Captions for Supporting Information Figures

Figure S1. ORTEP diagram of molecule 1 of [Fe(OEP)(CS)(Py)] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level.

Figure S2. ORTEP diagram of molecule 3 of [Fe(OEP)(CS)(Py3)] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level.

Figure S3. ORTEP diagram of [Fe(OEP)(CS)(CH_3OH)] displaying the atom labeling scheme. Thermal ellipsoids of all atoms are contoured at the 50% probability level.

Figure S4. Formal diagrams of the porphinato core displaying the perpendicular displacements, in units of 0.01Å, of the core atoms from the 24-atom mean plane of [Fe(OEP)(CS)(Py)] (molecule 1). Positive displacments ae towards the CS ligand.

Figure S5. Formal diagrams of the porphinato core displaying the perpendicular displacements, in units of 0.01Å, of the core atoms from the 24-atom mean plane of [Fe(OEP)(CS)(Py)] (molecule 2). Positive displacments ae towards the CS ligand.

Figure S6. Formal diagrams of the porphinato core displaying the perpendicular displacements, in units of 0.01Å, of the core atoms from the 24-atom mean plane of [Fe(OEP)(CS)(Py)] (molecule 3). Centrosymmetrically related atoms in the diagram have equal magnitude displacements but are of opposite sign.

Figure S7. Formal diagrams of the porphinato core displaying the perpendicular displacements, in units of 0.01Å, of the core atoms from the 24-atom mean plane of [Fe(OEP)(CS)(CH_3OH)]. Centrosymmetrically related atoms in the diagram have equal magnitude displacements but are of opposite sign.

Supporting Information Tables

Table S1. Complete Crystallographic Details for [Fe(OEP)(CS)(1-MeIm)].

Table S1. Crystal data and structure refinement for [Fe(OEP)(CS)(1-MeIm)]

Empirical formula	$C_{41}H_{50}FeN_6S$
Formula weight	714.78
Crystal system, Space group	Monoclinic, $P2_1/n$
Unit cell dimensions	a = 9.5906(5) Å α= 90^o
	b = 16.704(4) Å β= 100.453(7)^o
	c = 23.1417(6) Å γ = 90^o
Volume, Z	3645.9(8) Å^3, 4
Density (calculated)	1.302 g/cm^3
Wavelength	0.71073 Å
Absorption coefficient	0.509 mm^{-1}
F(000)	1520
Crystal size	0.22 x 0.14 x 0.03 mm^3
Temperature	130(2) K
Diffractometer	Enraf-Nonius FAST
Power setting	50kV, 40mA
Image time, sec	10
Increment, deg	0.15
Detector dist. mm	40
Detector tilt angle, deg	−25
Theta range for data collection	2.17 to 27.00^o
Index ranges	−7≤ h≤ 12, −21≤ k≤ 16, −29≤ l≤ 26
Reflection collected/unique	22290/7882 [R(int) = 0.0569]
Unique observed reflections	6057
Completeness to theta = 27.00^o	98.9 %
Absorption correction	DIFABS
Max. and min. transmission	1.000 and 0.7932
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	7882 / 0 / 442
Goodness-of-fit on F2	1.061
Final R indices [I>2σ(I)]	R1 = 0.0735, wR2 = 0.1742
R indices (all data)	R1 = 0.0987, wR2 = 0.1902
Largest diff. peak and hole	0.682 and −0.499 e.Å^{-3}

Table S2. Atomic coordinates ($\times 10^4$) and equivalent isotropic displacement parameters (Å^2 $\times 10^3$) for [Fe(OEP)(CS)(1-MeIm)][a]

Atom	x	y	z	U(eq)
Fe(1)	9446(1)	1116(1)	7745(1)	9(1)
C(1)	10433(3)	265(2)	7869(1)	12(1)
S(1)	11494(1)	-454(1)	7946(1)	22(1)
N(1)	10973(3)	1687(2)	8297(1)	11(1)
N(2)	10434(3)	1356(2)	7077(1)	11(1)
N(3)	7867(3)	592(2)	7191(1)	10(1)
N(4)	8342(3)	988(2)	8398(1)	11(1)
C(a1)	11104(3)	1747(2)	8896(2)	13(1)
C(a2)	12206(3)	2002(2)	8169(2)	13(1)
C(a3)	11659(3)	1791(2)	7099(2)	12(1)
C(a4)	10043(3)	1112(2)	6506(2)	12(1)
C(a5)	7822(3)	419(2)	6609(1)	12(1)
C(a6)	6590(3)	337(2)	7311(2)	11(1)
C(a7)	6980(3)	717(2)	8353(2)	13(1)
C(a8)	8774(4)	1187(2)	8976(2)	15(1)
C(b1)	12448(4)	2097(2)	9152(2)	15(1)
C(b2)	13137(3)	2260(2)	8700(2)	15(1)
C(b3)	11996(4)	1865(2)	6516(2)	14(1)
C(b4)	11010(4)	1429(2)	6151(2)	14(1)
C(b5)	6505(4)	26(2)	6360(2)	13(1)
C(b6)	5729(3)	-17(2)	6799(2)	13(1)
C(b7)	6527(4)	751(2)	8920(2)	14(1)
C(b8)	7648(4)	1047(2)	9308(2)	15(1)
C(m1)	12500(4)	2073(2)	7609(2)	15(1)
C(m2)	8847(4)	655(2)	6291(2)	13(1)
C(m3)	6161(3)	428(2)	7844(2)	13(1)
C(m4)	10077(4)	1512(2)	9210(2)	16(1)
C(11)	12943(4)	2242(3)	9800(2)	22(1)
C(12)	12224(5)	2963(3)	10032(2)	34(1)
C(21)	14570(4)	2635(2)	8730(2)	19(1)
C(22)	14522(4)	3538(3)	8692(2)	33(1)
C(31)	13208(4)	2339(2)	6361(2)	18(1)
C(32)	14533(4)	1852(3)	6350(2)	32(1)
C(41)	10920(4)	1274(2)	5507(2)	17(1)
C(42)	11569(4)	475(3)	5384(2)	24(1)
C(51)	6051(4)	-243(2)	5736(2)	18(1)
C(52)	6306(5)	-1131(3)	5644(2)	31(1)

Table S2. Continued...

Atom	x	y	z	U_{eq}
C(61)	4283(4)	-353(2)	6787(2)	17(1)
C(62)	4299(4)	-1151(2)	7110(2)	23(1)
C(71)	5109(4)	474(2)	9026(2)	19(1)
C(72)	5032(4)	-430(3)	9095(2)	30(1)
C(81)	7756(4)	1206(3)	9950(2)	25(1)
C(82)	8490(5)	539(3)	10342(2)	40(1)
N(5)	8325(3)	2198(2)	7541(1)	12(1)
C(91)	7598(4)	2649(2)	7887(2)	19(1)
C(92)	6948(4)	3272(2)	7574(2)	20(1)
N(6)	7268(3)	3205(2)	7023(1)	16(1)
C(93)	6745(4)	3716(2)	6520(2)	23(1)
C(94)	8098(3)	2557(2)	7025(2)	14(1)

[a] U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S3. Bond lengths for [Fe(OEP)(CS)(1-MeIm)][a].

bond	length Å	bond	length Å
Fe(1)–C(1)	1.703(4)	C(b3)–C(b4)	1.360(5)
Fe(1)–N(2)	1.996(3)	C(b3)–C(31)	1.502(5)
Fe(1)–N(3)	2.000(3)	C(b4)–C(41)	1.498(5)
Fe(1)–N(1)	2.002(3)	C(b5)–C(b6)	1.366(5)
Fe(1)–N(4)	2.006(3)	C(b5)–C(51)	1.500(5)
Fe(1)–N(5)	2.112(3)	C(b6)–C(61)	1.491(5)
C(1)–S(1)	1.563(4)	C(b7)–C(b8)	1.363(5)
N(1)–C(a1)	1.372(4)	C(b7)–C(71)	1.499(5)
N(1)–C(a2)	1.375(4)	C(b8)–C(81)	1.493(5)
N(2)–C(a4)	1.368(4)	C(m1)–H(m1)	0.9500
N(2)–C(a3)	1.374(4)	C(m2)–H(m2)	0.9500
N(3)–C(a5)	1.370(4)	C(m3)–H(m3)	0.9500
N(3)–C(a6)	1.373(4)	C(m4)–H(m4)	0.9500
N(4)–C(a7)	1.369(4)	C(11)–C(12)	1.532(6)
N(4)–C(a8)	1.369(5)	C(11)–H(11a)	0.9900
C(a1)–C(m4)	1.383(5)	C(11)–H(11b)	0.9900
C(a1)–C(b1)	1.442(5)	C(12)–H(12a)	0.9800
C(a2)–C(m1)	1.380(5)	C(12)–H(12b)	0.9800
C(a2)–C(b2)	1.448(5)	C(12)–H(12c)	0.9800
C(a3)–C(m1)	1.386(5)	C(21)–C(22)	1.511(6)
C(a3)–C(b3)	1.450(4)	C(21)–H(21a)	0.9900
C(a4)–C(m2)	1.393(5)	C(21)–H(21b)	0.9900
C(a4)–C(b4)	1.446(4)	C(22)–H(22a)	0.9800
C(a5)–C(m2)	1.387(5)	C(22)–H(22b)	0.9800
C(a5)–C(b5)	1.448(5)	C(22)–H(22c)	0.9800
C(a6)–C(m3)	1.377(5)	C(31)–C(32)	1.513(5)
C(a6)–C(b6)	1.443(5)	C(31)–H(31a)	0.9900
C(a7)–C(m3)	1.379(5)	C(31)–H(31b)	0.9900
C(a7)–C(b7)	1.455(5)	C(32)–H(32a)	0.9800
C(a8)–C(m4)	1.379(5)	C(32)–H(32b)	0.9800
C(a8)–C(b8)	1.454(5)	C(32)–H(32c)	0.9800
C(b1)–C(b2)	1.363(5)	C(41)–C(42)	1.522(5)
C(b1)–C(11)	1.508(5)	C(41)–H(41a)	0.9900
C(b2)–C(21)	1.501(5)	C(41)–H(41b)	0.9900
C(42)–H(42a)	0.9800	C(72)–H(72c)	0.9800
C(42)–H(42b)	0.9800	C(81)–C(82)	1.525(6)
C(42)–H(42c)	0.9800	C(81)–H(81a)	0.9900

Table S3. Continued...

bond	length Å	bond	length Å
C(51)–C(52)	1.525(6)	C(81)–H(81b)	0.9900
C(51)–H(51a)	0.9900	C(82)–H(82a)	0.9800
C(51)–H(51b)	0.9900	C(82)–H(82b)	0.9800
C(52)–H(52a)	0.9800	C(82)–H(82c)	0.9800
C(52)–H(52b)	0.9800	N(5)–C(94)	1.319(5)
C(52)–H(52c)	0.9800	N(5)–C(91)	1.379(4)
C(61)–C(62)	1.528(5)	C(91)–C(92)	1.354(5)
C(61)–H(61a)	0.9900	C(91)–H(91)	0.9500
C(61)–H(61b)	0.9900	C(92)–N(6)	1.368(5)
C(62)–H(62a)	0.9800	C(92)–H(92)	0.9500
C(62)–H(62b)	0.9800	N(6)–C(94)	1.343(5)
C(62)–H(62c)	0.9800	N(6)–C(93)	1.457(5)
C(71)–C(72)	1.521(6)	C(93)–H(93a)	0.9800
C(71)–H(71a)	0.9900	C(93)–H(93b)	0.9800
C(71)–H(71b)	0.9900	C(93)–H(93c)	0.9800
C(72)–H(72a)	0.9800	C(94)–H(94)	0.9500
C(72)–H(72b)	0.9800		

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S4. Bond angles for [Fe(OEP)(CS)(1-MeIm)][a].

angle	degree	angle	degree
C(1)–Fe(1)–N(2)	88.33(13)	C(1)–Fe(1)–N(3)	94.34(14)
N(2)–Fe(1)–N(3)	90.05(11)	C(1)–Fe(1)–N(1)	88.35(14)
N(2)–Fe(1)–N(1)	90.19(11)	N(3)–Fe(1)–N(1)	177.30(12)
C(1)–Fe(1)–N(4)	97.90(13)	N(2)–Fe(1)–N(4)	173.77(12)
N(3)–Fe(1)–N(4)	89.70(11)	N(1)–Fe(1)–N(4)	89.77(11)
C(1)–Fe(1)–N(5)	175.32(13)	N(2)–Fe(1)–N(5)	87.02(11)
N(3)–Fe(1)–N(5)	86.26(11)	N(1)–Fe(1)–N(5)	91.07(11)
N(4)–Fe(1)–N(5)	86.74(11)	S(1)–C(1)–Fe(1)	172.2(2)
C(a1)–N(1)–C(a2)	105.4(3)	C(a1)–N(1)–Fe(1)	126.9(2)
C(a2)–N(1)–Fe(1)	127.1(2)	C(a4)–N(2)–C(a3)	106.1(3)
C(a4)–N(2)–Fe(1)	127.1(2)	C(a3)–N(2)–Fe(1)	126.9(2)
C(a5)–N(3)–C(a6)	105.3(3)	C(a5)–N(3)–Fe(1)	127.5(2)
C(a6)–N(3)–Fe(1)	127.2(2)	C(a7)–N(4)–C(a8)	105.6(3)
C(a7)–N(4)–Fe(1)	127.3(2)	C(a8)–N(4)–Fe(1)	127.0(2)
N(1)–C(a1)–C(m4)	124.6(3)	N(1)–C(a1)–C(b1)	110.9(3)
C(m4)–C(a1)–C(b1)	124.6(3)	N(1)–C(a2)–C(m1)	124.5(3)
N(1)–C(a2)–C(b2)	110.6(3)	C(m1)–C(a2)–C(b2)	124.9(3)
N(2)–C(a3)–C(m1)	125.0(3)	N(2)–C(a3)–C(b3)	110.1(3)
C(m1)–C(a3)–C(b3)	124.8(3)	N(2)–C(a4)–C(m2)	124.9(3)
N(2)–C(a4)–C(b4)	110.4(3)	C(m2)–C(a4)–C(b4)	124.7(3)
N(3)–C(a5)–C(m2)	124.2(3)	N(3)–C(a5)–C(b5)	110.9(3)
C(m2)–C(a5)–C(b5)	124.7(3)	N(3)–C(a6)–C(m3)	124.8(3)
N(3)–C(a6)–C(b6)	111.0(3)	C(m3)–C(a6)–C(b6)	124.1(3)
N(4)–C(a7)–C(m3)	124.6(3)	N(4)–C(a7)–C(b7)	110.9(3)
C(m3)–C(a7)–C(b7)	124.5(3)	N(4)–C(a8)–C(m4)	124.9(3)
N(4)–C(a8)–C(b8)	110.8(3)	C(m4)–C(a8)–C(b8)	124.2(3)
C(b2)–C(b1)–C(a1)	106.7(3)	C(b2)–C(b1)–C(11)	128.5(3)
C(a1)–C(b1)–C(11)	124.8(3)	C(b1)–C(b2)–C(a2)	106.4(3)
C(b1)–C(b2)–C(21)	128.0(3)	C(a2)–C(b2)–C(21)	125.6(3)
C(b4)–C(b3)–C(a3)	106.6(3)	C(b4)–C(b3)–C(31)	128.0(3)
C(a3)–C(b3)–C(31)	125.4(3)	C(b3)–C(b4)–C(a4)	106.7(3)
C(b3)–C(b4)–C(41)	128.1(3)	C(a4)–C(b4)–C(41)	125.1(3)
C(b6)–C(b5)–C(a5)	106.4(3)	C(b6)–C(b5)–C(51)	126.8(3)
C(a5)–C(b5)–C(51)	126.8(3)	C(b5)–C(b6)–C(a6)	106.4(3)
C(b5)–C(b6)–C(61)	129.5(3)	C(a6)–C(b6)–C(61)	124.2(3)
C(b8)–C(b7)–C(a7)	106.3(3)	C(b8)–C(b7)–C(71)	129.4(3)
C(a7)–C(b7)–C(71)	124.3(3)	C(b7)–C(b8)–C(a8)	106.4(3)

Table S4. Continued...

angle	degree	angle	degree
C(b7)–C(b8)–C(81)	128.6(3)	C(a8)–C(b8)–C(81)	125.0(3)
C(a2)–C(m1)–C(a3)	125.7(3)	C(a2)–C(m1)–H(m1)	117.1
C(a3)–C(m1)–H(m1)	117.1	C(a5)–C(m2)–C(a4)	125.7(3)
C(a5)–C(m2)–H(m2)	117.2	C(a4)–C(m2)–H(m2)	117.2
C(a6)–C(m3)–C(a7)	125.9(3)	C(a6)–C(m3)–H(m3)	117.0
C(a7)–C(m3)–H(m3)	117.0	C(a8)–C(m4)–C(a1)	125.9(3)
C(a8)–C(m4)–H(m4)	117.1	C(a1)–C(m4)–H(m4)	117.1
C(b1)–C(11)–C(12)	113.2(3)	C(b1)–C(11)–H(11a)	108.9
C(12)–C(11)–H(11a)	108.9	C(b1)–C(11)–H(11b)	108.9
C(12)–C(11)–H(11b)	108.9	H(11a)–C(11)–H(11b)	107.8
C(11)–C(12)–H(12a)	109.5	C(11)–C(12)–H(12b)	109.5
H(12a)–C(12)–H(12b)	109.5	C(11)–C(12)–H(12c)	109.5
H(12a)–C(12)–H(12c)	109.5	H(12b)–C(12)–H(12c)	109.5
C(b2)–C(21)–C(22)	113.3(3)	C(b2)–C(21)–H(21a)	108.9
C(22)–C(21)–H(21a)	108.9	C(b2)–C(21)–H(21b)	108.9
C(22)–C(21)–H(21b)	108.9	H(21a)–C(21)–H(21b)	107.7
C(21)–C(22)–H(22a)	109.5	C(21)–C(22)–H(22b)	109.5
H(22a)–C(22)–H(22b)	109.5	C(21)–C(22)–H(22c)	109.5
H(22a)–C(22)–H(22c)	109.5	H(22b)–C(22)–H(22c)	109.5
C(b3)–C(31)–C(32)	114.2(3)	C(b3)–C(31)–H(31a)	108.7
C(32)–C(31)–H(31a)	108.7	C(b3)–C(31)–H(31b)	108.7
C(32)–C(31)–H(31b)	108.7	H(31a)–C(31)–H(31b)	107.6
C(31)–C(32)–H(32a)	109.5	C(31)–C(32)–H(32b)	109.5
H(32a)–C(32)–H(32b)	109.5	C(31)–C(32)–H(32c)	109.5
H(32a)–C(32)–H(32c)	109.5	H(32b)–C(32)–H(32c)	109.5
C(b4)–C(41)–C(42)	112.7(3)	C(b4)–C(41)–H(41a)	109.0
C(42)–C(41)–H(41a)	109.0	C(b4)–C(41)–H(41b)	109.0
C(42)–C(41)–H(41b)	109.0	H(41a)–C(41)–H(41b)	107.8
C(41)–C(42)–H(42a)	109.5	C(41)–C(42)–H(42b)	109.5
H(42a)–C(42)–H(42b)	109.5	C(41)–C(42)–H(42c)	109.5
H(42a)–C(42)–H(42c)	109.5	H(42b)–C(42)–H(42c)	109.5
C(b5)–C(51)–C(52)	113.6(3)	C(b5)–C(51)–H(51a)	108.9
C(52)–C(51)–H(51a)	108.9	C(b5)–C(51)–H(51b)	108.9
C(52)–C(51)–H(51b)	108.9	H(51a)–C(51)–H(51b)	107.7
C(51)–C(52)–H(52a)	109.5	C(51)–C(52)–H(52b)	109.5
H(52a)–C(52)–H(52b)	109.5	C(51)–C(52)–H(52c)	109.5
H(52a)–C(52)–H(52c)	109.5	H(52b)–C(52)–H(52c)	109.5
C(b6)–C(61)–C(62)	113.1(3)	C(b6)–C(61)–H(61a)	109.0

