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Supporting Information

Table S1. Complete Crystallographic Data for [Fe(OEP)(NO)] ($P2_1/c$)

formula	$C_{36}H_{44}FeN_5O$
FW	618.61
a, Å	14.950(2)
b, Å	22.361(2)
c, Å	9.6966(3)
β, deg	104.854(5)
V, Å^3	3133.3(4)
space group	$P2_1/c$
Z	4
D_c, g/cm^3	1.311
F(000)	1316
μ, mm^{-1}	0.519
detector distance, mm	40
detector tilt angle, deg	−25
image time, sec	10
increment, deg	0.20
crystal dimensions, mm	0.56 × 0.40 × 0.27
absorption correction	none
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	FAST (Enraf-Nonius)
θ range for collected data, deg	2.30–29.74
index range	$-20 \leq h \leq 20$
	$-16 \leq k \leq 30$
	$-10 \leq l \leq 13$
total data collected	22655
unique data	7890 (R_{int} = 0.0546)
unique observed data [I > 2σ(I)]	6949
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	7888 / 0 / 396
goodness-of-fit (based on F^2)	1.283
max($\Delta\rho$), e/Å^3	0.484
min($\Delta\rho$), e/Å^3	−0.484
final R indices [I > 2σ(I)]	R_1 = 0.0421, wR_2 = 0.1515
final R indices (all data)	R_1 = 0.0523, wR_2 = 0.1561

Table S2. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P2_1/c$)^a

atom	x	y	z	U(eq)
Fe(1)	0.25076(2)	0.53268(1)	0.23904(4)	0.0093(1)
N(1)	0.28638(14)	0.45054(9)	0.3205(2)	0.0114(4)
N(2)	0.37831(14)	0.54263(8)	0.2160(2)	0.0111(4)
N(3)	0.20909(14)	0.60033(9)	0.1041(2)	0.0109(4)
N(4)	0.11704(14)	0.51006(9)	0.2150(2)	0.0116(4)
N(5)	0.27246(14)	0.57710(9)	0.3890(2)	0.0137(4)
O(1)	0.3107(2)	0.61998(10)	0.4423(3)	0.0303(5)
C(m1)	0.4535(2)	0.45574(10)	0.3503(3)	0.0138(4)
C(m2)	0.3592(2)	0.63675(10)	0.0842(3)	0.0129(4)
C(m3)	0.0427(2)	0.59740(11)	0.0839(3)	0.0147(5)
C(m4)	0.1360(2)	0.41447(10)	0.3410(3)	0.0134(4)
C(a1)	0.2306(2)	0.40908(10)	0.3628(3)	0.0122(4)
C(a2)	0.3744(2)	0.42783(10)	0.3661(3)	0.0121(4)
C(a3)	0.4551(2)	0.50891(10)	0.2790(3)	0.0120(4)
C(a4)	0.4128(2)	0.59124(10)	0.1590(3)	0.0112(4)
C(a5)	0.2643(2)	0.64012(10)	0.0557(3)	0.0119(4)
C(a6)	0.1207(2)	0.62290(10)	0.0576(3)	0.0120(4)
C(a7)	0.0409(2)	0.54456(11)	0.1567(3)	0.0131(4)
C(a8)	0.0830(2)	0.46139(10)	0.2723(3)	0.0121(4)
C(b1)	0.2848(2)	0.35916(10)	0.4346(3)	0.0141(5)
C(b2)	0.3742(2)	0.37073(10)	0.4356(3)	0.0144(5)
C(b3)	0.5385(2)	0.53617(10)	0.2595(3)	0.0123(4)
C(b4)	0.5124(2)	0.58769(10)	0.1858(3)	0.0128(4)
C(b5)	0.2096(2)	0.68739(10)	−0.0270(3)	0.0126(4)
C(b6)	0.1202(2)	0.67666(10)	−0.0251(3)	0.0130(4)
C(b7)	−0.0425(2)	0.51751(11)	0.1776(3)	0.0139(4)
C(b8)	−0.0162(2)	0.46567(10)	0.2496(3)	0.0128(4)
C(11)	0.2471(2)	0.30503(11)	0.4914(3)	0.0189(5)
C(12)	0.2161(2)	0.25599(13)	0.3794(4)	0.0334(7)
C(21)	0.4580(2)	0.33234(11)	0.4913(3)	0.0200(5)
C(22)	0.4909(2)	0.30210(13)	0.3718(4)	0.0275(6)
C(31)	0.6336(2)	0.51049(11)	0.3099(3)	0.0150(5)
C(32)	0.6513(2)	0.45877(13)	0.2178(3)	0.0241(6)
C(41)	0.5734(2)	0.63217(11)	0.1388(3)	0.0187(5)

Table S2. Continued

atom	x	y	z	U(eq)
C(42)	0.5964(3)	0.6149(2)	−0.0004(4)	0.0421(9)
C(51)	0.2468(2)	0.73615(11)	−0.1023(3)	0.0179(5)
C(52)	0.2785(2)	0.71412(14)	−0.2315(3)	0.0279(6)
C(61)	0.0356(2)	0.71205(12)	−0.0968(3)	0.0173(5)
C(62)	0.0100(2)	0.7589(2)	0.0001(4)	0.0363(8)
C(71)	−0.1369(2)	0.54497(12)	0.1313(3)	0.0192(5)
C(72)	−0.1514(2)	0.59406(13)	0.2328(3)	0.0249(6)
C(81)	−0.0762(2)	0.42102(11)	0.2991(3)	0.0154(5)
C(82)	−0.0902(2)	0.43462(13)	0.4463(3)	0.0246(6)

