6)	63(8)	5(6)	-17(7)	-16(6)
C(21B)	41(8)	31(6)	141(15)	-28(8)	-21(9)	5(5)
C(22B)	95(12)	40(7)	88(11)	32(7)	-51(10)	-30(7)
Cl(1)	41(2)	45(2)	57(2)	16(1)	1(1)	2(1)
Cl(2)	43(2)	66(2)	43(2)	-6(2)	1(1)	-14(2)

Table 6. Hydrogen coordinates (x 10^4) and isotropic displacement parameters ($Å^2$ x 10^3) for 1.

	x	y	z	U(eq)
H(1AA)	412(5)	-846(5)	6620(7)	50
H(2AA)	-623(6)	-1359(5)	6295(7)	50
H(3AA)	-1639(6)	-786(5)	6815(9)	50
H(4AA)	-1507(5)	336(6)	7550(8)	50
H(6AA)	-591(5)	1472(5)	7604(8)	50
H(6AB)	-620(5)	1091(5)	8540(8)	50
H(9AA)	-454(6)	2224(6)	8724(10)	50
H(9AB)	91(6)	2464(6)	9433(10)	50
H(9AC)	71(6)	2829(6)	8478(10)	50
H(10A)	1171(6)	2582(7)	9706(8)	50
H(10B)	1323(6)	1763(7)	9902(8)	50
H(10C)	1897(6)	2271(7)	9541(8)	50
H(11A)	1157(7)	3053(5)	8081(10)	50
H(11B)	1892(7)	2745(5)	7992(10)	50
H(11C)	1338(7)	2524(5)	7288(10)	50
H(12A)	340(6)	260(6)	9429(7)	50
H(13A)	470(6)	-626(6)	10525(7)	50
H(14A)	1083(6)	-1698(6)	10186(8)	50
H(15A)	1710(6)	-1718(5)	8818(7)	50
H(17A)	2202(5)	-719(4)	7615(6)	50
H(17B)	1645(5)	-1180(4)	7141(6)	50
H(20A)	2373(6)	-927(6)	6152(7)	50
H(20B)	2119(6)	-696(6)	5191(7)	50
H(20C)	2721(6)	-282(6)	5645(7)	50
H(21A)	1747(7)	232(8)	4348(7)	50
H(21B)	1009(7)	150(8)	4716(7)	50
H(21C)	1259(7)	900(8)	4348(7)	50
H(22A)	2596(5)	949(6)	5342(9)	50
H(22B)	2111(5)	1619(6)	5287(9)	50
H(22C)	2346(5)	1326(6)	6230(9)	50
H(1BA)	272(5)	4600(5)	4259(6)	50
H(2BA)	265(6)	5488(6)	5362(6)	50
H(3BA)	920(6)	6546(6)	5174(7)	50
H(4BA)	1600(5)	6651(5)	3843(6)	50
H(6BA)	1611(5)	6154(5)	2172(7)	50
H(6BB)	2214(5)	5734(5)	2591(7)	50
H(9BA)	2403(6)	5946(6)	1222(8)	50
H(9BB)	2783(6)	5372(6)	629(8)	50
H(9BC)	2165(6)	5796(6)	229(8)	50
H(10D)	2653(5)	4199(6)	242(9)	50
H(10E)	2470(5)	3740(6)	1098(9)	50
H(10F)	2247(5)	3475(6)	137(9)	50
H(11D)	1868(7)	4875(8)	-690(8)	50
H(11E)	1393(7)	4200(8)	-796(8)	50
H(11F)	1109(7)	4925(8)	-396(8)	50
H(12B)	333(5)	5803(5)	1486(7)	50
H(13B)	-715(6)	6361(6)	1488(8)	50
H(14B)	-1630(6)	5724(6)	2050(9)	50
H(15C)	-1506(6)	4484(6)	2345(8)	50

H(17C)	-641(5)	3626(5)	3141(7)	50
H(17D)	-493(5)	3414(5)	2142(7)	50
H(20D)	-345(7)	2561(6)	3175(10)	50
H(20E)	217(7)	1962(6)	3168(10)	50

H(20F)	71(7)	2401(6)	4054(10)	50
H(21D)	1377(7)	1852(6)	2956(13)	50
H(21E)	1436(7)	2432(6)	2186(13)	50
H(21F)	2059(7)	2268(6)	2807(13)	50
H(22D)	1180(9)	2368(7)	4550(10)	50
H(22E)	1862(9)	2800(7)	4578(10)	50
H(22F)	1173(9)	3215(7)	4637(10)	50

Table 1. Crystal data and structure refinement for 1.

