Supporting Information for:

Models of the Cytochromes: Crystal Structures and EPR Spectral Characterization of Low-Spin Bis-Imidazole Complexes of (OETPP)Fe^{III} Having Intermediate Ligand Plane Dihedral Angles

Liliya A. Yatsunyk, Alice Dawson,[†] Michael D. Carducci, Gary S. Nichol and F. Ann Walker*

Contribution from the Department of Chemistry, University of Arizona, Tucson, AZ 85721-0041

Structure determination: experimental details

[(OETPP)Fe(HIm)$_2$]Cl A dark needle of $[FeN_8C_{66}H_{68}]^+Cl^-.5(CH_2Cl_2)$ having approximate dimensions of 0.34 x 0.27 x 0.22 mm^3 was mounted on a glass fiber in a random orientation. A total of 4686 frames at 1 detector setting covering $0 < 2\theta < 60^o$ were collected, having an omega scan width of 0.2º and an exposure time of 20 s. A total of 99450 reflections were integrated and retained of which 10891 were unique (<redundancy> = 9.13, Rint = 13.2%, Rsig = 8.4%). Of the unique reflections, 7226 (66.3%) were observed > 2σ(I). The final trigonal cell parameters of *a* = 21.7714(11)Å, *b* = 21.7714(11)Å, *c* = 27.6277(18)Å, α = 90º, β = 90º, γ = 120º, V = 11340.9(11) $Å^3$ are based on the refinement of the XYZ-centroids of 5425 reflections with I > 3σ(I) covering the range of 2.15º < θ < 19.6 º. An absorption correction was applied using the program Sadabs (Sheldrick, 2002). The absorption coefficient is 0.633 mm^{-1}. For Z = 6 and F.W. = 1489.21 the calculated density is 1.308 g cm^{-3}. Systematic absences and intensity

statistics indicate the space group to be $P3_221$ (154) which was consistent with the refinement. The porphyrin complexes form an open framework, with large channels in the structure. It was possible to identify what appeared to be dichloromethane solvent molecules within these channels from difference Fourier syntheses; however these could not be refined with reasonable structural parameters. Instead the residual electron density due to solvent was treated using the method of van der Sluis and Spek (1990); this gave a residual electron count per unit cell of 1158 electrons and a solvent accessible void of 3463.9 $Å^3$ centered on the origin. This was assumed to correspond to five molecules of CH_2Cl_2 per porphyrin complex for the calculation of molecular weight, density and F(000). The crystals were observed to break down rapidly on removal from the mother liquor, indicating the incorporation of a substantial amount of solvent in the lattice.

A resolution cut-off of 0.9 Å (23.3 º in 2θ) was applied during data processing. Higher angle data were very weak and worsened the refinement. Weak high angle data is common in systems with extensive solvent disorder.

The unit cell is doubled in *c* with respect to the 1-methylimidazole and 1-benzylimidazole crystal structures (Table 1). It is possible to index the diffraction pattern with a unit cell where *c* = 13.788 Å; this cell leaves a significant number of spots with *l* 0.5 from integer values (Figure S1). The structure can be refined using this smaller cell, giving a similar *R*-factor in the same space group with one half-molecule in the asymmetric unit. The porphyrin is disordered in this setting, with both imidazole ligands and both phenyls disordered over two positions with relative occupancies of 50:50 (in addition to the symmetry imposed disorder). The Cl anion in the larger cell is disordered over two positions close to x, x, 0.25; in the halved cell this position is x, x, 0.5 which is a special position. In the latter case the anion is no longer apparently disordered but the anisotropic displacement parameters are still unacceptable. For the larger unit cell, no large correlations in parameters were observed between the two porphyrin molecules. The spread in

standard uncertainties was similar to that seen for the smaller cell (due to the disorder the s.u.s for the smaller cell structure were larger). The MISSYM algorithm in Platon[1] was used to check for missed translational symmetry in the structure but did not find any. Overlaying the two independent molecules (Figure S2) gave a similar structure to the disordered Z = 0.5 structure. Given the improvement in the number of spots indexed and the removal of extensive disorder in the structure the larger cell was chosen as correct.

The asymmetric unit contains two crystallographically inequivalent half porphyrin molecules (**1** and **2**) each on a two-fold axis that lies along the N_{ax}-Fe-N_{ax} vector (Z = 2×0.5) with different orientations of axial ligands. Due to the symmetry of the molecule the HIm ligands are 2-fold disordered. The C-H and N-H groups could not be distinguished when the structure was refined in space group $P3_2$ (unlike the methyl imidazole case discussed below). The half-occupied C and N were constrained to have equal positions and thermal parameters. One of the imidazole ligands, D, was restrained to be flat. The chloride anion is disordered over two positions, the relative occupancies of which were fixed at 50:50 following refinement.

[(OETPP)Fe(N-BzIm)$_2$]Cl A dark block of $[FeC_{80}H_{80}N_8Cl].3[CH_2Cl_2]$ having approximate dimensions of 0.126 x 0.166 x 0.42 mm^3 was mounted on a glass fiber in a random orientation. A total of 3686 frames at 1 detector setting covering $0 < 2\theta < 60^\circ$ were collected, having an omega scan width of 0.2º and an exposure time of 20 s. A total of 61354 reflections were integrated and retained of which 5498 were unique (<redundancy> = 11.2, Rint = 17.5%, Rsig = 7.0%). Of the unique reflections, 4698 (85%) were observed > 2σ(I). The final trigonal cell parameters of *a* = 21.7519(8) Å, *b* = 21.7519(8) Å, *c* = 13.9290(10) Å, α = 90º, β = 90º, γ = 120º, V = 5707.5(5) Å^3 are based on the refinement of the XYZ-centroids of 4243 reflections with I > 3σ(I) covering the range of $2.15^\circ < \theta < 16.15^\circ$. Empirical absorption and decay

[1] Spek, A. L. *J. Appl. Cryst.* **2003**, *36,* 7-13.

corrections were applied using the program Sadabs (Sheldrick, 2002). The absorption coefficient is 0.494 mm^{-1}, Tmin = 0.925048, and Tmax = 1.0. For $Z = 3$ and F.W. = 1499.60 the calculated density is 1.309 g cm^{-3}. Systematic absences and intensity statistics indicate the space group to be $P3_221$ (#154) which was consistent with refinement. The structure contains large channels as in the imidazole and methyl imidazole cases. The benzyl groups penetrate far into these channels. The disorder of these groups slightly complicates the calculation of the void volume and residual electron density. This was modeled using the method of van der Sluis and Spek (1990). A solvent accessible void of 1181.5 $Å^3$ and a residual electron density of 385 e per unit cell were found; this is assumed to correspond to 3 molecules of CH_2Cl_2 per porphyrin.

Refinement of the structure in $P3_2$ indicated that the symmetry-imposed disorder in $P3_221$ is real and not an artifact of the symmetry of the porphyrin core. Due to the disorder the position occupied by N(3) in each of the imidazole ligands must in fact have occupancy 0.5N and 0.5C. However, including a carbon atom at this site (using positional constraints to ensure the N and C had equivalent coordinates) led to unstable refinement. Instead, the N atom at this position was refined with full occupancy. The phenyl group of the N-BzIm ligand A could be distinguished without difficulty. Constraints were used to impose a hexagonal shape on the group. The phenyl group of ligand B could not be so well distinguished; the atoms of the phenyl ring that could be identified from difference Fourier synthesis were used as the base atoms for a fitted hexagon group. The hexagon constraint was necessary throughout the refinement. Both benzyl groups were refined with isotropic thermal parameters. A common isotropic thermal parameter was refined for the phenyl ring of ligand A, via a free variable. This group has very large thermal parameters that possibly indicate unresolved disorder.

Anisotropic refinement of the pendant phenyl groups on the porphyrin core (in the positions initially obtained from direct methods) lead to unreasonable thermal parameters.

Instead each group was modeled to be disordered over two close-in-space positions; the relative occupancies were fixed at 50% following initial refinement of the occupancies. Distance restraints were applied to the C – C bond lengths, and similarity and rigid bond restraints were used in the refinement of the anisotropic thermal parameters.

The chloride anion was fixed to have 50% occupancy (this must be the case for charge balance); it does not occupy a special position in the structure. Restrained anisotropic refinement was used. The poor thermal parameters are likely to be a result of anion disorder within the channel.

[(OETPP)Fe(N-MeIm)$_2$]Cl A deep red block of $[FeC_{68}H_{72}N_8Cl].4[CHCl_3]$ having approximate dimensions of 0.10 x 0.19 x 0.41 mm^3 was mounted on a glass fiber in a random orientation. A total of 3736 frames at 1 detector setting covering $0 < 2\theta < 60^\circ$ were collected, having an omega scan width of 0.2º and an exposure time of 30 s. A total of 50794 reflections were integrated and retained of which 10854 were unique (<redundancy> = 4.7, Rint = 6.5%, Rsig = 6.9%). Of the unique reflections, 7815 (72.0%) were observed > 2σ(I). The final trigonal cell parameters of *a* = 21.7611(3) Å, *b* = 21.7611(3) Å, *c* = 13.8520(4) Å, α = 90º, β = 90º, γ = 120º, V = 5680.7(2) Å^3 are based on the refinement of the XYZ-centroids of 7374 reflections with I > 3σ(I) covering the range of $2.15^\circ < \theta < 21.08^\circ$. Empirical absorption and decay corrections were applied using the program Sadabs (Sheldrick, 2002). The absorption coefficient is 0.704 mm^{-1}, Tmin = 0.871758, and Tmax = 1.0. For Z = 3 and F.W. = 1570.11 the calculated density is 1.377g cm^{-3}. Systematic absences and intensity statistics indicate the space group to be $P3_2$ (#144) which was consistent with refinement. As in the imidazole case, the structure contains large voids. Residual electron density due to disordered chloroform molecules in these voids was treated using the method of van der Sluis and Spek (1990). A residual electron count per unit cell of 646 and a solvent accessible void of 1745.0 Å^3 was found. This corresponds to

approximately four molecules of chloroform per porphyrin complex.

There is some ambiguity regarding the space group for this compound. The bis-HIm and bis-N-BzIm (OETPP)Fe^{III} complexes crystallize in $P3_221$, where the two-fold axis along N_{ax}-Fe-N_{ax} vector relates one half of the complex to the other with axial ligands disordered about this axis. In the case of [(OETPP)Fe(N-MeIm)$_2$]Cl, although the porphyrin core maintains its two-fold symmetry the disorder of the axial ligands is more complex. For this reason the space group $P3_1$ was chosen over $P3_121$. Similarity restraints corresponding to a two-fold axis were used in refinement of the porphyrin core.

The first of these three crystal structures to be solved was that of [(OETPP)Fe(N-MeIm)$_2$]Cl, and from the first tentative solution there was a question as to whether the crystals might be merohedral twins, especially because of the large apparent void space that was, at that first solution, believed to have only one chloroform molecule per iron porphyrin complex unit. A number of tests were made at that time (2001) and since to verify whether or not the crystals were merohedral twins. For that complex two space groups were considered, $P3_121$ and $P3_1$, the latter of which yielded better R indices and RMS difference density. Diffraction spot shapes were also scrutinized carefully for signs of asymmetry; none was found. Then the powder diffraction data discussed below was obtained, to see if the unit cell was the same as found by single crystal techniques. Finally, a fresh model was created from the raw data. WinGX[2] was used to evaluate putative values of R(sym) in all Laue classes from the raw, uncorrected data. For [(OETPP)Fe(N-MeIm)$_2$]Cl it reported 0.072 for Laue class -3 but 0.121 for -3m. Increasing the space group symmetry from $P3_1$ to P3_121 effectively adds a two-fold rotation axis through the iron center and perpendicular to the porphyrin ring, with the iron located on the rotation axis. While the porphyrin core is compatible with this symmetry element (as evidenced by the data

[2] Farriguia, L. J. *J. Appl. Crystallogr*. **1999**, *32*, 837-838.

sets for the other two complexes) the axial ligands are not. The ligands suffer from both substitutional (exchanging places of the N and C atoms) and static/positional disorder. This second disorder is incompatible with the two-fold axis and the ligands could not be refined anisotropically. It is thus proposed that this rotation is a *pseudo*-symmetry element only, rather than a genuine symmetry element as found in the other two complexes (which are compatible with the two-fold rotation, since the axial ligands do not suffer from the same disorder). This is supported by the ADDSYM-EXT routine in PLATON, which does not detect missed symmetry in space group $P3_1$. For these reasons we are convinced that $P3_1$ is the correct space group for this complex.

Careful checking of the data sets for [(OETPP)Fe(HIm)$_2$]Cl and [(OETPP)Fe(N-BzIm)$_2$]Cl likewise showed that there is no indication of merohedral twinning in any of these three structures; all structures solved easily (were they twinned they would be difficult to solve). The mean E^2-1 test used in XPREP to determine centricity of the space groups reported 0.799 for [(OETPP)Fe(HIm)$_2$]Cl, 0.694 for [(OETPP)Fe(N-BzIm)$_2$]Cl, and 0.789 for [(OETPP)Fe(N-MeIm)$_2$]Cl. Expected values are 0.968 for a centrosymmetric space group and 0.736 for a non-centrosymmetric space group. While the value for [(OETPP)Fe(N-BzIm)$_2$]Cl is slightly lower than expected, it is not of the order of 0.4, which is often the case when a structure is affected by merohedral twinning.

There is one crystallographically independent molecule in this structure that occupies a general position. On one side of the porphyrin core, the axial ligand is disordered over two positions (A and C) with 0.584(12) occupancy of the major component A, and on the other side it is disordered over two positions (B and D) with the occupancy of the major component B of 0.772(10). These occupancies were freely refined. The angle between ligands A and C is 28.6(10)º and between B and D is 43.5(11)°. The axial ligands were refined using restrained

anisotropic thermal parameters, similarity and rigid bond restraints, and flat geometry. Distance restraints based on the geometry of other imidazole ligands in the Cambridge Structural Database were used.