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

Table S3. Bond Lengths for [Fe(OEP)(NO)] ($P2_1/c$)[a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.722(2)	C(a4)–C(b4)	1.447(3)
Fe(1)–N(2)	1.989(2)	C(a5)–C(b5)	1.447(3)
Fe(1)–N(3)	1.993(2)	C(a6)–C(b6)	1.444(3)
Fe(1)–N(1)	2.016(2)	C(a7)–C(b7)	1.446(3)
Fe(1)–N(4)	2.017(2)	C(a8)–C(b8)	1.446(3)
N(1)–C(a2)	1.373(3)	C(b1)–C(b2)	1.359(3)
N(1)–C(a1)	1.378(3)	C(b1)–C(11)	1.499(3)
N(2)–C(a4)	1.378(3)	C(b2)–C(21)	1.500(3)
N(2)–C(a3)	1.379(3)	C(b3)–C(b4)	1.359(3)
N(3)–C(a5)	1.375(3)	C(b3)–C(31)	1.494(3)
N(3)–C(a6)	1.378(3)	C(b4)–C(41)	1.497(3)
N(4)–C(a7)	1.371(3)	C(b5)–C(b6)	1.362(3)
N(4)–C(a8)	1.377(3)	C(b5)–C(51)	1.496(3)
N(5)–O(1)	1.167(3)	C(b6)–C(61)	1.503(3)
C(m1)–C(a3)	1.379(3)	C(b7)–C(b8)	1.358(3)
C(m1)–C(a2)	1.380(3)	C(b7)–C(71)	1.500(3)
C(m2)–C(a5)	1.376(3)	C(b8)–C(81)	1.500(3)
C(m2)–C(a4)	1.380(3)	C(11)–C(12)	1.529(4)
C(m3)–C(a7)	1.380(3)	C(21)–C(22)	1.528(4)
C(m3)–C(a6)	1.380(3)	C(31)–C(32)	1.525(4)
C(m4)–C(a8)	1.379(3)	C(41)–C(42)	1.526(4)
C(m4)–C(a1)	1.381(3)	C(51)–C(52)	1.530(4)
C(a1)–C(b1)	1.449(3)	C(61)–C(62)	1.520(4)
C(a2)–C(b2)	1.444(3)	C(71)–C(72)	1.526(4)
C(a3)–C(b3)	1.443(3)	C(81)–C(82)	1.527(4)

[a]The esd's of the least significant digits are given in parentheses.

Table S4. Bond Angles for [Fe(OEP)(NO)] ($P2_1/c$)[a]

angle	degree	angle	degree
N(5)–Fe(1)–N(2)	92.98(9)	N(3)–C(a6)–C(m3)	125.0(2)
N(5)–Fe(1)–N(3)	94.36(9)	N(3)–C(a6)–C(b6)	110.8(2)
N(2)–Fe(1)–N(3)	89.35(8)	C(m3)–C(a6)–C(b6)	124.2(2)
N(5)–Fe(1)–N(1)	102.77(9)	N(4)–C(a7)–C(m3)	124.8(2)
N(2)–Fe(1)–N(1)	88.93(8)	N(4)–C(a7)–C(b7)	111.2(2)
N(3)–Fe(1)–N(1)	162.85(8)	C(m3)–C(a7)–C(b7)	124.1(2)
N(5)–Fe(1)–N(4)	102.06(9)	N(4)–C(a8)–C(m4)	124.8(2)
N(2)–Fe(1)–N(4)	164.95(8)	N(4)–C(a8)–C(b8)	110.9(2)
N(3)–Fe(1)–N(4)	88.89(8)	C(m4)–C(a8)–C(b8)	124.3(2)
N(1)–Fe(1)–N(4)	88.35(8)	C(b2)–C(b1)–C(a1)	106.6(2)
C(a2)–N(1)–C(a1)	105.0(2)	C(b2)–C(b1)–C(11)	127.8(2)
C(a2)–N(1)–Fe(1)	126.7(2)	C(a1)–C(b1)–C(11)	125.6(2)
C(a1)–N(1)–Fe(1)	127.6(2)	C(b1)–C(b2)–C(a2)	106.5(2)
C(a4)–N(2)–C(a3)	104.7(2)	C(b1)–C(b2)–C(21)	128.5(2)
C(a4)–N(2)–Fe(1)	127.0(2)	C(a2)–C(b2)–C(21)	125.0(2)
C(a3)–N(2)–Fe(1)	127.1(2)	C(b4)–C(b3)–C(a3)	106.6(2)
C(a5)–N(3)–C(a6)	105.1(2)	C(b4)–C(b3)–C(31)	128.2(2)
C(a5)–N(3)–Fe(1)	126.9(2)	C(a3)–C(b3)–C(31)	125.2(2)
C(a6)–N(3)–Fe(1)	127.3(2)	C(b3)–C(b4)–C(a4)	106.5(2)
C(a7)–N(4)–C(a8)	104.9(2)	C(b3)–C(b4)–C(41)	127.4(2)
C(a7)–N(4)–Fe(1)	126.9(2)	C(a4)–C(b4)–C(41)	126.0(2)
C(a8)–N(4)–Fe(1)	127.6(2)	C(b6)–C(b5)–C(a5)	106.3(2)
O(1)–N(5)–Fe(1)	144.4(2)	C(b6)–C(b5)–C(51)	128.6(2)
C(a3)–C(m1)–C(a2)	124.8(2)	C(a5)–C(b5)–C(51)	125.1(2)
C(a5)–C(m2)–C(a4)	125.1(2)	C(b5)–C(b6)–C(a6)	106.8(2)
C(a7)–C(m3)–C(a6)	125.2(2)	C(b5)–C(b6)–C(61)	127.8(2)
C(a8)–C(m4)–C(a1)	125.4(2)	C(a6)–C(b6)–C(61)	125.4(2)
N(1)–C(a1)–C(m4)	124.8(2)	C(b8)–C(b7)–C(a7)	106.5(2)
N(1)–C(a1)–C(b1)	110.8(2)	C(b8)–C(b7)–C(71)	129.0(2)
C(m4)–C(a1)–C(b1)	124.5(2)	C(a7)–C(b7)–C(71)	124.5(2)
N(1)–C(a2)–C(m1)	125.1(2)	C(b7)–C(b8)–C(a8)	106.5(2)
N(1)–C(a2)–C(b2)	111.2(2)	C(b7)–C(b8)–C(81)	127.9(2)
C(m1)–C(a2)–C(b2)	123.7(2)	C(a8)–C(b8)–C(81)	125.5(2)
C(m1)–C(a3)–N(2)	125.0(2)	C(b1)–C(11)–C(12)	113.1(2)

Table S4. Continued

angle	degree	angle	degree
C(m1)–C(a3)–C(b3)	123.8(2)	C(b2)–C(21)–C(22)	112.4(2)
N(2)–C(a3)–C(b3)	111.1(2)	C(b3)–C(31)–C(32)	113.2(2)
N(2)–C(a4)–C(m2)	124.5(2)	C(b4)–C(41)–C(42)	113.2(2)
N(2)–C(a4)–C(b4)	111.0(2)	C(b5)–C(51)–C(52)	113.4(2)
C(m2)–C(a4)–C(b4)	124.5(2)	C(b6)–C(61)–C(62)	113.1(2)
N(3)–C(a5)–C(m2)	125.1(2)	C(b7)–C(71)–C(72)	112.3(2)
N(3)–C(a5)–C(b5)	111.0(2)	C(b8)–C(81)–C(82)	113.8(2)
C(m2)–C(a5)–C(b5)	123.9(2)		

[a]The esd's of the least significant digits are given in parentheses.