Table S4. Continued...

angle	degree	angle	degree
C(62)–C(61)–H(61a)	109.0	C(b6)–C(61)–H(61b)	109.0
C(62)–C(61)–H(61b)	109.0	H(61a)–C(61)–H(61b)	107.8
C(61)–C(62)–H(62a)	109.5	C(61)–C(62)–H(62b)	109.5
H(62a)–C(62)–H(62b)	109.5	C(61)–C(62)–H(62C)	109.5
H(62a)–C(62)–H(62c)	109.5	H(62b)–C(62)–H(62c)	109.5
C(b7)–C(71)–C(72)	112.8(3)	C(b7)–C(71)–H(71a)	109.0
C(72)–C(71)–H(71a)	109.0	C(b7)–C(71)–H(71b)	109.0
C(72)–C(71)–H(71b)	109.0	H(71a)–C(71)–H(71b)	107.8
C(71)–C(72)–H(72a)	109.5	C(71)–C(72)–H(72b)	109.5
H(72a)–C(72)–H(72b)	109.5	C(71)–C(72)–H(72c)	109.5
H(72a)–C(72)–H(72c)	109.5	H(72b)–C(72)–H(72c)	109.5
C(b8)–C(81)–C(82)	113.8(4)	C(b8)–C(81)–H(81a)	108.8
C(82)–C(81)–H(81a)	108.8	C(b8)–C(81)–H(81b)	108.8
C(82)–C(81)–H(81b)	108.8	H(81a)–C(81)–H(81b)	107.7
C(81)–C(82)–H(82a)	109.5	C(81)–C(82)–H(82b)	109.5
H(82a)–C(82)–H(82b)	109.5	C(81)–C(82)–H(82c)	109.5
H(82a)–C(82)–H(82c)	109.5	H(82b)–C(82)–H(82c)	109.5
C(94)–N(5)–C(91)	105.1(3)	C(94)–N(5)–Fe(1)	125.9(2)
C(91)–N(5)–Fe(1)	128.9(2)	C(92)–C(91)–N(5)	109.9(3)
C(92)–C(91)–H(91)	125.1	N(5)–C(91)–H(91)	125.1
C(91)–C(92)–N(6)	106.1(3)	C(91)–C(92)–H(92)	127.0
N(6)–C(92)–H(92)	127.0	C(94)–N(6)–C(92)	107.3(3)
C(94)–N(6)–C(93)	126.3(3)	C(92)–N(6)–C(93)	126.4(3)
N(6)–C(93)–H(93a)	109.5	N(6)–C(93)–H(93b)	109.5
H(93a)–C(93)–H(93b)	109.5	N(6)–C(93)–H(93c)	109.5
H(93a)–C(93)–H(93c)	109.5	H(93b)–C(93)–H(93c)	109.5
N(5)–C(94)–N(6)	111.7(3)	N(5)–C(94)–H(94)	124.2
N(6)–C(94)–H(94)	124.2		

[a] The estimated standard deviations of the least significant digits are given in parentheses.

Table S5. Anisotropic displacement parameters (Å^2 × 10^3) for [Fe(OEP)(CS)(1-MeIm)][a].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	10(1)	11(1)	8(1)	−1(1)	3(1)	−1(1)
C(1)	14(2)	16(2)	7(2)	−3(1)	4(1)	−5(1)
S(1)	23(1)	18(1)	25(1)	2(1)	5(1)	7(1)
N(1)	9(1)	12(1)	11(1)	−4(1)	3(1)	−4(1)
N(2)	11(1)	11(1)	12(1)	−1(1)	4(1)	1(1)
N(3)	12(1)	13(1)	7(1)	−2(1)	3(1)	−3(1)
N(4)	13(1)	11(1)	10(1)	−2(1)	3(1)	−2(1)
C(a1)	14(2)	14(2)	11(2)	−4(1)	1(1)	1(1)
C(a1)	11(2)	13(2)	13(2)	−1(1)	1(1)	−1(1)
C(a3)	12(2)	12(2)	13(2)	0(1)	6(1)	0(1)
C(a4)	13(2)	14(2)	11(2)	−2(1)	5(1)	1(1)
C(a5)	14(2)	16(2)	7(2)	−2(1)	1(1)	−2(1)
C(a6)	10(2)	10(2)	13(2)	−1(1)	2(1)	−1(1)
C(a7)	14(2)	13(2)	14(2)	1(1)	6(1)	−1(1)
C(a8)	16(2)	15(2)	14(2)	−1(1)	7(1)	0(1)
C(b1)	13(2)	16(2)	14(2)	−5(1)	1(1)	1(1)
C(b2)	10(2)	15(2)	18(2)	−3(1)	0(1)	0(1)
C(b3)	16(2)	16(2)	14(2)	1(1)	9(1)	2(1)
C(b4)	17(2)	13(2)	15(2)	4(1)	9(1)	6(1)
C(b5)	14(2)	14(2)	12(2)	−1(1)	0(1)	0(1)
C(b6)	12(2)	12(2)	13(2)	2(1)	0(1)	−1(1)
C(b7)	15(2)	16(2)	13(2)	2(1)	6(1)	0(1)
C(b8)	19(2)	18(2)	11(2)	1(1)	7(1)	3(1)
C(m1)	13(2)	12(2)	20(2)	−1(1)	7(1)	−1(1)
C(m2)	16(2)	15(2)	8(2)	1(1)	3(1)	3(1)
C(m3)	11(2)	16(2)	13(2)	1(1)	4(1)	−2(1)
C(m4)	20(2)	18(2)	9(2)	−2(1)	3(1)	−2(1)
C(11)	18(2)	30(2)	15(2)	−3(2)	−3(1)	−3(2)
C(12)	28(2)	43(3)	28(2)	−21(2)	1(2)	−5(2)
C(21)	12(2)	23(2)	22(2)	−4(2)	0(1)	−1(1)
C(22)	17(2)	26(2)	54(3)	4(2)	−1(2)	−8(2)
C(31)	19(2)	17(2)	22(2)	4(1)	10(1)	−2(1)
C(32)	17(2)	28(2)	51(3)	−6(2)	11(2)	−5(2)
C(41)	20(2)	23(2)	11(2)	2(1)	8(1)	2(1)
C(42)	23(2)	32(2)	19(2)	−5(2)	8(2)	3(2)
C(51)	12(2)	27(2)	13(2)	−1(1)	−1(1)	−1(1)
C(52)	38(2)	31(2)	23(2)	−13(2)	4(2)	−8(2)
C(61)	12(2)	21(2)	16(2)	3(1)	−1(1)	−3(1)

Table S5.Continued...

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(62)	14(2)	16(2)	37(2)	2(2)	5(2)	−3(1)
C(71)	17(2)	27(2)	16(2)	3(2)	8(1)	0(2)
C(72)	24(2)	33(2)	36(2)	13(2)	12(2)	−5(2)
C(81)	25(2)	37(2)	15(2)	−7(2)	10(2)	−6(2)
C(82)	35(2)	71(4)	16(2)	5(2)	7(2)	11(2)
N(5)	12(1)	13(2)	13(1)	1(1)	4(1)	−2(1)
C(91)	16(2)	24(2)	19(2)	−3(2)	9(1)	2(1)
C(92)	18(2)	24(2)	19(2)	1(2)	7(1)	5(2)
N(6)	16(1)	14(2)	18(2)	3(1)	3(1)	1(1)
C(93)	26(2)	18(2)	25(2)	7(2)	3(2)	1(2)
C(94)	12(2)	15(2)	16(2)	1(1)	3(1)	−2(1)

[a] The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form:
$-2\,\pi^2\,[\,h^2\,a^{*2}\,U_{11} + ... + 2\,h\,k\,a^*\,b^*\,U_{12}\,]$

Table S6. Hydrogen coordinates ($\times 10^4$) and isotropic displacement parameters ($Å^2 \times 10^3$) for [Fe(OEP)(CS)(1-MeIm)].

Atom	x	y	z	U(eq)
H(m1)	13354	2339	7570	17
H(m2)	8722	490	5892	15
H(m3)	5214	278	7863	16
H(m4)	10287	1582	9624	19
H(11a)	13981	2329	9876	26
H(11b)	12750	1758	10020	26
H(12a)	12490	3453	9846	51
H(12b)	12529	3002	10459	51
H(12c)	11192	2895	9939	51
H(21a)	15004	2425	8404	23
H(21b)	15185	2477	9103	23
H(22a)	14104	3700	8291	50
H(22b)	15486	3753	8794	50
H(22c)	13944	3747	8967	50
H(31a)	13443	2778	6650	22
H(31b)	12899	2586	5970	22
H(32a)	14856	1610	6737	47
H(32b)	15278	2201	6252	47
H(32c)	14323	1429	6053	47
H(41a)	11416	1709	5336	21
H(41b)	9912	1283	5312	21
H(42a)	12584	478	5550	36
H(42b)	11437	390	4958	36
H(42c)	11103	43	5563	36
H(51a)	6572	72	5482	22
H(51b)	5028	-128	5610	22
H(52a)	7324	-1244	5744	46
H(52b)	5958	-1271	5232	46
H(52c)	5802	-1448	5897	46
H(61a)	3815	-430	6373	20
H(61b)	3715	37	6967	20
H(62a)	4701	-1567	6891	34
H(62b)	3328	-1298	7145	34
H(62c)	4879	-1100	7504	34
H(71a)	4370	644	8692	23
H(71b)	4904	734	9385	23
H(72a)	5173	-691	8730	45

Table S6. Continued...

Atom	x	y	z	U(eq)
H(72b)	4100	-577	9179	45
H(72c)	5773	-604	9419	45
H(81a)	6790	1281	10035	30
H(81b)	8285	1711	10049	30
H(82a)	7974	36	10247	61
H(82b)	8503	675	10754	61
H(82c)	9465	478	10275	61
H(91)	7558	2540	8287	23
H(92)	6384	3674	7708	24
H(93a)	7262	3596	6202	35
H(93b)	6891	4278	6635	35
H(93c)	5731	3616	6385	35
H(94)	8475	2379	6695	17

Table S7. Crystal data and structure refinement for [Fe(OEP)(CS)(CH_3OH)]

Empirical formula	$C_{38}H_{52}FeN_4OS$
Formula weight	668.75
Temperature	100(2) K
Wavelength	0.71073 A
Crystal system	Triclinic
Space group	$P\bar{1}$
Unit cell dimensions	a = 9.0599(5) Åα=90.2610° (10)
	b = 9.4389(5) Åβ =100.3620° (10)
	c = 11.0676(6) Åγ =114.6640° (10)
Volume	842.72(8) $Å^3$
Z	1
Density (calculated)	1.318 g/cm^3
Absorption coefficient	0.546 mm^{-1}
F(000)	358
Crystal size	0.52 x 0.25 x 0.17 mm
Diffractometer	Bruker APEX
Theta range for data collection	2.38 to 28.28 °
Index ranges	-11≤h≤12, -12≤k≤12, -14≤l≤14
Reflections collected	9096
Independent reflections	4178 [R(int) = 0.0189]
Unique observed reflections	3956
Absorption correction	SADABS
Max. and min. transmission	1.0000 and 0.9163
Refinement method	Full-matrix least-squares on F^2
Data / restraints / parameters	4178 / 0 / 223
Goodness-of-fit on F^2	1.283
Final R indices [I¿2sigma(I)]	R1 = 0.0587, wR2 = 0.1395
R indices (all data)	R1 = 0.0608, wR2 = 0.1403
Largest diff. peak and hole	0.450 and -0.566e.A^{-3}

Table S8. Atomic coordinates and equivalent isotropic displacement parameters (Å^2) for [Fe(OEP)(CS)(CH_3OH)][a]

Atom	x	y	z	U(eq)
Fe(1)	-0.5000	-0.5000	0.5000	0.0216(2)
N(1)	-0.3870(3)	-0.6345(2)	0.56181(19)	0.0172(4)
C(a1)	-0.2738(3)	-0.6644(3)	0.5107(2)	0.0185(5)
S(1)	-0.1665(3)	-0.2321(2)	0.69425(19)	0.0256(4)
C(19)	-0.3231(14)	-0.3514(9)	0.6006(11)	0.0194(16)
O(51)	-0.3028(10)	-0.2978(6)	0.5926(7)	0.0209(13)
C(51)	-0.2022(10)	-0.2942(10)	0.7054(8)	0.0295(17)
C(b1)	-0.2188(3)	-0.7679(3)	0.5829(2)	0.0193(5)
N(2)	-0.6124(3)	-0.5419(2)	0.64366(19)	0.0181(4)
C(b2)	-0.2961(3)	-0.7972(3)	0.6801(2)	0.0196(5)
C(a2)	-0.3981(3)	-0.7115(3)	0.6680(2)	0.0189(5)
C(m1)	-0.4920(3)	-0.7058(3)	0.7518(2)	0.0199(5)
C(a3)	-0.5920(3)	-0.6272(3)	0.7410(2)	0.0192(5)
C(b3)	-0.6928(3)	-0.6263(3)	0.8288(2)	0.0213(5)
C(b4)	-0.7771(3)	-0.5419(3)	0.7829(2)	0.0209(5)
C(a4)	-0.7259(3)	-0.4888(3)	0.6682(2)	0.0194(5)
C(11)	-0.1044(3)	-0.8323(3)	0.5481(3)	0.0240(5)
C(12)	-0.1922(4)	-0.9640(3)	0.4440(3)	0.0272(6)
C(21)	-0.2860(3)	-0.9006(3)	0.7810(2)	0.0235(5)
C(22)	-0.4352(4)	-1.0590(3)	0.7631(3)	0.0325(7)
C(31)	-0.7019(4)	-0.7090(4)	0.9447(3)	0.0285(6)
C(32)	-0.8111(4)	-0.8840(4)	0.9213(3)	0.0364(7)
C(41)	-0.8991(3)	-0.5043(3)	0.8363(3)	0.0256(6)
C(42)	-0.8232(4)	-0.3408(4)	0.9039(3)	0.0352(7)
C(m2)	-0.7798(3)	-0.3948(3)	0.5952(2)	0.0201(5)

[a] U(eq) is defined as one third of the trace of the orthogonalized Uij tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S9. Bond lengths for [Fe(OEP)(CS)(CH_3OH)][a].

bond	length Å	bond	length Å
Fe(1)-C(19)	1.800(12)	Fe(1)–C(19)$^{\#1}$	1.801(12)
Fe(1)–N(1)$^{\#1}$	1.992(2)	Fe(1)–N(1)	1.992(2)
Fe(1)–N(2)$^{\#1}$	1.994(2)	Fe(1)–N(2)	1.994(2)
Fe(1)–O(51)$^{\#1}$	2.089(7)	Fe(1)–O(51)	2.089(7)
N(1)–C(a1)	1.379(3)	N(1)–C(a2)	1.382(3)
C(a1)–C(m2)$^{\#1}$	1.381(4)	C(a1)–C(b1)	1.453(3)
S(1)–C(19)	1.576(12)	O(51)–C(51)	1.398(11)
C(b1)–C(b2)	1.356(4)	C(b1)–C(11)	1.503(3)
N(2)–C(a3)	1.379(3)	N(2)–C(a4)	1.382(3)
C(b2)–C(a2)	1.452(3)	C(b2)–C(21)	1.501(4)
C(a2)–C(m1)	1.381(3)	C(m1)–C(a3)	1.382(4)
C(a3)–C(b3)	1.451(3)	C(b3)–C(b4)	1.359(4)
C(b3)–C(31)	1.502(4)	C(b4)–C(a4)	1.450(3)
C(b4)–C(41)	1.503(3)	C(a4)–C(m2)	1.380(4)
C(11)–C(12)	1.529(4)	C(21)–C(22)	1.522(4)
C(31)–C(32)	1.521(4)	C(41)–C(42)	1.528(4)
C(m2)–C(a1)$^{\#1}$	1.381(4)		

[a] The estimated standard deviations of the least significant digits are given in parentheses.Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x-1,-y-1,-z+1

Table S10. Bond angles for [Fe(OEP)(CS)(CH_3OH)][a].

angle	degree	angle	degree
C(19)–Fe(1)–C(19)$^{\#1}$	180.0(5)	C(19)–Fe(1)–N(1)$^{\#1}$	97.5(3)
C(19)$^{\#1}$–Fe(1)–N(1)$^{\#1}$	82.5(3)	C(19)–Fe(1)–N(1)	82.4(3)
C(19)$^{\#1}$–Fe(1)–N(1)	97.6(3)	N(1)$^{\#1}$–Fe(1)–N(1)	179.999(1)
C(19)–Fe(1)–N(2)$^{\#1}$	92.9(3)	C(19)$^{\#1}$–Fe(1)–N(2)$^{\#1}$	87.1(3)
N(1)$^{\#1}$–Fe(1)–N(2)$^{\#1}$	89.72(8)	N(1)–Fe(1)–N(2)$^{\#1}$	90.28(8)
C(19)–Fe(1)–N(2)	87.1(3)	C(19)$^{\#1}$–Fe(1)–N(2)	92.9(3)
N(1)$^{\#1}$–Fe(1)–N(2)	90.28(8)	N(1)–Fe(1)–N(2)	89.72(8)
N(2)$^{\#1}$–Fe(1)–N(2)	180.00(11)	C(19)–Fe(1)–O(51)$^{\#1}$	168.8(4)
C(19)$^{\#1}$–Fe(1)–O(51)$^{\#1}$	11.2(4)	N(1)$^{\#1}$–Fe(1)–O(51)$^{\#1}$	92.34(19)
N(1)–Fe(1)–O(51)$^{\#1}$	87.67(19)	N(2)$^{\#1}$–Fe(1)–O(51)$^{\#1}$	92.4(2)
N(2)–Fe(1)–O(51)$^{\#1}$	87.6(2)	C(19)–Fe(1)–O(51)	11.2(4)
C(19)$^{\#1}$–Fe(1)–O(51)	168.8(4)	N(1)$^{\#1}$–Fe(1)–O(51)	87.66(19)
N(1)–Fe(1)–O(51)	92.33(19)	N(2)$^{\#1}$–Fe(1)–O(51)	87.6(2)
N(2)–Fe(1)–O(51)	92.4(2)	O(51)$^{\#1}$–Fe(1)–O(51)	180.0
C(a1)–N(1)–C(a2)	104.9(2)	C(a1)–N(1)–Fe(1)	127.22(17)
C(a2)–N(1)–Fe(1)	127.78(16)	N(1)–C(a1)–C(m2)$^{\#1}$	124.8(2)
N(1)–C(a1)–C(b1)	110.9(2)	C(m2)$^{\#1}$–C(a1)–C(b1)	124.3(2)
S(1)–C(19)–Fe(1)	175.4(6)	C(51)–O(51)–Fe(1)	124.2(5)
C(b2)–C(b1)–C(a1)	106.6(2)	C(b2)–C(b1)–C(11)	128.8(2)
C(a1)–C(b1)–C(11)	124.5(2)	C(a3)–N(2)–C(a4)	105.1(2)
C(a3)–N(2)–Fe(1)	127.74(17)	C(a4)–N(2)–Fe(1)	127.13(17)
C(b1)–C(b2)–C(a2)	106.7(2)	C(b1)–C(b2)–C(21)	128.4(2)
C(a2)–C(b2)–C(21)	124.9(2)	C(m1)–C(a2)–N(1)	124.5(2)
C(m1)–C(a2)–C(b2)	124.8(2)	N(1)–C(a2)–C(b2)	110.8(2)
C(a2)–C(m1)–C(a3)	125.7(2)	N(2)–C(a3)–C(m1)	124.5(2)
N(2)–C(a3)–C(b3)	110.8(2)	C(m1)–C(a3)–C(b3)	124.6(2)
C(b4)–C(b3)–C(a3)	106.6(2)	C(b4)–C(b3)–C(31)	128.5(2)
C(a3)–C(b3)–C(31)	124.9(2)	C(b3)–C(b4)–C(a4)	106.8(2)
C(b3)–C(b4)–C(41)	129.0(2)	C(a4)–C(b4)–C(41)	124.2(2)
C(m2)–C(a4)–N(2)	124.7(2)	C(m2)–C(a4)–C(b4)	124.6(2)
N(2)–C(a4)–C(b4)	110.6(2)	C(b1)–C(11)–C(12)	112.1(2)
C(b2)–C(21)–C(22)	113.3(2)	C(b3)–C(31)–C(32)	113.0(2)
C(b4)–C(41)–C(42)	113.4(2)	C(a4)–C(m2)–C(a1)$^{\#1}$	125.7(2)

[a] The estimated standard deviations of the least significant digits are given in parentheses. Symmetry transformations used to generate equivalent atoms:

$^{\#1}$ -x-1,-y-1,-z+1

Table S11. Anisotropic displacement parameters (Å^2) for [Fe(OEP)(CS)(CH_3OH)][a].

Atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0289(3)	0.0170(3)	0.0289(3)	0.0090(2)	0.0179(2)	0.0145(2)
N(1)	0.0167(10)	0.0172(10)	0.0174(10)	-0.0001(8)	0.0033(8)	0.0070(8)
C(a1)	0.0157(11)	0.0169(11)	0.0207(12)	-0.0046(9)	0.0006(9)	0.0062(9)
S(1)	0.0222(9)	0.0230(9)	0.0255(8)	-0.0029(8)	-0.0001(6)	0.0059(8)
C(19)	0.026(4)	0.015(4)	0.023(3)	0.007(3)	0.009(2)	0.013(4)
O(51)	0.024(3)	0.020(3)	0.021(2)	0.002(3)	0.0060(18)	0.011(3)
C(51)	0.027(4)	0.027(4)	0.027(4)	-0.003(4)	0.000(3)	0.006(4)
C(b1)	0.0150(11)	0.0183(11)	0.0212(12)	-0.0040(9)	-0.0019(9)	0.0059(9)
N(2)	0.0168(10)	0.0194(10)	0.0189(10)	0.0006(8)	0.0057(8)	0.0076(8)
C(b2)	0.0163(11)	0.0173(11)	0.0216(12)	-0.0031(9)	-0.0014(9)	0.0059(9)
C(a2)	0.0169(11)	0.0158(11)	0.0211(12)	-0.0004(9)	0.0010(9)	0.0053(9)
C(m1)	0.0204(12)	0.0195(11)	0.0181(12)	0.0024(9)	0.0024(9)	0.0073(10)
C(a3)	0.0177(11)	0.0196(11)	0.0181(12)	-0.0005(9)	0.0035(9)	0.0058(9)
C(b3)	0.0196(12)	0.0228(12)	0.0193(12)	-0.0003(9)	0.0057(9)	0.0062(10)
C(b4)	0.0184(12)	0.0225(12)	0.0194(12)	-0.0025(9)	0.0056(9)	0.0056(10)
C(a4)	0.0168(11)	0.0166(11)	0.0233(12)	-0.0029(9)	0.0062(9)	0.0047(9)
C(11)	0.0226(13)	0.0281(13)	0.0238(13)	-0.0034(10)	0.0003(10)	0.0149(11)
C(12)	0.0307(15)	0.0289(14)	0.0257(14)	-0.0055(11)	-0.0034(11)	0.0199(12)
C(21)	0.0230(13)	0.0243(13)	0.0225(13)	-0.0005(10)	-0.0009(10)	0.0117(11)
C(22)	0.0303(15)	0.0267(14)	0.0381(17)	0.0099(12)	0.0001(12)	0.0125(12)
C(31)	0.0283(14)	0.0365(15)	0.0221(13)	0.0050(11)	0.0090(11)	0.0136(12)
C(32)	0.0260(15)	0.0376(17)	0.0386(17)	0.0178(14)	0.0056(13)	0.0072(13)
C(41)	0.0216(13)	0.0314(14)	0.0259(13)	0.0032(11)	0.0112(11)	0.0107(11)
C(42)	0.0272(15)	0.0461(18)	0.0324(16)	-0.0140(14)	0.0059(12)	0.0158(14)
C(m2)	0.0141(11)	0.0196(12)	0.0257(13)	-0.0039(10)	0.0046(9)	0.0062(9)

[a] The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form:
$-2\,\pi^2\,[\,h^2\,a^{*2}\,U_{11} + \ldots + 2\,h\,k\,a^*\,b^*\,U_{12}\,]$

Table S12. Hydrogen coordinates and isotropic displacement parameters (Å^2) for [Fe(OEP)(CS)(CH_3OH)].

Atom	x	y	z	U(eq)
H(51)	-0.2293	-0.2690	0.5322	0.025
H(51a)	-0.1220	-0.2055	0.7609	0.035
H(51b)	-0.1647	-0.3693	0.6890	0.035
H(51c)	-0.2764	-0.3553	0.7543	0.035
H(m1)	-0.4819	-0.7604	0.8228	0.024
H(11a)	-0.0227	-0.7544	0.5244	0.029
H(11b)	-0.0779	-0.8782	0.6177	0.029
H(12a)	-0.2954	-1.0522	0.4611	0.033
H(12b)	-0.2137	-0.9283	0.3745	0.033
H(12c)	-0.1162	-0.9948	0.4262	0.033
H(21a)	-0.2597	-0.8492	0.8584	0.028
H(22b)	-0.1971	-0.9169	0.7793	0.028
H(22a)	-0.4259	-1.1195	0.8312	0.039
H(22b)	-0.4574	-1.1215	0.6764	0.039
H(22c)	-0.5224	-1.0412	0.7756	0.039
H(31a)	-0.5880	-0.6802	0.9873	0.034
H(31b)	-0.7368	-0.6613	0.9989	0.034
H(32a)	-0.7552	-0.9291	0.8759	0.044
H(32b)	-0.8218	-0.9555	0.9719	0.044
H(32c)	-0.9325	-0.9117	0.8775	0.044
H(41a)	-0.9455	-0.5756	0.8798	0.031
H(41b)	-0.9801	-0.5186	0.7852	0.031
H(42a)	-0.8995	-0.3207	0.9356	0.042
H(42b)	-0.7640	-0.2677	0.8603	0.042
H(42c)	-0.7555	-0.3425	0.9544	0.042
H(m2)	-0.8545	-0.3696	0.6188	0.024

Table S13. Complete Crystallographic Details for [Fe(OEP)(CS)(Py)]

formula	$C_{42}H_{49}FeN_5S$
FW, amu	711.77
a, Å	13.9073(6)
b, Å	16.2624(7)
c, Å	22.0709(9)
α, deg	70.5860(10)
β, deg	77.2420(10)
γ, deg	77.9590(10)
V, Å^3	4541.8(3)
space group	$P\bar{1}$
Z	5
D_c, g/cm^3	1.301
F(000)	1890
μ, mm^{-1}	0.510
crystal dimensions, mm	0.3 × 0.2 × 0.2
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	100(2)
diffractometer	Enraf Bruker Apex CCD
θ range for collected data, deg	1.87–28.29
index range	$-18 \leq h \leq 18$
	$-21 \leq k \leq 21$
	$-29 \leq l \leq 29$
total data collected	49146
absorption correction	SADABS
Max. and min. transmission	1.0000 and 0.9086
unique data	22494 (R_{int} = 0.023)
unique observed data [I > 2σ(I)]	18114
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	22494/0/1370
goodness-of-fit (pased on F^2)	1.029
final R indices [I > 2σ(I)]	R_1 = 0.0458, wR_2 = 0.1106
final R indices (all data)	R_1 = 0.0587, wR_2 = 0.1185

Table S14. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(CS)(Py)][a]

atom	x	y	z	U(eq)
Fe(1)_1	−0.09618(2)	0.76543(2)	0.92497(1)	0.0271(1)
S(1)_1	0.13752(4)	0.73055(4)	0.94298(3)	0.0392(1)
N(1)_1	−0.14592(11)	0.68330(10)	1.01145(7)	0.0247(3)
N(2)_1	−0.13042(14)	0.86500(11)	0.96409(8)	0.0391(4)
N(3)_1	−0.05788(13)	0.84990(10)	0.83678(8)	0.0338(4)
N(4)_1	−0.07095(11)	0.66713(9)	0.88508(7)	0.0230(3)
N(5)_1	−0.24637(12)	0.79352(10)	0.90595(8)	0.0313(4)
C(a2)_1	−0.18041(15)	0.70211(12)	1.06958(9)	0.0291(4)
C(m1)_1	−0.1869(2)	0.78426(14)	1.07740(10)	0.0483(6)
C(a3)_1	−0.1638(2)	0.86005(15)	1.02842(12)	0.0582(8)
C(b3)_1	−0.1996(3)	0.9541(2)	1.03115(19)	0.0256(7)
C(b4)_1	−0.1692(3)	1.0099(2)	0.97205(18)	0.0223(7)
C(31)_1	−0.2495(4)	0.9749(3)	1.0945(2)	0.0341(8)
C(32)_1	−0.1800(4)	0.9577(4)	1.1413(3)	0.0480(12)
C(31)_1	−0.1626(4)	1.1059(3)	0.9550(2)	0.0252(8)
C(42)_1	−0.0597(3)	1.1248(2)	0.95654(19)	0.0278(7)
C(b3a)_1	−0.1487(3)	0.9371(3)	1.0444(2)	0.0264(8)
C(b4a)_1	−0.1219(3)	0.9947(3)	0.9852(2)	0.0255(8)
C(41a)_1	−0.1790(4)	0.9546(3)	1.1085(2)	0.0375(11)
C(32a)_1	−0.2927(4)	0.9688(3)	1.1317(3)	0.0529(15)
C(41a)_1	−0.1095(4)	1.0906(3)	0.9688(2)	0.0324(9)
C(42a)_1	−0.2010(4)	1.1495(3)	0.9467(2)	0.0393(10)
C(a4)_1	−0.1190(2)	0.95191(14)	0.93234(12)	0.0527(7)
C(m2)_1	−0.0857(2)	0.98606(14)	0.86648(12)	0.0531(7)
C(a5)_1	−0.0567(2)	0.93868(14)	0.82181(11)	0.0477(6)
C(b5)_1	−0.0308(3)	0.9782(2)	0.74948(16)	0.0256(6)
C(b6)_1	−0.0065(3)	0.9097(2)	0.72348(16)	0.0238(6)
C(51)_1	−0.0217(3)	1.0732(2)	0.71448(16)	0.0286(6)
C(52)_1	0.0837(3)	1.0955(2)	0.7020(2)	0.0434(8)
C(61)_1	0.0329(3)	0.9121(2)	0.65395(17)	0.0303(7)
C(62)_1	0.1449(3)	0.8795(3)	0.64420(18)	0.0456(8)
C(b5a)_1	0.0132(5)	0.9681(4)	0.7632(3)	0.0289(12)
C(b6a)_1	0.0340(5)	0.9011(4)	0.7363(3)	0.0253(12)
C(51a)_1	0.0419(5)	1.0605(4)	0.7323(3)	0.0344(12)

Table S14. Continued...

atom	x	y	z	U(eq)
C(52a)_1	−0.0408(6)	1.1227(5)	0.7001(3)	0.0429(15)
C(61a)_1	0.0815(5)	0.9025(4)	0.6672(3)	0.0280(13)
C(62a)_1	0.0067(5)	0.9174(5)	0.6208(3)	0.0391(14)
C(a6)_1	−0.01887(17)	0.82921(13)	0.77973(10)	0.0386(5)
C(m3)_1	−0.00491(15)	0.74558(12)	0.77317(9)	0.0316(4)
C(a7)_1	−0.02863(13)	0.66992(12)	0.82201(9)	0.0245(3)
C(b7)_1	−0.01314(12)	0.58302(11)	0.81377(8)	0.0228(3)
C(b8)_1	−0.04666(12)	0.52739(11)	0.87251(8)	0.0217(3)
C(a8)_1	−0.08136(12)	0.58001(11)	0.91689(8)	0.0212(3)
C(m4)_1	−0.11906(12)	0.54670(11)	0.98214(8)	0.0213(3)
C(a1)_1	−0.15021(12)	0.59494(11)	1.02598(8)	0.0212(3)
C(b1)_1	−0.19082(12)	0.55811(11)	1.09421(8)	0.0214(3)
C(b2)_1	−0.21053(13)	0.62496(12)	1.12099(9)	0.0252(4)
C(71)_1	0.03065(13)	0.55998(12)	0.75185(8)	0.0255(4)
C(72)_1	−0.04822(15)	0.55106(15)	0.71728(10)	0.0356(4)
C(81)_1	−0.04903(13)	0.43037(11)	0.88983(9)	0.0235(3)
C(82)_1	−0.15320(13)	0.40862(12)	0.89516(9)	0.0284(4)
C(11)_1	−0.20812(13)	0.46404(11)	1.12590(8)	0.0233(3)
C(12)_1	−0.30576(14)	0.44638(13)	1.11498(9)	0.0296(4)
C(21)_1	−0.26153(15)	0.62497(13)	1.18833(9)	0.0305(4)
C(22)_1	−0.37096(17)	0.66430(16)	1.19015(11)	0.0490(6)
C(1)_1	0.02471(15)	0.74570(12)	0.93692(9)	0.0300(4)
C(2)_1	−0.32358(16)	0.81177(13)	0.95090(11)	0.0384(5)
C(3)_1	−0.42117(17)	0.83240(14)	0.94014(12)	0.0460(6)
C(4)_1	−0.44173(17)	0.83421(14)	0.88140(12)	0.0462(6)
C(5)_1	−0.36364(17)	0.81473(14)	0.83507(11)	0.0427(5)
C(6)_1	−0.26761(2)	0.79477(1)	0.84911(1)	0.0361(4)
Fe(1)_2	0.29602(2)	0.60481(1)	0.30865(1)	0.0193(1)
S(1)_2	0.51471(2)	0.52877(1)	0.35244(1)	0.0345(1)
N(1)_2	0.31618(2)	0.73053(1)	0.26296(1)	0.0277(3)
N(2)_2	0.24109(2)	0.63435(1)	0.39206(1)	0.0212(3)
N(3)_2	0.26598(2)	0.48140(1)	0.35212(1)	0.0195(3)
N(4)_2	0.34329(2)	0.57746(1)	0.22358(1)	0.0215(3)
N(5)_2	0.14649(2)	0.64437(1)	0.28697(1)	0.0234(3)

Table S14. Continued...

atom	x	y	z	U(eq)
C(a2)_2	0.29482(18)	0.79869(13)	0.28972(10)	0.0395(5)
C(m1)_2	0.25703(18)	0.79089(13)	0.35457(10)	0.0394(5)
C(a3)_2	0.23232(14)	0.71429(12)	0.40243(9)	0.0266(4)
C(b3)_2	0.19373(15)	0.70800(13)	0.47029(9)	0.0302(4)
C(b4)_2	0.18028(13)	0.62295(12)	0.50093(8)	0.0242(3)
C(a4)_2	0.21033(12)	0.57732(11)	0.45171(8)	0.0215(3)
C(m2)_2	0.20585(13)	0.48922(11)	0.46329(8)	0.0231(3)
C(a5)_2	0.23284(12)	0.44411(11)	0.41727(8)	0.0213(3)
C(b5)_2	0.23338(13)	0.35029(11)	0.43179(8)	0.0233(3)
C(b6)_2	0.26940(13)	0.33057(11)	0.37495(8)	0.0226(3)
C(a6)_2	0.29015(12)	0.41271(11)	0.32599(8)	0.0203(3)
C(m3)_2	0.33166(12)	0.42002(11)	0.26149(8)	0.0217(3)
C(a7)_2	0.35768(12)	0.49604(11)	0.21427(8)	0.0211(3)
C(b7)_2	0.40649(13)	0.49996(12)	0.14808(8)	0.0236(3)
C(b8)_2	0.42159(13)	0.58515(12)	0.11754(8)	0.0253(4)
C(a8)_2	0.38257(14)	0.63285(12)	0.16505(8)	0.0256(4)
C(m4)_2	0.38599(16)	0.72104(13)	0.15329(9)	0.0329(4)
C(a1)_2	0.35386(17)	0.76703(13)	0.19852(9)	0.0362(5)
C(b1)_2	0.3460(2)	0.86371(19)	0.18181(14)	0.0261(6)
C(b2)_2	0.3087(2)	0.88357(18)	0.23834(14)	0.0272(6)
C(11)_2	0.3829(3)	0.9239(2)	0.11691(15)	0.0316(6)
C(12)_2	0.4950(3)	0.9265(2)	0.10390(15)	0.0372(7)
C(21)_2	0.2924(3)	0.97125(18)	0.25086(15)	0.0329(6)
C(22)_2	0.3796(3)	0.98263(19)	0.27747(16)	0.0407(7)
C(b1a)_2	0.3900(6)	0.8491(5)	0.1935(4)	0.0241(15)
C(b2a)_2	0.3546(6)	0.8674(5)	0.2501(4)	0.0239(14)
C(11a)_2	0.4444(8)	0.9088(5)	0.1295(4)	0.0318(15)
C(12a)_2	0.3742(8)	0.9493(7)	0.0827(6)	0.054(3)
C(21a)_2	0.3487(6)	0.9527(4)	0.2649(4)	0.0235(13)
C(22a)_2	0.2446(5)	1.0049(5)	0.2703(4)	0.0310(15)
C(31)_2	0.1752(2)	0.78275(15)	0.49923(11)	0.0503(7)
C(32)_2	0.0938(3)	0.8450(2)	0.48941(19)	0.0291(8)
C(31a)_2	0.2420(4)	0.7991(3)	0.5243(3)	0.0478(11)
C(41)_2	0.14289(14)	0.57992(12)	0.57153(9)	0.0282(4)

Table S14. Continued...

atom	x	y	z	U(eq)
C(42)_2	0.22597(16)	0.52578(14)	0.60979(9)	0.0354(4)
C(51)_2	0.19804(15)	0.29021(12)	0.49763(9)	0.0309(4)
C(52)_2	0.08475(18)	0.29694(18)	0.51274(11)	0.0506(6)
C(61)_2	0.28847(15)	0.24265(11)	0.36287(9)	0.0278(4)
C(62)_2	0.20837(18)	0.22735(15)	0.33186(12)	0.0450(5)
C(71)_2	0.43269(13)	0.42363(12)	0.12056(8)	0.0259(4)
C(72)_2	0.34943(14)	0.41222(12)	0.09040(9)	0.0275(4)
C(81)_2	0.46914(15)	0.62446(13)	0.04862(9)	0.0314(4)
C(82)_2	0.39435(16)	0.67521(14)	0.00313(9)	0.0359(4)
C(1)_2	0.41185(13)	0.56965(11)	0.32960(8)	0.0234(3)
C(2)_2	0.12896(16)	0.69111(12)	0.22655(9)	0.0304(4)
C(3)_2	0.03463(17)	0.71961(13)	0.21079(10)	0.0381(5)
C(4)_2	−0.04677(17)	0.70031(14)	0.25884(11)	0.0391(5)
C(5)_2	−0.03036(15)	0.65252(13)	0.32157(11)	0.0357(4)
C(6)_2	0.06659(14)	0.62584(12)	0.33334(9)	0.0284(4)
Fe(1)_3	0.50000(14)	0.00000(12)	0.50000(9)	0.0463(1)
N(5)_3	0.3615(2)	0.0153(2)	0.48746(13)	0.020(2)
C(2)_3	0.3416(2)	0.00230(19)	0.43363(13)	0.0299(8)
C(3)_3	0.24535(19)	0.01625(17)	0.42315(12)	0.0347(9)
C(4)_3	0.16905(18)	0.04326(17)	0.46650(12)	0.0340(8)
C(5)_3	0.18896(18)	0.05630(16)	0.52034(12)	0.0315(8)
C(6)_3	0.2852(2)	0.04235(18)	0.53081(12)	0.0293(8)
S(1)_3	0.25746(9)	0.01593(8)	0.47383(8)	0.0596(4)
C(1)_3	0.3683(6)	0.0132(5)	0.4850(4)	0.046(4)
N(1)_3	0.46553(14)	0.10003(10)	0.53829(8)	0.0363(4)
N(2)_3	0.53632(13)	0.08354(10)	0.41166(7)	0.0321(4)
C(a1)_3	0.4487(3)	0.0937(2)	0.60484(16)	0.0270(7)
C(b1)_3	0.4362(3)	0.18059(19)	0.61269(14)	0.0263(6)
C(m2)_3	0.4331(3)	0.0169(2)	0.65492(16)	0.0334(7)
C(11)_3	0.4103(2)	0.20022(19)	0.67702(16)	0.0304(6)
C(12)_3	0.2991(3)	0.2138(3)	0.6996(2)	0.0446(8)
C(1a)_3	0.3993(5)	0.1010(4)	0.5971(3)	0.0239(11)
C(2a)_3	0.3822(4)	0.1882(3)	0.6045(3)	0.0219(10)
C(10b)_3	0.3765(6)	0.0253(4)	0.6458(3)	0.0334(14)

Table S14. Continued...

atom	x	y	z	U(eq)
C(11a)_3	0.3303(4)	0.2111(3)	0.6652(3)	0.0282(12)
C(12a)_3	0.3921(6)	0.1899(5)	0.7189(3)	0.0515(19)
C(b2)_3	0.44265(17)	0.23995(12)	0.55042(10)	0.0359(5)
C(a2)_3	0.47153(14)	0.18734(11)	0.50583(9)	0.0253(4)
C(m1)_3	0.50217(12)	0.22119(11)	0.43985(8)	0.0222(3)
C(a3)_3	0.53349(13)	0.17284(11)	0.39595(8)	0.0236(3)
C(b3)_3	0.56630(15)	0.21094(12)	0.32673(9)	0.0288(4)
C(b4)_3	0.5799(4)	0.1432(6)	0.2998(4)	0.0255(10)
C(a4)_3	0.5581(4)	0.0661(4)	0.3518(3)	0.0287(10)
C(41)_3	0.6203(6)	0.1472(4)	0.2309(2)	0.0344(11)
C(42)_3	0.7398(6)	0.1298(5)	0.2140(3)	0.056(2)
C(8a)_3	0.6132(11)	0.1431(10)	0.3039(8)	0.056(4)
C(9a)_3	0.5957(7)	0.0598(8)	0.3588(5)	0.032(2)
C(41a)_3	0.7082(14)	0.1379(9)	0.2289(8)	0.101(6)
C(42a)_3	0.6308(17)	0.1455(13)	0.2119(9)	0.114(7)
C(21)_3	0.44281(15)	0.33729(12)	0.53152(9)	0.0298(4)
C(22)_3	0.54771(16)	0.36096(14)	0.51900(11)	0.0381(5)
C(31)_3	0.57443(15)	0.30686(12)	0.29328(9)	0.0291(4)
C(32)_3	0.66995(16)	0.33361(14)	0.29835(11)	0.0390(5)

[a] U(eg) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor. The estimated standard deviations of the least significant digits are given in parentheses.