Identification code	hj963
Empirical formula	$C_{42}H_{72}Cl_2Fe_2N_{12}O_2S_4$ $[Fe(III)(DITIm)_2]Cl\cdot\frac{1}{2}\epsilon+c$ $\cdot\frac{1}{2}H_2$
Formula weight	1087.96
Temperature	183 K (2)
Wavelength	0.71073 Å
Crystal system	Monoclinic
Space group	~~c1c1~~ Cc
Unit cell dimensions	a = 24.792(4) Å α = 90° b = 14.364(3) Å β = 124.91(2)° c = 17.527(3) Å γ = 90°
Volume	5118(1) Å^3
Z	8
Density (calculated)	2.824 Mg/m^3
Absorption coefficient	1.765 mm^{-1}
F(000)	4592
Crystal size	.2 x .3 x .4 mm
θ range for data collection	1.74 to 22.51°
Index ranges	$-26 \le h \le 13$, $-13 \le k \le 15$, $-7 \le \ell \le 18$
Reflections collected	4756
Independent reflections	3356 (R_{int} = 0.0427)
Absorption correction	Semi-empirical from ψ-scans
Max. and min. transmission	0.520 and 0.944
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	3292 / 0 / 575
Goodness-of-fit on F^2	1.075
Final R indices [I>2σ(I)]	R1 = 0.0387, wR2 = 0.1117
R indices (all data)	R1 = 0.0431, wR2 = 0.1216
Absolute structure parameter	0.04(2)
Largest diff. peak and hole	0.362 and -0.266 eÅ^{-3}

Table 2. Atomic coordinates [x 10^4] and equivalent isotropic displacement parameters [$Å^2$ x 10^3] for 1. U(eq) is defined as one third of the trace of the orthogonalized U_{ij} tensor.

	x	y	z	U(eq)
Fe(1)	2189	1747(1)	1781	18(1)
S(1A)	1514(1)	831(1)	1877(2)	24(1)
S(2A)	2628(1)	2370(1)	3173(2)	24(1)
N(1A)	1786(3)	1149(4)	483(5)	20(2)
N(2A)	1060(3)	759(4)	-975(5)	24(2)
N(3A)	2903(3)	817(4)	2436(4)	17(2)
N(4A)	2778(3)	2545(4)	1580(5)	21(2)
N(5A)	3641(4)	3198(4)	1758(5)	28(2)
N(6A)	1491(4)	2700(4)	1275(4)	20(2)
C(1A)	1265(4)	1427(6)	-329(6)	26(2)
C(2A)	1481(5)	6(6)	-550(6)	25(2)
C(3A)	1918(4)	252(5)	358(5)	17(2)
C(4A)	2436(4)	-325(5)	1136(6)	28(2)
C(5A)	3030(4)	214(6)	1873(6)	27(2)
C(6A)	1008(4)	2601(5)	1342(5)	19(2)
C(7A)	534(5)	3378(6)	1149(7)	36(2)
C(8A)	861(5)	1655(5)	1584(7)	26(2)
C(9A)	211(5)	1304(7)	768(8)	52(3)
C(10A)	855(6)	1747(7)	2461(8)	48(3)
C(11A)	3098(5)	3731(6)	1101(7)	32(2)
C(12A)	3426(5)	2508(6)	2026(6)	25(2)
C(13A)	2578(5)	3326(5)	1001(6)	23(2)
C(14A)	1583(4)	3643(5)	1008(6)	26(2)
C(15A)	1883(4)	3625(6)	466(6)	29(2)
C(16A)	3258(4)	737(5)	3326(6)	24(2)
C(17A)	3795(5)	26(6)	3862(6)	34(2)
C(18A)	3163(4)	1407(6)	3902(6)	22(2)
C(19A)	3827(5)	1836(6)	4666(7)	35(2)
C(20A)	2848(5)	910(6)	4328(6)	32(2)
Fe(2)	2718(1)	-3323(1)	2800(1)	20(1)
S(1B)	2091(1)	-4045(1)	1460(2)	28(1)
S(2B)	3219(1)	-2430(1)	2357(2)	27(1)
N(1B)	2325(4)	-4101(4)	3338(5)	22(2)
N(2B)	1611(4)	-4800(5)	3497(5)	28(2)
N(3B)	1991(4)	-2390(4)	2282(5)	22(2)
N(4B)	3256(4)	-2694(4)	4088(5)	22(2)
N(5B)	4084(4)	-2140(5)	5428(5)	26(2)
N(6B)	3437(4)	-4243(4)	3181(5)	22(2)
C(1B)	1714(5)	-4101(6)	3105(7)	29(2)
C(2B)	2183(5)	-5280(6)	4032(6)	34(2)
C(3B)	2626(4)	-4851(5)	3929(6)	24(2)
C(4B)	3326(5)	-5074(6)	4351(7)	36(2)
C(5B)	3479(5)	-5146(6)	3628(7)	34(2)
C(6B)	1502(5)	-2412(5)	1424(7)	25(2)
C(7B)	959(4)	-1687(5)	962(6)	27(2)
C(8B)	1417(5)	-3206(5)	788(6)	27(2)
C(9B)	1460(5)	-2816(6)	6(6)	35(2)
C(10B)	761(5)	-3708(6)	389(7)	38(2)

