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Table S1. Crystal Data and Intensity Data Collection Parameters for $[Fe(OEP)Cl]ClO_4 \cdot CH_2Cl_2$

Parameter	Value
empirical formula	$C_{37}H_{46}FeCl_4O_4N_4$
formula weight, Daltons	808.46
crystal dimensions, mm	0.074 x 0.27 x 0.31
crystal color and shape	deep brown diamond shaped plate
temperature, deg K	123 ± 2
crystal system	monoclinic
space group	*C2/c* (No. 15)
a, Å	27.454 (7)
b, Å	15.322 (3)
c, Å	19.802 (3)
β, degrees	116.14 (2)
V, A^3	7477.4
lattice parameter refinement	25 reflns; $9.2° < 2\theta < 32.8°$
Z	8
calculated density, g/cm^3	1.44
μ(MoKα), cm^{-1}	7.34
diffractometer	Enraf-Nonius CAD4
radiation	graphite crystal, incident beam monochromated MoKα, $\bar{\lambda}$=0.71073 Å
attenuator	Zr foil, factor 19.3
take-off angle, deg	2.8
crystal-detector distance, cm	21
omega width at half-height, deg	0.21
scan type	$\theta/2\theta$
scan rate, deg/min in omega	4.12
scan width, deg	0.85+0.34tanθ
2θ maximum, deg	56.8
$\sin\theta/\lambda$ maximum	0.669
total data measured	11146
unique data, measured	9178
Fo>3σ(Fo)	5787
corrections, on I	Lorentz-polarization linear decay (correction: 1.000 to 1.034) absorption (transmission; 0.798 to 1.000)
reflection averaging (1968 pairs)	$R_{merge}(I)=0.040$; $R_{merge}(F)=0.026$
refinement	full-matrix least-squares
hydrogen atom	fixed: d[CH]=0.95Å; B[H]=1.1B[attached C]
minimization function	$\Sigma w(\lvert F_o\rvert - \lvert F_c\rvert)^2$
p, weight=$[\sigma^2(F)^2+p^2F^2]^{-1/2}$	0.04
anomalous dispérsion	Fe,Cl
data:variable ratio	12.8
discrepency indices, R_1	0.069
R_2	0.063
goodness of fit	1.45
convergence, largest shift/error	0.01
high peak in final diff. map	0.64(16)$e^-/Å^3$
computer hardware	VAXstation 3200 and VAXstation 4000-90