Table S5. Anisotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P2_1/c$)[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0077(2)	0.0094(2)	0.0110(2)	0.0004(1)	0.0026(1)	0.0005(1)
N(1)	0.0095(9)	0.0106(8)	0.0143(10)	0.0005(7)	0.0034(8)	0.0008(7)
N(2)	0.0095(9)	0.0113(9)	0.0126(10)	0.0011(7)	0.0031(8)	0.0005(7)
N(3)	0.0091(9)	0.0125(8)	0.0103(9)	0.0008(7)	0.0009(8)	0.0009(7)
N(4)	0.0094(9)	0.0130(9)	0.0126(10)	−0.0007(7)	0.0029(8)	−0.0002(7)
N(5)	0.0128(9)	0.0145(9)	0.0138(10)	0.0009(7)	0.0033(8)	0.0024(7)
O(1)	0.0373(13)	0.0222(10)	0.0322(12)	−0.0119(9)	0.0105(10)	−0.0085(9)
C(m1)	0.0107(10)	0.0138(10)	0.0173(12)	0.0015(8)	0.0045(9)	0.0020(8)
C(m2)	0.0130(11)	0.0109(10)	0.0149(12)	0.0017(8)	0.0039(9)	−0.0004(8)
C(m3)	0.0098(10)	0.0175(11)	0.0163(12)	0.0014(9)	0.0027(9)	0.0029(8)
C(m4)	0.0125(11)	0.0111(10)	0.0181(12)	−0.0017(8)	0.0064(9)	−0.0029(8)
C(a1)	0.0128(10)	0.0103(9)	0.0136(11)	−0.0012(8)	0.0033(9)	−0.0005(8)
C(a2)	0.0114(10)	0.0117(10)	0.0130(11)	0.0009(8)	0.0026(9)	0.0016(8)
C(a3)	0.0096(10)	0.0129(10)	0.0136(11)	−0.0003(8)	0.0030(9)	0.0011(8)
C(a4)	0.0089(10)	0.0123(10)	0.0117(11)	0.0002(8)	0.0012(9)	−0.0006(8)
C(a5)	0.0139(11)	0.0106(9)	0.0110(11)	0.0003(8)	0.0029(9)	0.0009(8)
C(a6)	0.0111(10)	0.0147(10)	0.0088(11)	−0.0005(8)	0.0000(9)	0.0026(8)
C(a7)	0.0096(10)	0.0173(11)	0.0126(11)	−0.0018(8)	0.0029(9)	0.0003(8)
C(a8)	0.0094(10)	0.0137(10)	0.0133(11)	−0.0041(8)	0.0030(9)	−0.0022(8)
C(b1)	0.0145(11)	0.0109(10)	0.0173(12)	0.0012(8)	0.0046(10)	0.0004(8)
C(b2)	0.0150(11)	0.0110(10)	0.0177(12)	0.0019(8)	0.0053(10)	0.0010(8)
C(b3)	0.0089(10)	0.0140(10)	0.0135(11)	−0.0008(8)	0.0019(9)	−0.0008(8)
C(b4)	0.0103(10)	0.0130(10)	0.0144(12)	0.0002(8)	0.0022(9)	−0.0015(8)
C(b5)	0.0143(11)	0.0113(10)	0.0113(11)	−0.0003(8)	0.0018(9)	0.0018(8)
C(b6)	0.0142(11)	0.0142(10)	0.0097(11)	0.0004(8)	0.0014(9)	0.0038(8)
C(b7)	0.0087(10)	0.0181(11)	0.0148(12)	−0.0025(9)	0.0026(9)	−0.0008(8)
C(b8)	0.0094(10)	0.0159(10)	0.0132(11)	−0.0050(8)	0.0031(9)	−0.0017(8)
C(11)	0.0158(12)	0.0137(11)	0.0269(14)	0.0053(9)	0.0050(11)	−0.0014(9)
C(12)	0.033(2)	0.0172(13)	0.049(2)	−0.0059(13)	0.009(2)	−0.0080(11)
C(21)	0.0158(12)	0.0166(11)	0.0270(15)	0.0083(10)	0.0043(11)	0.0031(9)
C(22)	0.0234(14)	0.0193(13)	0.040(2)	0.0015(11)	0.0083(13)	0.0094(10)
C(31)	0.0092(10)	0.0157(10)	0.0191(12)	0.0016(9)	0.0016(9)	0.0004(8)
C(32)	0.0150(12)	0.0238(13)	0.035(2)	−0.0061(11)	0.0086(12)	0.0031(10)
C(41)	0.0110(11)	0.0162(11)	0.0279(14)	0.0063(10)	0.0033(10)	−0.0022(8)

Table S5. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(42)	0.039(2)	0.066(2)	0.023(2)	0.003(2)	0.010(2)	−0.029(2)
C(51)	0.0181(12)	0.0141(10)	0.0209(13)	0.0055(9)	0.0037(10)	0.0017(9)
C(52)	0.035(2)	0.0289(14)	0.0230(15)	0.0101(11)	0.0133(13)	0.0062(12)
C(61)	0.0163(12)	0.0200(11)	0.0145(12)	0.0030(9)	0.0016(10)	0.0062(9)
C(62)	0.028(2)	0.040(2)	0.036(2)	−0.0124(14)	0.0000(14)	0.0175(13)
C(71)	0.0093(10)	0.0235(12)	0.0236(14)	0.0016(10)	0.0022(10)	0.0004(9)
C(72)	0.0165(12)	0.0248(13)	0.035(2)	0.0020(11)	0.0089(12)	0.0071(10)
C(81)	0.0119(10)	0.0151(10)	0.0206(13)	−0.0051(9)	0.0067(10)	−0.0041(8)
C(82)	0.0284(14)	0.0259(13)	0.0230(14)	−0.0058(11)	0.0130(12)	−0.0099(11)