The pendant phenyl rings of the porphyrin core are disordered over two positions. Their refinement was performed in the same way as for the [(OETPP)Fe(N-BzIm)$_2$]Cl complex.

Figure S1

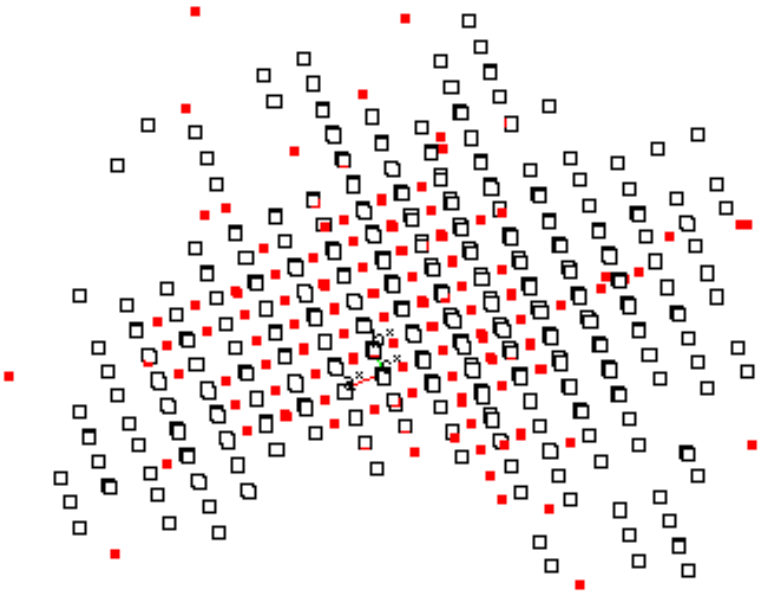


Figure S1. A reciprocal lattice view of the reflection array, indexed using the 21, 21, 13 Å unit cell, viewed along *c**. White squares represent indexed reflections and red (full) squares reflections which are not indexed. The doubling of *c* is clear.

Figure S2

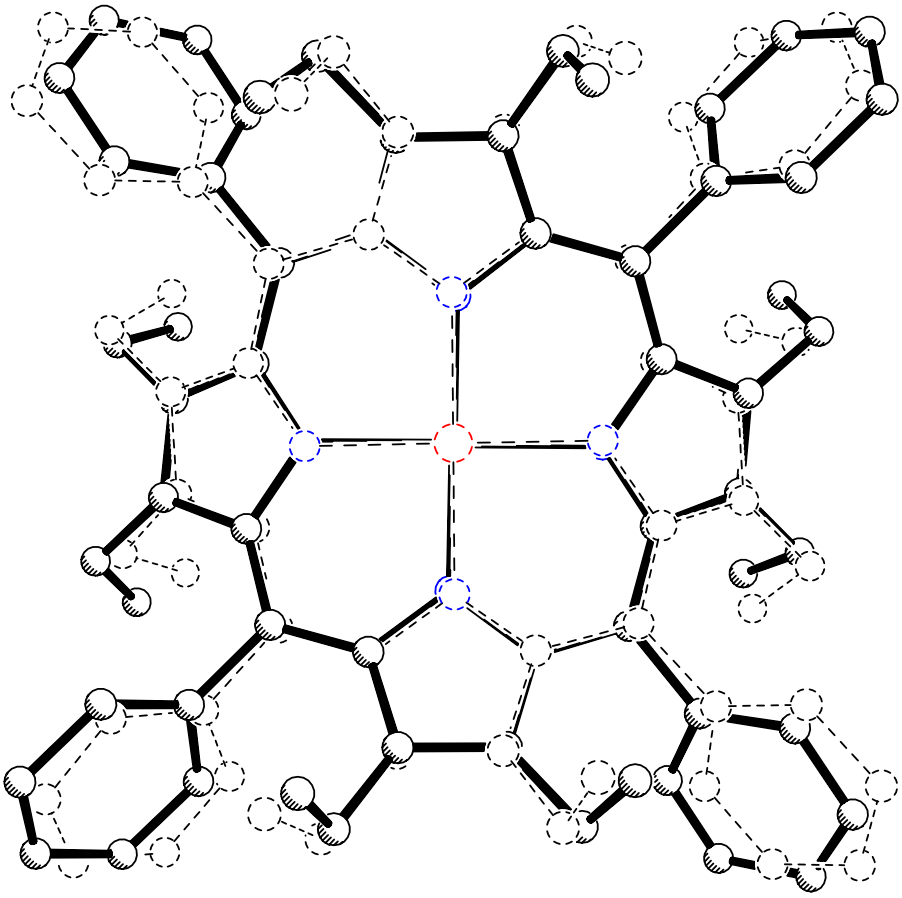
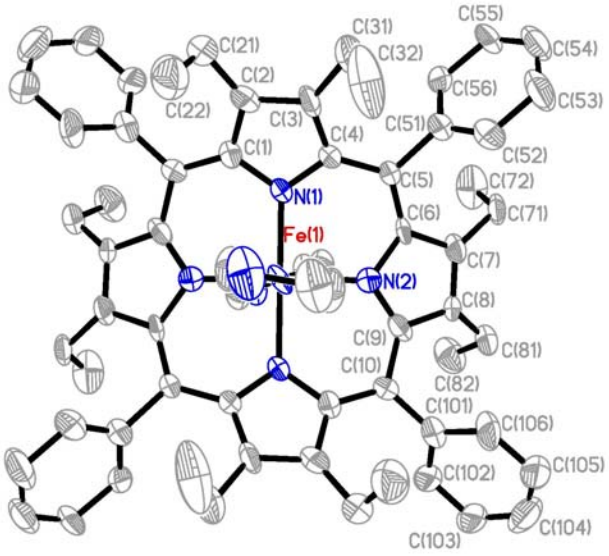
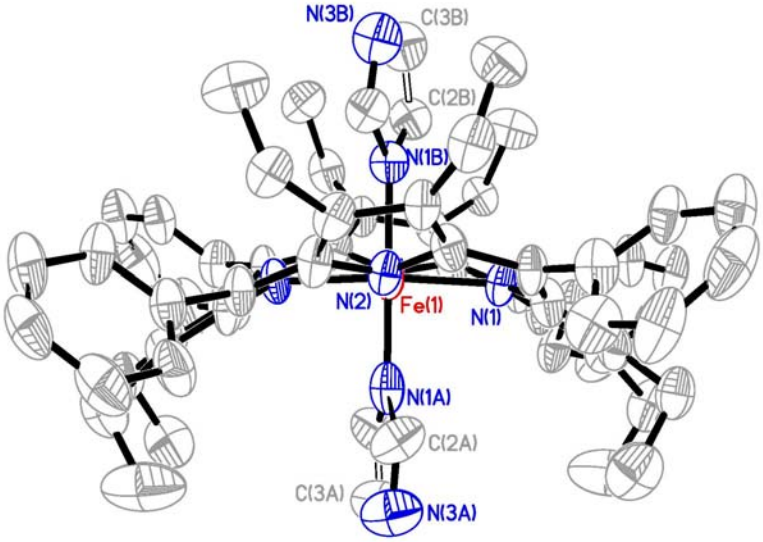


Figure S2. Overlay of the porphyrin cores of the two independent molecules of [(OETPP)Fe(HIm)$_2$]Cl. Molecule **2** - full lines, molecule **1** – dashed lines. The core atoms fit with an average deviation of 0.2312Å.

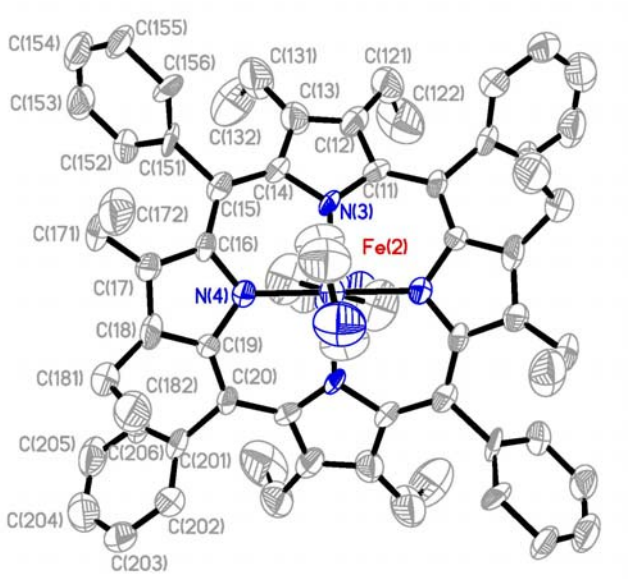
S3a


C(55)
C(31)
C(21)
C(32)
C(54)
C(2)
C(56)
C(22)
C(53)
C(3)
C(51)
C(4)
C(1)
C(52)
C(5)
C(72)
N(1)
C(6)
C(71)
Fe(1)
C(7)
N(2)
C(8)
C(9)
C(81)
C(10)
C(82)
C(101)
C(106)
C(105)
C(102)
C(103)
C(104)

S3b


N(3B)
C(3B)
C(2B)
N(1B)
N(2)
Fe(1)
N(1)
N(1A)
C(2A)
C(3A)
N(3A)

S3c



S3d

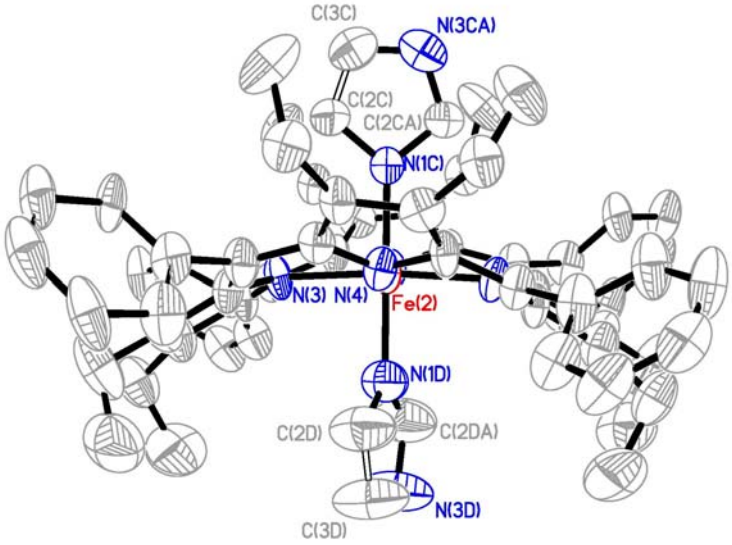
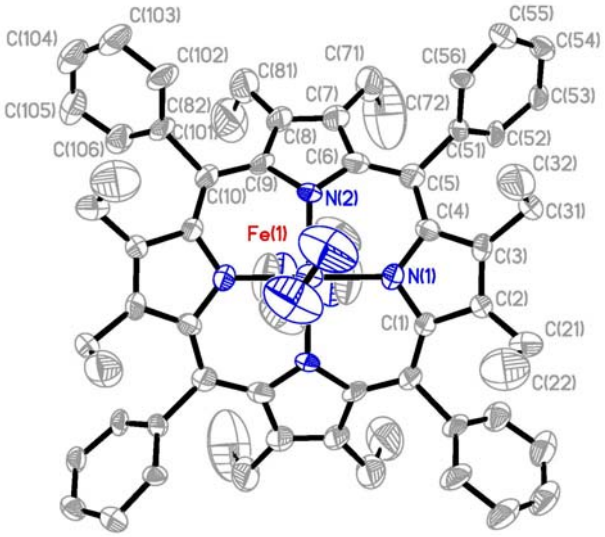


Figure S3. Thermal ellipsoid plots of the porphyrin macrocycle of [(OETPP)Fe(HIm)$_2$]Cl, with the numbering scheme for unique atoms: Molecule 1: a) top view; b) side-on view. Molecule 2: c) top view; d) side-on view. Thermal ellipsoids are shown at 50% probability and H-atoms are omitted for clarity.

4a



4b

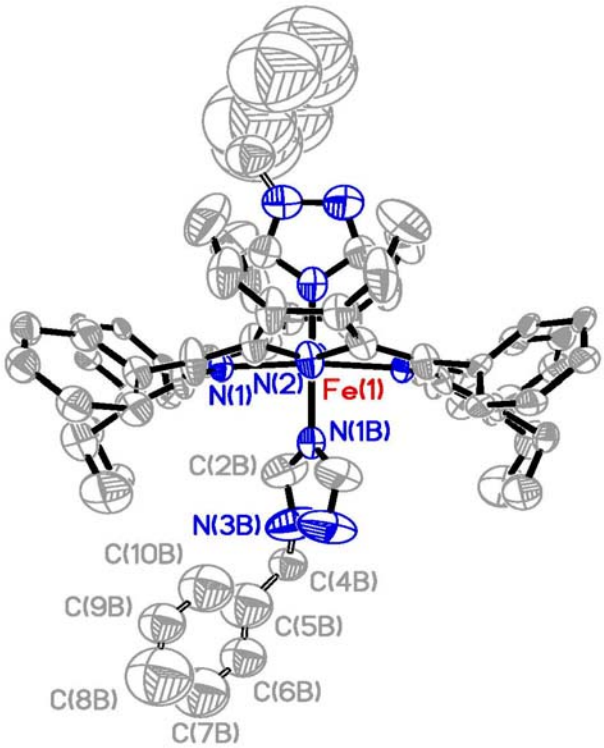


Figure S4. Thermal ellipsoid plots of the porphyrin macrocycle of [(OETPP)Fe(N-BzIm)$_2$]Cl, with the numbering scheme for unique atoms: a) top view; b) side-on view. Thermal ellipsoids are shown at 50% probability and H-atoms are omitted for clarity.