Table S2. Fractional Coordinates

Atom	x	y	z
Fe	0.46348(2)	0.27537(4)	0.13434(3)
Cl(1)	0.42926(4)	0.27829(8)	0.01160(6)
N(1)	0.4910(1)	0.1493(2)	0.1602(2)
N(2)	0.3993(1)	0.2402(2)	0.1562(2)
N(3)	0.4507(1)	0.4008(2)	0.1592(2)
N(4)	0.5428(1)	0.3105(2)	0.1641(2)
C(a1)	0.5366(2)	0.1158(3)	0.1591(2)
C(a2)	0.4600(2)	0.0778(3)	0.1597(2)
C(a3)	0.3815(2)	0.1580(3)	0.1578(2)
C(a4)	0.3577(2)	0.2945(3)	0.1522(2)
C(a5)	0.4040(2)	0.4343(3)	0.1559(2)
C(a6)	0.4818(2)	0.4732(3)	0.1598(2)
C(a7)	0.5613(2)	0.3921(3)	0.1638(2)
C(a8)	0.5833(2)	0.2555(3)	0.1639(2)
C(b1)	0.5350(2)	0.0205(3)	0.1566(2)
C(b2)	0.4873(2)	-0.0027(3)	0.1566(2)
C(b3)	0.3280(2)	0.1586(3)	0.1557(2)
C(b4)	0.3125(1)	0.2427(3)	0.1499(2)
C(b5)	0.4050(2)	0.5292(3)	0.1561(2)
C(b6)	0.4525(2)	0.5534(3)	0.1561(2)
C(b7)	0.6139(2)	0.3920(3)	0.1644(2)
C(b8)	0.6280(2)	0.3071(3)	0.1653(2)
C(m1)	0.4103(2)	0.0815(3)	0.1603(2)
C(m2)	0.3598(2)	0.3839(3)	0.1519(2)
C(m3)	0.5326(2)	0.4688(3)	0.1626(2)
C(m4)	0.5800(2)	0.1661(3)	0.1613(2)
C(11)	0.5768(2)	-0.0372(3)	0.1516(2)
C(12)	0.5646(2)	-0.0615(4)	0.0713(3)
C(21)	0.4636(2)	-0.0919(3)	0.1524(2)
C(22)	0.4185(2)	-0.1141(3)	0.0742(3)
C(31)	0.2974(2)	0.0787(3)	0.1589(2)
C(32)	0.2662(2)	0.0337(3)	0.0828(3)
C(41)	0.2591(2)	0.2787(3)	0.1415(2)
C(42)	0.2177(2)	0.2912(3)	0.0596(3)
C(51)	0.3608(2)	0.5881(3)	0.1544(2)
C(52)	0.3221(2)	0.6171(3)	0.0750(3)
C(61)	0.4736(2)	0.6422(3)	0.1528(2)
C(62)	0.4705(2)	0.6623(3)	0.0743(3)
C(71)	0.6446(2)	0.4723(3)	0.1617(2)
C(72)	0.6234(2)	0.5121(3)	0.0833(3)
C(81)	0.6795(2)	0.2720(3)	0.1671(2)
C(82)	0.6778(2)	0.2672(3)	0.0892(2)
Cl(2)	0.22140(4)	0.47393(7)	-0.33943(6)
O(1)	0.2172(1)	0.5434(2)	-0.2926(2)
O(2)	0.2428(1)	0.5083(2)	-0.3885(2)
O(3)	0.2574(1)	0.4070(2)	-0.2920(2)

Table S2 -- continued

Atom	x	y	z
O(4)	0.1685(1)	0.4371(2)	-0.3835(2)
C(9)	0.3269(2)	0.2233(3)	-0.2535(3)
Cl(3)	0.38519(6)	0.26991(9)	-0.18160(7)
Cl(4)	0.34107(6)	0.17498(9)	-0.32390(7)

a. Estimated standard deviations in the least significant digits are given in parentheses.

Table S3. General Atomic Displacement Parameters (in Å^2)[a]