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

Table S6. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P2_1/c$)[a]

atom	x	y	z	U(eq)
H(m1)	0.5111(2)	0.43692(10)	0.3916(3)	0.017
H(m2)	0.3903(2)	0.66820(10)	0.0496(3)	0.015
H(m3)	−0.0143(2)	0.61785(11)	0.0492(3)	0.018
H(m4)	0.1048(2)	0.38328(10)	0.3763(3)	0.016
H(11A)	0.1937(2)	0.31711(11)	0.5279(3)	0.023
H(11B)	0.2952(2)	0.28866(11)	0.5724(3)	0.023
H(12A)	0.1917(18)	0.2220(5)	0.4222(9)	0.050
H(12B)	0.2691(5)	0.2429(9)	0.3448(22)	0.050
H(12C)	0.1678(14)	0.2717(4)	0.2994(14)	0.050
H(21A)	0.4432(2)	0.30126(11)	0.5548(3)	0.024
H(21B)	0.5086(2)	0.35731(11)	0.5488(3)	0.024
H(22A)	0.5398(12)	0.2732(8)	0.4131(4)	0.041
H(22B)	0.5152(16)	0.3324(2)	0.3180(17)	0.041
H(22C)	0.4389(4)	0.2813(10)	0.3077(16)	0.041
H(31A)	0.6428(2)	0.49629(11)	0.4092(3)	0.018
H(31B)	0.6795(2)	0.54242(11)	0.3102(3)	0.018
H(32A)	0.7139(6)	0.4431(7)	0.2573(15)	0.036
H(32B)	0.6454(17)	0.4729(3)	0.1203(7)	0.036
H(32C)	0.6060(11)	0.4270(5)	0.2168(21)	0.036
H(41A)	0.6317(2)	0.63623(11)	0.2146(3)	0.022
H(41B)	0.5423(2)	0.67161(11)	0.1266(3)	0.022
H(42A)	0.6380(18)	0.6449(8)	−0.0239(18)	0.063
H(42B)	0.5393(4)	0.6131(14)	−0.0773(8)	0.063
H(42C)	0.6268(19)	0.5757(7)	0.0105(11)	0.063
H(51A)	0.2997(2)	0.75536(11)	−0.0342(3)	0.022
H(51B)	0.1982(2)	0.76689(11)	−0.1343(3)	0.022
H(52A)	0.3010(17)	0.7481(2)	−0.2770(17)	0.042
H(52B)	0.2263(5)	0.6953(10)	−0.2999(13)	0.042
H(52C)	0.3284(12)	0.6849(9)	−0.2003(5)	0.042
H(61A)	−0.0171(2)	0.68427(12)	−0.1297(3)	0.021
H(61B)	0.0466(2)	0.73213(12)	−0.1820(3)	0.021
H(62A)	−0.0414(13)	0.7832(8)	−0.0548(8)	0.054
H(62B)	0.0635(6)	0.7847(8)	0.0391(25)	0.054
H(62C)	−0.0087(19)	0.7390(2)	0.0784(18)	0.054

Table S6. Continued

atom	x	y	z	U(eq)
H(71A)	−0.1842(2)	0.51343(12)	0.1262(3)	0.023
H(71B)	−0.1458(2)	0.56203(12)	0.0345(3)	0.023
H(72A)	−0.2126(7)	0.6121(7)	0.1958(14)	0.037
H(72B)	−0.1036(10)	0.6248(6)	0.2407(20)	0.037
H(72C)	−0.1473(17)	0.5768(2)	0.3271(8)	0.037
H(81A)	−0.0479(2)	0.38090(11)	0.3011(3)	0.018
H(81B)	−0.1374(2)	0.41978(11)	0.2291(3)	0.018
H(82A)	−0.1276(14)	0.4029(6)	0.4736(12)	0.037
H(82B)	−0.1222(15)	0.4730(5)	0.4437(7)	0.037
H(82C)	−0.0300(2)	0.4366(11)	0.5162(6)	0.037

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

Table S7. Complete Crystallographic Data for [Fe(OEP)(NO)] ($P\bar{1}$)

formula	$C_{36}H_{44}FeN_5O$
FW	618.61
a, Å	10.4204(1)
b, Å	10.5562(7)
c, Å	14.0425(7)
α, deg	79.830(5)
β, deg	89.585(4)
γ, deg	80.264(4)
V, Å^3	1498.10(13)
space group	$P\bar{1}$
Z	2
D_c, g/cm^3	1.371
F(000)	658
μ, mm^{-1}	0.542
detector distance, mm	40
detector tilt angle, deg	−25 and −60
image time, sec	10
increment, deg	0.20
power setting	50 kV, 30 mA and 50 kV, 40 mA
crystal dimensions, mm	0.40 × 0.33 × 0.27
absorption correction	DIFABS
rel. trans. coeffic. (I)	1.00–0.74
radiation	MoKα, $\bar{\lambda}$ = 0.71073 Å
temperature, K	130(2)
diffractometer	FAST (Enraf-Nonius)
θ range for collected data, deg	2.44–44.50
index range	$-19 \leq h \leq 20$
	$-21 \leq k \leq 21$
	$-28 \leq l \leq 28$
total data collected	44013
unique data	20616 (R_{int} = 0.045)
unique observed data [I > 2σ(I)]	17208
refinement method	Full-matrix least-squares on F^2
data/restraints/parameters	20575/0/396
goodness-of-fit (based on F^2)	1.024
max($\Delta\rho$), e/Å^3	1.507
min($\Delta\rho$), e/Å^3	−1.026
final R indices [I > 2σ(I)]	R_1 = 0.0412, wR_2 = 0.1059
final R indices (all data)	R_1 = 0.0535, wR_2 = 0.1128