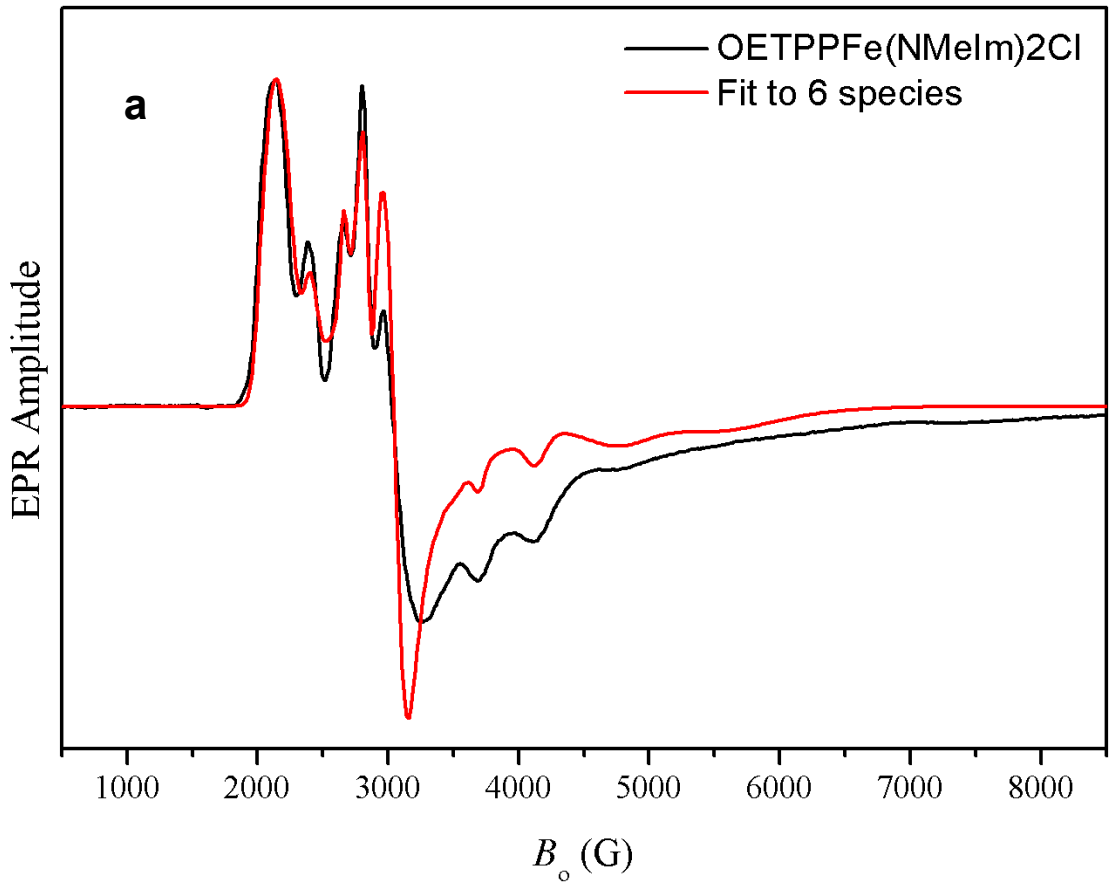


Figure S5. a) Simulation (red trace) of the EPR spectrum of crushed crystals of [OETPPFe(N-MeIm)$_2$]Cl and comparison to the experimental spectrum (black trace) from Figure 5. b) (next page) The species utilized for the simulation are (1) a "large g_{max}" species representing 13% of the crystalline sample, with g = 3.3, 2.01, 1.05 and linewidths of those features of 80, 1000 and 1000 G, respectively; (2) a "large g_{max}" species representing 10% of the crystalline sample, with g = 3.2, 2.08, 1.2 and linewidths of those features of 80, 1000 and 1000 G, respectively; (3) a normal rhombic species representing 45% of the crystalline sample, with g = 3.14, 2.19, 1.18 and linewidths of those features of 160, 170 and 800 G, respectively; (4) a normal rhombic species representing 32% of the crystalline sample, with g = 3.04, 3.20, 1.39 and linewidths of those features of 150, 170, and 500 G, respectively; (5) a normal rhombic species representing 10% of

the signal intensity and probably arising from the frozen mother liquor that accompanied the crystalline sample to prevent decomposition of the crystals, with g = 2.79, 2.36, 1.62 and linewidths of those features of 100, 70 and 150 G, respectively; and (6) a somewhat compressed normal rhombic signal representing 2% of the signal intensity, whose origin is not known, with g = 2.52, 2.31, 1.81 and linewidths of those features of 50, 60 and 80 G, respectively ; the percentages of the last two species were adjusted so as to best account for the observed spectral features. Although the percentages add up to 112%, they are only scaling factors for the relative contributions of each. The lack of agreement in the baseline between the high-field side of the experimental and calculated spectra is likely caused by molecular oxygen in the EPR tube, since the tube was not sealed.

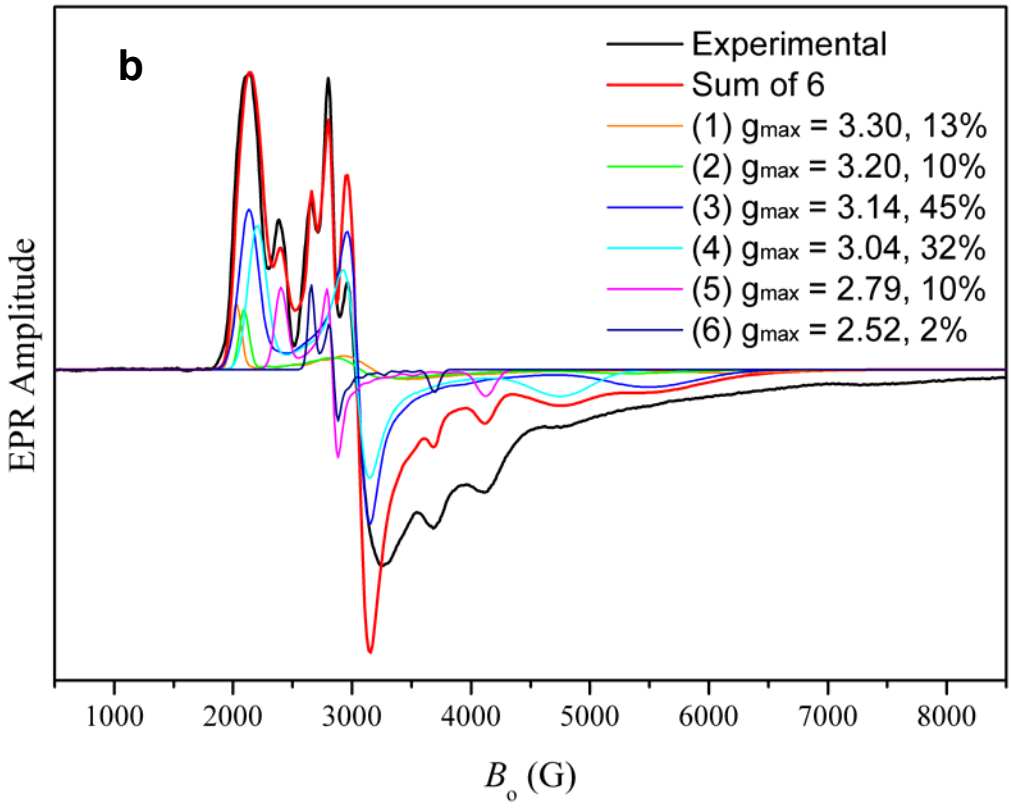


Table S1. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [(OETPP)Fe(HIm)$_2$]Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	0	4183(1)	8333	40(1)
N(1)	-971(2)	3656(2)	8599(2)	39(1)
C(1)	-1569(3)	3220(3)	8322(2)	45(2)
C(2)	-2072(3)	2618(3)	8584(2)	47(2)
C(21)	-2714(3)	1970(4)	8408(2)	56(2)
C(22)	-2479(5)	1514(4)	8108(3)	85(2)
C(3)	-1773(3)	2706(3)	9046(2)	43(2)
C(31)	-2057(4)	2111(4)	9438(2)	69(2)
C(32)	-1648(7)	1738(6)	9441(3)	121(4)
C(4)	-1124(3)	3359(4)	9054(2)	44(2)
C(5)	-699(3)	3723(3)	9458(2)	40(2)
C(51)	-994(3)	3481(3)	9961(2)	48(2)
C(52)	-691(4)	3196(4)	10253(2)	62(2)
C(53)	-944(5)	2968(4)	10729(2)	73(2)
C(54)	-1490(4)	3086(4)	10889(2)	68(2)
C(55)	-1776(4)	3358(4)	10603(2)	64(2)
C(56)	-1538(3)	3573(4)	10126(2)	55(2)
N(2)	384(2)	4412(3)	9002(2)	39(1)
C(6)	-12(3)	4296(3)	9412(2)	42(2)
C(7)	411(3)	4824(3)	9774(2)	44(2)
C(71)	147(3)	4987(4)	10238(2)	44(2)
C(72)	-223(5)	5406(4)	10167(3)	78(2)
C(8)	1079(3)	5249(3)	9581(2)	39(1)
C(81)	1620(3)	5939(4)	9782(2)	55(2)
C(82)	1686(4)	6571(4)	9480(2)	68(2)
C(9)	1049(3)	4936(3)	9107(2)	44(2)
C(10)	1651(3)	5078(3)	8818(2)	43(2)
C(101)	2345(4)	5450(4)	9051(2)	56(2)
C(102)	2884(3)	6101(4)	8886(2)	58(2)
C(103)	3537(4)	6464(4)	9108(3)	70(2)
C(104)	3653(4)	6141(5)	9504(3)	86(2)
C(105)	3151(4)	5465(5)	9674(3)	80(2)
C(106)	2504(4)	5135(4)	9441(2)	64(2)
N(1A)	0	3294(4)	8333	51(2)
C(2A)	307(4)	3071(5)	8655(2)	66(2)
N(3A)	191(5)	2428(4)	8548(2)	83(2)
C(3A)	191(5)	2428(4)	8548(2)	83(2)
N(1B)	0	5101(3)	8333	41(2)
C(2B)	22(3)	5496(4)	8715(2)	52(2)
N(3B)	19(4)	6071(4)	8572(2)	65(2)
C(3B)	19(4)	6071(4)	8572(2)	65(2)
Fe(2)	0	4005(1)	3333	38(1)
N(3)	980(2)	4451(3)	3079(2)	40(1)
C(11)	1538(3)	4525(3)	3348(2)	43(2)
C(12)	2035(4)	4446(4)	3043(2)	57(2)
C(121)	2638(4)	4347(5)	3200(3)	75(2)
C(122)	2356(5)	3602(6)	3401(4)	121(4)

C(13)	1830(3)	4437(4)	2576(2)	54(2)
C(131)	2162(5)	4315(6)	2150(3)	96(3)
C(132)	1862(7)	3575(6)	1997(4)	124(4)
C(14)	1155(3)	4433(3)	2592(2)	44(2)
C(15)	732(3)	4450(4)	2215(2)	50(2)
C(151)	1056(3)	4633(4)	1723(2)	51(2)
C(152)	835(4)	4120(4)	1363(2)	67(2)
C(153)	1157(4)	4285(5)	899(2)	78(2)
C(154)	1673(4)	4976(5)	807(3)	81(2)
C(155)	1892(4)	5498(5)	1143(2)	70(2)
C(156)	1577(3)	5317(4)	1612(2)	59(2)
N(4)	-356(2)	3867(3)	2674(2)	40(1)
C(16)	17(3)	4249(3)	2274(2)	38(1)
C(17)	-416(3)	4348(3)	1929(2)	44(2)
C(171)	-220(4)	4825(4)	1510(2)	56(2)
C(172)	57(5)	5588(4)	1658(3)	85(3)
C(18)	-1100(3)	3938(3)	2108(2)	46(2)
C(181)	-1750(4)	3959(4)	1920(2)	54(2)
C(182)	-1928(4)	4381(5)	2230(3)	81(2)
C(19)	-1062(3)	3634(3)	2549(2)	39(2)
C(20)	-1609(3)	3106(3)	2826(2)	40(1)
C(201)	-2300(3)	2650(4)	2555(2)	56(2)
C(202)	-2926(3)	2621(4)	2663(2)	72(2)
C(203)	-3529(4)	2199(4)	2378(2)	78(2)
C(204)	-3473(4)	1818(4)	2006(3)	75(2)
C(205)	-2856(4)	1819(4)	1905(2)	73(2)
C(206)	-2295(4)	2236(4)	2177(2)	62(2)
N(1C)	0	4906(3)	3333	38(2)
C(2C)	470(4)	5538(4)	3123(3)	70(2)
N(3C)	290(4)	6024(4)	3208(3)	86(2)
C(3C)	290(4)	6024(4)	3208(3)	86(2)
N(1D)	0	3099(4)	3333	68(2)
C(2D)	-31(5)	2720(5)	2930(4)	108(3)
N(3D)	-19(3)	2133(4)	3087(3)	120(3)
C(3D)	-19(3)	2133(4)	3087(3)	120(3)
Cl(5)	1386(5)	1752(4)	2711(3)	152(3)
Cl(5A)	2013(5)	2033(5)	2412(3)	156(3)

Table S2. Bond lengths [Å] and angles [°] for [(OETPP)Fe(HIm)$_2$]Cl.