Name	U_{11}	U_{22}	U_{33}	U_{12}	U_{13}	U_{23}
Fe	0.0094(2)	0.0080(3)	0.0142(2)	0.0009(2)	0.0051(2)	-0.0003(3)
Cl(1)	0.0249(4)	0.0230(6)	0.0154(4)	0.0003(5)	0.0062(3)	0.0001(5)
N(1)	0.012(1)	0.008(2)	0.018(1)	0.000(1)	0.007(1)	0.000(1)
N(2)	0.013(1)	0.009(2)	0.016(1)	0.001(1)	0.0083(9)	-0.002(1)
N(3)	0.012(1)	0.012(2)	0.016(1)	-0.001(1)	0.007(1)	0.000(1)
N(4)	0.011(1)	0.011(2)	0.015(1)	-0.001(1)	0.004(1)	0.001(1)
C(a1)	0.015(2)	0.011(2)	0.015(2)	0.003(2)	0.008(1)	0.002(2)
C(a2)	0.015(2)	0.013(2)	0.012(2)	0.001(2)	0.003(1)	0.002(2)
C(a3)	0.010(1)	0.015(2)	0.013(2)	0.000(2)	0.004(1)	-0.001(2)
C(a4)	0.012(1)	0.011(2)	0.016(2)	0.002(1)	0.006(1)	-0.002(2)
C(a5)	0.010(1)	0.013(2)	0.013(2)	0.000(2)	0.005(1)	-0.002(2)
C(a6)	0.017(2)	0.006(2)	0.013(2)	0.002(2)	0.004(1)	0.002(2)
C(a7)	0.012(2)	0.010(2)	0.013(2)	0.001(2)	0.003(1)	0.002(2)
C(a8)	0.011(1)	0.013(2)	0.014(2)	0.003(1)	0.005(1)	0.003(2)
C(b1)	0.018(2)	0.008(2)	0.012(2)	0.005(2)	0.007(1)	0.003(2)
C(b2)	0.013(2)	0.009(2)	0.015(2)	0.002(2)	0.004(1)	0.001(2)
C(b3)	0.014(2)	0.018(2)	0.011(2)	-0.000(2)	0.006(1)	-0.001(2)
C(b4)	0.011(1)	0.017(2)	0.013(2)	-0.001(2)	0.006(1)	-0.001(2)
C(b5)	0.014(2)	0.016(2)	0.011(2)	0.000(2)	0.004(1)	-0.001(2)
C(b6)	0.015(2)	0.010(2)	0.015(2)	0.001(2)	0.007(1)	-0.002(2)
C(b7)	0.012(1)	0.017(2)	0.009(2)	-0.001(2)	0.004(1)	0.000(2)
C(b8)	0.012(1)	0.010(2)	0.012(2)	0.003(2)	0.005(1)	0.002(2)
C(m1)	0.013(2)	0.012(2)	0.015(2)	0.002(2)	0.005(1)	0.001(2)
C(m2)	0.014(2)	0.010(2)	0.015(2)	-0.001(2)	0.007(1)	-0.001(2)
C(m3)	0.014(2)	0.009(2)	0.017(2)	-0.004(2)	0.005(1)	-0.002(2)
C(m4)	0.013(2)	0.016(2)	0.014(2)	0.005(2)	0.006(1)	0.003(2)
C(11)	0.019(2)	0.009(2)	0.028(2)	0.006(2)	0.013(1)	0.005(2)
C(12)	0.026(2)	0.033(3)	0.031(2)	0.004(2)	0.017(1)	-0.005(2)
C(21)	0.018(2)	0.010(2)	0.022(2)	0.002(2)	0.007(1)	0.002(2)
C(22)	0.024(2)	0.016(2)	0.023(2)	-0.003(2)	0.006(2)	-0.004(2)
C(31)	0.018(2)	0.011(2)	0.026(2)	-0.002(2)	0.011(1)	0.001(2)
C(32)	0.031(2)	0.015(2)	0.028(2)	-0.012(2)	0.004(2)	-0.004(2)
C(41)	0.015(1)	0.014(2)	0.020(2)	-0.000(2)	0.009(1)	-0.001(2)
C(42)	0.015(2)	0.028(3)	0.028(2)	0.006(2)	0.002(2)	-0.003(2)
C(51)	0.018(2)	0.008(2)	0.017(2)	0.003(2)	0.007(1)	0.000(2)
C(52)	0.020(2)	0.030(3)	0.021(2)	0.011(2)	0.005(1)	0.005(2)
C(61)	0.017(2)	0.012(2)	0.025(2)	-0.002(2)	0.008(1)	0.000(2)
C(62)	0.027(2)	0.014(2)	0.031(2)	0.000(2)	0.015(1)	0.006(2)
C(71)	0.012(2)	0.015(2)	0.028(2)	-0.001(2)	0.009(1)	-0.000(2)
C(72)	0.032(2)	0.020(2)	0.033(2)	0.002(2)	0.019(1)	0.006(2)
C(81)	0.013(1)	0.019(2)	0.018(2)	0.001(2)	0.008(1)	0.002(2)
C(82)	0.027(2)	0.030(3)	0.020(2)	0.011(2)	0.012(1)	0.005(2)
Cl(2)	0.0139(4)	0.0133(5)	0.0298(4)	-0.0017(4)	0.0121(3)	0.0009(4)
O(1)	0.030(1)	0.017(2)	0.033(1)	-0.000(1)	0.018(1)	-0.006(1)
O(2)	0.029(1)	0.021(2)	0.038(1)	-0.001(1)	0.023(1)	0.002(1)
O(3)	0.019(1)	0.016(2)	0.035(2)	0.005(1)	0.009(1)	0.005(1)
O(4)	0.014(1)	0.023(2)	0.038(2)	-0.004(1)	0.010(1)	0.003(1)
C(9)	0.021(2)	0.021(2)	0.034(2)	0.000(2)	0.012(1)	-0.001(2)
Cl(3)	0.0512(7)	0.0218(6)	0.0228(6)	0.0007(6)	0.0006(5)	0.0007(6)
Cl(4)	0.0546(7)	0.0212(6)	0.0256(6)	0.0041(6)	0.0137(5)	-0.0016(5)