Table S8. Atomic Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P\bar{1}$)[a]

atom	x	y	z	U(eq)
Fe(1)	0.13244(1)	0.07844(1)	0.24465(1)	0.0100(1)
N(1)	−0.02234(6)	0.07010(6)	0.33189(4)	0.0121(1)
N(2)	0.07551(6)	0.27180(6)	0.20974(5)	0.0120(1)
N(3)	0.30661(6)	0.09828(6)	0.18926(4)	0.0113(1)
N(4)	0.21045(6)	−0.10226(6)	0.31335(4)	0.0116(1)
N(5)	0.07437(7)	0.04902(7)	0.13689(5)	0.0162(1)
O(1)	0.07532(11)	0.08194(10)	0.05305(6)	0.0356(2)
C(m1)	−0.14034(7)	0.29194(7)	0.28157(6)	0.0140(1)
C(m2)	0.25763(7)	0.32724(7)	0.10967(5)	0.0132(1)
C(m3)	0.42401(7)	−0.12441(7)	0.23861(5)	0.0128(1)
C(m4)	0.02696(7)	−0.15802(7)	0.41240(5)	0.0136(1)
C(a1)	−0.05222(7)	−0.03716(7)	0.39311(5)	0.0127(1)
C(a2)	−0.12866(7)	0.16632(7)	0.33344(5)	0.0128(1)
C(a3)	−0.04525(7)	0.34112(7)	0.22432(5)	0.0129(1)
C(a4)	0.13667(7)	0.35897(7)	0.14878(5)	0.0125(1)
C(a5)	0.33602(7)	0.20535(7)	0.12773(5)	0.0120(1)
C(a6)	0.41237(6)	0.00103(7)	0.18659(5)	0.0115(1)
C(a7)	0.33046(7)	−0.17227(7)	0.29849(5)	0.0120(1)
C(a8)	0.14972(7)	−0.18823(7)	0.37554(5)	0.0123(1)
C(b1)	−0.17869(7)	−0.00762(7)	0.43508(5)	0.0133(1)
C(b2)	−0.22703(7)	0.11934(7)	0.39707(5)	0.0132(1)
C(b3)	−0.05960(7)	0.47376(7)	0.17247(5)	0.0137(1)
C(b4)	0.05453(7)	0.48619(7)	0.12633(5)	0.0132(1)
C(b5)	0.46121(7)	0.17472(7)	0.08456(5)	0.0123(1)
C(b6)	0.50975(6)	0.04760(7)	0.12191(5)	0.0120(1)
C(b7)	0.34622(7)	−0.30367(7)	0.35267(5)	0.0127(1)
C(b8)	0.23270(7)	−0.31407(7)	0.40044(5)	0.0130(1)
C(11)	−0.24189(8)	−0.10133(8)	0.50521(6)	0.0160(1)
C(12)	−0.31257(9)	−0.18786(10)	0.45485(7)	0.0209(1)
C(21)	−0.35752(7)	0.19613(8)	0.41335(6)	0.0157(1)
C(22)	−0.46103(8)	0.18403(10)	0.34014(7)	0.0206(1)
C(31)	−0.17947(7)	0.57536(8)	0.16913(6)	0.0164(1)
C(32)	−0.19508(9)	0.63836(9)	0.25929(7)	0.0207(1)
C(41)	0.08806(8)	0.60633(8)	0.06446(6)	0.0159(1)

Table S8. Continued

atom	x	y	z	U(eq)
C(42)	0.14420(11)	0.69562(11)	0.12137(8)	0.0264(2)
C(51)	0.52245(8)	0.26771(8)	0.01287(6)	0.0162(1)
C(52)	0.59550(10)	0.35515(10)	0.06024(8)	0.0233(2)
C(61)	0.63852(7)	−0.02994(8)	0.10165(5)	0.0143(1)
C(62)	0.75070(8)	−0.01467(10)	0.16601(8)	0.0223(2)
C(71)	0.46464(7)	−0.40624(8)	0.35382(6)	0.0166(1)
C(72)	0.47602(9)	−0.46767(9)	0.26264(7)	0.0223(2)
C(81)	0.19733(8)	−0.43172(8)	0.46437(6)	0.0176(1)
C(82)	0.12911(11)	−0.51416(11)	0.40865(9)	0.0281(2)

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

Table S9. Bond Lengths for [Fe(OEP)(NO)] ($P\bar{1}$)[a]

bond	length (Å)	bond	length (Å)
Fe(1)–N(5)	1.7307(7)	C(a4)–C(b4)	1.4495(10)
Fe(1)–N(3)	1.9985(6)	C(a5)–C(b5)	1.4453(9)
Fe(1)–N(2)	2.0000(6)	C(a6)–C(b6)	1.4471(9)
Fe(1)–N(4)	2.0167(6)	C(a7)–C(b7)	1.4429(10)
Fe(1)–N(1)	2.0226(6)	C(a8)–C(b8)	1.4445(10)
N(1)–C(a2)	1.3735(9)	C(b1)–C(b2)	1.3630(11)
N(1)–C(a1)	1.3746(9)	C(b1)–C(11)	1.4997(10)
N(2)–C(a4)	1.3777(9)	C(b2)–C(21)	1.4988(10)
N(2)–C(a3)	1.3778(9)	C(b3)–C(b4)	1.3649(10)
N(3)–C(a5)	1.3734(9)	C(b3)–C(31)	1.4976(10)
N(3)–C(a6)	1.3785(9)	C(b4)–C(41)	1.4972(10)
N(4)–C(a7)	1.3754(9)	C(b5)–C(b6)	1.3629(10)
N(4)–C(a8)	1.3758(9)	C(b5)–C(51)	1.4959(10)
N(5)–O(1)	1.1677(11)	C(b6)–C(61)	1.5022(9)
C(m1)–C(a2)	1.3818(11)	C(b7)–C(b8)	1.3666(10)
C(m1)–C(a3)	1.3830(10)	C(b7)–C(71)	1.4959(10)
C(m2)–C(a4)	1.3837(9)	C(b8)–C(81)	1.4968(10)
C(m2)–C(a5)	1.3854(10)	C(11)–C(12)	1.5297(12)
C(m3)–C(a6)	1.3809(10)	C(21)–C(22)	1.5316(12)
C(m3)–C(a7)	1.3846(10)	C(31)–C(32)	1.5262(12)
C(m4)–C(a1)	1.3809(10)	C(41)–C(42)	1.5260(13)
C(m4)–C(a8)	1.3845(9)	C(51)–C(52)	1.5283(13)
C(a1)–C(b1)	1.4478(9)	C(61)–C(62)	1.5297(12)
C(a2)–C(b2)	1.4482(10)	C(71)–C(72)	1.5293(13)
C(a3)–C(b3)	1.4435(10)	C(81)–C(82)	1.527(2)

[a]The esd's of the least significant digits are given in parentheses.