Fe(1)-N(1A)	1.936(9)	C(82)-H(82A)	0.9800
Fe(1)-N(1)#1	1.975(4)	C(82)-H(82B)	0.9800
Fe(1)-N(1)	1.975(4)	C(82)-H(82C)	0.9800
Fe(1)-N(2)#1	1.985(4)	C(9)-C(10)	1.431(8)
Fe(1)-N(2)	1.985(4)	C(10)-C(1)#1	1.423(8)
Fe(1)-N(1B)	1.998(7)	C(10)-C(101)	1.459(8)
N(1)-C(4)	1.376(7)	C(101)-C(102)	1.389(9)
N(1)-C(1)	1.394(7)	C(101)-C(106)	1.410(9)
C(1)-C(2)	1.417(8)	C(102)-C(103)	1.378(9)
C(1)-C(10)#1	1.423(8)	C(102)-H(102)	0.9500
C(2)-C(3)	1.403(8)	C(103)-C(104)	1.389(11)
C(2)-C(21)	1.487(9)	C(103)-H(103)	0.9500
C(21)-C(22)	1.562(9)	C(104)-C(105)	1.405(11)
C(21)-H(21A)	0.9900	C(104)-H(104)	0.9500
C(21)-H(21B)	0.9900	C(105)-C(106)	1.379(10)
C(22)-H(22A)	0.9800	C(105)-H(105)	0.9500
C(22)-H(22B)	0.9800	C(106)-H(106)	0.9500
C(22)-H(22C)	0.9800	N(1A)-C(2A)#1	1.341(8)
C(3)-C(4)	1.417(9)	N(1A)-C(2A)	1.341(8)
C(3)-C(31)	1.558(8)	C(2A)-N(3A)	1.325(10)
C(31)-C(32)	1.476(10)	C(2A)-H(2A)	0.9500
C(31)-H(31A)	0.9900	N(3A)-N(3A)#1	1.389(14)
C(31)-H(31B)	0.9900	N(1B)-C(2B)#1	1.347(8)
C(32)-H(32A)	0.9800	N(1B)-C(2B)	1.347(8)
C(32)-H(32B)	0.9800	C(2B)-N(3B)	1.315(9)
C(32)-H(32C)	0.9800	C(2B)-H(2B)	0.9500
C(4)-C(5)	1.414(8)	N(3B)-N(3B)#1	1.322(11)
C(5)-C(6)	1.395(8)	Fe(2)-N(4)	1.943(4)
C(5)-C(51)	1.509(8)	Fe(2)-N(4)#2	1.943(4)
C(51)-C(52)	1.371(9)	Fe(2)-N(1C)	1.962(7)
C(51)-C(56)	1.375(9)	Fe(2)-N(1D)	1.973(9)
C(52)-C(53)	1.416(9)	Fe(2)-N(3)	1.979(4)
C(52)-H(52)	0.9500	Fe(2)-N(3)#2	1.979(4)
C(53)-C(54)	1.406(11)	N(3)-C(11)	1.362(7)
C(53)-H(53)	0.9500	N(3)-C(14)	1.404(7)
C(54)-C(55)	1.315(10)	C(11)-C(20)#2	1.410(7)
C(54)-H(54)	0.9500	C(11)-C(12)	1.448(8)
C(55)-C(56)	1.405(8)	C(12)-C(13)	1.362(9)
C(55)-H(55)	0.9500	C(12)-C(121)	1.496(9)
C(56)-H(56)	0.9500	C(121)-C(122)	1.524(12)
N(2)-C(9)	1.351(7)	C(121)-H(12A)	0.9900
N(2)-C(6)	1.369(7)	C(121)-H(12B)	0.9900
C(6)-C(7)	1.454(8)	C(122)-H(12C)	0.9800
C(7)-C(8)	1.382(8)	C(122)-H(12D)	0.9800
C(7)-C(71)	1.519(8)	C(122)-H(12E)	0.9800
C(71)-C(72)	1.502(9)	C(13)-C(14)	1.466(9)
C(71)-H(71A)	0.9900	C(13)-C(131)	1.474(10)
C(71)-H(71B)	0.9900	C(131)-C(132)	1.467(11)
C(72)-H(72A)	0.9800	C(131)-H(13A)	0.9900
C(72)-H(72B)	0.9800	C(131)-H(13B)	0.9900
C(72)-H(72C)	0.9800	C(132)-H(13C)	0.9800
C(8)-C(9)	1.463(8)	C(132)-H(13D)	0.9800
C(8)-C(81)	1.477(9)	C(132)-H(13E)	0.9800
C(81)-C(82)	1.554(9)	C(14)-C(15)	1.403(9)
C(81)-H(81A)	0.9900	C(15)-C(16)	1.400(8)
C(81)-H(81B)	0.9900	C(15)-C(151)	1.490(8)

C(151)-C(156)	1.381(9)
C(151)-C(152)	1.391(9)
C(152)-C(153)	1.418(9)
C(152)-H(152)	0.9500
C(153)-C(154)	1.378(12)
C(153)-H(153)	0.9500
C(154)-C(155)	1.355(10)
C(154)-H(154)	0.9500
C(155)-C(156)	1.426(8)
C(155)-H(155)	0.9500
C(156)-H(156)	0.9500
N(4)-C(16)	1.378(7)
N(4)-C(19)	1.401(7)
C(16)-C(17)	1.431(8)
C(17)-C(18)	1.390(8)
C(17)-C(171)	1.468(8)
C(171)-C(172)	1.511(10)
C(171)-H(17A)	0.9900
C(171)-H(17B)	0.9900
C(172)-H(17C)	0.9800
C(172)-H(17D)	0.9800
C(172)-H(17E)	0.9800
C(18)-C(19)	1.407(8)
C(18)-C(181)	1.529(9)
C(181)-C(182)	1.445(9)
C(181)-H(18A)	0.9900
C(181)-H(18B)	0.9900
C(182)-H(18C)	0.9800
C(182)-H(18D)	0.9800
C(182)-H(18E)	0.9800
C(19)-C(20)	1.398(8)
C(20)-C(11)#2	1.410(7)
C(20)-C(201)	1.522(6)
C(201)-C(202)	1.364(8)
C(201)-C(206)	1.382(8)
C(202)-C(203)	1.408(9)
C(202)-H(202)	0.9500
C(203)-C(204)	1.365(9)
C(203)-H(203)	0.9500
C(204)-C(205)	1.370(10)
C(204)-H(204)	0.9500
C(205)-C(206)	1.332(8)
C(205)-H(205)	0.9500
C(206)-H(206)	0.9500
N(1C)-C(2C)	1.366(8)
N(1C)-C(2C)#2	1.366(8)
C(2C)-N(3C)	1.320(10)
C(2C)-H(2C)	0.9500
N(3C)-N(3C)#2	1.293(14)
N(1D)-C(2D)	1.368(10)
N(1D)-C(2D)#2	1.368(10)
C(2D)-N(3D)	1.362(12)
C(2D)-H(2D)	0.9500
N(3D)-N(3D)#2	1.363(16)
N(1A)-Fe(1)-N(1)#1	87.35(15)
N(1A)-Fe(1)-N(1)	87.35(15)
N(1)#1-Fe(1)-N(1)	174.7(3)
N(1A)-Fe(1)-N(2)#1	92.32(15)
N(1)#1-Fe(1)-N(2)#1	89.70(18)
N(1)-Fe(1)-N(2)#1	90.52(18)
N(1A)-Fe(1)-N(2)	92.32(15)
N(1)#1-Fe(1)-N(2)	90.52(18)
N(1)-Fe(1)-N(2)	89.70(18)
N(2)#1-Fe(1)-N(2)	175.4(3)
N(1A)-Fe(1)-N(1B)	180.000(4)
N(1)#1-Fe(1)-N(1B)	92.65(15)
N(1)-Fe(1)-N(1B)	92.65(15)
N(2)#1-Fe(1)-N(1B)	87.68(15)
N(2)-Fe(1)-N(1B)	87.68(15)
C(4)-N(1)-C(1)	105.0(4)
C(4)-N(1)-Fe(1)	123.3(4)
C(1)-N(1)-Fe(1)	123.7(3)
N(1)-C(1)-C(2)	112.0(5)
N(1)-C(1)-C(10)#1	120.8(5)
C(2)-C(1)-C(10)#1	126.9(5)
C(3)-C(2)-C(1)	104.4(5)
C(3)-C(2)-C(21)	125.4(6)
C(1)-C(2)-C(21)	129.5(5)
C(2)-C(21)-C(22)	109.0(5)
C(2)-C(21)-H(21A)	109.9
C(22)-C(21)-H(21A)	109.9
C(2)-C(21)-H(21B)	109.9
C(22)-C(21)-H(21B)	109.9
H(21A)-C(21)-H(21B)	108.3
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(2)-C(3)-C(4)	108.2(5)
C(2)-C(3)-C(31)	123.7(6)
C(4)-C(3)-C(31)	127.3(5)
C(32)-C(31)-C(3)	111.3(7)
C(32)-C(31)-H(31A)	109.4
C(3)-C(31)-H(31A)	109.4
C(32)-C(31)-H(31B)	109.4
C(3)-C(31)-H(31B)	109.4
H(31A)-C(31)-H(31B)	108.0
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
N(1)-C(4)-C(5)	121.5(5)
N(1)-C(4)-C(3)	110.1(5)
C(5)-C(4)-C(3)	128.2(5)
C(6)-C(5)-C(4)	122.4(5)
C(6)-C(5)-C(51)	118.4(5)
C(4)-C(5)-C(51)	119.2(5)
C(52)-C(51)-C(56)	121.0(6)
C(52)-C(51)-C(5)	118.9(6)
C(56)-C(51)-C(5)	120.1(6)
C(51)-C(52)-C(53)	120.9(7)

C(51)-C(52)-H(52)	119.5
C(53)-C(52)-H(52)	119.5
C(54)-C(53)-C(52)	116.4(7)
C(54)-C(53)-H(53)	121.8
C(52)-C(53)-H(53)	121.8
C(55)-C(54)-C(53)	121.8(6)
C(55)-C(54)-H(54)	119.1
C(53)-C(54)-H(54)	119.1
C(54)-C(55)-C(56)	122.3(7)
C(54)-C(55)-H(55)	118.9
C(56)-C(55)-H(55)	118.9
C(51)-C(56)-C(55)	117.6(7)
C(51)-C(56)-H(56)	121.2
C(55)-C(56)-H(56)	121.2
C(9)-N(2)-C(6)	106.8(5)
C(9)-N(2)-Fe(1)	123.4(4)
C(6)-N(2)-Fe(1)	125.1(4)
N(2)-C(6)-C(5)	122.5(5)
N(2)-C(6)-C(7)	109.3(5)
C(5)-C(6)-C(7)	128.0(5)
C(8)-C(7)-C(6)	107.6(5)
C(8)-C(7)-C(71)	124.4(5)
C(6)-C(7)-C(71)	127.0(5)
C(72)-C(71)-C(7)	114.3(5)
C(72)-C(71)-H(71A)	108.7
C(7)-C(71)-H(71A)	108.7
C(72)-C(71)-H(71B)	108.7
C(7)-C(71)-H(71B)	108.7
H(71A)-C(71)-H(71B)	107.6
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(7)-C(8)-C(9)	104.3(5)
C(7)-C(8)-C(81)	124.9(5)
C(9)-C(8)-C(81)	129.6(5)
C(8)-C(81)-C(82)	111.9(5)
C(8)-C(81)-H(81A)	109.2
C(82)-C(81)-H(81A)	109.2
C(8)-C(81)-H(81B)	109.2
C(82)-C(81)-H(81B)	109.2
H(81A)-C(81)-H(81B)	107.9
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
N(2)-C(9)-C(10)	122.8(5)
N(2)-C(9)-C(8)	111.4(5)
C(10)-C(9)-C(8)	125.1(5)
C(1)#1-C(10)-C(9)	121.1(5)
C(1)#1-C(10)-C(101)	121.3(5)
C(9)-C(10)-C(101)	117.1(5)
C(102)-C(101)-C(106)	117.3(6)
C(102)-C(101)-C(10)	122.3(6)
C(106)-C(101)-C(10)	120.3(6)
C(101)-C(102)-C(103)	122.8(7)
C(101)-C(102)-H(102)	118.6
C(103)-C(102)-H(102)	118.6
C(104)-C(103)-C(102)	117.2(8)
C(104)-C(103)-H(103)	121.4
C(102)-C(103)-H(103)	121.4
C(103)-C(104)-C(105)	123.4(7)
C(103)-C(104)-H(104)	118.3
C(105)-C(104)-H(104)	118.3
C(106)-C(105)-C(104)	116.5(8)
C(106)-C(105)-H(105)	121.7
C(104)-C(105)-H(105)	121.7
C(105)-C(106)-C(101)	122.5(8)
C(105)-C(106)-H(106)	118.7
C(101)-C(106)-H(106)	118.7
C(2A)#1-N(1A)-C(2A)	104.5(9)
C(2A)#1-N(1A)-Fe(1)	127.7(5)
C(2A)-N(1A)-Fe(1)	127.7(5)
N(3A)-C(2A)-N(1A)	111.7(7)
N(3A)-C(2A)-H(2A)	124.2
N(1A)-C(2A)-H(2A)	124.2
C(2A)-N(3A)-N(3A)#1	106.0(4)
C(2B)#1-N(1B)-C(2B)	103.3(8)
C(2B)#1-N(1B)-Fe(1)	128.4(4)
C(2B)-N(1B)-Fe(1)	128.4(4)
N(3B)-C(2B)-N(1B)	110.9(6)
N(3B)-C(2B)-H(2B)	124.6
N(1B)-C(2B)-H(2B)	124.6
N(3B)#1-N(3B)-C(2B)	107.5(4)
N(4)-Fe(2)-N(4)#2	174.9(3)
N(4)-Fe(2)-N(1C)	87.47(15)
N(4)#2-Fe(2)-N(1C)	87.47(15)
N(4)-Fe(2)-N(1D)	92.53(15)
N(4)#2-Fe(2)-N(1D)	92.53(15)
N(1C)-Fe(2)-N(1D)	180.000(2)
N(4)-Fe(2)-N(3)	89.52(18)
N(4)#2-Fe(2)-N(3)	90.73(18)
N(1C)-Fe(2)-N(3)	92.77(16)
N(1D)-Fe(2)-N(3)	87.23(16)
N(4)-Fe(2)-N(3)#2	90.73(18)
N(4)#2-Fe(2)-N(3)#2	89.52(18)
N(1C)-Fe(2)-N(3)#2	92.77(16)
N(1D)-Fe(2)-N(3)#2	87.23(16)
N(3)-Fe(2)-N(3)#2	174.5(3)
C(11)-N(3)-C(14)	106.7(4)
C(11)-N(3)-Fe(2)	122.9(3)
C(14)-N(3)-Fe(2)	124.6(4)
N(3)-C(11)-C(20)#2	121.5(5)
N(3)-C(11)-C(12)	110.2(5)
C(20)#2-C(11)-C(12)	128.1(5)
C(13)-C(12)-C(11)	107.0(6)
C(13)-C(12)-C(121)	125.2(6)
C(11)-C(12)-C(121)	127.7(6)
C(12)-C(121)-C(122)	110.1(7)
C(12)-C(121)-H(12A)	109.6
C(122)-C(121)-H(12A)	109.6
C(12)-C(121)-H(12B)	109.6