C(11B)	3506(5)	-1727(5)	5219(7)	30(2)
C(12B)	3890(5)	-2712(6)	4716(7)	29(2)
C(13B)	3016(4)	-2088(5)	4416(6)	20(2)
C(14B)	2300(5)	-1849(6)	3847(6)	27(2)

C(15B)	2014(5)	-1593(6)	2843(6)	32(2)
C(16B)	3848(5)	-4103(5)	2968(6)	28(2)
C(17B)	4404(5)	-4774(6)	3240(7)	39(3)
C(18B)	3791(5)	-3259(5)	2413(7)	31(2)
C(19B)	4448(5)	-2783(7)	2842(8)	52(3)
C(20B)	3533(6)	-3599(6)	1417(7)	42(3)
Cl(1)	4901(1)	-4160(1)	6868(2)	29(1)
Cl(2)	4992(1)	-1810(2)	8694(2)	37(1)
C(1S)	13(5)	4447(6)	2928(7)	43(3)
C(2S)	-409(6)	4870(8)	1958(7)	58(3)
O(1S)	548(3)	5024(4)	3551(4)	37(2)
O(2S)	331(3)	7103(4)	2204(4)	38(2)

Table 3. Selected bond lengths [Å] and angles [°] for 1.

Fe(1)-N(6A)	1.974(7)	Fe(1)-N(3A)	1.978(7)
Fe(1)-N(4A)	2.039(7)	Fe(1)-N(1A)	2.076(7)
Fe(1)-S(1A)	2.209(2)	Fe(1)-S(2A)	2.213(2)
N(6A)-Fe(1)-N(3A)	172.9(3)	N(6A)-Fe(1)-N(4A)	93.6(3)
N(3A)-Fe(1)-N(4A)	89.4(3)	N(6A)-Fe(1)-N(1A)	92.7(3)
N(3A)-Fe(1)-N(1A)	93.8(3)	N(4A)-Fe(1)-N(1A)	89.2(3)
N(6A)-Fe(1)-S(1A)	86.5(2)	N(3A)-Fe(1)-S(1A)	91.1(2)
N(4A)-Fe(1)-S(1A)	175.0(2)	N(1A)-Fe(1)-S(1A)	85.8(2)
N(6A)-Fe(1)-S(2A)	88.1(2)	N(3A)-Fe(1)-S(2A)	85.5(2)
N(4A)-Fe(1)-S(2A)	90.8(2)	N(1A)-Fe(1)-S(2A)	179.3(2)
S(1A)-Fe(1)-S(2A)	94.17(9)		

Symmetry transformations used to generate equivalent atoms:

Table 4. Bond lengths [Å] and angles [°] for 1.