Table S10. Bond Angles for [Fe(OEP)(NO)] ($P\bar{1}$)[a]

angle	degree	angle	degree
N(5)–Fe(1)–N(3)	92.20(3)	N(3)–C(a6)–C(m3)	124.56(6)
N(5)–Fe(1)–N(2)	93.65(3)	N(3)–C(a6)–C(b6)	111.06(6)
N(3)–Fe(1)–N(2)	89.48(2)	C(m3)–C(a6)–C(b6)	124.38(6)
N(5)–Fe(1)–N(4)	102.63(3)	N(4)–C(a7)–C(m3)	124.85(6)
N(3)–Fe(1)–N(4)	88.94(2)	N(4)–C(a7)–C(b7)	111.15(6)
N(2)–Fe(1)–N(4)	163.69(3)	C(m3)–C(a7)–C(b7)	123.99(6)
N(5)–Fe(1)–N(1)	103.01(3)	N(4)–C(a8)–C(m4)	124.91(6)
N(3)–Fe(1)–N(1)	164.78(3)	N(4)–C(a8)–C(b8)	111.12(6)
N(2)–Fe(1)–N(1)	88.89(3)	C(m4)–C(a8)–C(b8)	123.94(6)
N(4)–Fe(1)–N(1)	88.38(2)	C(b2)–C(b1)–C(a1)	106.33(6)
C(a2)–N(1)–C(a1)	104.88(6)	C(b2)–C(b1)–C(11)	128.04(6)
C(a2)–N(1)–Fe(1)	127.02(5)	C(a1)–C(b1)–C(11)	125.62(7)
C(a1)–N(1)–Fe(1)	127.63(5)	C(b1)–C(b2)–C(a2)	106.37(6)
C(a4)–N(2)–C(a3)	104.94(6)	C(b1)–C(b2)–C(21)	127.88(7)
C(a4)–N(2)–Fe(1)	127.06(5)	C(a2)–C(b2)–C(21)	125.71(7)
C(a3)–N(2)–Fe(1)	126.68(5)	C(b4)–C(b3)–C(a3)	106.92(6)
C(a5)–N(3)–C(a6)	105.02(5)	C(b4)–C(b3)–C(31)	127.52(7)
C(a5)–N(3)–Fe(1)	126.24(5)	C(a3)–C(b3)–C(31)	125.55(7)
C(a6)–N(3)–Fe(1)	127.34(5)	C(b3)–C(b4)–C(a4)	106.02(6)
C(a7)–N(4)–C(a8)	104.93(6)	C(b3)–C(b4)–C(41)	127.12(7)
C(a7)–N(4)–Fe(1)	127.06(5)	C(a4)–C(b4)–C(41)	126.86(6)
C(a8)–N(4)–Fe(1)	127.54(5)	C(b6)–C(b5)–C(a5)	106.78(6)
O(1)–N(5)–Fe(1)	142.74(8)	C(b6)–C(b5)–C(51)	128.00(6)
C(a2)–C(m1)–C(a3)	125.34(6)	C(a5)–C(b5)–C(51)	125.23(6)
C(a4)–C(m2)–C(a5)	125.37(7)	C(b5)–C(b6)–C(a6)	106.19(6)
C(a6)–C(m3)–C(a7)	125.37(6)	C(b5)–C(b6)–C(61)	127.60(6)
C(a1)–C(m4)–C(a8)	125.21(7)	C(a6)–C(b6)–C(61)	126.21(6)
N(1)–C(a1)–C(m4)	124.91(6)	C(b8)–C(b7)–C(a7)	106.45(6)
N(1)–C(a1)–C(b1)	111.20(6)	C(b8)–C(b7)–C(71)	128.02(7)
C(m4)–C(a1)–C(b1)	123.89(7)	C(a7)–C(b7)–C(71)	125.54(6)
N(1)–C(a2)–C(m1)	124.57(6)	C(b7)–C(b8)–C(a8)	106.35(6)
N(1)–C(a2)–C(b2)	111.20(6)	C(b7)–C(b8)–C(81)	127.87(7)
C(m1)–C(a2)–C(b2)	124.23(6)	C(a8)–C(b8)–C(81)	125.77(6)
N(2)–C(a3)–C(m1)	125.10(7)	C(b1)–C(11)–C(12)	112.56(7)

Table S10. Continued

angle	degree	angle	degree
N(2)–C(a3)–C(b3)	110.92(6)	C(b2)–C(21)–C(22)	112.16(6)
C(m1)–C(a3)–C(b3)	123.98(6)	C(b3)–C(31)–C(32)	113.46(7)
N(2)–C(a4)–C(m2)	124.38(6)	C(b4)–C(41)–C(42)	113.73(7)
N(2)–C(a4)–C(b4)	111.17(6)	C(b5)–C(51)–C(52)	113.10(7)
C(m2)–C(a4)–C(b4)	124.36(7)	C(b6)–C(61)–C(62)	113.65(6)
N(3)–C(a5)–C(m2)	124.99(6)	C(b7)–C(71)–C(72)	113.23(7)
N(3)–C(a5)–C(b5)	110.94(6)	C(b8)–C(81)–C(82)	112.51(7)
C(m2)–C(a5)–C(b5)	124.06(6)		

[a]The esd's of the least significant digits are given in parentheses.

Table S11. Anisotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P\bar{1}$)[a]