C(122)-C(121)-H(12B)	109.6
H(12A)-C(121)-H(12B)	108.2
C(121)-C(122)-H(12C)	109.5
C(121)-C(122)-H(12D)	109.5
H(12C)-C(122)-H(12D)	109.5
C(121)-C(122)-H(12E)	109.5
H(12C)-C(122)-H(12E)	109.5
H(12D)-C(122)-H(12E)	109.5
C(12)-C(13)-C(14)	107.0(5)
C(12)-C(13)-C(131)	125.0(6)
C(14)-C(13)-C(131)	127.1(6)
C(13)-C(131)-C(132)	116.0(9)
C(13)-C(131)-H(13A)	108.3
C(132)-C(131)-H(13A)	108.3
C(13)-C(131)-H(13B)	108.3
C(132)-C(131)-H(13B)	108.3
H(13A)-C(131)-H(13B)	107.4
C(131)-C(132)-H(13C)	109.5
C(131)-C(132)-H(13D)	109.5
H(13C)-C(132)-H(13D)	109.5
C(131)-C(132)-H(13E)	109.5
H(13C)-C(132)-H(13E)	109.5
H(13D)-C(132)-H(13E)	109.5
C(15)-C(14)-N(3)	121.4(5)
C(15)-C(14)-C(13)	130.2(5)
N(3)-C(14)-C(13)	108.3(5)
C(16)-C(15)-C(14)	123.1(5)
C(16)-C(15)-C(151)	119.4(5)
C(14)-C(15)-C(151)	117.2(5)
C(156)-C(151)-C(152)	118.4(6)
C(156)-C(151)-C(15)	121.0(6)
C(152)-C(151)-C(15)	120.6(6)
C(151)-C(152)-C(153)	120.9(8)
C(151)-C(152)-H(152)	119.5
C(153)-C(152)-H(152)	119.5
C(154)-C(153)-C(152)	118.2(8)
C(154)-C(153)-H(153)	120.9
C(152)-C(153)-H(153)	120.9
C(155)-C(154)-C(153)	122.8(7)
C(155)-C(154)-H(154)	118.6
C(153)-C(154)-H(154)	118.6
C(154)-C(155)-C(156)	118.2(7)
C(154)-C(155)-H(155)	120.9
C(156)-C(155)-H(155)	120.9
C(151)-C(156)-C(155)	121.4(7)
C(151)-C(156)-H(156)	119.3
C(155)-C(156)-H(156)	119.3
C(16)-N(4)-C(19)	103.3(4)
C(16)-N(4)-Fe(2)	126.1(4)
C(19)-N(4)-Fe(2)	124.6(4)
N(4)-C(16)-C(15)	120.6(5)
N(4)-C(16)-C(17)	113.0(5)
C(15)-C(16)-C(17)	126.1(5)
C(18)-C(17)-C(16)	103.9(5)
C(18)-C(17)-C(171)	125.0(6)
C(16)-C(17)-C(171)	130.6(6)
C(17)-C(171)-C(172)	112.3(5)
C(17)-C(171)-H(17A)	109.1
C(172)-C(171)-H(17A)	109.1
C(17)-C(171)-H(17B)	109.1
C(172)-C(171)-H(17B)	109.1
H(17A)-C(171)-H(17B)	107.9
C(171)-C(172)-H(17C)	109.5
C(171)-C(172)-H(17D)	109.5
H(17C)-C(172)-H(17D)	109.5
C(171)-C(172)-H(17E)	109.5
H(17C)-C(172)-H(17E)	109.5
H(17D)-C(172)-H(17E)	109.5
C(17)-C(18)-C(19)	108.3(5)
C(17)-C(18)-C(181)	124.7(5)
C(19)-C(18)-C(181)	125.6(5)
C(182)-C(181)-C(18)	111.3(5)
C(182)-C(181)-H(18A)	109.4
C(18)-C(181)-H(18A)	109.4
C(182)-C(181)-H(18B)	109.4
C(18)-C(181)-H(18B)	109.4
H(18A)-C(181)-H(18B)	108.0
C(181)-C(182)-H(18C)	109.5
C(181)-C(182)-H(18D)	109.5
H(18C)-C(182)-H(18D)	109.5
C(181)-C(182)-H(18E)	109.5
H(18C)-C(182)-H(18E)	109.5
H(18D)-C(182)-H(18E)	109.5
N(4)-C(19)-C(20)	119.5(5)
N(4)-C(19)-C(18)	110.8(5)
C(20)-C(19)-C(18)	129.3(5)
C(19)-C(20)-C(11)#2	123.5(5)
C(19)-C(20)-C(201)	115.2(4)
C(11)#2-C(20)-C(201)	121.3(5)
C(202)-C(201)-C(206)	117.9(6)
C(202)-C(201)-C(20)	124.1(6)
C(206)-C(201)-C(20)	118.0(6)
C(201)-C(202)-C(203)	119.4(7)
C(201)-C(202)-H(202)	120.3
C(203)-C(202)-H(202)	120.3
C(204)-C(203)-C(202)	118.6(7)
C(204)-C(203)-H(203)	120.7
C(202)-C(203)-H(203)	120.7
C(203)-C(204)-C(205)	122.6(8)
C(203)-C(204)-H(204)	118.7
C(205)-C(204)-H(204)	118.7
C(206)-C(205)-C(204)	116.7(8)
C(206)-C(205)-H(205)	121.7
C(204)-C(205)-H(205)	121.7
C(205)-C(206)-C(201)	124.6(7)
C(205)-C(206)-H(206)	117.7
C(201)-C(206)-H(206)	117.7
C(2C)-N(1C)-C(2C)#2	101.6(8)
C(2C)-N(1C)-Fe(2)	129.2(4)
C(2C)#2-N(1C)-Fe(2)	129.2(4)
N(3C)-C(2C)-N(1C)	111.0(7)
N(3C)-C(2C)-H(2C)	124.5
N(1C)-C(2C)-H(2C)	124.5
N(3C)#2-N(3C)-C(2C)	108.2(4)
C(2D)-N(1D)-C(2D)#2	109.3(11)
C(2D)-N(1D)-Fe(2)	125.4(5)

C(2D)#2-N(1D)-Fe(2)	125.4(5)	N(1D)-C(2D)-H(2D)	126.6
N(3D)-C(2D)-N(1D)	106.8(9)	C(2D)-N(3D)-N(3D)#2	108.6(6)
N(3D)-C(2D)-H(2D)	126.6		

Symmetry transformations used to generate equivalent atoms:
#1 -x,-x+y,-z+5/3 #2 -x,-x+y,-z+2/3

Table S3. Anisotropic displacement parameters ($Å^2$ x 10^3) for [(OETPP)Fe(HIm)$_2$]Cl. The anisotropic displacement factor exponent takes the form: $-2\pi^2 [h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	37(1)	58(1)	19(1)	1(1)	2(1)	19(1)
N(1)	33(3)	50(3)	20(2)	2(2)	3(2)	11(2)
C(1)	38(3)	69(4)	25(3)	1(3)	0(3)	24(3)
C(2)	44(4)	57(4)	33(3)	1(3)	12(3)	21(3)
C(21)	45(4)	67(5)	42(4)	3(3)	1(3)	17(4)
C(22)	92(6)	79(6)	64(5)	-11(4)	-5(4)	28(5)
C(3)	56(4)	53(4)	17(3)	1(3)	2(3)	24(4)
C(31)	72(5)	81(5)	40(4)	17(4)	-6(4)	28(4)
C(32)	235(13)	126(8)	54(5)	-7(5)	-27(7)	131(9)
C(4)	29(3)	68(4)	24(3)	5(3)	3(2)	16(3)
C(5)	32(3)	57(4)	20(3)	1(3)	1(2)	14(3)
C(51)	41(4)	61(4)	29(3)	0(3)	3(3)	16(3)
C(52)	54(4)	70(5)	48(4)	25(3)	8(3)	21(4)
C(53)	98(6)	69(5)	32(3)	13(3)	5(4)	26(4)
C(54)	79(5)	62(5)	28(3)	6(3)	10(3)	10(4)
C(55)	59(4)	84(5)	23(3)	3(3)	11(3)	16(4)
C(56)	36(4)	84(5)	28(3)	-10(3)	-1(3)	19(3)
N(2)	32(3)	54(3)	31(3)	2(2)	1(2)	21(3)
C(6)	40(4)	74(4)	12(3)	7(3)	-2(2)	28(4)
C(7)	50(4)	65(4)	21(3)	-7(3)	-1(3)	31(4)
C(71)	51(4)	70(4)	19(3)	0(3)	-8(3)	36(4)
C(72)	108(7)	88(6)	62(5)	-12(4)	-16(5)	66(5)
C(8)	32(3)	60(4)	19(3)	3(3)	-5(3)	19(3)
C(81)	56(4)	85(5)	27(3)	0(3)	-2(3)	37(4)
C(82)	86(5)	56(5)	48(4)	-5(3)	5(4)	26(4)
C(9)	47(4)	53(4)	22(3)	4(3)	7(3)	17(3)
C(10)	32(3)	60(4)	29(3)	3(3)	6(2)	16(3)
C(101)	54(4)	76(5)	28(3)	0(3)	0(3)	26(3)
C(102)	38(4)	81(5)	43(4)	-15(3)	-2(3)	22(3)
C(103)	40(4)	99(6)	52(4)	-30(4)	-10(3)	19(4)
C(104)	54(4)	137(7)	76(5)	-44(5)	-28(4)	55(4)
C(105)	60(5)	145(7)	46(4)	-13(4)	-7(3)	59(5)
C(106)	77(5)	87(5)	29(3)	-17(3)	-11(3)	42(4)
N(1A)	49(5)	78(4)	16(4)	5(2)	10(3)	25(2)
C(2A)	79(5)	91(6)	48(4)	-16(4)	-20(4)	59(5)
N(3A)	122(7)	92(6)	57(4)	-3(4)	-8(4)	71(6)
C(3A)	122(7)	92(6)	57(4)	-3(4)	-8(4)	71(6)
N(1B)	53(4)	55(3)	15(3)	-1(2)	-2(3)	26(2)
C(2B)	58(4)	67(5)	37(4)	5(3)	-5(3)	36(4)
N(3B)	76(5)	83(5)	38(3)	2(3)	-5(3)	40(4)
C(3B)	76(5)	83(5)	38(3)	2(3)	-5(3)	40(4)
Fe(2)	39(1)	53(1)	17(1)	1(1)	2(1)	19(1)
N(3)	38(3)	68(4)	15(2)	-2(2)	8(2)	27(3)
C(11)	33(3)	59(4)	31(3)	5(3)	10(3)	19(3)
C(12)	56(4)	82(5)	35(4)	4(3)	10(3)	36(4)
C(121)	61(5)	115(6)	64(5)	-7(4)	-10(4)	56(5)
C(122)	106(8)	129(8)	159(10)	19(7)	-32(7)	81(7)
C(13)	50(4)	71(5)	45(4)	-11(3)	-5(3)	34(4)
C(131)	71(6)	170(9)	73(6)	-34(6)	-13(5)	81(6)
C(132)	170(11)	139(8)	92(7)	13(7)	36(7)	99(9)
C(14)	43(4)	59(4)	23(3)	8(3)	9(3)	20(3)
C(15)	49(4)	66(5)	26(3)	-4(3)	6(3)	22(4)

C(151)	61(4)	82(5)	11(3)	7(3)	0(3)	36(4)
C(152)	59(4)	97(5)	31(3)	-9(3)	-6(3)	29(4)
C(153)	63(5)	155(7)	32(4)	-6(4)	4(3)	65(5)
C(154)	75(5)	161(7)	34(4)	21(4)	14(4)	80(5)
C(155)	57(4)	125(6)	32(4)	32(4)	15(3)	50(4)
C(156)	50(4)	76(4)	25(3)	3(3)	18(3)	14(3)
N(4)	37(3)	47(3)	26(3)	-2(2)	0(2)	13(2)
C(16)	46(4)	49(4)	17(3)	-11(2)	-2(3)	21(3)
C(17)	41(4)	56(4)	26(3)	-15(3)	1(3)	17(3)
C(171)	69(5)	72(5)	25(3)	6(3)	-4(3)	33(4)
C(172)	96(6)	56(5)	62(5)	13(4)	-12(4)	6(5)
C(18)	62(4)	54(4)	21(3)	-8(3)	-5(3)	28(4)
C(181)	54(4)	73(5)	35(4)	4(3)	1(3)	31(4)
C(182)	81(6)	133(8)	61(5)	8(5)	3(4)	77(6)
C(19)	28(3)	56(4)	25(3)	-5(3)	1(2)	16(3)
C(20)	39(3)	49(4)	20(3)	-9(3)	-2(2)	13(3)
C(201)	51(4)	84(5)	19(3)	7(3)	3(3)	23(4)
C(202)	48(4)	115(6)	44(4)	16(4)	5(3)	33(4)
C(203)	44(4)	104(6)	49(4)	11(4)	8(3)	10(4)
C(204)	70(5)	70(5)	61(5)	8(4)	-12(4)	17(4)
C(205)	83(5)	63(5)	40(4)	-5(3)	-8(4)	11(4)
C(206)	65(4)	72(5)	29(3)	-1(3)	-9(3)	19(4)
N(1C)	37(4)	45(3)	28(4)	-2(2)	-4(3)	19(2)
C(2C)	70(5)	49(5)	94(6)	8(4)	25(4)	32(4)
N(3C)	81(6)	52(4)	113(7)	1(4)	6(5)	24(4)
C(3C)	81(6)	52(4)	113(7)	1(4)	6(5)	24(4)
N(1D)	100(5)	70(3)	45(4)	11(2)	21(4)	50(2)
C(2D)	160(6)	81(5)	96(5)	-9(4)	0(5)	70(5)
N(3D)	197(8)	79(5)	107(6)	-7(4)	-23(6)	87(5)
C(3D)	197(8)	79(5)	107(6)	-7(4)	-23(6)	87(5)
Cl(5)	165(7)	141(6)	124(5)	-1(4)	-6(5)	57(5)
Cl(5A)	160(7)	145(6)	182(7)	26(5)	9(5)	90(5)