Table S15. Bond Lengths for [Fe(OEP)(CS)(Py)][a]

bond	length (Å)	bond	length (Å)
Fe(1)_1–C(1)_1	1.707(2)	C(b4)_2–C(a4)_2	1.453(2)
Fe(1)_1–N(1)_1	2.0034(15)	C(b4)_2–C(41)_2	1.503(2)
Fe(1)_1–N(4)_1	2.0048(14)	C(a4)_2–C(m2)_2	1.382(2)
Fe(1)_1–N(2)_1	2.0050(16)	C(m2)_2–C(a5)_2	1.387(2)
Fe(1)_1–N(3)_1	2.0072(16)	C(a5)_2–C(b5)_2	1.450(2)
Fe(1)_1–N(5)_1	2.1469(18)	C(b5)_2–C(b6)_2	1.360(2)
S(1)_1–C(1)_1	1.565(2)	C(b5)_2–C(51)_2	1.500(2)
N(1)_1–C(a1)_1	1.376(2)	C(b6)_2–C(a6)_2	1.449(2)
N(1)_1–C(a2)_1	1.378(2)	C(b6)_2–C(61)_2	1.500(2)
N(2)_1–C(a3)_1	1.374(3)	C(a6)_2–C(m3)_2	1.388(2)
N(2)_1–C(a4)_1	1.378(3)	C(m3)_2–C(a7)_2	1.382(2)
N(3)_1–C(a5)_1	1.373(2)	C(a7)_2–C(b7)_2	1.455(2)
N(3)_1–C(a6)_1	1.377(2)	C(b7)_2–C(b8)_2	1.362(2)
N(4)_1–C(a7)_1	1.376(2)	C(b7)_2–C(71)_2	1.502(2)
N(4)_1–C(a8)_1	1.379(2)	C(b8)_2–C(a8)_2	1.453(2)
N(5)_1–C(6)_1	1.3438(17)	C(b8)_2–C(81)_2	1.498(2)
N(5)_1–C(2)_1	1.348(2)	C(a8)_2–C(m4)_2	1.379(3)
C(a2)_1–C(m1)_1	1.385(3)	C(m4)_2–C(a1)_2	1.384(3)
C(a2)_1–C(b2)_1	1.449(2)	C(a1)_2–C(b1)_2	1.477(3)
C(m1)_1–C(a3)_1	1.385(3)	C(a1)_2–C(b1a)_2	1.484(8)
C(a3)_1–C(b3a)_1	1.474(4)	C(b1)_2–C(b2)_2	1.357(4)
C(a3)_1–C(b3)_1	1.523(4)	C(b1)_2–C(11)_2	1.492(4)
C(b3)_1–C(b4)_1	1.354(5)	C(b2)_2–C(21)_2	1.503(4)
C(b3)_1–C(31)_1	1.530(5)	C(11)_2–C(12)_2	1.529(4)
C(b4)_1–C(a4)_1	1.466(4)	C(21)_2–C(22)_2	1.527(4)
C(b4)_1–C(41)_1	1.497(5)	C(b1a)_2–C(b2a)_2	1.345(10)
C(31)_1–C(32)_1	1.488(6)	C(b1a)_2–C(11a)_2	1.559(11)
C(41)_1–C(42)_1	1.535(6)	C(b2a)_2–C(21a)_2	1.510(9)
C(b3a)_1–C(b4a)_1	1.356(6)	C(11a)_2–C(12a)_2	1.478(13)
C(b3a)_1–C(41a)_1	1.488(6)	C(21a)_2–C(22a)_2	1.519(10)
C(b4a)_1–C(41a)_1	1.517(6)	C(31)_2–C(31a)_2	1.291(5)
C(b4a)_1–C(a4)_1	1.535(4)	C(31)_2–C(32)_2	1.356(4)
C(31a)_1–C(32a)_1	1.544(7)	C(41)_2–C(42)_2	1.528(3)
C(41a)_1–C(42a)_1	1.493(6)	C(51)_2–C(52)_2	1.525(3)

Table S15. Continued...

bond	length (Å)	bond	length (Å)
C(a4)_1–C(m2)_1	1.382(3)	C(61)_2–C(62)_2	1.529(3)
C(m2)_1–C(a5)_1	1.389(3)	C(71)_2–C(72)_2	1.527(2)
C(a5)_1–C(b5a)_1	1.440(6)	C(81)_2–C(82)_2	1.524(3)
C(a5)_1–C(b5)_1	1.500(4)	C(2)_2–C(3)_2	1.378(3)
C(b5)_1–C(b6)_1	1.366(5)	C(3)_2–C(4)_2	1.379(3)
C(b5)_1–C(51)_1	1.499(4)	C(4)_2–C(5)_2	1.387(3)
C(b6)_1–C(a6)_1	1.484(4)	C(5)_2–C(6)_2	1.382(3)
C(b6)_1–C(61)_1	1.501(5)	Fe(1)_3–C(1)_3	1.889(8)
C(51)_1–C(52)_1	1.528(4)	Fe(1)_3–C(1)_3#1	1.889(8)
C(61)_1–C(62)_1	1.529(5)	Fe(1)_3–N(5)_3	1.959(3)
C(b5a)_1–C(b6a)_1	1.359(9)	Fe(1)_3–N(5)_3#1	1.959(3)
C(b5a)_1–C(51a)_1	1.527(8)	Fe(1)_3–N(2)_3#1	1.998(2)
C(b6a)_1–C(a6)_1	1.459(6)	Fe(1)_3–N(2)_3	1.998(2)
C(b6a)_1–C(61a)_1	1.516(8)	Fe(1)_3–N(1)_3	2.000(2)
C(51a)_1–C(52a)_1	1.500(9)	Fe(1)_3–N(1)_3#1	2.000(2)
C(61a)_1–C(62a)_1	1.546(9)	N(5)_3–C(2)_3	1.3677(17)
C(a6)_1–C(m3)_1	1.384(3)	N(5)_3–C(6)_3	1.3679(17)
C(m3)_1–C(a7)_1	1.384(3)	C(2)_3–C(3)_3	1.3678(17)
C(a7)_1–C(b7)_1	1.450(2)	C(3)_3–C(4)_3	1.3679(17)
C(b7)_1–C(b8)_1	1.359(2)	C(4)_3–C(5)_3	1.3677(17)
C(b7)_1–C(71)_1	1.502(2)	C(5)_3–C(6)_3	1.3679(17)
C(b8)_1–C(a8)_1	1.449(2)	S(1)_3–C(1)_3	1.604(8)
C(b8)_1–C(81)_1	1.501(2)	N(1)_3–C(a2)_3	1.372(2)
C(a8)_1–C(m4)_1	1.382(2)	N(1)_3–C(a1)_3	1.407(3)
C(m4)_1–C(a1)_1	1.385(2)	N(1)_3–C(1a)_3	1.418(6)
C(a1)_1–C(b1)_1	1.453(2)	N(2)_3–C(a3)_3	1.370(2)
C(b1)_1–C(b2)_1	1.356(2)	N(2)_3–C(9a)_3	1.390(11)
C(b1)_1–C(11)_1	1.502(2)	N(2)_3–C(a4)_3	1.397(6)
C(b2)_1–C(21)_1	1.499(2)	C(a1)_3–C(m2)_3	1.384(5)
C(71)_1–C(72)_1	1.522(3)	C(a1)_3–C(b1)_3	1.451(4)
C(81)_1–C(82)_1	1.532(2)	C(b1)_3–C(b2)_3	1.389(4)
C(11)_1–C(12)_1	1.529(2)	C(b1)_3–C(11)_3	1.508(4)
C(21)_1–C(22)_1	1.520(3)	C(m2)_3–C(a4)_3#1	1.384(7)
C(2)_1–C(3)_1	1.382(3)	C(11)_3–C(12)_3	1.509(5)

Table S15. Continued...

bond	length (Å)	bond	length (Å)
C(3)_1–C(4)_1	1.378(4)	C(1a)_3–C(10b)_3	1.380(8)
C(4)_1–C(5)_1	1.381(3)	C(1a)_3–C(2a)_3	1.446(7)
C(5)_1–C(6)_1	1.386(2)	C(2a)_3–C(b2)_3	1.423(6)
Fe(1)_2–C(1)_2	1.7043(18)	C(2a)_3–C(11a)_3	1.499(7)
Fe(1)_2–N(3)_2	2.0039	C(10b)_3–C(9a)_3#1	1.389(13)
Fe(1)_2–N(2)_2	2.0043	C(11a)_3–C(12a)_3	1.523(9)
Fe(1)_2–N(1)_2	2.0048	C(b2)_3–C(a2)_3	1.450(2)
Fe(1)_2–N(4)_2	2.0108	C(b2)_3–C(21)_3	1.497(2)
Fe(1)_2–N(5)_2	2.1550	C(a2)_3–C(m1)_3	1.377(2)
S(1)_2–C(1)_2	1.5626(18)	C(m1)_3–C(a3)_3	1.387(2)
N(1)_2–C(a2)_2	1.3734(19)	C(a3)_3–C(b3)_3	1.451(2)
N(1)_2–C(a1)_2	1.3744(19)	C(b3)_3–C(8a)_3	1.350(17)
N(2)_2–C(a3)_2	1.3699(17)	C(b3)_3–C(b4)_3	1.378(8)
N(2)_2–C(a4)_2	1.3716(17)	C(b3)_3–C(31)_3	1.504(2)
N(3)_2–C(a6)_2	1.3710(16)	C(b4)_3–C(a4)_3	1.425(11)
N(3)_2–C(a5)_2	1.3754(16)	C(b4)_3–C(41)_3	1.485(9)
N(4)_2–C(a7)_2	1.3739(16)	C(a4)_3–C(m2)_3#1	1.384(7)
N(4)_2–C(a8)_2	1.3779(17)	C(41)_3–C(42)_3	1.606(11)
N(5)_2–C(6)_2	1.3436(19)	C(8a)_3–C(9a)_3	1.511(18)
N(5)_2–C(2)_2	1.3446(18)	C(8a)_3–C(41a)_3	1.89(2)
C(a2)_2–C(m1)_2	1.384(3)	C(8a)_3–C(42a)_3	1.98(2)
C(a2)_2–C(b2a)_2	1.457(7)	C(9a)_3–C(10b)_3#1	1.389(13)
C(a2)_2–C(b2)_2	1.484(3)	C(41a)_3–C(42a)_3	1.19(3)
C(m1)_2–C(a3)_2	1.389(3)	C(21)_3–C(22)_3	1.529(3)
C(a3)_2–C(b3)_2	1.452(2)	C(31)_3–C(32)_3	1.518(3)
C(b3)_2–C(b4)_2	1.355(3)		
C(b3)_2–C(31)_2	1.505(3)		

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S16. Bond Angles for [Fe(OEP)(CS)(Py)][a]

angle	degree	angle	degree
C(1)_1–Fe(1)_1–N(1)_1	95.12(8)	N(2)_2–C(a4)_2–C(b4)_2	110.59(13)
C(1)_1–Fe(1)_1–N(4)_1	91.11(7)	C(m2)_2–C(a4)_2–C(b4)_2	124.50(16)
N(1)_1–Fe(1)_1–N(4)_1	89.94(6)	C(a4)_2–C(m2)_2–C(a5)_2	125.85(16)
C(1)_1–Fe(1)_1–N(2)_1	92.51(8)	N(3)_2–C(a5)_2–C(m2)_2	124.81(14)
N(1)_1–Fe(1)_1–N(2)_1	89.64(6)	N(3)_2–C(a5)_2–C(b5)_2	110.68(13)
N(4)_1–Fe(1)_1–N(2)_1	176.38(7)	C(m2)_2–C(a5)_2–C(b5)_2	124.47(15)
C(1)_1–Fe(1)_1–N(3)_1	89.60(8)	C(b6)_2–C(b5)_2–C(a5)_2	106.69(15)
N(1)_1–Fe(1)_1–N(3)_1	175.27(7)	C(b6)_2–C(b5)_2–C(51)_2	128.71(16)
N(4)_1–Fe(1)_1–N(3)_1	89.92(6)	C(a5)_2–C(b5)_2–C(51)_2	124.59(16)
N(2)_1–Fe(1)_1–N(3)_1	90.20(7)	C(b5)_2–C(b6)_2–C(a6)_2	106.24(14)
C(1)_1–Fe(1)_1–N(5)_1	177.66(8)	C(b5)_2–C(b6)_2–C(61)_2	128.86(16)
N(1)_1–Fe(1)_1–N(5)_1	87.20(6)	C(a6)_2–C(b6)_2–C(61)_2	124.87(15)
N(4)_1–Fe(1)_1–N(5)_1	88.67(6)	N(3)_2–C(a6)_2–C(m3)_2	124.68(14)
N(2)_1–Fe(1)_1–N(5)_1	87.71(7)	N(3)_2–C(a6)_2–C(b6)_2	111.17(13)
N(3)_1–Fe(1)_1–N(5)_1	88.07(7)	C(m3)_2–C(a6)_2–C(b6)_2	124.13(15)
C(a1)_1–N(1)_1–C(a2)_1	105.01(14)	C(a7)_2–C(m3)_2–C(a6)_2	125.89(15)
C(a1)_1–N(1)_1–Fe(1)_1	127.26(11)	N(4)_2–C(a7)_2–C(m3)_2	124.93(14)
C(a2)_1–N(1)_1–Fe(1)_1	127.71(12)	N(4)_2–C(a7)_2–C(b7)_2	110.80(13)
C(a3)_1–N(2)_1–C(a4)_1	105.76(16)	C(m3)_2–C(a7)_2–C(b7)_2	124.26(15)
C(a3)_1–N(2)_1–Fe(1)_1	127.36(14)	C(b8)_2–C(b7)_2–C(a7)_2	106.38(15)
C(a4)_1–N(2)_1–Fe(1)_1	126.76(13)	C(b8)_2–C(b7)_2–C(71)_2	128.23(16)
C(a5)_1–N(3)_1–C(a6)_1	105.64(16)	C(a7)_2–C(b7)_2–C(71)_2	125.38(15)
C(a5)_1–N(3)_1–Fe(1)_1	127.30(14)	C(b7)_2–C(b8)_2–C(a8)_2	106.73(15)
C(a6)_1–N(3)_1–Fe(1)_1	126.83(13)	C(b7)_2–C(b8)_2–C(81)_2	127.99(16)
C(a7)_1–N(4)_1–C(a8)_1	105.30(14)	C(a8)_2–C(b8)_2–C(81)_2	125.29(16)
C(a7)_1–N(4)_1–Fe(1)_1	127.27(12)	N(4)_2–C(a8)_2–C(m4)_2	124.91(15)
C(a8)_1–N(4)_1–Fe(1)_1	127.03(11)	N(4)_2–C(a8)_2–C(b8)_2	110.58(14)
C(6)_1–N(5)_1–C(2)_1	117.21(17)	C(m4)_2–C(a8)_2–C(b8)_2	124.51(16)
C(6)_1–N(5)_1–Fe(1)_1	122.00(10)	C(a8)_2–C(m4)_2–C(a1)_2	125.68(17)
C(2)_1–N(5)_1–Fe(1)_1	120.78(15)	N(1)_2–C(a1)_2–C(m4)_2	124.75(16)
N(1)_1–C(a2)_1–C(m1)_1	124.38(17)	N(1)_2–C(a1)_2–C(b1)_2	111.21(18)
N(1)_1–C(a2)_1–C(b2)_1	110.94(15)	C(m4)_2–C(a1)_2–C(b1)_2	123.75(19)
C(m1)_1–C(a2)_1–C(b2)_1	124.68(17)	N(1)_2–C(a1)_2–C(b1a)_2	107.1(3)
C(a3)_1–C(m1)_1–C(a2)_1	125.79(19)	C(m4)_2–C(a1)_2–C(b1a)_2	124.2(3)

Table S16. Continued...