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
Fe(1)	0.0089(1)	0.0091(1)	0.0120(1)	−0.0018(1)	0.0014(1)	−0.0018(1)
N(1)	0.0106(2)	0.0113(2)	0.0144(2)	−0.0021(2)	0.0026(2)	−0.0024(2)
N(2)	0.0109(2)	0.0098(2)	0.0150(2)	−0.0019(2)	0.0021(2)	−0.0013(2)
N(3)	0.0102(2)	0.0098(2)	0.0136(2)	−0.0012(2)	0.0017(2)	−0.0020(2)
N(4)	0.0109(2)	0.0104(2)	0.0131(2)	−0.0012(2)	0.0018(2)	−0.0020(2)
N(5)	0.0156(2)	0.0162(3)	0.0172(2)	−0.0041(2)	−0.0006(2)	−0.0027(2)
O(1)	0.0494(5)	0.0428(5)	0.0174(3)	−0.0040(3)	−0.0038(3)	−0.0174(4)
C(m1)	0.0112(2)	0.0128(3)	0.0176(3)	−0.0029(2)	0.0027(2)	−0.0008(2)
C(m2)	0.0125(2)	0.0110(3)	0.0156(3)	−0.0008(2)	0.0025(2)	−0.0022(2)
C(m3)	0.0106(2)	0.0114(3)	0.0154(2)	−0.0009(2)	0.0015(2)	−0.0010(2)
C(m4)	0.0126(2)	0.0127(3)	0.0150(2)	−0.0006(2)	0.0031(2)	−0.0029(2)
C(a1)	0.0114(2)	0.0136(3)	0.0134(2)	−0.0024(2)	0.0029(2)	−0.0031(2)
C(a2)	0.0106(2)	0.0130(3)	0.0151(2)	−0.0036(2)	0.0027(2)	−0.0024(2)
C(a3)	0.0118(2)	0.0111(3)	0.0154(3)	−0.0024(2)	0.0016(2)	−0.0011(2)
C(a4)	0.0121(2)	0.0104(2)	0.0146(2)	−0.0014(2)	0.0016(2)	−0.0016(2)
C(a5)	0.0109(2)	0.0111(2)	0.0137(2)	−0.0013(2)	0.0020(2)	−0.0025(2)
C(a6)	0.0102(2)	0.0105(2)	0.0137(2)	−0.0017(2)	0.0013(2)	−0.0020(2)
C(a7)	0.0112(2)	0.0104(2)	0.0138(2)	−0.0011(2)	0.0007(2)	−0.0015(2)
C(a8)	0.0120(2)	0.0117(3)	0.0127(2)	−0.0006(2)	0.0014(2)	−0.0024(2)
C(b1)	0.0123(2)	0.0146(3)	0.0138(2)	−0.0035(2)	0.0033(2)	−0.0039(2)
C(b2)	0.0112(2)	0.0148(3)	0.0144(2)	−0.0043(2)	0.0029(2)	−0.0029(2)
C(b3)	0.0127(2)	0.0116(3)	0.0158(3)	−0.0020(2)	0.0007(2)	0.0000(2)
C(b4)	0.0136(2)	0.0104(2)	0.0149(2)	−0.0014(2)	0.0009(2)	−0.0012(2)
C(b5)	0.0116(2)	0.0122(3)	0.0135(2)	−0.0023(2)	0.0026(2)	−0.0031(2)
C(b6)	0.0105(2)	0.0126(3)	0.0131(2)	−0.0029(2)	0.0019(2)	−0.0024(2)
C(b7)	0.0123(2)	0.0115(3)	0.0133(2)	−0.0002(2)	0.0002(2)	−0.0011(2)
C(b8)	0.0134(2)	0.0114(3)	0.0131(2)	0.0006(2)	0.0002(2)	−0.0023(2)
C(11)	0.0163(3)	0.0179(3)	0.0151(3)	−0.0037(2)	0.0054(2)	−0.0059(2)
C(12)	0.0223(3)	0.0211(4)	0.0221(3)	−0.0050(3)	0.0035(3)	−0.0106(3)
C(21)	0.0121(2)	0.0187(3)	0.0171(3)	−0.0063(2)	0.0038(2)	−0.0019(2)
C(22)	0.0149(3)	0.0247(4)	0.0227(3)	−0.0075(3)	−0.0006(2)	−0.0015(2)
C(31)	0.0142(3)	0.0143(3)	0.0187(3)	−0.0013(2)	0.0001(2)	0.0017(2)
C(32)	0.0205(3)	0.0174(3)	0.0219(3)	−0.0044(3)	0.0028(2)	0.0038(2)
C(41)	0.0166(3)	0.0119(3)	0.0181(3)	0.0003(2)	0.0006(2)	−0.0024(2)

Table S11. Continued

atom	U_{11}	U_{22}	U_{33}	U_{23}	U_{13}	U_{12}
C(42)	0.0326(5)	0.0208(4)	0.0286(4)	−0.0037(3)	−0.0011(3)	−0.0129(3)
C(51)	0.0164(3)	0.0154(3)	0.0164(3)	−0.0009(2)	0.0055(2)	−0.0040(2)
C(52)	0.0223(4)	0.0187(4)	0.0297(4)	−0.0007(3)	0.0028(3)	−0.0098(3)
C(61)	0.0113(2)	0.0153(3)	0.0164(3)	−0.0043(2)	0.0026(2)	−0.0015(2)
C(62)	0.0139(3)	0.0237(4)	0.0298(4)	−0.0087(3)	−0.0032(3)	−0.0004(2)
C(71)	0.0139(3)	0.0145(3)	0.0186(3)	0.0013(2)	0.0001(2)	0.0012(2)
C(72)	0.0227(4)	0.0169(3)	0.0252(4)	−0.0042(3)	0.0039(3)	0.0026(3)
C(81)	0.0169(3)	0.0149(3)	0.0183(3)	0.0039(2)	0.0015(2)	−0.0025(2)
C(82)	0.0291(4)	0.0203(4)	0.0349(5)	0.0026(3)	−0.0038(4)	−0.0120(3)

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

Table S12. Hydrogen Atom Coordinates and Equivalent Isotropic Displacement Parameters (Å^2) for [Fe(OEP)(NO)] ($P\bar{1}$)[a]