Table S4. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [(OETPP)Fe(HIm)$_2$]Cl.

	x	y	z	U(eq)
H(21A)	-3001	2104	8203	68
H(21B)	-3008	1692	8686	68
H(22A)	-2899	1087	7989	127
H(22B)	-2200	1379	8314	127
H(22C)	-2189	1792	7833	127
H(31A)	-2026	2323	9760	82
H(31B)	-2563	1767	9372	82
H(32A)	-1838	1368	9690	181
H(32B)	-1149	2077	9511	181
H(32C)	-1686	1520	9124	181
H(52)	-306	3151	10135	74
H(53)	-756	2748	10930	88
H(54)	-1656	2967	11212	81
H(55)	-2157	3410	10722	77
H(56)	-1745	3775	9926	65
H(71A)	-184	4533	10400	53
H(71B)	556	5253	10458	53
H(72A)	-376	5490	10482	118
H(72B)	-637	5141	9958	118
H(72C)	104	5862	10016	118
H(81A)	2085	5959	9787	66
H(81B)	1493	5980	10119	66
H(82A)	2049	7018	9624	101
H(82B)	1229	6558	9479	101
H(82C)	1821	6537	9147	101
H(102)	2799	6304	8608	69
H(103)	3893	6916	8996	84
H(104)	4094	6391	9668	103
H(105)	3251	5247	9936	96
H(106)	2151	4678	9548	77
H(2A)	575	3340	8926	79
H(3A)	339	2153	8729	99
H(2B)	37	5375	9044	62
H(3B)	40	6433	8775	78
H(12A)	2919	4701	3451	90
H(12B)	2953	4422	2920	90
H(12C)	2755	3542	3502	182
H(12D)	2084	3252	3150	182
H(12E)	2049	3531	3679	182
H(13A)	2673	4509	2220	115
H(13B)	2128	4589	1875	115
H(13C)	2119	3553	1713	186
H(13D)	1360	3378	1915	186
H(13E)	1906	3299	2261	186
H(152)	463	3651	1429	80
H(153)	1021	3929	658	94
H(154)	1883	5092	495	97
H(155)	2247	5970	1069	83
H(156)	1728	5675	1853	70
H(17A)	-641	4669	1300	68
H(17B)	148	4793	1320	68

H(17C)	180	5886	1368	128
H(17D)	479	5748	1861	128
H(17E)	-310	5623	1841	128
H(18A)	-1652	4161	1589	65
H(18B)	-2158	3470	1902	65
H(18C)	-2346	4384	2101	122
H(18D)	-1528	4868	2244	122
H(18E)	-2033	4177	2557	122
H(202)	-2953	2883	2929	87
H(203)	-3967	2179	2444	94
H(204)	-3877	1542	1809	90
H(205)	-2830	1536	1653	88
H(206)	-1862	2250	2108	75
H(2C)	873	5617	2941	84
H(3C)	543	6504	3104	103
H(2D)	-57	2842	2604	130
H(3D)	-36	1770	2887	144

Table S5. Torsion angles [°] for [(OETPP)Fe(HIm)$_2$]Cl.

N(1A)-Fe(1)-N(1)-C(4)	67.1(5)
N(1)#1-Fe(1)-N(1)-C(4)	67.1(5)
N(2)#1-Fe(1)-N(1)-C(4)	159.4(5)
N(2)-Fe(1)-N(1)-C(4)	-25.2(5)
N(1B)-Fe(1)-N(1)-C(4)	-112.9(5)
N(1A)-Fe(1)-N(1)-C(1)	-76.9(5)
N(1)#1-Fe(1)-N(1)-C(1)	-76.9(5)
N(2)#1-Fe(1)-N(1)-C(1)	15.4(5)
N(2)-Fe(1)-N(1)-C(1)	-169.2(5)
N(1B)-Fe(1)-N(1)-C(1)	103.1(5)
C(4)-N(1)-C(1)-C(2)	-5.0(7)
Fe(1)-N(1)-C(1)-C(2)	144.5(4)
C(4)-N(1)-C(1)-C(10)#1	169.8(6)
Fe(1)-N(1)-C(1)-C(10)#1	-40.7(8)
N(1)-C(1)-C(2)-C(3)	1.8(7)
C(10)#1-C(1)-C(2)-C(3)	-172.6(6)
N(1)-C(1)-C(2)-C(21)	-168.7(6)
C(10)#1-C(1)-C(2)-C(21)	16.8(11)
C(3)-C(2)-C(21)-C(22)	-97.7(7)
C(1)-C(2)-C(21)-C(22)	71.0(9)
C(1)-C(2)-C(3)-C(4)	2.1(7)
C(21)-C(2)-C(3)-C(4)	173.2(6)
C(1)-C(2)-C(3)-C(31)	-167.9(6)
C(21)-C(2)-C(3)-C(31)	3.1(10)
C(2)-C(3)-C(31)-C(32)	97.1(8)
C(4)-C(3)-C(31)-C(32)	-71.0(9)
C(1)-N(1)-C(4)-C(5)	-168.3(6)
Fe(1)-N(1)-C(4)-C(5)	42.1(8)
C(1)-N(1)-C(4)-C(3)	6.3(7)
Fe(1)-N(1)-C(4)-C(3)	-143.4(4)
C(2)-C(3)-C(4)-N(1)	-5.4(7)
C(31)-C(3)-C(4)-N(1)	164.2(6)
C(2)-C(3)-C(4)-C(5)	168.6(6)
C(31)-C(3)-C(4)-C(5)	-21.8(11)
N(1)-C(4)-C(5)-C(6)	-18.1(10)
C(3)-C(4)-C(5)-C(6)	168.4(6)
N(1)-C(4)-C(5)-C(51)	162.5(6)
C(3)-C(4)-C(5)-C(51)	-10.9(10)
C(6)-C(5)-C(51)-C(52)	-66.0(8)
C(4)-C(5)-C(51)-C(52)	113.4(7)
C(6)-C(5)-C(51)-C(56)	111.4(7)
C(4)-C(5)-C(51)-C(56)	-69.1(9)
C(56)-C(51)-C(52)-C(53)	2.0(11)
C(5)-C(51)-C(52)-C(53)	179.4(6)
C(51)-C(52)-C(53)-C(54)	-3.3(11)
C(52)-C(53)-C(54)-C(55)	3.6(11)
C(53)-C(54)-C(55)-C(56)	-2.6(12)
C(52)-C(51)-C(56)-C(55)	-0.7(10)
C(5)-C(51)-C(56)-C(55)	-178.1(6)
C(54)-C(55)-C(56)-C(51)	1.0(11)
N(1A)-Fe(1)-N(2)-C(9)	110.0(5)
N(1)#1-Fe(1)-N(2)-C(9)	22.6(5)
N(1)-Fe(1)-N(2)-C(9)	-162.6(5)
N(2)#1-Fe(1)-N(2)-C(9)	-70.0(5)
N(1B)-Fe(1)-N(2)-C(9)	-70.0(5)
N(1A)-Fe(1)-N(2)-C(6)	-97.5(5)
N(1)#1-Fe(1)-N(2)-C(6)	175.1(5)
N(1)-Fe(1)-N(2)-C(6)	-10.2(5)

N(2)#1-Fe(1)-N(2)-C(6)	82.5(5)
N(1B)-Fe(1)-N(2)-C(6)	82.5(5)
C(9)-N(2)-C(6)-C(5)	-170.5(6)
Fe(1)-N(2)-C(6)-C(5)	33.3(8)
C(9)-N(2)-C(6)-C(7)	6.1(7)
Fe(1)-N(2)-C(6)-C(7)	-150.1(4)
C(4)-C(5)-C(6)-N(2)	-21.3(10)
C(51)-C(5)-C(6)-N(2)	158.1(5)
C(4)-C(5)-C(6)-C(7)	162.9(6)
C(51)-C(5)-C(6)-C(7)	-17.7(10)
N(2)-C(6)-C(7)-C(8)	-1.9(7)
C(5)-C(6)-C(7)-C(8)	174.4(6)
N(2)-C(6)-C(7)-C(71)	167.0(6)
C(5)-C(6)-C(7)-C(71)	-16.7(10)
C(8)-C(7)-C(71)-C(72)	91.1(8)
C(6)-C(7)-C(71)-C(72)	-76.0(9)
C(6)-C(7)-C(8)-C(9)	-2.7(6)
C(71)-C(7)-C(8)-C(9)	-172.0(6)
C(6)-C(7)-C(8)-C(81)	165.8(6)
C(71)-C(7)-C(8)-C(81)	-3.4(9)
C(7)-C(8)-C(81)-C(82)	-104.1(7)
C(9)-C(8)-C(81)-C(82)	61.4(9)
C(6)-N(2)-C(9)-C(10)	163.2(6)
Fe(1)-N(2)-C(9)-C(10)	-40.1(8)
C(6)-N(2)-C(9)-C(8)	-8.0(7)
Fe(1)-N(2)-C(9)-C(8)	148.7(4)
C(7)-C(8)-C(9)-N(2)	6.8(7)
C(81)-C(8)-C(9)-N(2)	-161.0(6)
C(7)-C(8)-C(9)-C(10)	-164.2(6)
C(81)-C(8)-C(9)-C(10)	28.0(10)
N(2)-C(9)-C(10)-C(1)#1	14.8(10)
C(8)-C(9)-C(10)-C(1)#1	-175.2(6)
N(2)-C(9)-C(10)-C(101)	-157.4(6)
C(8)-C(9)-C(10)-C(101)	12.6(10)
C(1)#1-C(10)-C(101)-C(102)	67.8(9)
C(9)-C(10)-C(101)-C(102)	-120.1(7)
C(1)#1-C(10)-C(101)-C(106)	-108.4(7)
C(9)-C(10)-C(101)-C(106)	63.8(9)
C(106)-C(101)-C(102)-C(103)	-4.9(10)
C(10)-C(101)-C(102)-C(103)	178.8(6)
C(101)-C(102)-C(103)-C(104)	2.2(10)
C(102)-C(103)-C(104)-C(105)	2.0(12)
C(103)-C(104)-C(105)-C(106)	-3.1(12)
C(104)-C(105)-C(106)-C(101)	0.1(11)
C(102)-C(101)-C(106)-C(105)	3.7(10)
C(10)-C(101)-C(106)-C(105)	-180.0(6)
N(1)#1-Fe(1)-N(1A)-C(2A)#1	-101.3(4)
N(1)-Fe(1)-N(1A)-C(2A)#1	78.7(4)
N(2)#1-Fe(1)-N(1A)-C(2A)#1	-11.7(4)
N(2)-Fe(1)-N(1A)-C(2A)#1	168.3(4)
N(1B)-Fe(1)-N(1A)-C(2A)#1	57(100)
N(1)#1-Fe(1)-N(1A)-C(2A)	78.7(4)
N(1)-Fe(1)-N(1A)-C(2A)	-101.3(4)
N(2)#1-Fe(1)-N(1A)-C(2A)	168.3(4)
N(2)-Fe(1)-N(1A)-C(2A)	-11.7(4)
N(1B)-Fe(1)-N(1A)-C(2A)	-123(100)
C(2A)#1-N(1A)-C(2A)-N(3A)	-1.1(4)
Fe(1)-N(1A)-C(2A)-N(3A)	178.9(4)

N(1A)-C(2A)-N(3A)-N(3A)#1	2.6(11)
N(1A)-Fe(1)-N(1B)-C(2B)#1	-88(100)
N(1)#1-Fe(1)-N(1B)-C(2B)#1	70.4(4)
N(1)-Fe(1)-N(1B)-C(2B)#1	-109.6(4)
N(2)#1-Fe(1)-N(1B)-C(2B)#1	-19.2(4)
N(2)-Fe(1)-N(1B)-C(2B)#1	160.8(4)
N(1A)-Fe(1)-N(1B)-C(2B)	92(100)
N(1)#1-Fe(1)-N(1B)-C(2B)	-109.6(4)
N(1)-Fe(1)-N(1B)-C(2B)	70.4(4)
N(2)#1-Fe(1)-N(1B)-C(2B)	160.8(4)
N(2)-Fe(1)-N(1B)-C(2B)	-19.2(4)
C(2B)#1-N(1B)-C(2B)-N(3B)	-0.5(4)
Fe(1)-N(1B)-C(2B)-N(3B)	179.5(4)
N(1B)-C(2B)-N(3B)-N(3B)#1	1.3(10)
N(4)-Fe(2)-N(3)-C(11)	-161.5(5)
N(4)#2-Fe(2)-N(3)-C(11)	23.5(5)
N(1C)-Fe(2)-N(3)-C(11)	111.0(5)
N(1D)-Fe(2)-N(3)-C(11)	-69.0(5)
N(3)#2-Fe(2)-N(3)-C(11)	-69.0(5)
N(4)-Fe(2)-N(3)-C(14)	-12.1(5)
N(4)#2-Fe(2)-N(3)-C(14)	172.9(5)
N(1C)-Fe(2)-N(3)-C(14)	-99.6(5)
N(1D)-Fe(2)-N(3)-C(14)	80.4(5)
N(3)#2-Fe(2)-N(3)-C(14)	80.4(5)
C(14)-N(3)-C(11)-C(20)#2	166.1(6)
Fe(2)-N(3)-C(11)-C(20)#2	-39.9(8)
C(14)-N(3)-C(11)-C(12)	-8.8(7)
Fe(2)-N(3)-C(11)-C(12)	145.2(5)
N(3)-C(11)-C(12)-C(13)	9.6(8)
C(20)#2-C(11)-C(12)-C(13)	-164.9(6)
N(3)-C(11)-C(12)-C(121)	-167.0(7)
C(20)#2-C(11)-C(12)-C(121)	18.5(12)
C(13)-C(12)-C(121)-C(122)	-103.3(9)
C(11)-C(12)-C(121)-C(122)	72.7(10)
C(11)-C(12)-C(13)-C(14)	-6.1(8)
C(121)-C(12)-C(13)-C(14)	170.7(7)
C(11)-C(12)-C(13)-C(131)	-175.6(8)
C(121)-C(12)-C(13)-C(131)	1.1(13)
C(12)-C(13)-C(131)-C(132)	90.1(10)
C(14)-C(13)-C(131)-C(132)	-77.3(11)
C(11)-N(3)-C(14)-C(15)	-171.9(6)
Fe(2)-N(3)-C(14)-C(15)	34.6(8)
C(11)-N(3)-C(14)-C(13)	5.0(7)
Fe(2)-N(3)-C(14)-C(13)	-148.5(5)
C(12)-C(13)-C(14)-C(15)	177.4(7)
C(131)-C(13)-C(14)-C(15)	-13.4(13)
C(12)-C(13)-C(14)-N(3)	0.9(8)
C(131)-C(13)-C(14)-N(3)	170.2(8)
N(3)-C(14)-C(15)-C(16)	-22.2(10)
C(13)-C(14)-C(15)-C(16)	161.7(7)
N(3)-C(14)-C(15)-C(151)	163.1(6)
C(13)-C(14)-C(15)-C(151)	-13.0(11)
C(16)-C(15)-C(151)-C(156)	113.2(7)
C(14)-C(15)-C(151)-C(156)	-71.8(9)
C(16)-C(15)-C(151)-C(152)	-66.2(9)
C(14)-C(15)-C(151)-C(152)	108.7(8)
C(156)-C(151)-C(152)-C(153)	2.7(10)
C(15)-C(151)-C(152)-C(153)	-177.8(7)