angle	degree	angle	degree
N(2)_1–C(a3)_1–C(m1)_1	124.82(18)	C(b1)_2–C(a1)_2–C(b1a)_2	26.7(3)
N(2)_1–C(a3)_1–C(b3a)_1	112.9(2)	C(b2)_2–C(b1)_2–C(a1)_2	106.0(2)
C(m1)_1–C(a3)_1–C(b3a)_1	120.5(2)	C(b2)_2–C(b1)_2–C(11)_2	128.1(3)
N(2)_1–C(a3)_1–C(b3)_1	107.0(2)	C(a1)_2–C(b1)_2–C(11)_2	125.6(3)
C(m1)_1–C(a3)_1–C(b3)_1	125.8(2)	C(b1)_2–C(b2)_2–C(a2)_2	106.5(2)
C(b3a)_1–C(a3)_1–C(b3)_1	30.37(18)	C(b1)_2–C(b2)_2–C(21)_2	128.9(3)
C(b4)_1–C(b3)_1–C(a3)_1	108.2(3)	C(a2)_2–C(b2)_2–C(21)_2	124.4(2)
C(b4)_1–C(b3)_1–C(31)_1	129.1(3)	C(b1)_2–C(11)_2–C(12)_2	114.2(3)
C(a3)_1–C(b3)_1–C(31)_1	122.3(3)	C(b2)_2–C(21)_2–C(22)_2	111.5(3)
C(b3)_1–C(b4)_1–C(a4)_1	104.4(3)	C(b2a)_2–C(b1a)_2–C(a1)_2	107.5(6)
C(b3)_1–C(b4)_1–C(41)_1	128.0(3)	C(b2a)_2–C(b1a)_2–C(11a)_2	127.5(7)
C(a4)_1–C(b4)_1–C(41)_1	125.8(3)	C(a1)_2–C(b1a)_2–C(11a)_2	124.4(6)
C(32)_1–C(31)_1–C(b3)_1	113.6(4)	C(b1a)_2–C(b2a)_2–C(a2)_2	105.7(6)
C(b4)_1–C(41)_1–C(42)_1	113.9(4)	C(b1a)_2–C(b2a)_2–C(21a)_2	128.5(7)
C(b4a)_1–C(b3a)_1–C(a3)_1	103.5(3)	C(a2)_2–C(b2a)_2–C(21a)_2	123.5(6)
C(b4a)_1–C(b3a)_1–C(41a)_1	128.0(4)	C(12a)_2–C(11a)_2–C(b1a)_2	109.1(8)
C(a3)_1–C(b3a)_1–C(31a)_1	127.1(3)	C(b2a)_2–C(21a)_2–C(22a)_2	114.2(7)
C(b3a)_1–C(b4a)_1–C(41a)_1	128.7(4)	C(31a)_2–C(31)_2–C(32)_2	116.6(3)
C(b3a)_1–C(b4a)_1–C(a4)_1	108.8(3)	C(31a)_2–C(31)_2–C(b3)_2	122.3(3)
C(41a)_1–C(b4a)_1–C(a4)_1	122.0(3)	C(32)_2–C(31)_2–C(b3)_2	120.1(3)
C(b3a)_1–C(31a)_1–C(32a)_1	114.7(5)	C(b4)_2–C(41)_2–C(42)_2	113.25(15)
C(42a)_1–C(41a)_1–C(b4a)_1	110.3(4)	C(b5)_2–C(51)_2–C(52)_2	112.22(17)
N(2)_1–C(a4)_1–C(m2)_1	125.17(18)	C(b6)_2–C(61)_2–C(62)_2	114.04(16)
N(2)_1–C(a4)_1–C(b4)_1	112.2(2)	C(b7)_2–C(71)_2–C(72)_2	113.43(15)
C(m2)_1–C(a4)_1–C(b4)_1	121.0(2)	C(b8)_2–C(81)_2–C(82)_2	113.60(16)
N(2)_1–C(a4)_1–C(b4a)_1	106.6(2)	S(1)_2–C(1)_2–Fe(1)_2	174.57(12)
C(m2)_1–C(a4)_1–C(b4a)_1	126.3(2)	N(5)_2–C(2)_2–C(3)_2	123.27(18)
C(b4)_1–C(a4)_1–C(b4a)_1	28.41(17)	C(2)_2–C(3)_2–C(4)_2	119.20(19)
C(a4)_1–C(m2)_1–C(a5)_1	125.88(19)	C(3)_2–C(4)_2–C(5)_2	118.46(19)
N(3)_1–C(a5)_1–C(m2)_1	124.59(19)	C(6)_2–C(5)_2–C(4)_2	118.8(2)
N(3)_1–C(a5)_1–C(b5a)_1	110.1(3)	N(5)_2–C(6)_2–C(5)_2	123.26(17)
C(m2)_1–C(a5)_1–C(b5a)_1	121.1(3)	C(1)_3–Fe(1)_3–C(1)_3#1	180.00(14)
N(3)_1–C(a5)_1–C(b5)_1	109.9(2)	C(1)_3#1–Fe(1)_3–N(5)_3	177.8(3)
C(m2)_1–C(a5)_1–C(b5)_1	125.1(2)		

Table S16. Continued...

angle	degree	angle	degree
C(b5a)_1–C(a5)_1–C(b5)_1	27.8(3)	C(1)_3–Fe(1)_3–N(5)_3#1	177.8(3)
C(b6)_1–C(b5)_1–C(51)_1	127.2(3)		
C(b6)_1–C(b5)_1–C(a5)_1	106.7(3)	N(5)_3–Fe(1)_3–N(5)_3#1	180.00(18)
C(51)_1–C(b5)_1–C(a5)_1	125.7(3)	C(1)_3–Fe(1)_3–N(2)_3#1	89.7(2)
C(b5)_1–C(b6)_1–C(a6)_1	105.4(3)	C(1)_3#1–Fe(1)_3–N(2)_3#1	90.3(2)
C(b5)_1–C(b6)_1–C(61)_1	128.4(3)	N(5)_3–Fe(1)_3–N(2)_3#1	88.51(13)
C(a6)_1–C(b6)_1–C(61)_1	126.0(3)	N(5)_3#1–Fe(1)_3–N(2)_3#1	91.49(13)
C(b5)_1–C(51)_1–C(52)_1	114.5(3)	C(1)_3–Fe(1)_3–N(2)_3	90.3(2)
C(b6)_1–C(61)_1–C(62)_1	111.1(3)	C(1)_3#1–Fe(1)_3–N(2)_3	89.7(2)
C(b6a)_1–C(b5a)_1–C(a5)_1	104.8(5)	N(5)_3–Fe(1)_3–N(2)_3	91.49(13)
C(b6a)_1–C(b5a)_1–C(51a)_1	127.5(5)	N(5)_3#1–Fe(1)_3–N(2)_3	88.51(13)
C(a5)_1–C(b5a)_1–C(51a)_1	126.8(5)	N(2)_3#1–Fe(1)_3–N(2)_3	180.00(13)
C(b5a)_1–C(b6a)_1–C(a6)_1	108.5(5)	C(1)_3–Fe(1)_3–N(1)_3	91.8(2)
C(b5a)_1–C(b6a)_1–C(61a)_1	128.7(6)	C(1)_3#1–Fe(1)_3–N(1)_3	88.2(2)
C(a6)_1–C(b6a)_1–C(61a)_1	121.3(5)	N(5)_3–Fe(1)_3–N(1)_3	89.90(12)
C(52a)_1–C(51a)_1–C(b5a)_1	110.3(6)	N(5)_3#1–Fe(1)_3–N(1)_3	90.10(12)
C(b6a)_1–C(61a)_1–C(62a)_1	114.7(5)	N(2)_3#1–Fe(1)_3–N(1)_3	89.77(10)
N(3)_1–C(a6)_1–C(m3)_1	124.92(17)	N(2)_3–Fe(1)_3–N(1)_3	90.23(10)
N(3)_1–C(a6)_1–C(b6a)_1	107.2(3)	C(1)_3–Fe(1)_3–N(1)_3#1	88.2(2)
C(m3)_1–C(a6)_1–C(b6a)_1	124.9(3)	C(1)_3#1–Fe(1)_3–N(1)_3#1	91.8(2)
N(3)_1–C(a6)_1–C(b6)_1	111.4(2)	N(5)_3–Fe(1)_3–N(1)_3#1	90.10(12)
C(m3)_1–C(a6)_1–C(b6)_1	123.1(2)	N(5)_3#1–Fe(1)_3–N(1)_3#1	89.90(12)
C(b6a)_1–C(a6)_1–C(b6)_1	25.6(2)	N(2)_3#1–Fe(1)_3–N(1)_3#1	90.23(10)
C(a7)_1–C(m3)_1–C(a6)_1	125.98(17)	N(2)_3–Fe(1)_3–N(1)_3#1	89.77(10)
N(4)_1–C(a7)_1–C(m3)_1	124.47(16)	N(1)_3–Fe(1)_3–N(1)_3#1	180.00(16)
N(4)_1–C(a7)_1–C(b7)_1	110.70(15)	C(2)_3–N(5)_3–C(6)_3	120.0
C(m3)_1–C(a7)_1–C(b7)_1	124.83(16)	C(2)_3–N(5)_3–Fe(1)_3	119.61(15)
C(b8)_1–C(b7)_1–C(a7)_1	106.67(15)	C(6)_3–N(5)_3–Fe(1)_3	120.34(15)
C(b8)_1–C(b7)_1–C(71)_1	127.09(15)	N(5)_3–C(2)_3–C(3)_3	120.0
C(a7)_1–C(b7)_1–C(71)_1	126.24(16)	C(2)_3–C(3)_3–C(4)_3	120.0
C(b7)_1–C(b8)_1–C(a8)_1	106.64(15)	C(5)_3–C(4)_3–C(3)_3	120.0
C(b7)_1–C(b8)_1–C(81)_1	127.97(15)	C(4)_3–C(5)_3–C(6)_3	120.0
C(a8)_1–C(b8)_1–C(81)_1	125.39(15)	C(5)_3–C(6)_3–N(5)_3	120.0
N(4)_1–C(a8)_1–C(m4)_1	125.06(15)	S(1)_3–C(1)_3–Fe(1)_3	175.4(5)

Table S16. Continued...

angle	degree	angle	degree
N(4)_1–C(a8)_1–C(b8)_1	110.68(14)	C(a2)_3–N(1)_3–C(a1)_3	105.26(18)
C(m4)_1–C(a8)_1–C(b8)_1	124.26(15)	C(a2)_3–N(1)_3–C(1a)_3	104.2(3)
C(a8)_1–C(m4)_1–C(a1)_1	125.48(16)	C(a1)_3–N(1)_3–C(1a)_3	29.6(2)
N(1)_1–C(a1)_1–C(m4)_1	125.02(15)	C(a2)_3–N(1)_3–Fe(1)_3	127.05(13)
N(1)_1–C(a1)_1–C(b1)_1	110.84(14)	C(a1)_3–N(1)_3–Fe(1)_3	126.69(17)
C(m4)_1–C(a1)_1–C(b1)_1	124.13(15)	C(1a)_3–N(1)_3–Fe(1)_3	125.5(3)
C(b2)_1–C(b1)_1–C(a1)_1	106.57(15)	C(a3)_3–N(2)_3–C(9a)_3	105.5(5)
C(b2)_1–C(b1)_1–C(11)_1	128.68(15)	C(a3)_3–N(2)_3–C(a4)_3	104.8(3)
C(a1)_1–C(b1)_1–C(11)_1	124.74(14)	C(9a)_3–N(2)_3–C(a4)_3	23.1(4)
C(b1)_1–C(b2)_1–C(a2)_1	106.60(15)	C(a3)_3–N(2)_3–Fe(1)_3	127.09(13)
C(b1)_1–C(b2)_1–C(21)_1	128.57(16)	C(9a)_3–N(2)_3–Fe(1)_3	125.1(5)
C(a2)_1–C(b2)_1–C(21)_1	124.63(16)	C(a4)_3–N(2)_3–Fe(1)_3	127.7(3)
C(b7)_1–C(71)_1–C(72)_1	112.79(15)	C(m2)_3–C(a1)_3–N(1)_3	124.2(3)
C(b8)_1–C(81)_1–C(82)_1	113.05(15)	C(m2)_3–C(a1)_3–C(b1)_3	125.2(3)
C(b1)_1–C(11)_1–C(12)_1	113.19(15)	N(1)_3–C(a1)_3–C(b1)_3	110.1(3)
C(b2)_1–C(21)_1–C(22)_1	112.03(17)	C(b2)_3–C(b1)_3–C(a1)_3	106.4(2)
S(1)_1–C(1)_1–Fe(1)_1	176.24(13)	C(b2)_3–C(b1)_3–C(11)_3	128.2(2)
N(5)_1–C(2)_1–C(3)_1	122.8(2)	C(a1)_3–C(b1)_3–C(11)_3	125.1(3)
C(4)_1–C(3)_1–C(2)_1	119.4(2)	C(a1)_3–C(m2)_3–C(a4)_3#1	126.0(4)
C(3)_1–C(4)_1–C(5)_1	118.6(2)	C(b1)_3–C(11)_3–C(12)_3	111.8(3)
C(4)_1–C(5)_1–C(6)_1	118.9(2)	C(10b)_3–C(1a)_3–N(1)_3	123.1(5)
N(5)_1–C(6)_1–C(5)_1	123.11(12)	C(10b)_3–C(1a)_3–C(2a)_3	125.3(5)
C(1)_2–Fe(1)_2–N(3)_2	88.30(6)	N(1)_3–C(1a)_3–C(2a)_3	109.7(4)
C(1)_2–Fe(1)_2–N(2)_2	91.69(5)	C(b2)_3–C(2a)_3–C(1a)_3	106.4(4)
N(3)_2–Fe(1)_2–N(2)_2	90.1	C(b2)_3–C(2a)_3–C(11a)_3	127.1(4)
C(1)_2–Fe(1)_2–N(1)_2	95.95(6)	C(1a)_3–C(2a)_3–C(11a)_3	125.0(5)
N(3)_2–Fe(1)_2–N(1)_2	175.7	C(1a)_3–C(10b)_3–C(9a)_3#1	125.4(7)
N(2)_2–Fe(1)_2–N(1)_2	90.2	C(2a)_3–C(11a)_3–C(12a)_3	116.4(5)
C(1)_2–Fe(1)_2–N(4)_2	91.59(5)	C(b1)_3–C(b2)_3–C(2a)_3	32.4(2)
N(3)_2–Fe(1)_2–N(4)_2	90.0	C(b1)_3–C(b2)_3–C(a2)_3	106.18(18)
N(2)_2–Fe(1)_2–N(4)_2	176.7	C(2a)_3–C(b2)_3–C(a2)_3	103.7(2)
N(1)_2–Fe(1)_2–N(4)_2	89.5	C(b1)_3–C(b2)_3–C(21)_3	127.49(19)
C(1)_2–Fe(1)_2–N(5)_2	176.94(6)	C(2a)_3–C(b2)_3–C(21)_3	127.2(2)
N(3)_2–Fe(1)_2–N(5)_2	89.2	C(a2)_3–C(b2)_3–C(21)_3	125.06(17)

Table S16. Continued...

angle	degree	angle	degree
N(2)_2–Fe(1)_2–N(5)_2	86.6	N(1)_3–C(a2)_3–C(m1)_3	125.00(15)
N(1)_2–Fe(1)_2–N(5)_2	86.6	N(1)_3–C(a2)_3–C(b2)_3	111.04(16)
N(4)_2–Fe(1)_2–N(5)_2	90.2	C(m1)_3–C(a2)_3–C(b2)_3	123.96(16)
C(a2)_2–N(1)_2–C(a1)_2	105.33(12)	C(a2)_3–C(m1)_3–C(a3)_3	125.75(16)
C(a2)_2–N(1)_2–Fe(1)_2	127.02(8)	N(2)_3–C(a3)_3–C(m1)_3	124.86(16)
C(a1)_2–N(1)_2–Fe(1)_2	127.64(8)	N(2)_3–C(a3)_3–C(b3)_3	111.04(15)
C(a3)_2–N(2)_2–C(a4)_2	105.55(10)	C(m1)_3–C(a3)_3–C(b3)_3	124.09(16)
C(a3)_2–N(2)_2–Fe(1)_2	127.28(7)	C(8a)_3–C(b3)_3–C(b4)_3	20.7(6)
C(a4)_2–N(2)_2–Fe(1)_2	127.05(7)	C(8a)_3–C(b3)_3–C(a3)_3	106.3(6)
C(a6)_2–N(3)_2–C(a5)_2	105.19(10)	C(b4)_3–C(b3)_3–C(a3)_3	105.8(4)
C(a6)_2–N(3)_2–Fe(1)_2	127.11(7)	C(8a)_3–C(b3)_3–C(31)_3	126.2(6)
C(a5)_2–N(3)_2–Fe(1)_2	126.83(7)	C(b4)_3–C(b3)_3–C(31)_3	129.1(4)
C(a7)_2–N(4)_2–C(a8)_2	105.51(10)	C(a3)_3–C(b3)_3–C(31)_3	125.00(16)
C(a7)_2–N(4)_2–Fe(1)_2	126.68(7)	C(b3)_3–C(b4)_3–C(a4)_3	107.1(6)
C(a8)_2–N(4)_2–Fe(1)_2	127.10(7)	C(b3)_3–C(b4)_3–C(41)_3	126.5(6)
C(6)_2–N(5)_2–C(2)_2	116.98(12)	C(a4)_3–C(b4)_3–C(41)_3	126.0(7)
C(6)_2–N(5)_2–Fe(1)_2	121.74(8)	C(m2)_3#1–C(a4)_3–N(2)_3	124.1(5)
C(2)_2–N(5)_2–Fe(1)_2	121.26(9)	C(m2)_3#1–C(a4)_3–C(b4)_3	124.8(6)
N(1)_2–C(a2)_2–C(m1)_2	124.89(17)	N(2)_3–C(a4)_3–C(b4)_3	110.7(5)
N(1)_2–C(a2)_2–C(b2a)_2	109.3(3)	C(b4)_3–C(41)_3–C(42)_3	114.9(5)
C(m1)_2–C(a2)_2–C(b2a)_2	121.1(3)	C(b3)_3–C(8a)_3–C(9a)_3	106.5(11)
N(1)_2–C(a2)_2–C(b2)_2	110.53(18)	C(b3)_3–C(8a)_3–C(41a)_3	132.1(10)
C(m1)_2–C(a2)_2–C(b2)_2	124.3(2)	C(9a)_3–C(8a)_3–C(41a)_3	120.0(11)
C(b2a)_2–C(a2)_2–C(b2)_2	27.9(3)	C(b3)_3–C(8a)_3–C(42a)_3	124.4(11)
C(a2)_2–C(m1)_2–C(a3)_2	125.92(18)	C(9a)_3–C(8a)_3–C(42a)_3	121.1(12)
N(2)_2–C(a3)_2–C(m1)_2	124.64(15)	C(41a)_3–C(8a)_3–C(42a)_3	35.6(8)
N(2)_2–C(a3)_2–C(b3)_2	110.73(14)	C(10b)_3#1–C(9a)_3–N(2)_3	126.0(9)
C(m1)_2–C(a3)_2–C(b3)_2	124.63(17)	C(10b)_3#1–C(9a)_3–C(8a)_3	125.4(11)
C(b4)_2–C(b3)_2–C(a3)_2	106.54(15)	N(2)_3–C(9a)_3–C(8a)_3	108.1(10)
C(b4)_2–C(b3)_2–C(31)_2	128.17(17)	C(42a)_3–C(41a)_3–C(8a)_3	76.2(14)
C(a3)_2–C(b3)_2–C(31)_2	125.29(17)	C(41a)_3–C(42a)_3–C(8a)_3	68.2(16)
C(b3)_2–C(b4)_2–C(a4)_2	106.59(15)	C(b2)_3–C(21)_3–C(22)_3	112.51(17)
C(b3)_2–C(b4)_2–C(41)_2	128.98(16)	C(b3)_3–C(31)_3–C(32)_3	113.93(17)
C(a4)_2–C(b4)_2–C(41)_2	124.44(16)	N(2)_2–C(a4)_2–C(m2)_2	124.89(14)

[a]The estimated standard deviations of the least significant digits are given in parentheses.