a. Estimated standard deviations in the least significant digits are given in parentheses. The form of the anisotropic displacement parameter is: $\exp[-2\pi^2\{h^2a^{*2}U_{11}+k^2b^{*2}U_{22}+l^2c^{*2}U_{33}+2hka^*b^*U_{12}+2hla^*c^*U_{13}+2klb^*c^*U_{23}\}]$ where a^*, b^*, and c^* are reciprocal lattice constants.

Table S4. Fractional Monoclinic Coordinates and Isotropic Thermal Parameters (Å^2) for the Fixed Hydrogen Contributions[a]

Atom	x	y	z	B_{iso}
H(m1)	0.394	0.028	0.163	1.2
H(m2)	0.329	0.415	0.149	1.1
H(m3)	0.550	0.523	0.164	1.2
H(m4)	0.610	0.135	0.161	1.3
H(11a)	0.579	-0.089	0.179	1.6
H(11b)	0.611	-0.008	0.174	1.6
H(12a)	0.593	-0.098	0.072	2.5
H(12b)	0.531	-0.091	0.048	2.5
H(12c)	0.563	-0.010	0.044	2.5
H(21a)	0.449	-0.095	0.188	1.5
H(21b)	0.492	-0.134	0.165	1.5
H(22a)	0.405	-0.171	0.075	1.9
H(22b)	0.390	-0.073	0.061	1.9
H(22c)	0.433	-0.112	0.038	1.9
H(31a)	0.272	0.095	0.177	1.6
H(31b)	0.323	0.038	0.192	1.6
H(32a)	0.248	-0.016	0.089	2.4
H(32b)	0.240	0.073	0.049	2.4
H(32c)	0.291	0.016	0.064	2.4
H(41a)	0.266	0.334	0.166	1.4
H(41b)	0.244	0.239	0.165	1.4
H(42a)	0.185	0.314	0.058	2.3
H(42b)	0.232	0.331	0.036	2.3
H(42c)	0.211	0.237	0.034	2.3
H(51a)	0.377	0.638	0.184	1.3
H(51b)	0.341	0.558	0.175	1.3
H(52a)	0.295	0.654	0.077	2.2
H(52b)	0.342	0.648	0.053	2.2
H(52c)	0.305	0.567	0.045	2.2
H(61a)	0.510	0.646	0.189	1.6
H(61b)	0.453	0.684	0.164	1.6
H(62a)	0.484	0.719	0.075	2.0
H(62b)	0.492	0.621	0.063	2.0
H(62c)	0.434	0.659	0.037	2.0
H(71a)	0.682	0.457	0.178	1.6
H(71b)	0.642	0.515	0.195	1.6
H(72a)	0.644	0.562	0.085	2.3
H(72b)	0.626	0.471	0.050	2.3
H(72c)	0.586	0.528	0.066	2.3
H(81a)	0.686	0.215	0.188	1.4
H(81b)	0.709	0.309	0.198	1.4
H(82a)	0.711	0.245	0.093	2.2
H(82b)	0.649	0.230	0.058	2.2
H(82c)	0.672	0.324	0.068	2.2
H(9a)	0.300	0.268	-0.276	2.2
H(9b)	0.313	0.180	-0.232	2.2

a. Hydrogens idealized with d[C-H]=0.95Å and B[H]=1.1B[C].