C(151)-C(152)-C(153)-C(154)	-2.9(11)
C(152)-C(153)-C(154)-C(155)	1.3(11)
C(153)-C(154)-C(155)-C(156)	0.4(11)
C(152)-C(151)-C(156)-C(155)	-0.9(10)
C(15)-C(151)-C(156)-C(155)	179.6(6)
C(154)-C(155)-C(156)-C(151)	-0.6(11)
N(4)#2-Fe(2)-N(4)-C(16)	69.5(5)
N(1C)-Fe(2)-N(4)-C(16)	69.5(5)
N(1D)-Fe(2)-N(4)-C(16)	-110.5(5)
N(3)-Fe(2)-N(4)-C(16)	-23.3(5)
N(3)#2-Fe(2)-N(4)-C(16)	162.2(5)
N(4)#2-Fe(2)-N(4)-C(19)	-78.6(5)
N(1C)-Fe(2)-N(4)-C(19)	-78.6(5)
N(1D)-Fe(2)-N(4)-C(19)	101.4(5)
N(3)-Fe(2)-N(4)-C(19)	-171.4(5)
N(3)#2-Fe(2)-N(4)-C(19)	14.1(5)
C(19)-N(4)-C(16)-C(15)	-166.9(5)
Fe(2)-N(4)-C(16)-C(15)	39.7(7)
C(19)-N(4)-C(16)-C(17)	8.1(6)
Fe(2)-N(4)-C(16)-C(17)	-145.4(4)
C(14)-C(15)-C(16)-N(4)	-15.5(9)
C(151)-C(15)-C(16)-N(4)	159.2(6)
C(14)-C(15)-C(16)-C(17)	170.3(6)
C(151)-C(15)-C(16)-C(17)	-15.1(10)
N(4)-C(16)-C(17)-C(18)	-6.5(6)
C(15)-C(16)-C(17)-C(18)	168.1(6)
N(4)-C(16)-C(17)-C(171)	166.6(6)
C(15)-C(16)-C(17)-C(171)	-18.8(10)
C(18)-C(17)-C(171)-C(172)	97.7(8)
C(16)-C(17)-C(171)-C(172)	-74.1(9)
C(16)-C(17)-C(18)-C(19)	2.0(6)
C(171)-C(17)-C(18)-C(19)	-171.6(6)
C(16)-C(17)-C(18)-C(181)	169.1(5)
C(171)-C(17)-C(18)-C(181)	-4.5(9)
C(17)-C(18)-C(181)-C(182)	-100.5(7)
C(19)-C(18)-C(181)-C(182)	64.4(9)
C(16)-N(4)-C(19)-C(20)	166.8(5)
Fe(2)-N(4)-C(19)-C(20)	-39.2(8)
C(16)-N(4)-C(19)-C(18)	-6.6(6)
Fe(2)-N(4)-C(19)-C(18)	147.4(4)
C(17)-C(18)-C(19)-N(4)	2.9(7)
C(181)-C(18)-C(19)-N(4)	-164.0(6)
C(17)-C(18)-C(19)-C(20)	-169.7(6)
C(181)-C(18)-C(19)-C(20)	23.4(10)
N(4)-C(19)-C(20)-C(11)#2	27.1(9)
C(18)-C(19)-C(20)-C(11)#2	-160.9(6)
N(4)-C(19)-C(20)-C(201)	-152.1(5)
C(18)-C(19)-C(20)-C(201)	19.9(10)
C(19)-C(20)-C(201)-C(202)	-117.0(7)
C(11)#2-C(20)-C(201)-C(202)	63.8(10)
C(19)-C(20)-C(201)-C(206)	63.4(8)
C(11)#2-C(20)-C(201)-C(206)	-115.8(7)
C(206)-C(201)-C(202)-C(203)	-2.6(11)
C(20)-C(201)-C(202)-C(203)	177.8(6)
C(201)-C(202)-C(203)-C(204)	1.3(11)
C(202)-C(203)-C(204)-C(205)	1.5(12)
C(203)-C(204)-C(205)-C(206)	-2.7(12)
C(204)-C(205)-C(206)-C(201)	1.3(11)

C(202)-C(201)-C(206)-C(205)	1.3(11)
C(20)-C(201)-C(206)-C(205)	-179.0(6)
N(4)-Fe(2)-N(1C)-C(2C)	-77.0(5)
N(4)#2-Fe(2)-N(1C)-C(2C)	103.0(5)
N(1D)-Fe(2)-N(1C)-C(2C)	33(40)
N(3)-Fe(2)-N(1C)-C(2C)	12.4(5)
N(3)#2-Fe(2)-N(1C)-C(2C)	-167.6(5)
N(4)-Fe(2)-N(1C)-C(2C)#2	103.0(5)
N(4)#2-Fe(2)-N(1C)-C(2C)#2	-77.0(5)
N(1D)-Fe(2)-N(1C)-C(2C)#2	-147(40)
N(3)-Fe(2)-N(1C)-C(2C)#2	-167.6(5)
N(3)#2-Fe(2)-N(1C)-C(2C)#2	12.4(5)
C(2C)#2-N(1C)-C(2C)-N(3C)	0.5(5)
Fe(2)-N(1C)-C(2C)-N(3C)	-179.5(5)
N(1C)-C(2C)-N(3C)-N(3C)#2	-1.3(13)
N(4)-Fe(2)-N(1D)-C(2D)	17.2(5)
N(4)#2-Fe(2)-N(1D)-C(2D)	-162.8(5)
N(1C)-Fe(2)-N(1D)-C(2D)	-93(100)
N(3)-Fe(2)-N(1D)-C(2D)	-72.2(5)
N(3)#2-Fe(2)-N(1D)-C(2D)	107.8(5)
N(4)-Fe(2)-N(1D)-C(2D)#2	-162.8(5)
N(4)#2-Fe(2)-N(1D)-C(2D)#2	17.2(5)
N(1C)-Fe(2)-N(1D)-C(2D)#2	87(100)
N(3)-Fe(2)-N(1D)-C(2D)#2	107.8(5)
N(3)#2-Fe(2)-N(1D)-C(2D)#2	-72.2(5)
C(2D)#2-N(1D)-C(2D)-N(3D)	0.02(9)
Fe(2)-N(1D)-C(2D)-N(3D)	-179.98(9)
N(1D)-C(2D)-N(3D)-N(3D)#2	-0.1(2)

_____

Symmetry transformations used to generate equivalent atoms:
#1 -x,-x+y,-z+5/3 #2 -x,-x+y,-z+2/3

Table S6. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [(OETPP)Fe(N-MeIm)$_2$]Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	-1(1)	4117(1)	8839(1)	49(1)
N(1)	-974(3)	3604(3)	9362(3)	50(1)
C(1)	-1540(3)	3151(4)	8808(4)	66(2)
C(2)	-2034(4)	2568(4)	9410(5)	76(2)
C(21)	-2639(4)	1856(5)	9033(6)	99(3)
C(22)	-2333(6)	1432(6)	8608(9)	137(4)
C(3)	-1805(3)	2694(3)	10327(4)	60(2)
C(31)	-2139(5)	2161(5)	11143(6)	104(3)
C(32)	-1779(7)	1766(6)	11328(9)	146(4)
C(4)	-1140(3)	3352(4)	10305(4)	60(2)
C(5)	-723(3)	3759(4)	11094(4)	58(2)
N(2)	361(3)	4338(3)	10154(3)	52(1)
C(6)	-16(3)	4300(3)	10975(4)	50(2)
C(7)	420(3)	4833(3)	11664(4)	50(2)
C(71)	202(4)	5050(4)	12589(4)	59(2)
C(72)	-156(5)	5505(5)	12323(6)	86(2)
C(8)	1092(3)	5191(4)	11289(4)	58(2)
C(81)	1675(4)	5861(4)	11667(5)	80(2)
C(82)	1797(6)	6465(5)	10979(6)	123(3)
C(9)	1059(3)	4840(4)	10389(4)	65(2)
C(10)	1614(3)	4904(5)	9825(5)	76(2)
C(51)	-1036(8)	3651(9)	12095(12)	34(4)
C(52)	-839(10)	3311(11)	12771(11)	49(4)
C(53)	-1107(9)	3199(9)	13720(11)	58(4)
C(54)	-1639(9)	3349(9)	13932(12)	65(4)
C(55)	-1870(9)	3666(10)	13266(11)	61(4)
C(56)	-1567(8)	3804(9)	12349(12)	45(4)
C(5AA)	-1006(11)	3455(11)	12073(15)	51(5)
C(5BB)	-672(12)	3214(13)	12696(13)	61(5)
C(5CC)	-983(10)	2984(10)	13611(13)	74(5)
C(5DD)	-1476(10)	3155(10)	13939(12)	64(4)
C(5EE)	-1770(10)	3454(10)	13345(12)	63(4)
C(5FF)	-1553(10)	3562(10)	12382(13)	60(5)
C(101)	2281(9)	4988(9)	10376(13)	84(4)
C(102)	2265(9)	4560(11)	11135(11)	90(4)
C(103)	2867(8)	4751(11)	11692(13)	104(4)
C(104)	3461(12)	5392(10)	11446(16)	118(5)
C(105)	3530(10)	5846(12)	10714(14)	107(4)
C(106)	2919(8)	5572(10)	10152(12)	95(4)
C(10A)	2337(6)	5362(7)	10262(8)	49(3)
C(10B)	2868(5)	6006(7)	9921(9)	61(3)
C(10C)	3529(6)	6317(9)	10374(10)	75(3)
C(10D)	3599(10)	5985(9)	11204(12)	97(5)
C(10E)	3097(7)	5339(9)	11573(10)	76(4)
C(10F)	2480(6)	5075(8)	11062(8)	62(3)
N(3)	968(2)	4561(3)	8322(3)	51(1)
C(11)	1533(3)	4669(4)	8849(4)	65(2)
C(12)	2036(3)	4584(5)	8274(5)	77(2)
C(121)	2644(4)	4493(6)	8620(7)	93(2)
C(122)	2362(6)	3785(7)	9071(9)	125(3)

C(13)	1789(4)	4464(5)	7349(4)	79(2)
C(131)	2134(5)	4307(5)	6524(7)	106(3)
C(132)	1820(7)	3549(6)	6347(10)	147(4)
C(14)	1138(3)	4485(4)	7354(4)	54(2)
C(15)	723(3)	4470(4)	6579(4)	56(2)
N(4)	-376(2)	3976(3)	7511(3)	50(1)
C(16)	19(3)	4309(4)	6680(4)	49(2)
C(17)	-412(3)	4420(3)	5992(4)	54(2)
C(171)	-189(3)	4858(3)	5094(4)	57(2)
C(172)	134(5)	5664(4)	5337(7)	99(3)
C(18)	-1092(3)	4096(4)	6382(4)	58(2)
C(181)	-1676(4)	4194(5)	6029(5)	80(2)
C(182)	-1765(5)	4713(6)	6686(7)	109(3)
C(19)	-1047(3)	3794(4)	7302(4)	67(2)
C(20)	-1614(4)	3282(4)	7841(5)	85(3)
C(151)	986(10)	4464(7)	5613(12)	52(4)
C(152)	692(10)	3876(8)	4997(10)	60(4)
C(153)	934(9)	3940(8)	4051(9)	64(4)
C(154)	1458(8)	4601(8)	3751(10)	59(3)
C(155)	1769(8)	5206(8)	4318(10)	53(3)
C(156)	1523(9)	5096(7)	5266(10)	51(4)
C(15A)	1048(9)	4695(7)	5578(11)	43(3)
C(15B)	821(9)	4153(7)	4892(9)	50(3)
C(15C)	1130(8)	4279(8)	3967(9)	57(3)
C(15D)	1645(7)	4973(7)	3773(11)	56(3)
C(15E)	1893(7)	5543(8)	4422(9)	50(3)
C(15F)	1554(8)	5374(7)	5321(10)	46(3)
C(201)	-2341(6)	3060(7)	7418(8)	57(3)
C(202)	-2881(5)	3154(7)	7748(8)	59(3)
C(203)	-3533(6)	2788(8)	7270(10)	81(4)
C(204)	-3656(8)	2328(9)	6491(12)	93(4)
C(205)	-3108(7)	2259(9)	6105(12)	90(4)
C(206)	-2479(7)	2617(8)	6614(10)	75(4)
C(20A)	-2285(11)	2743(12)	7345(14)	105(4)
C(20B)	-2912(9)	2732(11)	7547(15)	107(4)
C(20C)	-3506(11)	2227(11)	7013(14)	115(4)
C(20D)	-3421(13)	1907(13)	6205(15)	119(4)
C(20E)	-2832(10)	1885(11)	5856(14)	119(4)
C(20F)	-2362(8)	2337(12)	6542(14)	111(4)
N(1A)	2(3)	5036(3)	8837(3)	66(1)
C(2A)	-406(6)	5159(7)	9433(8)	69(2)
N(3A)	-190(5)	5883(6)	9309(7)	72(2)
C(3A)	-400(7)	6346(7)	9732(9)	87(2)
C(4A)	232(8)	6090(8)	8502(9)	72(2)
C(5A)	440(6)	5616(5)	8303(8)	70(2)
C(2C)	157(10)	5476(8)	8092(8)	78(3)
N(3C)	92(8)	6069(8)	8323(10)	82(3)
C(3C)	214(12)	6630(10)	7719(14)	113(5)
C(4C)	0(13)	6063(9)	9294(11)	77(3)
C(5C)	-130(11)	5396(8)	9554(8)	70(2)
N(1B)	4(3)	3221(3)	8840(4)	77(1)
C(2B)	43(7)	2870(6)	9608(7)	92(2)
N(3B)	-2(5)	2243(6)	9326(7)	102(2)
C(3B)	22(7)	1748(7)	9950(11)	135(4)
C(4B)	-28(8)	2239(7)	8324(8)	102(2)
C(5B)	-50(8)	2827(6)	8041(7)	95(2)
C(2D)	-427(16)	2655(10)	8340(20)	81(3)
N(3D)	-281(12)	2127(12)	8613(17)	85(3)