Table S17. Anisotropic Displacement Parameters (Å^2) for [Fe(OEP)(CS)(Py)][a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)_1	0.0362(2)	0.0219(1)	0.0242(1)	−0.0122(1)	0.0089(1)	−0.0127(1)
S(1)_1	0.0358(3)	0.0385(3)	0.0469(3)	−0.0221(2)	0.0087(2)	−0.0139(2)
N(1)_1	0.0299(8)	0.0228(7)	0.0237(7)	−0.0124(6)	0.0063(6)	−0.0110(6)
N(2)_1	0.0599(12)	0.0257(8)	0.0315(9)	−0.0165(7)	0.0190(8)	−0.0211(8)
N(3)_1	0.0460(10)	0.0233(8)	0.0304(9)	−0.0127(7)	0.0116(7)	−0.0128(7)
N(4)_1	0.0274(7)	0.0221(7)	0.0210(7)	−0.0099(6)	0.0031(6)	−0.0087(6)
N(5)_1	0.0379(9)	0.0191(7)	0.0302(8)	−0.0059(6)	0.0064(7)	−0.0054(6)
C(a2)_1	0.0371(10)	0.0272(9)	0.0260(9)	−0.0140(7)	0.0064(7)	−0.0135(8)
C(m1)_1	0.0831(18)	0.0349(11)	0.0294(11)	−0.0215(9)	0.0240(11)	−0.0297(11)
C(a3)_1	0.102(2)	0.0353(12)	0.0397(13)	−0.0268(10)	0.0338(13)	−0.0374(13)
C(b3)_1	0.035(2)	0.0185(17)	0.0262(19)	−0.0127(14)	−0.0057(17)	0.0004(16)
C(b4)_1	0.0221(19)	0.0204(17)	0.0268(19)	−0.0109(14)	−0.0056(15)	−0.0007(15)
C(31)_1	0.044(2)	0.0236(18)	0.037(2)	−0.0132(16)	−0.007(2)	−0.0031(17)
C(32)_1	0.050(3)	0.054(3)	0.044(3)	−0.024(3)	−0.009(2)	0.001(2)
C(31)_1	0.032(2)	0.0100(18)	0.029(2)	−0.0082(15)	−0.0017(17)	0.0069(16)
C(42)_1	0.034(2)	0.0162(16)	0.036(2)	−0.0090(14)	−0.0025(16)	−0.0104(15)
C(b3a)_1	0.031(2)	0.0223(19)	0.028(2)	−0.0100(15)	−0.0046(17)	−0.0045(16)
C(b4a)_1	0.028(2)	0.0205(19)	0.031(2)	−0.0122(16)	−0.0034(17)	−0.0047(16)
C(31a)_1	0.062(4)	0.031(2)	0.029(2)	−0.020(2)	0.003(2)	−0.021(2)
C(32a)_1	0.074(4)	0.043(3)	0.038(3)	−0.029(2)	0.033(3)	−0.019(2)
C(41a)_1	0.036(3)	0.027(2)	0.033(2)	−0.0107(17)	−0.008(2)	0.005(2)
C(42a)_1	0.036(3)	0.034(3)	0.048(3)	−0.011(2)	−0.003(2)	−0.012(2)
C(a4)_1	0.0848(18)	0.0278(10)	0.0440(13)	−0.0231(10)	0.0307(12)	−0.0281(11)
C(m2)_1	0.0846(18)	0.0247(10)	0.0439(13)	−0.0175(9)	0.0294(12)	−0.0257(11)
C(a5)_1	0.0724(16)	0.0263(10)	0.0365(12)	−0.0123(9)	0.0247(11)	−0.0211(10)
C(b5)_1	0.0252(16)	0.0273(15)	0.0229(16)	−0.0040(12)	−0.0045(12)	−0.0063(13)
C(b6)_1	0.0259(17)	0.0253(15)	0.0207(15)	−0.0049(12)	−0.0050(13)	−0.0072(14)
C(51)_1	0.0347(18)	0.0175(15)	0.0289(16)	−0.0037(12)	−0.0015(13)	−0.0028(13)
C(52)_1	0.0409(19)	0.0245(15)	0.062(2)	−0.0096(15)	0.0019(17)	−0.0146(14)
C(61)_1	0.031(2)	0.0286(16)	0.029(2)	−0.0053(13)	0.0001(16)	−0.0091(15)
C(62)_1	0.055(2)	0.048(2)	0.0361(18)	−0.0111(16)	−0.0050(17)	−0.0164(18)
C(b5a)_1	0.038(4)	0.025(3)	0.022(3)	−0.007(2)	0.003(3)	−0.011(3)
C(b6a)_1	0.026(3)	0.028(3)	0.021(3)	−0.005(2)	−0.003(2)	−0.008(3)
C(51a)_1	0.045(4)	0.033(3)	0.028(3)	−0.010(2)	−0.003(3)	−0.012(3)

Table S17. Continued...

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(52a)_1	0.057(4)	0.032(4)	0.044(4)	−0.012(3)	−0.011(3)	−0.012(3)
C(61a)_1	0.023(3)	0.023(3)	0.029(3)	−0.009(2)	0.021(3)	−0.006(2)
C(62a)_1	0.051(4)	0.053(4)	0.021(3)	−0.020(3)	0.006(3)	−0.022(3)
C(a6)_1	0.0542(13)	0.0287(10)	0.0279(10)	−0.0110(8)	0.0166(9)	−0.0159(9)
C(m3)_1	0.0412(11)	0.0289(9)	0.0242(9)	−0.0132(8)	0.0102(8)	−0.0118(8)
C(a7)_1	0.0265(9)	0.0259(9)	0.0234(8)	−0.0116(7)	0.0015(7)	−0.0077(7)
C(b7)_1	0.0219(8)	0.0262(8)	0.0245(8)	−0.0134(7)	0.0002(6)	−0.0070(7)
C(b8)_1	0.0205(8)	0.0249(8)	0.0234(8)	−0.0125(7)	0.0000(6)	−0.0066(6)
C(a8)_1	0.0211(8)	0.0220(8)	0.0243(8)	−0.0115(7)	−0.0020(6)	−0.0062(6)
C(m4)_1	0.0219(8)	0.0219(8)	0.0225(8)	−0.0089(6)	−0.0012(6)	−0.0071(6)
C(a1)_1	0.0215(8)	0.0219(8)	0.0224(8)	−0.0091(6)	−0.0008(6)	−0.0073(6)
C(b1)_1	0.0209(8)	0.0248(8)	0.0203(8)	−0.0090(6)	0.0001(6)	−0.0071(6)
C(b2)_1	0.0268(9)	0.0265(9)	0.0244(9)	−0.0116(7)	0.0028(7)	−0.0094(7)
C(71)_1	0.0283(9)	0.0267(9)	0.0233(8)	−0.0126(7)	0.0042(7)	−0.0086(7)
C(72)_1	0.0374(11)	0.0490(12)	0.0256(10)	−0.0173(9)	−0.0021(8)	−0.0108(9)
C(81)_1	0.0256(8)	0.0242(8)	0.0245(8)	−0.0133(7)	0.0013(7)	−0.0078(7)
C(82)_1	0.0301(9)	0.0308(9)	0.0290(9)	−0.0140(8)	0.0015(7)	−0.0131(7)
C(11)_1	0.0273(9)	0.0247(8)	0.0194(8)	−0.0076(6)	−0.0005(6)	−0.0089(7)
C(12)_1	0.0298(9)	0.0307(9)	0.0305(10)	−0.0088(8)	−0.0011(7)	−0.0138(8)
C(21)_1	0.0410(11)	0.0289(9)	0.0232(9)	−0.0125(7)	0.0060(8)	−0.0127(8)
C(22)_1	0.0460(13)	0.0470(13)	0.0370(12)	−0.0108(10)	0.0145(10)	0.0041(10)
C(1)_1	0.0427(11)	0.0252(9)	0.0248(9)	−0.0142(7)	0.0108(8)	−0.0175(8)
C(2)_1	0.0421(12)	0.0249(9)	0.0402(12)	−0.0095(8)	0.0101(9)	−0.0060(8)
C(3)_1	0.0428(12)	0.0296(11)	0.0503(14)	−0.0065(10)	0.0136(10)	−0.0039(9)
C(4)_1	0.0393(12)	0.0272(10)	0.0544(15)	0.0045(9)	0.0001(10)	−0.0023(9)
C(5)_1	0.0442(12)	0.0296(10)	0.0410(12)	0.0036(9)	−0.0039(10)	−0.0036(9)
C(6)_1	0.0422(11)	0.0256(9)	0.0319(10)	−0.0032(8)	0.0032(8)	−0.0053(8)
Fe(1)_2	0.0244(1)	0.0190(1)	0.0162(1)	−0.0063(1)	−0.0011(1)	−0.0074(1)
S(1)_2	0.0268(2)	0.0438(3)	0.0362(3)	−0.0163(2)	−0.0066(2)	−0.0038(2)
N(1)_2	0.0405(9)	0.0234(7)	0.0212(7)	−0.0080(6)	0.0014(6)	−0.0139(6)
N(2)_2	0.0247(7)	0.0222(7)	0.0183(7)	−0.0080(5)	−0.0015(5)	−0.0059(6)
N(3)_2	0.0229(7)	0.0197(7)	0.0172(7)	−0.0065(5)	−0.0018(5)	−0.0056(5)
N(4)_2	0.0278(7)	0.0222(7)	0.0167(7)	−0.0066(5)	−0.0014(5)	−0.0093(6)
N(5)_2	0.0315(8)	0.0184(7)	0.0227(7)	−0.0069(6)	−0.0065(6)	−0.0051(6)

Table S17. Continued...

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(a2)_2	0.0632(14)	0.0275(10)	0.0301(10)	−0.0124(8)	0.0080(9)	−0.0219(10)
C(m1)_2	0.0626(14)	0.0272(10)	0.0322(11)	−0.0168(8)	0.0082(9)	−0.0187(9)
C(a3)_2	0.0329(9)	0.0262(9)	0.0240(9)	−0.0127(7)	0.0011(7)	−0.0090(7)
C(b3)_2	0.0379(10)	0.0306(9)	0.0253(9)	−0.0151(8)	0.0022(8)	−0.0084(8)
C(b4)_2	0.0255(8)	0.0286(9)	0.0203(8)	−0.0118(7)	−0.0011(6)	−0.0035(7)
C(a4)_2	0.0217(8)	0.0245(8)	0.0188(8)	−0.0079(6)	−0.0033(6)	−0.0025(6)
C(m2)_2	0.0263(8)	0.0236(8)	0.0167(8)	−0.0045(6)	−0.0014(6)	−0.0029(7)
C(a5)_2	0.0231(8)	0.0210(8)	0.0187(8)	−0.0038(6)	−0.0023(6)	−0.0056(6)
C(b5)_2	0.0264(8)	0.0204(8)	0.0221(8)	−0.0043(6)	−0.0042(7)	−0.0049(6)
C(b6)_2	0.0267(8)	0.0201(8)	0.0216(8)	−0.0057(6)	−0.0043(6)	−0.0055(6)
C(a6)_2	0.0227(8)	0.0193(8)	0.0204(8)	−0.0069(6)	−0.0036(6)	−0.0046(6)
C(m3)_2	0.0261(8)	0.0210(8)	0.0209(8)	−0.0097(6)	−0.0034(6)	−0.0043(6)
C(a7)_2	0.0239(8)	0.0230(8)	0.0187(8)	−0.0087(6)	−0.0024(6)	−0.0056(6)
C(b7)_2	0.0253(8)	0.0297(9)	0.0189(8)	−0.0100(7)	−0.0011(6)	−0.0085(7)
C(b8)_2	0.0289(9)	0.0307(9)	0.0195(8)	−0.0096(7)	−0.0001(7)	−0.0117(7)
C(a8)_2	0.0317(9)	0.0284(9)	0.0184(8)	−0.0075(7)	0.0006(7)	−0.0123(7)
C(m4)_2	0.0494(12)	0.0294(9)	0.0202(9)	−0.0069(7)	0.0058(8)	−0.0199(9)
C(a1)_2	0.0571(13)	0.0271(9)	0.0247(9)	−0.0066(8)	0.0063(9)	−0.0230(9)
C(b1)_2	0.0355(17)	0.0203(13)	0.0237(14)	0.0005(10)	−0.0122(12)	−0.0107(12)
C(b2)_2	0.0347(16)	0.0192(13)	0.0296(14)	−0.0020(10)	−0.0126(13)	−0.0091(12)
C(11)_2	0.050(2)	0.0217(14)	0.0233(15)	0.0030(11)	−0.0108(15)	−0.0175(13)
C(12)_2	0.0426(18)	0.0331(15)	0.0314(16)	−0.0024(12)	0.0034(13)	−0.0177(13)
C(21)_2	0.0400(18)	0.0208(13)	0.0390(16)	−0.0037(12)	−0.0145(15)	−0.0067(13)
C(22)_2	0.0557(19)	0.0253(14)	0.0472(18)	−0.0086(13)	−0.0226(15)	−0.0082(13)
C(b1a)_2	0.030(4)	0.021(3)	0.019(4)	−0.003(3)	−0.005(3)	−0.002(3)
C(b2a)_2	0.029(4)	0.018(3)	0.024(4)	−0.007(3)	−0.003(3)	−0.004(3)
C(11a)_2	0.040(5)	0.028(4)	0.033(4)	−0.015(3)	−0.009(4)	−0.005(4)
C(12a)_2	0.051(6)	0.043(6)	0.062(7)	−0.003(5)	−0.009(6)	−0.017(5)
C(21a)_2	0.029(4)	0.019(3)	0.025(3)	−0.011(3)	0.001(3)	−0.009(3)
C(22a)_2	0.030(4)	0.022(3)	0.037(4)	−0.013(3)	0.010(3)	−0.004(3)
C(31)_2	0.0884(19)	0.0379(12)	0.0287(11)	−0.0205(9)	0.0178(11)	−0.0301(12)
C(32)_2	0.0320(19)	0.0236(17)	0.039(2)	−0.0215(16)	−0.0057(16)	0.0006(14)
C(31a)_2	0.054(3)	0.040(2)	0.059(3)	−0.027(2)	−0.017(2)	−0.001(2)
C(41)_2	0.0322(10)	0.0309(9)	0.0223(9)	−0.0140(7)	0.0031(7)	−0.0045(7)

Table S17. Continued...

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(42)_2	0.0422(11)	0.0409(11)	0.0216(9)	−0.0118(8)	−0.0030(8)	−0.0015(9)
C(51)_2	0.0432(11)	0.0237(9)	0.0225(9)	−0.0037(7)	−0.0004(8)	−0.0085(8)
C(52)_2	0.0492(14)	0.0596(15)	0.0331(12)	−0.0008(11)	0.0076(10)	−0.0236(12)
C(61)_2	0.0390(10)	0.0210(8)	0.0239(9)	−0.0067(7)	−0.0025(7)	−0.0082(7)
C(62)_2	0.0550(14)	0.0380(12)	0.0557(14)	−0.0268(11)	−0.0148(11)	−0.0094(10)
C(71)_2	0.0300(9)	0.0288(9)	0.0204(8)	−0.0115(7)	0.0013(7)	−0.0067(7)
C(72)_2	0.0329(10)	0.0266(9)	0.0263(9)	−0.0123(7)	−0.0007(7)	−0.0089(7)
C(81)_2	0.0391(11)	0.0362(10)	0.0206(9)	−0.0101(8)	0.0052(7)	−0.0171(8)
C(82)_2	0.0469(12)	0.0396(11)	0.0205(9)	−0.0059(8)	0.0027(8)	−0.0188(9)
C(1)_2	0.0292(9)	0.0258(8)	0.0179(8)	−0.0098(6)	0.0035(6)	−0.0120(7)
C(2)_2	0.0456(11)	0.0229(9)	0.0243(9)	−0.0081(7)	−0.0110(8)	−0.0012(8)
C(3)_2	0.0568(14)	0.0281(10)	0.0336(11)	−0.0117(8)	−0.0232(10)	0.0053(9)
C(4)_2	0.0417(12)	0.0338(11)	0.0505(13)	−0.0189(10)	−0.0252(10)	0.0046(9)
C(5)_2	0.0317(10)	0.0331(10)	0.0447(12)	−0.0120(9)	−0.0101(9)	−0.0054(8)
C(6)_2	0.0314(9)	0.0248(9)	0.0289(9)	−0.0050(7)	−0.0082(7)	−0.0058(7)
Fe(1)_3	0.0915(4)	0.0180(2)	0.0210(2)	−0.0092(2)	0.0200(2)	−0.0159(2)
N(5)_3	0.042(4)	0.012(4)	0.010(3)	−0.002(2)	−0.006(3)	−0.009(3)
C(2)_3	0.047(2)	0.0215(17)	0.0224(18)	−0.0079(14)	−0.0023(16)	−0.0083(15)
C(3)_3	0.060(3)	0.0274(19)	0.0209(18)	−0.0041(15)	−0.0129(18)	−0.0146(18)
C(4)_3	0.042(2)	0.0242(18)	0.034(2)	−0.0017(15)	−0.0069(17)	−0.0107(16)
C(5)_3	0.041(2)	0.0227(17)	0.0258(18)	−0.0035(14)	0.0008(16)	−0.0067(15)
C(6)_3	0.043(2)	0.0208(16)	0.0198(17)	−0.0036(13)	0.0005(15)	−0.0065(15)
S(1)_3	0.0391(6)	0.0387(6)	0.0798(10)	0.0160(6)	−0.0109(6)	−0.0150(5)
C(1)_3	0.039(5)	0.025(6)	0.050(6)	−0.002(4)	0.023(4)	0.000(4)
N(1)_3	0.0629(12)	0.0202(7)	0.0206(8)	−0.0087(6)	0.0119(7)	−0.0105(7)
N(2)_3	0.0528(10)	0.0190(7)	0.0206(7)	−0.0078(6)	0.0083(7)	−0.0092(7)
C(a1)_3	0.0382(19)	0.0224(15)	0.0213(15)	−0.0120(11)	0.0046(15)	−0.0070(15)
C(b1)_3	0.0324(17)	0.0234(14)	0.0251(15)	−0.0127(11)	0.0025(13)	−0.0070(13)
C(m2)_3	0.056(2)	0.0239(15)	0.0182(14)	−0.0091(12)	0.0055(16)	−0.0093(16)
C(11)_3	0.0405(18)	0.0257(14)	0.0261(16)	−0.0125(12)	0.0014(13)	−0.0066(12)
C(12)_3	0.042(2)	0.056(2)	0.039(2)	−0.0249(18)	0.0030(17)	−0.0075(17)
C(1a)_3	0.028(3)	0.019(2)	0.022(3)	−0.0070(19)	0.000(2)	−0.001(2)
C(2a)_3	0.020(3)	0.021(2)	0.026(3)	−0.0118(19)	−0.003(2)	0.001(2)
C(10b)_3	0.052(4)	0.023(3)	0.019(3)	−0.010(2)	0.009(3)	−0.001(3)

Table S17. Continued...

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(11a)_3	0.032(3)	0.024(3)	0.023(3)	−0.014(2)	0.013(2)	0.000(2)
C(12a)_3	0.067(5)	0.059(4)	0.025(3)	−0.023(3)	−0.005(3)	0.013(4)
C(b2)_3	0.0566(13)	0.0212(9)	0.0265(10)	−0.0113(7)	0.0079(9)	−0.0074(8)
C(a2)_3	0.0317(9)	0.0191(8)	0.0245(9)	−0.0093(7)	0.0016(7)	−0.0043(7)
C(m1)_3	0.0243(8)	0.0176(7)	0.0236(8)	−0.0063(6)	−0.0021(6)	−0.0027(6)
C(a3)_3	0.0289(9)	0.0195(8)	0.0204(8)	−0.0053(6)	0.0007(7)	−0.0055(7)
C(b3)_3	0.0386(10)	0.0215(8)	0.0212(9)	−0.0043(7)	0.0038(7)	−0.0060(7)
C(b4)_3	0.031(2)	0.028(2)	0.0188(17)	−0.0090(14)	0.0019(18)	−0.0109(18)
C(a4)_3	0.041(3)	0.0245(19)	0.0187(18)	−0.0067(14)	0.001(2)	−0.007(2)
C(41)_3	0.069(3)	0.0230(18)	0.0085(13)	−0.0073(12)	0.0120(15)	−0.0164(19)
C(42)_3	0.072(4)	0.049(3)	0.030(2)	−0.0197(19)	0.031(2)	−0.001(2)
C(8a)_3	0.098(12)	0.020(4)	0.031(6)	−0.002(4)	0.032(7)	−0.025(7)
C(9a)_3	0.051(6)	0.020(3)	0.017(4)	−0.004(3)	0.007(4)	−0.004(5)
C(41a)_3	0.109(14)	0.039(6)	0.152(16)	0.025(8)	−0.076(12)	−0.037(8)
C(42a)_3	0.103(11)	0.040(6)	0.156(19)	−0.014(12)	0.039(15)	−0.009(7)
C(21)_3	0.0395(10)	0.0206(8)	0.0287(9)	−0.0117(7)	0.0007(8)	−0.0029(7)
C(22)_3	0.0432(12)	0.0346(11)	0.0440(12)	−0.0204(9)	−0.0124(9)	−0.0020(9)
C(31)_3	0.0393(10)	0.0210(8)	0.0216(9)	−0.0037(7)	0.0008(7)	−0.0038(7)
C(32)_3	0.0464(12)	0.0302(10)	0.0347(11)	−0.0025(8)	−0.0007(9)	−0.0121(9)

[a]The estimated standard deviations of the least significant digits are given in parentheses. The anisotropic displacement factor exponent takes the form: $-2\ \pi^2\ [h^2a^{*2}\ U_{11} + ... + 2\ h\ k\ a^*\ b^*\ U_{12}]$.