Fe(1)-N(6A)	1.974(7)	Fe(1)-N(3A)	1.978(7)
Fe(1)-N(4A)	2.039(7)	Fe(1)-N(1A)	2.076(7)
Fe(1)-S(1A)	2.209(2)	Fe(1)-S(2A)	2.213(2)
S(1A)-C(8A)	1.825(9)	S(2A)-C(18A)	1.834(9)
N(1A)-C(1A)	1.323(11)	N(1A)-C(3A)	1.379(10)
N(2A)-C(1A)	1.343(11)	N(2A)-C(2A)	1.387(11)
N(3A)-C(16A)	1.283(10)	N(3A)-C(5A)	1.476(11)
N(4A)-C(12A)	1.325(11)	N(4A)-C(13A)	1.398(11)
N(5A)-C(12A)	1.333(11)	N(5A)-C(11A)	1.396(12)
N(6A)-C(6A)	1.276(11)	N(6A)-C(14A)	1.493(11)
C(2A)-C(3A)	1.362(12)	C(3A)-C(4A)	1.479(12)
C(4A)-C(5A)	1.503(12)	C(6A)-C(7A)	1.513(13)
C(6A)-C(8A)	1.528(12)	C(8A)-C(9A)	1.503(14)
C(8A)-C(10A)	1.551(14)	C(11A)-C(13A)	1.331(13)
C(13A)-C(15A)	1.478(13)	C(14A)-C(15A)	1.506(13)
C(16A)-C(18A)	1.508(12)	C(16A)-C(17A)	1.507(12)
C(18A)-C(20A)	1.530(13)	C(18A)-C(19A)	1.536(13)
Fe(2)-N(3B)	1.998(7)	Fe(2)-N(6B)	2.003(7)
Fe(2)-N(1B)	2.036(7)	Fe(2)-N(4B)	2.060(7)
Fe(2)-S(1B)	2.198(2)	Fe(2)-S(2B)	2.212(2)
S(1B)-C(8B)	1.837(9)	S(2B)-C(18B)	1.811(10)
N(1B)-C(1B)	1.324(12)	N(1B)-C(3B)	1.380(10)
N(2B)-C(1B)	1.320(11)	N(2B)-C(2B)	1.359(11)
N(3B)-C(6B)	1.284(11)	N(3B)-C(15B)	1.488(11)
N(4B)-C(12B)	1.306(12)	N(4B)-C(13B)	1.353(11)
N(5B)-C(12B)	1.333(12)	N(5B)-C(11B)	1.391(13)
N(6B)-C(16B)	1.285(12)	N(6B)-C(5B)	1.487(11)
C(2B)-C(3B)	1.358(13)	C(3B)-C(4B)	1.482(13)
C(4B)-C(5B)	1.519(14)	C(6B)-C(7B)	1.518(12)
C(6B)-C(8B)	1.524(13)	C(8B)-C(9B)	1.538(14)
C(8B)-C(10B)	1.535(13)	C(11B)-C(13B)	1.330(12)
C(13B)-C(14B)	1.497(13)	C(14B)-C(15B)	1.519(13)
C(16B)-C(18B)	1.509(13)	C(16B)-C(17B)	1.518(13)
C(18B)-C(19B)	1.511(14)	C(18B)-C(20B)	1.555(14)
C(1S)-O(1S)	1.408(11)	C(1S)-C(2S)	1.52(2)

N(6A)-Fe(1)-N(3A)	172.9(3)	N(6A)-Fe(1)-N(4A)	93.6(3)
N(3A)-Fe(1)-N(4A)	89.4(3)	N(6A)-Fe(1)-N(1A)	92.7(3)