atom	x	y	z	U(eq)
H(m1)	−0.22022(7)	0.34920(7)	0.28556(6)	0.017
H(m2)	0.28955(7)	0.39457(7)	0.06693(5)	0.016
H(m3)	0.50266(7)	−0.18265(7)	0.23284(5)	0.015
H(m4)	−0.00538(7)	−0.22584(7)	0.45431(5)	0.016
H(11A)	−0.30500(8)	−0.05144(8)	0.54368(6)	0.019
H(11B)	−0.17450(8)	−0.15746(8)	0.55042(6)	0.019
H(12A)	−0.3480(9)	−0.2504(7)	0.50363(7)	0.031
H(12B)	−0.2512(3)	−0.2353(8)	0.4149(6)	0.031
H(12C)	−0.3838(6)	−0.13328(14)	0.4137(6)	0.031
H(21A)	−0.34983(7)	0.28927(8)	0.40836(6)	0.019
H(21B)	−0.38554(7)	0.16475(8)	0.47958(6)	0.019
H(22A)	−0.5438(3)	0.2379(8)	0.3519(5)	0.031
H(22B)	−0.4724(7)	0.0926(2)	0.3472(5)	0.031
H(22C)	−0.4331(5)	0.2138(10)	0.27439(7)	0.031
H(31A)	−0.25678(7)	0.53470(8)	0.16128(6)	0.020
H(31B)	−0.17648(7)	0.64428(8)	0.11174(6)	0.020
H(32A)	−0.2766(5)	0.7013(7)	0.2537(3)	0.031
H(32B)	−0.1216(5)	0.6835(9)	0.2654(4)	0.031
H(32C)	−0.1971(10)	0.57070(15)	0.31662(10)	0.031
H(41A)	0.00858(8)	0.65611(8)	0.02867(6)	0.019
H(41B)	0.15213(8)	0.57977(8)	0.01625(6)	0.019
H(42A)	0.1636(10)	0.7721(6)	0.07672(12)	0.040
H(42B)	0.2244(6)	0.6480(4)	0.1556(7)	0.040
H(42C)	0.0806(5)	0.7241(9)	0.1683(6)	0.040
H(51A)	0.45376(8)	0.32339(8)	−0.03145(6)	0.019
H(51B)	0.58389(8)	0.21726(8)	−0.02636(6)	0.019
H(52A)	0.6281(9)	0.4179(7)	0.00995(8)	0.035
H(52B)	0.6689(6)	0.30126(14)	0.0994(6)	0.035
H(52C)	0.5363(3)	0.4023(8)	0.1017(6)	0.035
H(61A)	0.65964(7)	−0.00219(8)	0.03310(5)	0.017
H(61B)	0.63060(7)	−0.12345(8)	0.11090(5)	0.017
H(62A)	0.8311(2)	−0.0690(8)	0.1501(5)	0.033
H(62B)	0.7309(5)	−0.0423(10)	0.23408(8)	0.033
H(62C)	0.7620(7)	0.0770(2)	0.1551(6)	0.033

Table S12. Continued

atom	x	y	z	U(eq)
H(71A)	0.46231(7)	−0.47574(8)	0.41093(6)	0.020
H(71B)	0.54305(7)	−0.36686(8)	0.36075(6)	0.020
H(72A)	0.5569(5)	−0.5313(8)	0.2664(4)	0.033
H(72B)	0.4770(10)	−0.3993(2)	0.20562(9)	0.033
H(72C)	0.4015(5)	−0.5118(9)	0.2575(4)	0.033
H(81A)	0.13936(8)	−0.40312(8)	0.51550(6)	0.021
H(81B)	0.27739(8)	−0.48617(8)	0.49635(6)	0.021
H(82A)	0.1071(10)	−0.5892(6)	0.4535(2)	0.042
H(82B)	0.1872(4)	−0.5451(9)	0.3593(6)	0.042
H(82C)	0.0493(6)	−0.4610(3)	0.3774(7)	0.042

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

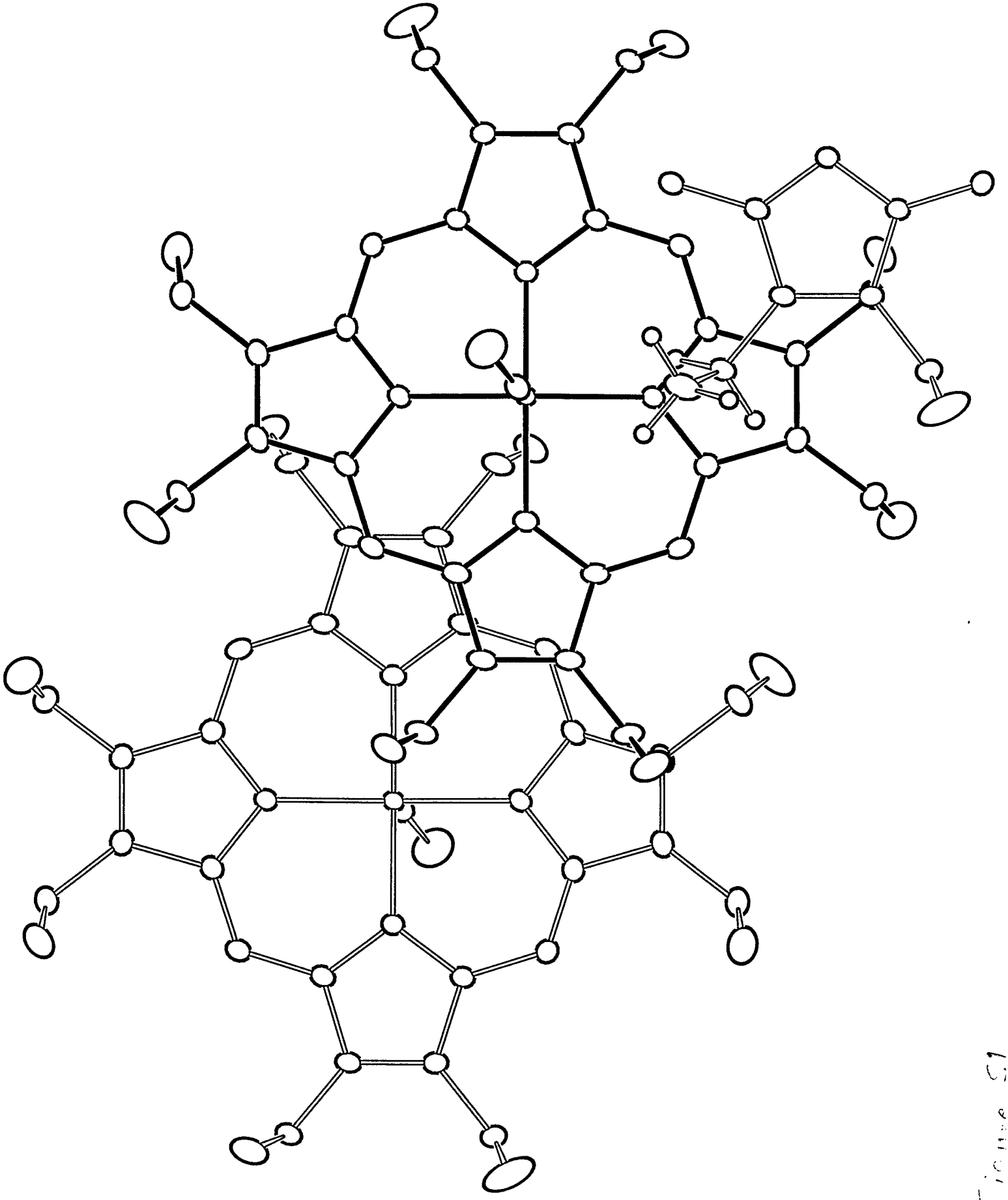

Figure S1