Table S18. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(CS)(Py)][a]

atom	x	y	z	U(eq)
H(m1)_1	−0.2092	0.7889	1.1207	0.058
H(31a)_1	−0.3010	0.9381	1.1104	0.041
H(31b)_1	−0.2763	1.0357	1.0771	0.041
H(32a)_1	−0.2151	0.9734	1.1795	0.058
H(32b)_1	−0.1519	0.8965	1.1535	0.058
H(32c)_1	−0.1276	0.9930	1.1206	0.058
H(41a)_1	−0.2154	1.1287	0.9840	0.030
H(41b)_1	−0.1788	1.1231	0.9120	0.030
H(42a)_1	−0.0575	1.1871	0.9410	0.033
H(42b)_1	−0.0465	1.1018	1.0005	0.033
H(42c)_1	−0.0102	1.0962	0.9292	0.033
H(31c)_1	−0.1468	1.0025	1.1063	0.045
H(31d)_1	−0.1465	0.8991	1.1329	0.045
H(32d)_1	−0.3083	0.9720	1.1755	0.063
H(32e)_1	−0.3205	1.0230	1.1030	0.063
H(32f)_1	−0.3203	0.9208	1.1293	0.063
H(41c)_1	−0.0507	1.0976	0.9363	0.039
H(41d)_1	−0.0973	1.0897	1.0102	0.039
H(42d)_1	−0.1934	1.2095	0.9393	0.047
H(42e)_1	−0.2114	1.1425	0.9073	0.047
H(42f)_1	−0.2573	1.1346	0.9802	0.047
H(m2)_1	−0.0828	1.0482	0.8501	0.064
H(51a)_1	−0.0650	1.1090	0.7393	0.034
H(51b)_1	−0.0441	1.0885	0.6735	0.034
H(52a)_1	0.0841	1.1571	0.6792	0.052
H(52b)_1	0.1062	1.0818	0.7429	0.052
H(52c)_1	0.1273	1.0611	0.6762	0.052
H(61a)_1	0.0205	0.9715	0.6261	0.036
H(61b)_1	−0.0015	0.8759	0.6419	0.036
H(62a)_1	0.1690	0.8814	0.5996	0.055
H(62b)_1	0.1791	0.9163	0.6558	0.055
H(62c)_1	0.1570	0.8200	0.6717	0.055
H(51c)_1	0.1001	1.0584	0.6997	0.041
H(51d)_1	0.0572	1.0814	0.7645	0.041

Table S18. Continued...

atom	x	y	z	U(eq)
H(52d)_1	−0.0232	1.1808	0.6798	0.051
H(52e)_1	−0.0553	1.1014	0.6679	0.051
H(52f)_1	−0.0985	1.1245	0.7331	0.051
H(61c)_1	0.1246	0.8476	0.6687	0.034
H(61d)_1	0.1221	0.9487	0.6489	0.034
H(62d)_1	0.0422	0.9171	0.5783	0.047
H(62e)_1	−0.0332	0.8706	0.6378	0.047
H(62f)_1	−0.0357	0.9729	0.6178	0.047
H(m3)_1	0.0246	0.7392	0.7310	0.038
H(m4)_1	−0.1239	0.4849	0.9986	0.026
H(71a)_1	0.0760	0.5058	0.7614	0.031
H(71b)_1	0.0679	0.6054	0.7229	0.031
H(72a)_1	−0.0168	0.5366	0.6780	0.043
H(72b)_1	−0.0848	0.5049	0.7457	0.043
H(72c)_1	−0.0930	0.6054	0.7068	0.043
H(81a)_1	−0.0262	0.4014	0.9308	0.028
H(81b)_1	−0.0039	0.4076	0.8575	0.028
H(82a)_1	−0.1507	0.3460	0.9065	0.034
H(82b)_1	−0.1983	0.4302	0.9281	0.034
H(82c)_1	−0.1759	0.4364	0.8540	0.034
H(11a)_1	−0.2092	0.4497	1.1719	0.028
H(11b)_1	−0.1536	0.4261	1.1094	0.028
H(12a)_1	−0.3131	0.3856	1.1365	0.036
H(12b)_1	−0.3608	0.4832	1.1323	0.036
H(12c)_1	−0.3046	0.4593	1.0691	0.036
H(21a)_1	−0.2287	0.6583	1.2041	0.037
H(21b)_1	−0.2560	0.5655	1.2167	0.037
H(22a)_1	−0.4010	0.6630	1.2339	0.059
H(22b)_1	−0.3767	0.7241	1.1624	0.059
H(22c)_1	−0.4043	0.6305	1.1751	0.059
H(2a)_1	−0.3102	0.8097	0.9923	0.046
H(3a)_1	−0.4739	0.8456	0.9733	0.055
H(4a)_1	−0.5089	0.8488	0.8727	0.055
H(5a)_1	−0.3753	0.8145	0.7939	0.051

Table S18. Continued...

atom	x	y	z	U(eq)
H(6a)_1	−0.2138	0.7814	0.8166	0.043
H(m1)_2	0.2472	0.8431	0.3677	0.047
H(m2)_2	0.1821	0.4562	0.5072	0.028
H(m3)_2	0.3436	0.3674	0.2486	0.026
H(m4)_2	0.4132	0.7533	0.1100	0.039
H(11a)_2	0.3486	0.9825	0.1138	0.038
H(11b)_2	0.3666	0.9059	0.0836	0.038
H(12a)_2	0.5139	0.9663	0.0616	0.045
H(12b)_2	0.5117	0.9457	0.1365	0.045
H(12c)_2	0.5299	0.8683	0.1059	0.045
H(21a)_2	0.2324	0.9754	0.2818	0.040
H(21b)_2	0.2839	1.0178	0.2112	0.040
H(22a)_2	0.3671	1.0388	0.2853	0.049
H(22b)_2	0.3875	0.9366	0.3175	0.049
H(22c)_2	0.4394	0.9793	0.2462	0.049
H(11c)_2	0.5021	0.8753	0.1113	0.038
H(11d)_2	0.4654	0.9559	0.1380	0.038
H(12d)_2	0.4047	0.9868	0.0424	0.064
H(12e)_2	0.3538	0.9015	0.0745	0.064
H(12f)_2	0.3170	0.9827	0.1013	0.064
H(21c)_2	0.3910	0.9902	0.2313	0.028
H(21d)_2	0.3722	0.9399	0.3053	0.028
H(22d)_2	0.2428	1.0584	0.2802	0.037
H(22e)_2	0.2214	1.0186	0.2297	0.037
H(22f)_2	0.2025	0.9679	0.3043	0.037
H(31a)_2	0.1184	0.7733	0.5331	0.060
H(31b)_2	0.1554	0.8353	0.4659	0.060
H(31c)_2	0.2330	0.8122	0.4835	0.060
H(31d)_2	0.1721	0.7573	0.5455	0.060
H(32a)_2	0.0932	0.8879	0.5108	0.035
H(32b)_2	0.0963	0.8736	0.4435	0.035
H(32c)_2	0.0346	0.8179	0.5067	0.035
H(31e)_2	0.2148	0.8493	0.5396	0.057
H(31f)_2	0.2603	0.7493	0.5600	0.057

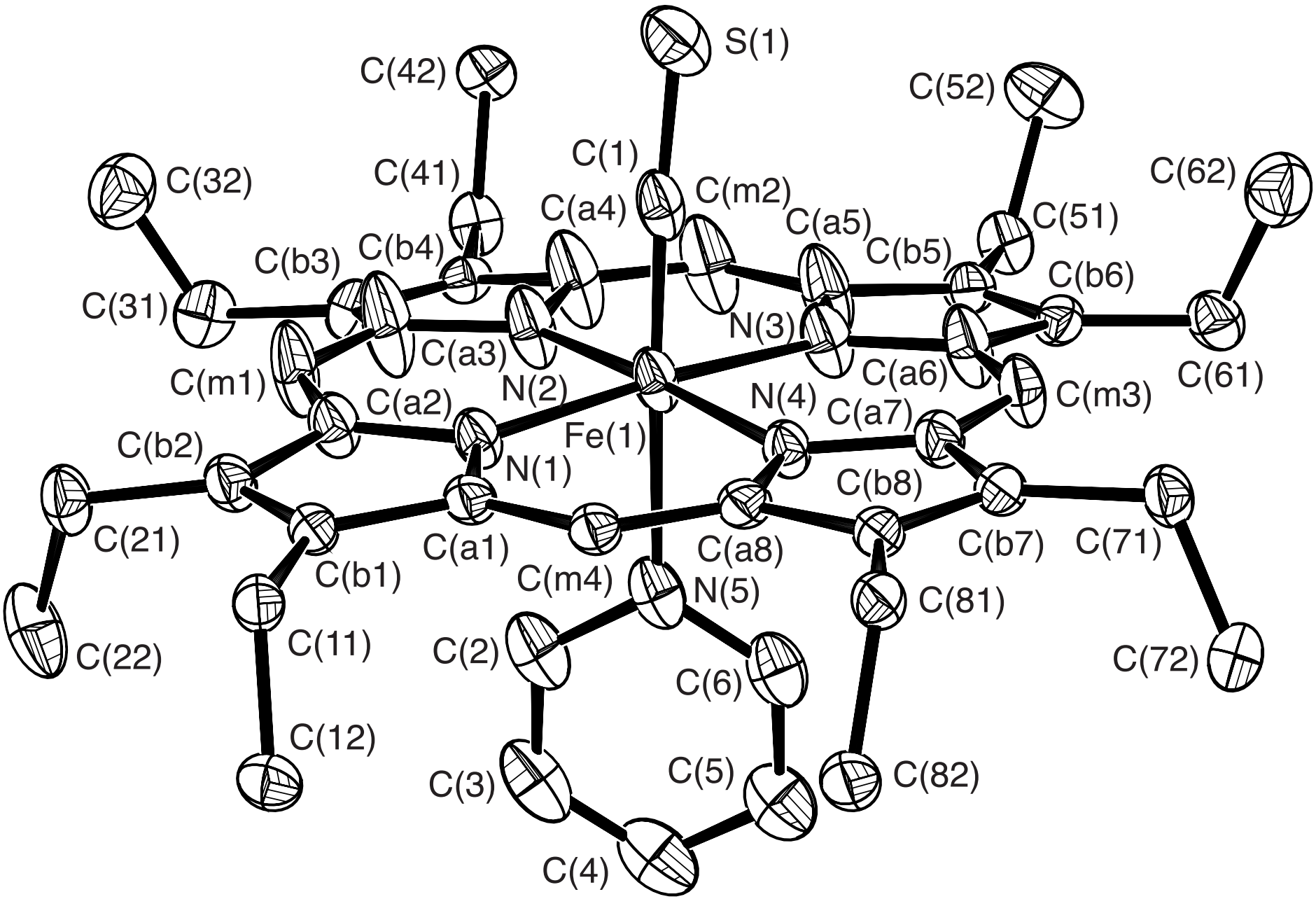
Table S18. Continued...

atom	x	y	z	U(eq)
H(31g)_2	0.2999	0.8119	0.4918	0.057
H(41a)_2	0.0967	0.5419	0.5744	0.034
H(41b)_2	0.1075	0.6246	0.5911	0.034
H(42a)_2	0.1976	0.4999	0.6543	0.042
H(42b)_2	0.2608	0.4800	0.5912	0.042
H(42c)_2	0.2717	0.5637	0.6080	0.042
H(51a)_2	0.2212	0.3045	0.5303	0.037
H(51b)_2	0.2265	0.2306	0.4992	0.037
H(52a)_2	0.0654	0.2574	0.5551	0.061
H(52b)_2	0.0561	0.3563	0.5120	0.061
H(52c)_2	0.0614	0.2816	0.4807	0.061
H(61a)_2	0.2931	0.1974	0.4037	0.033
H(61b)_2	0.3516	0.2374	0.3349	0.033
H(62a)_2	0.2249	0.1700	0.3256	0.054
H(62b)_2	0.1453	0.2311	0.3600	0.054
H(62c)_2	0.2044	0.2716	0.2905	0.054
H(71a)_2	0.4485	0.3705	0.1546	0.031
H(71b)_2	0.4913	0.4323	0.0880	0.031
H(72a)_2	0.3708	0.3627	0.0737	0.033
H(72b)_2	0.2910	0.4021	0.1229	0.033
H(72c)_2	0.3342	0.4645	0.0556	0.033
H(81a)_2	0.5092	0.5780	0.0326	0.038
H(81b)_2	0.5126	0.6637	0.0478	0.038
H(82a)_2	0.4293	0.6984	−0.0401	0.043
H(82b)_2	0.3516	0.6361	0.0028	0.043
H(82c)_2	0.3550	0.7228	0.0181	0.043
H(2a)_2	0.1851	0.7048	0.1927	0.036
H(3a)_2	0.0256	0.7528	0.1670	0.046
H(4a)_2	−0.1132	0.7196	0.2489	0.047
H(5a)_2	−0.0853	0.6380	0.3562	0.043
H(6a)_2	0.0779	0.5924	0.3767	0.034
H(2a)_3	0.3945	−0.0164	0.4036	0.036
H(3a)_3	0.2315	0.0072	0.3858	0.042
H(4a)_3	0.1023	0.0529	0.4592	0.041

Table S18. Continued...

atom	x	y	z	U(eq)
H(5a_3	0.1360	0.0750	0.5504	0.038
H(6a_3	0.2990	0.0514	0.5682	0.035
H(12y)_3	0.4175	0.0209	0.6985	0.040
H(11a)_3	0.4369	0.2521	0.6728	0.037
H(11b)_3	0.4405	0.1520	0.7093	0.037
H(12a)_3	0.2850	0.2261	0.7405	0.053
H(12b)_3	0.2689	0.2626	0.6677	0.053
H(12c)_3	0.2725	0.1616	0.7044	0.053
H(12z)_3	0.3459	0.0313	0.6879	0.040
H(11c)_3	0.2746	0.1792	0.6836	0.034
H(11d)_3	0.3047	0.2729	0.6537	0.034
H(12d)_3	0.3543	0.2059	0.7564	0.062
H(12e)_3	0.4168	0.1280	0.7314	0.062
H(12f)_3	0.4471	0.2226	0.7012	0.062
H(m1)_3	0.5017	0.2838	0.4226	0.027
H(41a)_3	0.5966	0.2040	0.2033	0.041
H(41b)_3	0.5944	0.1039	0.2208	0.041
H(42a)_3	0.7594	0.1332	0.1688	0.067
H(42b)_3	0.7668	0.1737	0.2227	0.067
H(42c)_3	0.7645	0.0724	0.2404	0.067
H(41c)_3	0.7556	0.0850	0.2323	0.121
H(41d)_3	0.7417	0.1888	0.2107	0.121
H(42d)_3	0.6580	0.1464	0.1678	0.137
H(42e)_3	0.5977	0.0947	0.2335	0.137
H(42f)_3	0.5839	0.1980	0.2121	0.137
H(21a)_3	0.4024	0.3597	0.5655	0.036
H(22b)_3	0.4135	0.3652	0.4928	0.036
H(22a)_3	0.5438	0.4238	0.5069	0.046
H(22b)_3	0.5769	0.3342	0.5579	0.046
H(22c)_3	0.5882	0.3398	0.4844	0.046
H(31a)_3	0.5185	0.3417	0.3117	0.035
H(31b)_3	0.5707	0.3197	0.2481	0.035
H(32a)_3	0.6703	0.3953	0.2760	0.047
H(32b)_3	0.6735	0.3224	0.3434	0.047
H(32c)_3	0.7263	0.3001	0.2791	0.047

[a] U(eq) is defined as one third of the trace of the orthogonalized $\mathbf{U}_{ij}$ tensor the estimated standard deviations of the least significant digits are given in parentheses.