N(3A)-Fe(1)-N(1A)	93.8(3)	N(4A)-Fe(1)-N(1A)	89.2(3)
N(6A)-Fe(1)-S(1A)	86.5(2)	N(3A)-Fe(1)-S(1A)	91.1(2)
N(4A)-Fe(1)-S(1A)	175.0(2)	N(1A)-Fe(1)-S(1A)	85.8(2)
N(6A)-Fe(1)-S(2A)	88.1(2)	N(3A)-Fe(1)-S(2A)	85.5(2)
N(4A)-Fe(1)-S(2A)	90.8(2)	N(1A)-Fe(1)-S(2A)	179.3(2)
S(1A)-Fe(1)-S(2A)	94.17(9)	C(8A)-S(1A)-Fe(1)	100.4(3)
C(18A)-S(2A)-Fe(1)	99.6(3)	C(1A)-N(1A)-C(3A)	106.6(7)
C(1A)-N(1A)-Fe(1)	128.0(6)	C(3A)-N(1A)-Fe(1)	123.6(5)
C(1A)-N(2A)-C(2A)	107.4(7)	C(16A)-N(3A)-C(5A)	120.0(7)
C(16A)-N(3A)-Fe(1)	121.9(6)	C(5A)-N(3A)-Fe(1)	118.1(5)
C(12A)-N(4A)-C(13A)	105.5(7)	C(12A)-N(4A)-Fe(1)	128.4(5)
C(13A)-N(4A)-Fe(1)	125.8(6)	C(12A)-N(5A)-C(11A)	107.9(7)
C(6A)-N(6A)-C(14A)	116.7(7)	C(6A)-N(6A)-Fe(1)	120.6(5)
C(14A)-N(6A)-Fe(1)	121.2(6)	N(1A)-C(1A)-N(2A)	110.9(7)
C(3A)-C(2A)-N(2A)	106.1(7)	C(2A)-C(3A)-N(1A)	109.0(7)
C(2A)-C(3A)-C(4A)	128.5(7)	N(1A)-C(3A)-C(4A)	122.4(7)
C(3A)-C(4A)-C(5A)	114.2(7)	N(3A)-C(5A)-C(4A)	113.4(7)
N(6A)-C(6A)-C(7A)	123.2(7)	N(6A)-C(6A)-C(8A)	120.7(7)
C(7A)-C(6A)-C(8A)	116.1(8)	C(9A)-C(8A)-C(6A)	109.2(7)
C(9A)-C(8A)-C(10A)	110.9(9)	C(6A)-C(8A)-C(10A)	109.8(7)
C(9A)-C(8A)-S(1A)	110.2(6)	C(6A)-C(8A)-S(1A)	109.9(6)
C(10A)-C(8A)-S(1A)	106.7(6)	C(13A)-C(11A)-N(5A)	105.8(7)
N(4A)-C(12A)-N(5A)	110.8(7)	C(11A)-C(13A)-N(4A)	110.0(8)
C(11A)-C(13A)-C(15A)	130.2(8)	N(4A)-C(13A)-C(15A)	119.6(8)
N(6A)-C(14A)-C(15A)	113.7(7)	C(13A)-C(15A)-C(14A)	115.0(7)
N(3A)-C(16A)-C(18A)	119.7(8)	N(3A)-C(16A)-C(17A)	124.4(7)
C(18A)-C(16A)-C(17A)	115.9(8)	C(16A)-C(18A)-C(20A)	110.3(7)
C(16A)-C(18A)-C(19A)	109.8(8)	C(20A)-C(18A)-C(19A)	110.7(7)
C(16A)-C(18A)-S(2A)	110.0(6)	C(20A)-C(18A)-S(2A)	108.9(6)
C(19A)-C(18A)-S(2A)	107.0(6)	N(3B)-Fe(2)-N(6B)	173.4(3)
N(3B)-Fe(2)-N(1B)	91.8(3)	N(6B)-Fe(2)-N(1B)	93.1(3)
N(3B)-Fe(2)-N(4B)	93.1(3)	N(6B)-Fe(2)-N(4B)	91.7(3)
N(1B)-Fe(2)-N(4B)	85.1(3)	N(3B)-Fe(2)-S(1B)	85.9(2)
N(6B)-Fe(2)-S(1B)	89.7(2)	N(1B)-Fe(2)-S(1B)	90.1(2)
N(4B)-Fe(2)-S(1B)	175.1(2)	N(3B)-Fe(2)-S(2B)	89.6(2)
N(6B)-Fe(2)-S(2B)	85.9(2)	N(1B)-Fe(2)-S(2B)	174.3(2)
N(4B)-Fe(2)-S(2B)	89.4(2)	S(1B)-Fe(2)-S(2B)	95.44(9)
C(8B)-S(1B)-Fe(2)	101.7(3)	C(18B)-S(2B)-Fe(2)	100.3(3)
C(1B)-N(1B)-C(3B)	105.2(7)	C(1B)-N(1B)-Fe(2)	128.6(6)
C(3B)-N(1B)-Fe(2)	125.4(6)	C(1B)-N(2B)-C(2B)	108.0(8)

C(6B)-N(3B)-C(15B)	116.5(7)	C(6B)-N(3B)-Fe(2)	121.2(6)
C(15B)-N(3B)-Fe(2)	122.2(6)	C(12B)-N(4B)-C(13B)	105.3(7)

C(12B)-N(4B)-Fe(2)	128.9(6)	C(13B)-N(4B)-Fe(2)	125.6(6)
C(12B)-N(5B)-C(11B)	104.6(8)	C(16B)-N(6B)-C(5B)	117.6(7)
C(16B)-N(6B)-Fe(2)	120.1(6)	C(5B)-N(6B)-Fe(2)	122.1(6)
N(2B)-C(1B)-N(1B)	111.6(8)	N(2B)-C(2B)-C(3B)	106.4(7)
C(2B)-C(3B)-N(1B)	108.9(8)	C(2B)-C(3B)-C(4B)	129.9(8)
N(1B)-C(3B)-C(4B)	121.2(8)	C(3B)-C(4B)-C(5B)	112.3(8)
N(6B)-C(5B)-C(4B)	113.9(7)	N(3B)-C(6B)-C(7B)	124.3(8)
N(3B)-C(6B)-C(8B)	121.2(8)	C(7B)-C(6B)-C(8B)	114.5(8)
C(6B)-C(8B)-C(9B)	109.2(6)	C(6B)-C(8B)-C(10B)	110.5(8)
C(9B)-C(8B)-C(10B)	111.2(8)	C(6B)-C(8B)-S(1B)	109.2(6)
C(9B)-C(8B)-S(1B)	108.0(7)	C(10B)-C(8B)-S(1B)	108.7(6)
C(13B)-C(11B)-N(5B)	106.9(8)	N(4B)-C(12B)-N(5B)	113.1(8)
C(11B)-C(13B)-N(4B)	110.1(8)	C(11B)-C(13B)-C(14B)	129.2(8)
N(4B)-C(13B)-C(14B)	120.4(7)	C(13B)-C(14B)-C(15B)	114.6(8)
N(3B)-C(15B)-C(14B)	113.3(7)	N(6B)-C(16B)-C(18B)	121.1(8)
N(6B)-C(16B)-C(17B)	122.4(8)	C(18B)-C(16B)-C(17B)	116.5(8)
C(19B)-C(18B)-C(16B)	111.5(9)	C(19B)-C(18B)-C(20B)	109.5(8)
C(16B)-C(18B)-C(20B)	107.3(7)	C(19B)-C(18B)-S(2B)	108.4(6)
C(16B)-C(18B)-S(2B)	110.2(7)	C(20B)-C(18B)-S(2B)	109.9(7)
O(1S)-C(1S)-C(2S)	111.8(8)		

Symmetry transformations used to generate equivalent atoms:

Table 5. Anisotropic displacement parameters [$Å^2 \times 10^3$] for 1.

The anisotropic displacement factor exponent takes the form:

$-2\pi^2 [(ha^*)^2 U_{11} + ... + 2hka^* b^* U_{12}]$

	U11	U22	U33	U23	U13	U12
Fe(1)	18(1)	17(1)	18(1)	1(1)	9(1)	0(1)
S(1A)	22(1)	20(1)	28(1)	3(1)	14(1)	1(1)
S(2A)	25(1)	23(1)	21(1)	-2(1)	12(1)	0(1)
N(1A)	18(5)	19(4)	16(4)	4(3)	6(4)	5(3)
N(2A)	21(5)	27(4)	16(4)	-6(4)	6(4)	-4(4)
N(3A)	27(5)	15(4)	12(5)	-1(3)	12(4)	-2(3)
N(4A)	17(5)	19(4)	19(4)	1(3)	6(4)	-1(3)
N(5A)	23(5)	28(4)	36(5)	-2(4)	18(4)	-2(4)
N(6A)	22(5)	21(4)	15(4)	0(3)	10(4)	0(3)
C(1A)	25(6)	27(5)	28(6)	5(5)	17(6)	5(4)
C(2A)	27(6)	26(5)	17(5)	-3(4)	9(5)	-2(4)
C(3A)	18(5)	18(5)	15(5)	-1(4)	9(5)	-1(4)
C(4A)	34(6)	24(5)	40(6)	2(4)	29(5)	4(5)
C(5A)	23(6)	31(5)	22(5)	5(4)	10(5)	10(4)
C(6A)	15(5)	26(5)	9(5)	6(3)	2(4)	5(4)
C(7A)	33(7)	37(5)	37(6)	6(4)	19(5)	6(5)
C(8A)	32(6)	17(5)	36(6)	-2(4)	23(5)	-9(4)
C(9A)	27(7)	34(5)	77(8)	19(5)	19(6)	-7(5)
C(10A)	69(9)	46(6)	55(8)	19(5)	52(7)	26(5)
C(11A)	44(7)	21(5)	42(6)	-8(5)	31(6)	-9(6)
C(12A)	24(6)	29(5)	27(5)	2(4)	18(5)	0(4)
C(13A)	23(6)	22(5)	27(6)	-8(4)	17(5)	-4(4)
C(14A)	21(5)	21(5)	30(5)	3(4)	11(5)	-2(4)
C(15A)	34(7)	22(5)	21(5)	8(4)	10(5)	-5(4)
C(16A)	27(6)	21(5)	31(7)	3(4)	22(6)	-3(4)
C(17A)	34(6)	39(5)	29(5)	14(4)	18(5)	16(5)
C(18A)	21(5)	25(4)	20(5)	-5(4)	11(5)	-5(4)
C(19A)	26(6)	44(5)	26(6)	-7(4)	10(5)	-6(4)
C(20A)	35(6)	42(5)	26(5)	14(4)	22(5)	9(4)
Fe(2)	22(1)	19(1)	20(1)	0(1)	12(1)	0(1)
S(1B)	30(2)	20(1)	26(1)	-3(1)	12(1)	2(1)
S(2B)	37(2)	19(1)	35(1)	0(1)	26(1)	-2(1)
N(1B)	23(5)	19(4)	19(4)	4(3)	9(4)	4(3)
N(2B)	31(5)	29(4)	30(4)	2(3)	21(4)	-1(4)
N(3B)	23(5)	23(4)	23(5)	-5(3)	14(4)	-8(3)
N(4B)	12(5)	26(4)	18(4)	3(3)	3(4)	1(3)
N(5B)	22(5)	33(4)	20(4)	2(4)	10(4)	-2(4)
N(6B)	24(5)	27(4)	17(4)	-4(3)	12(4)	-5(3)
C(1B)	26(7)	34(6)	34(6)	-3(4)	22(5)	-1(4)
C(2B)	33(6)	37(5)	23(5)	5(4)	11(5)	2(6)
C(3B)	29(6)	22(4)	21(5)	2(4)	15(5)	-1(5)
C(4B)	33(6)	35(5)	37(6)	23(4)	18(5)	15(5)
C(5B)	39(6)	27(5)	48(6)	19(5)	31(5)	19(5)
C(6B)	23(6)	23(5)	35(6)	4(4)	20(6)	1(4)
C(7B)	21(6)	22(5)	32(6)	0(4)	12(5)	3(4)
C(8B)	30(6)	29(5)	23(5)	0(4)	15(5)	-5(4)
C(9B)	34(6)	41(5)	24(6)	3(4)	12(5)	17(5)
C(10B)	35(7)	36(5)	41(6)	-6(5)	21(5)	0(5)

C(11B)	41(7)	22(5)	27(6)	-5(4)	20(6)	-2(5)
C(12B)	34(7)	29(5)	28(6)	-3(5)	20(6)	2(4)
C(13B)	26(6)	14(4)	22(6)	-4(4)	15(5)	-2(4)
C(14B)	28(7)	33(5)	23(5)	-9(4)	15(5)	-1(4)