S(1)
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C(52)
C(1)
C(41)
C(62)
C(32)
C(m2)
C(a4)
C(a5)
C(51)
C(b3)
C(b4)
C(b5)
C(b6)
C(31)
N(3)
C(a3)
C(a6)
C(61)
C(m1)
N(2)
N(4)
C(m3)
C(a2)
C(a7)
Fe(1)
C(b2)
N(1)
C(b8)
C(21)
C(a1)
C(a8)
C(b7)
C(71)
C(b1)
C(m4)
N(5)
C(81)
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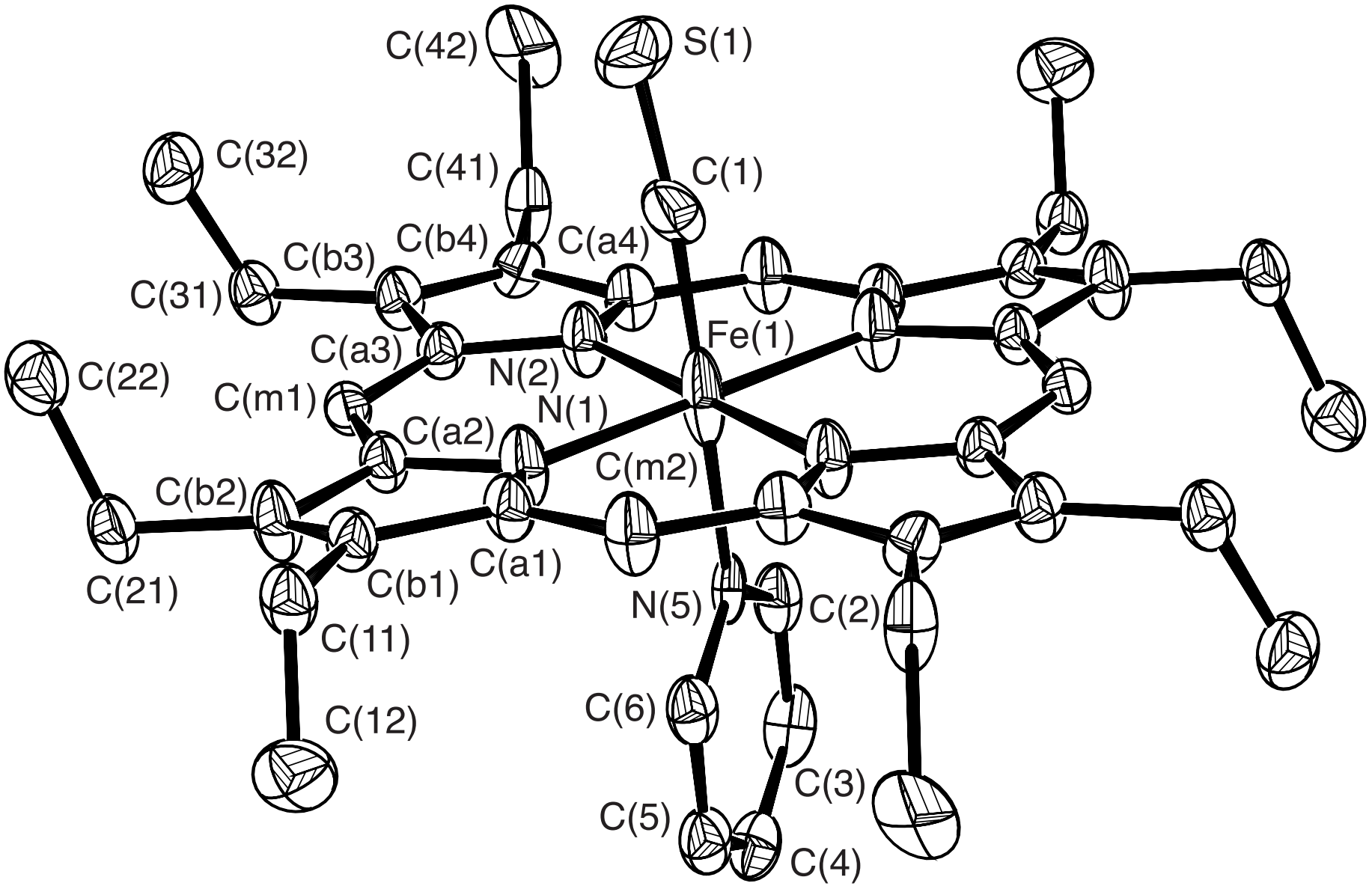
C(2)
C(6)
C(72)
C(12)
C(3)
C(5)
C(82)
C(4)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C(32)
C(41)
C(1)
C(b4)
C(a4)
C(b3)
C(31)
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Fe(1)
C(22)
N(2)
C(m1)
N(1)
C(a2)
C(m2)
C(b2)
C(21)
C(b1)
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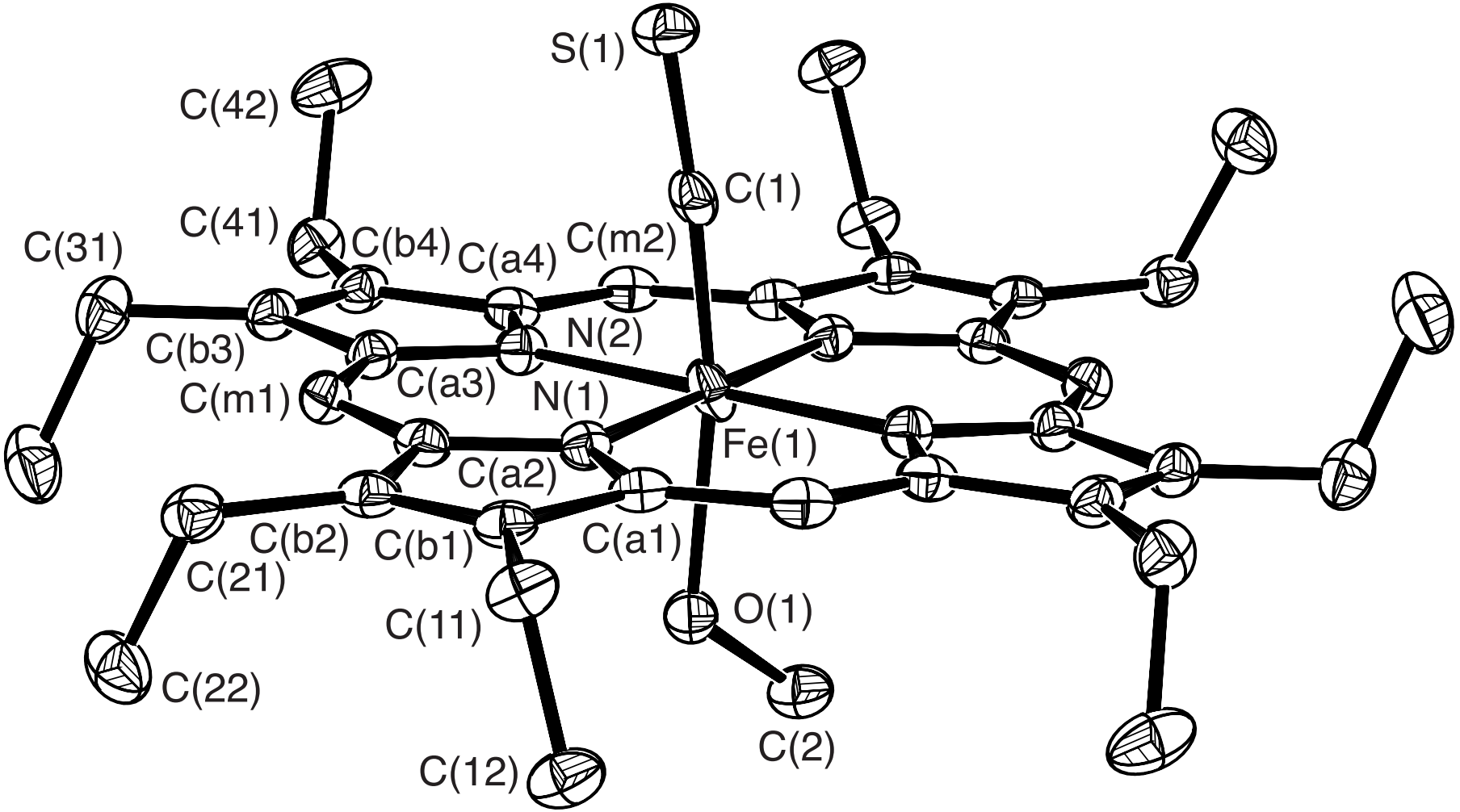
N(5)
C(2)
C(11)
C(6)
C(12)
C(3)
C(5)
C(4)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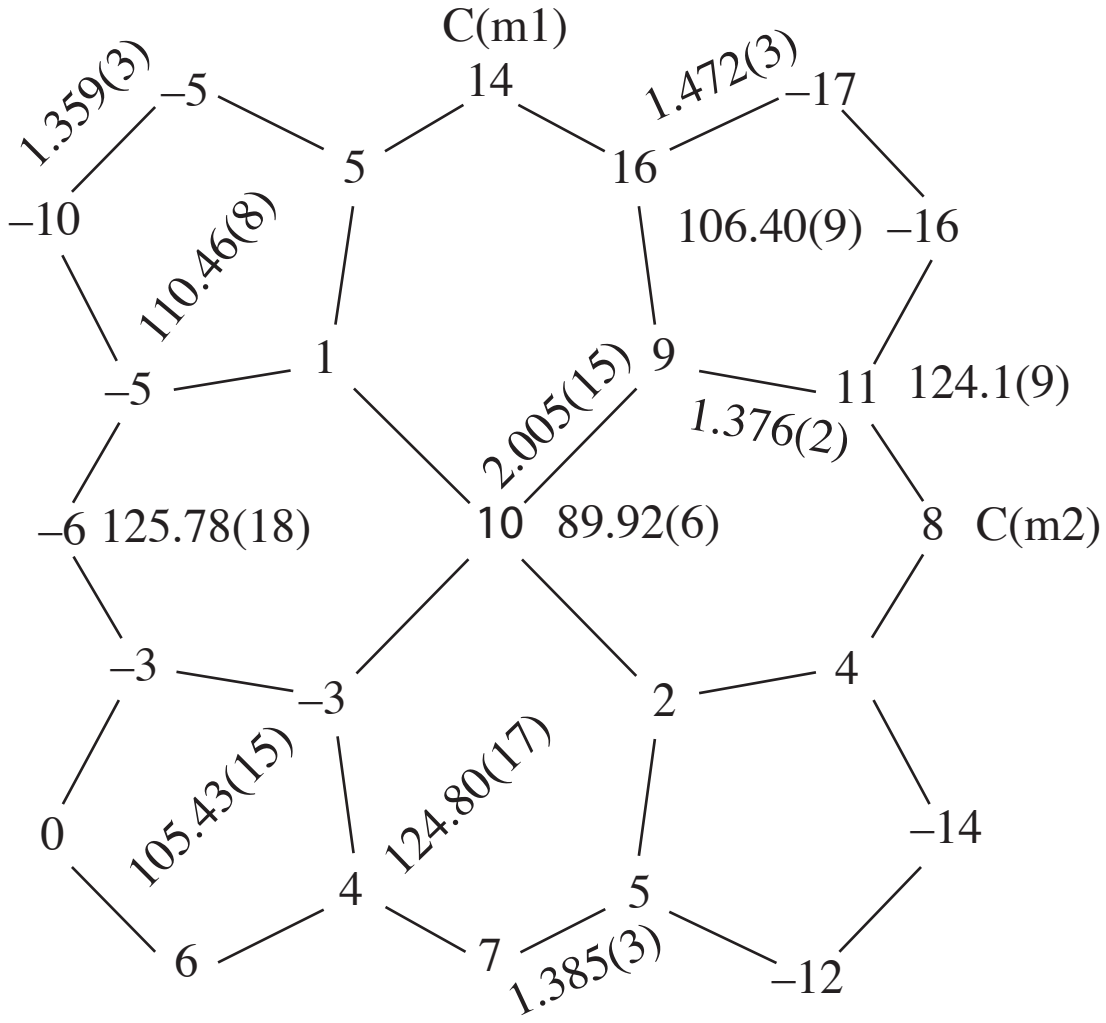
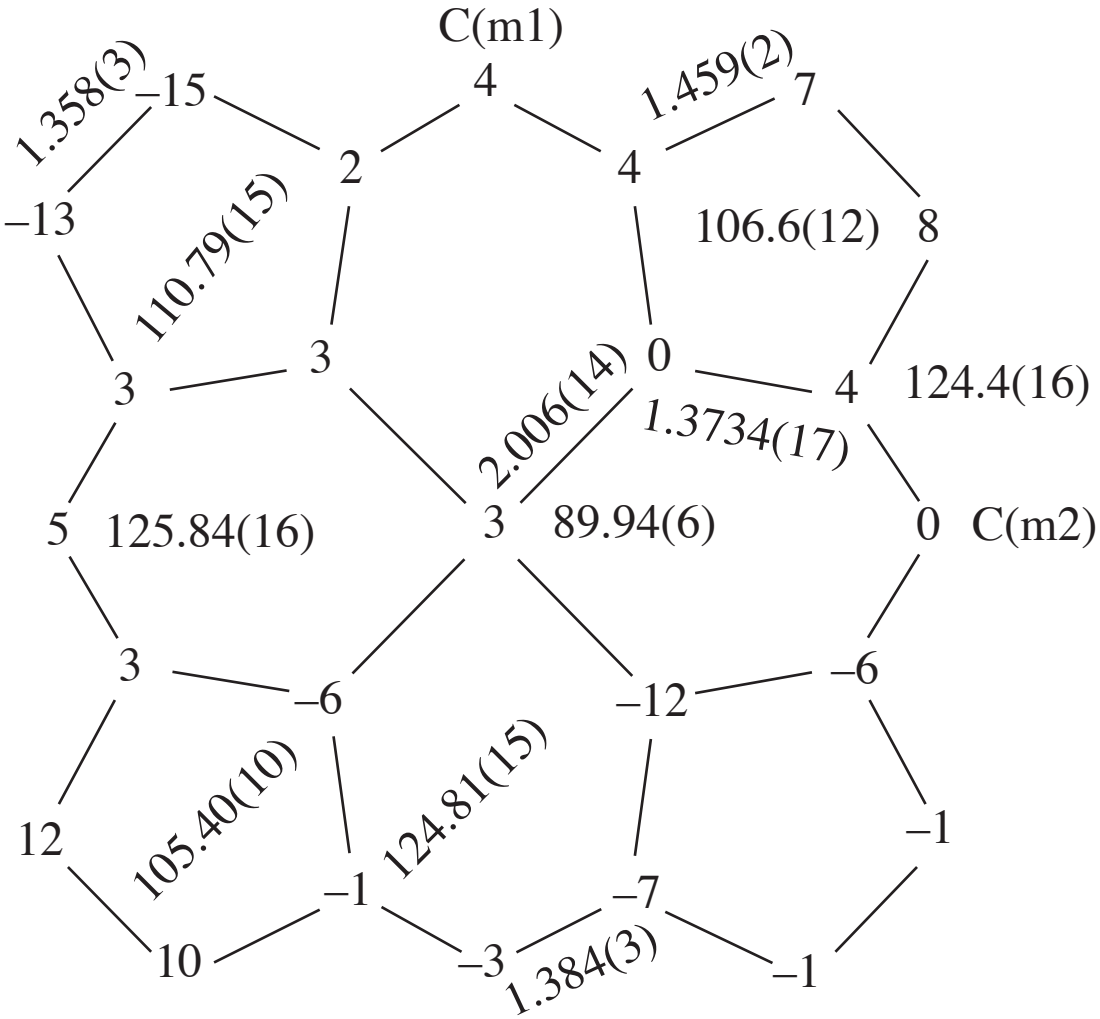
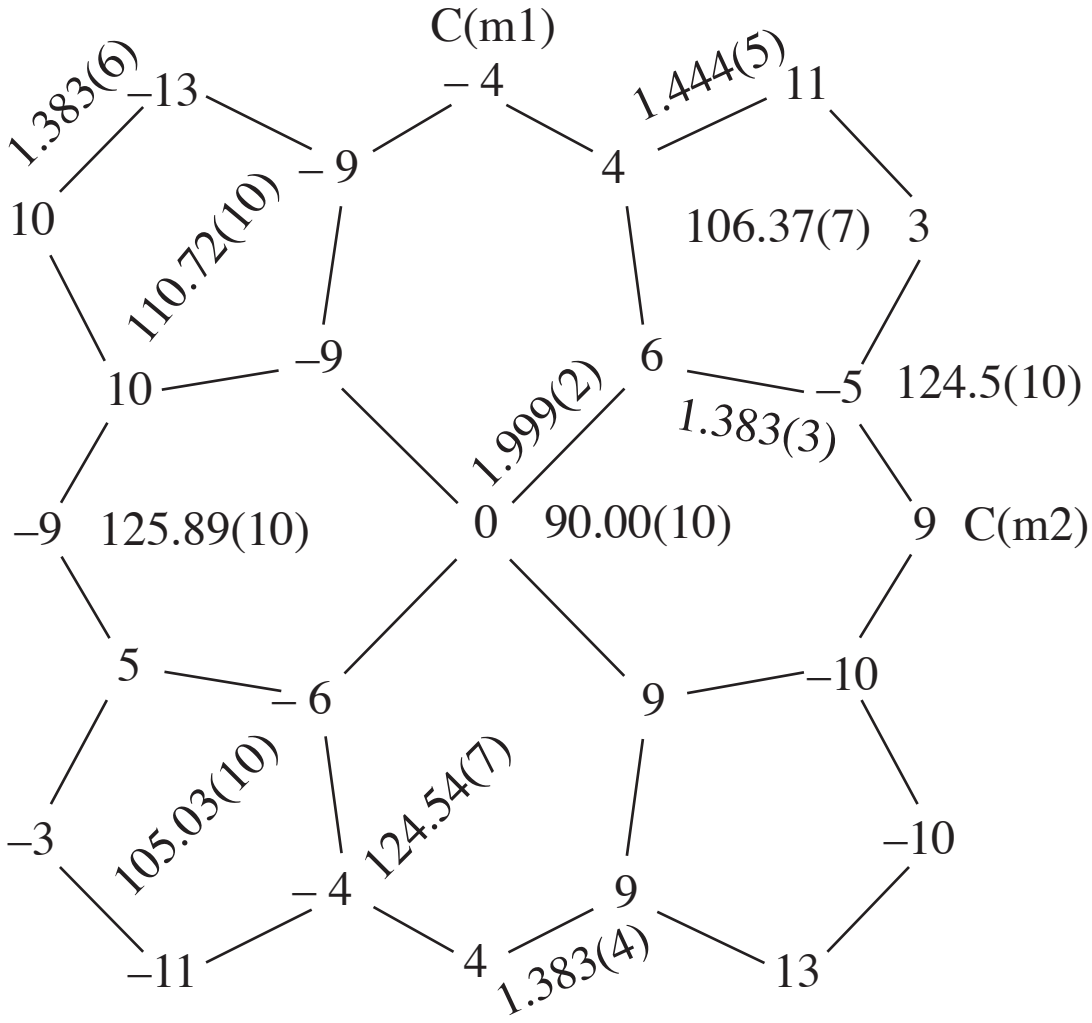
C(1)
C(41)
C(b4)
C(a4)
C(m2)
C(31)
N(2)
C(b3)
C(a3)
N(1)
C(m1)
Fe(1)
C(a2)
C(b2)
C(b1)
C(a1)
C(21)
C(11)
O(1)
C(22)
C(2)
C(12)



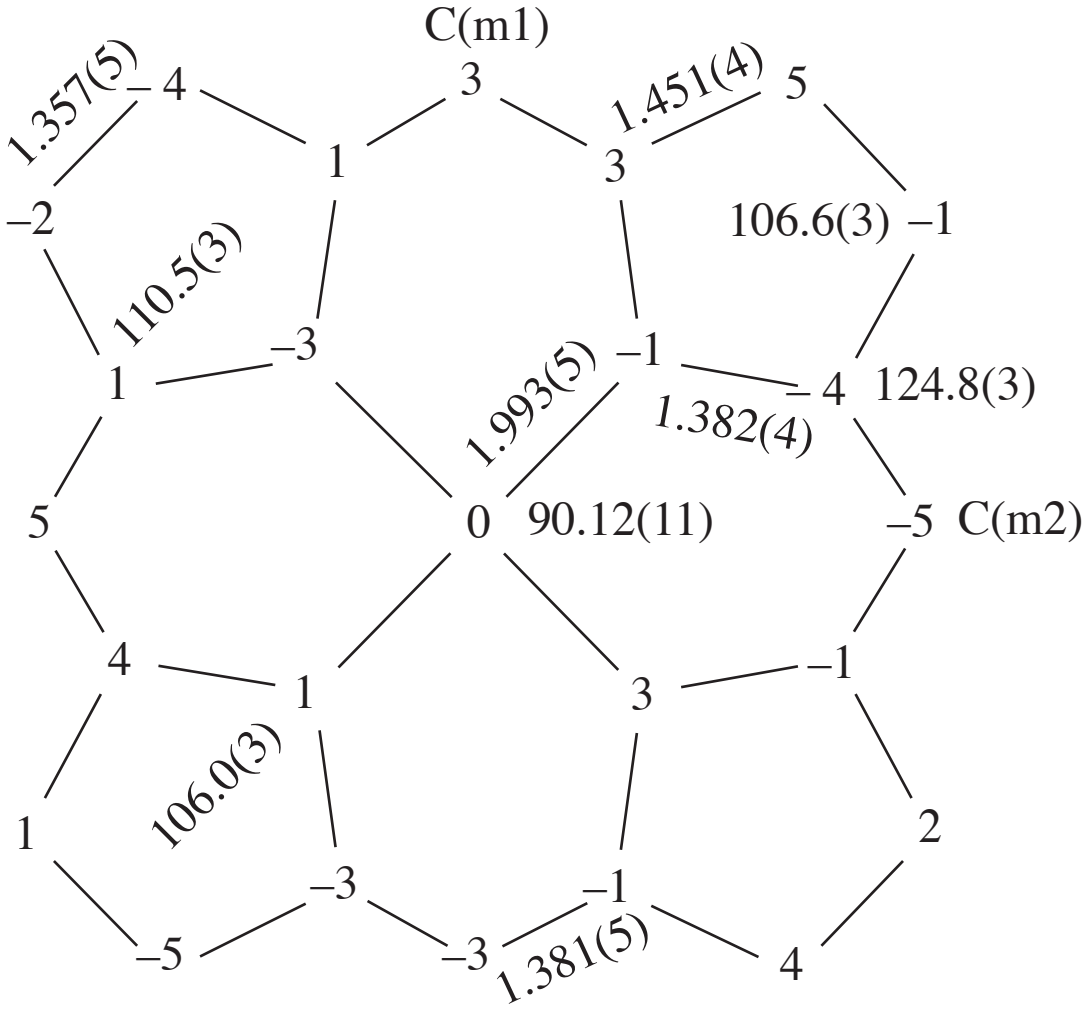
24-atom mean plane for [Fe(OEP)(CS)(Py)] - Molecule 1



24-atom mean plane for [Fe(OEP)(CS)(Py)] - Molecule 2



24-atom mean plane for [Fe(OEP)(CS)(Py)] - Molecule 3



24-atom mean plane for [Fe(OEP)(CS)(CH3OH)]