C(3D)	-599(18)	1426(13)	8280(30)	99(6)
C(4D)	295(17)	2427(16)	9220(30)	82(3)
C(5D)	370(18)	3056(15)	9490(20)	80(3)
Cl(1)	-953(5)	2193(5)	5873(6)	298(4)

Table S7. Bond lengths [Å] and angles [°] for [(OETPP)Fe(N-MeIm)$_2$]Cl.

Fe(1)-N(2)	1.947(5)	C(52)-H(162)	0.9500
Fe(1)-N(1B)	1.956(6)	C(53)-C(54)	1.384(10)
Fe(1)-N(3)	1.964(5)	C(53)-H(163)	0.9500
Fe(1)-N(1)	1.973(5)	C(54)-C(55)	1.387(10)
Fe(1)-N(4)	1.973(4)	C(54)-H(164)	0.9500
Fe(1)-N(1A)	1.996(5)	C(55)-C(56)	1.392(10)
N(1)-C(1)	1.365(7)	C(55)-H(165)	0.9500
N(1)-C(4)	1.392(7)	C(56)-H(166)	0.9500
C(1)-C(20)	1.395(9)	C(5AA)-C(5BB)	1.387(10)
C(1)-C(2)	1.448(8)	C(5AA)-C(5FF)	1.392(10)
C(2)-C(3)	1.343(8)	C(5BB)-C(5CC)	1.405(10)
C(2)-C(21)	1.537(9)	C(5BB)-H(172)	0.9500
C(21)-C(22)	1.503(13)	C(5CC)-C(5DD)	1.376(10)
C(21)-H(13A)	0.9900	C(5CC)-H(173)	0.9500
C(21)-H(13B)	0.9900	C(5DD)-C(5EE)	1.388(10)
C(22)-H(13C)	0.9800	C(5DD)-H(174)	0.9500
C(22)-H(13D)	0.9800	C(5EE)-C(5FF)	1.394(10)
C(22)-H(13E)	0.9800	C(5EE)-H(175)	0.9500
C(3)-C(4)	1.439(8)	C(5FF)-H(176)	0.9500
C(3)-C(31)	1.519(9)	C(101)-C(106)	1.369(10)
C(31)-C(32)	1.448(8)	C(101)-C(102)	1.394(10)
C(31)-H(14A)	0.9900	C(102)-C(103)	1.393(10)
C(31)-H(14B)	0.9900	C(102)-H(262)	0.9500
C(32)-H(14C)	0.9800	C(103)-C(104)	1.389(11)
C(32)-H(14D)	0.9800	C(103)-H(263)	0.9500
C(32)-H(14E)	0.9800	C(104)-C(105)	1.371(10)
C(4)-C(5)	1.414(8)	C(104)-H(264)	0.9500
C(5)-C(6)	1.403(8)	C(105)-C(106)	1.392(10)
C(5)-C(5AA)	1.50(2)	C(105)-H(265)	0.9500
C(5)-C(51)	1.511(16)	C(106)-H(266)	0.9500
N(2)-C(6)	1.379(7)	C(10A)-C(10B)	1.378(10)
N(2)-C(9)	1.395(8)	C(10A)-C(10F)	1.381(10)
C(6)-C(7)	1.434(8)	C(10B)-C(10C)	1.397(9)
C(7)-C(8)	1.370(8)	C(10B)-H(272)	0.9500
C(7)-C(71)	1.521(8)	C(10C)-C(10D)	1.405(10)
C(71)-C(72)	1.578(10)	C(10C)-H(273)	0.9500
C(71)-H(23A)	0.9900	C(10D)-C(10E)	1.377(10)
C(71)-H(23B)	0.9900	C(10D)-H(274)	0.9500
C(72)-H(23C)	0.9800	C(10E)-C(10F)	1.364(10)
C(72)-H(23D)	0.9800	C(10E)-H(275)	0.9500
C(72)-H(23E)	0.9800	C(10F)-H(276)	0.9500
C(8)-C(9)	1.446(9)	N(3)-C(11)	1.345(7)
C(8)-C(81)	1.469(9)	N(3)-C(14)	1.422(7)
C(81)-C(82)	1.536(11)	C(11)-C(12)	1.440(9)
C(81)-H(24F)	0.9900	C(12)-C(13)	1.363(9)
C(81)-H(24G)	0.9900	C(12)-C(121)	1.510(9)
C(82)-H(24H)	0.9800	C(121)-C(122)	1.482(13)
C(82)-H(24I)	0.9800	C(121)-H(33A)	0.9900
C(82)-H(24J)	0.9800	C(121)-H(33B)	0.9900
C(9)-C(10)	1.386(8)	C(122)-H(33C)	0.9800
C(10)-C(11)	1.424(9)	C(122)-H(33D)	0.9800
C(10)-C(10A)	1.506(13)	C(122)-H(33E)	0.9800
C(10)-C(101)	1.567(19)	C(13)-C(14)	1.442(9)
C(51)-C(52)	1.388(10)	C(13)-C(131)	1.497(9)
C(51)-C(56)	1.399(10)	C(131)-C(132)	1.456(8)
C(52)-C(53)	1.408(10)	C(131)-H(34A)	0.9900

C(131)-H(34B)	0.9900	C(204)-C(205)	1.381(10)
C(132)-H(34C)	0.9800	C(204)-H(464)	0.9500
C(132)-H(34D)	0.9800	C(205)-C(206)	1.383(10)
C(132)-H(34E)	0.9800	C(205)-H(465)	0.9500
C(14)-C(15)	1.393(8)	C(206)-H(466)	0.9500
C(15)-C(16)	1.398(8)	C(20A)-C(20F)	1.378(10)
C(15)-C(151)	1.457(17)	C(20A)-C(20B)	1.380(10)
C(15)-C(15A)	1.521(16)	C(20B)-C(20C)	1.415(10)
N(4)-C(19)	1.340(8)	C(20B)-H(472)	0.9500
N(4)-C(16)	1.402(7)	C(20C)-C(20D)	1.378(10)
C(16)-C(17)	1.439(8)	C(20C)-H(473)	0.9500
C(17)-C(18)	1.392(7)	C(20D)-C(20E)	1.394(10)
C(17)-C(171)	1.492(8)	C(20D)-H(474)	0.9500
C(171)-C(172)	1.565(10)	C(20E)-C(20F)	1.383(10)
C(171)-H(43A)	0.9900	C(20E)-H(475)	0.9500
C(171)-H(43B)	0.9900	C(20F)-H(476)	0.9500
C(172)-H(43C)	0.9800	N(1A)-C(2C)	1.332(9)
C(172)-H(43D)	0.9800	N(1A)-C(2A)	1.334(8)
C(172)-H(43E)	0.9800	N(1A)-C(5A)	1.360(5)
C(18)-C(19)	1.460(9)	N(1A)-C(5C)	1.381(5)
C(18)-C(181)	1.472(9)	C(2A)-N(3A)	1.411(14)
C(181)-C(182)	1.537(11)	C(2A)-H(2A)	0.9500
C(181)-H(44A)	0.9900	N(3A)-C(4A)	1.372(9)
C(181)-H(44B)	0.9900	N(3A)-C(3A)	1.425(14)
C(182)-H(44C)	0.9800	C(3A)-H(3A1)	0.9800
C(182)-H(44D)	0.9800	C(3A)-H(3A2)	0.9800
C(182)-H(44E)	0.9800	C(3A)-H(3A3)	0.9800
C(19)-C(20)	1.396(8)	C(4A)-C(5A)	1.347(12)
C(20)-C(20A)	1.51(2)	C(4A)-H(4A)	0.9500
C(20)-C(201)	1.523(14)	C(5A)-H(5A)	0.9500
C(151)-C(156)	1.371(10)	C(2C)-N(3C)	1.404(16)
C(151)-C(152)	1.398(10)	C(2C)-H(2C)	0.9500
C(152)-C(153)	1.393(10)	N(3C)-C(4C)	1.359(10)
C(152)-H(362)	0.9500	N(3C)-C(3C)	1.392(16)
C(153)-C(154)	1.380(10)	C(3C)-H(3C1)	0.9800
C(153)-H(363)	0.9500	C(3C)-H(3C2)	0.9800
C(154)-C(155)	1.385(10)	C(3C)-H(3C3)	0.9800
C(154)-H(364)	0.9500	C(4C)-C(5C)	1.381(13)
C(155)-C(156)	1.393(10)	C(4C)-H(4C)	0.9500
C(155)-H(365)	0.9500	C(5C)-H(5C)	0.9500
C(156)-H(366)	0.9500	N(1B)-C(2D)	1.314(10)
C(15A)-C(15F)	1.376(10)	N(1B)-C(2B)	1.337(8)
C(15A)-C(15B)	1.398(10)	N(1B)-C(5D)	1.364(10)
C(15B)-C(15C)	1.407(10)	N(1B)-C(5B)	1.368(8)
C(15B)-H(372)	0.9500	C(2B)-N(3B)	1.375(13)
C(15C)-C(15D)	1.385(10)	C(2B)-H(2B)	0.9500
C(15C)-H(373)	0.9500	N(3B)-C(4B)	1.389(9)
C(15D)-C(15E)	1.402(10)	N(3B)-C(3B)	1.402(14)
C(15D)-H(374)	0.9500	C(3B)-H(3B1)	0.9800
C(15E)-C(15F)	1.401(9)	C(3B)-H(3B2)	0.9800
C(15E)-H(375)	0.9500	C(3B)-H(3B3)	0.9800
C(15F)-H(376)	0.9500	C(4B)-C(5B)	1.361(11)
C(201)-C(202)	1.368(10)	C(4B)-H(4B)	0.9500
C(201)-C(206)	1.403(10)	C(5B)-H(5B)	0.9500
C(202)-C(203)	1.398(10)	C(2D)-N(3D)	1.392(18)
C(202)-H(462)	0.9500	C(2D)-H(2D)	0.9500
C(203)-C(204)	1.404(10)	N(3D)-C(4D)	1.374(11)
C(203)-H(463)	0.9500	N(3D)-C(3D)	1.400(19)

C(3D)-H(3D1)	0.9800
C(3D)-H(3D2)	0.9800
C(3D)-H(3D3)	0.9800
C(4D)-C(5D)	1.348(14)
C(4D)-H(4D)	0.9500
C(5D)-H(5D)	0.9500
N(2)-Fe(1)-N(1B)	92.5(2)
N(2)-Fe(1)-N(3)	91.04(19)
N(1B)-Fe(1)-N(3)	87.2(2)
N(2)-Fe(1)-N(1)	89.03(19)
N(1B)-Fe(1)-N(1)	88.5(2)
N(3)-Fe(1)-N(1)	175.7(2)
N(2)-Fe(1)-N(4)	174.4(2)
N(1B)-Fe(1)-N(4)	93.1(2)
N(3)-Fe(1)-N(4)	89.72(18)
N(1)-Fe(1)-N(4)	90.63(18)
N(2)-Fe(1)-N(1A)	87.4(2)
N(1B)-Fe(1)-N(1A)	179.6(3)
N(3)-Fe(1)-N(1A)	92.4(2)
N(1)-Fe(1)-N(1A)	91.8(2)
N(4)-Fe(1)-N(1A)	87.0(2)
C(1)-N(1)-C(4)	106.3(5)
C(1)-N(1)-Fe(1)	121.9(4)
C(4)-N(1)-Fe(1)	124.1(4)
N(1)-C(1)-C(20)	123.1(5)
N(1)-C(1)-C(2)	108.4(5)
C(20)-C(1)-C(2)	128.4(5)
C(3)-C(2)-C(1)	109.2(5)
C(3)-C(2)-C(21)	124.8(6)
C(1)-C(2)-C(21)	125.0(6)
C(22)-C(21)-C(2)	109.4(8)
C(22)-C(21)-H(13A)	109.8
C(2)-C(21)-H(13A)	109.8
C(22)-C(21)-H(13B)	109.8
C(2)-C(21)-H(13B)	109.8
H(13A)-C(21)-H(13B)	108.2
C(21)-C(22)-H(13C)	109.5
C(21)-C(22)-H(13D)	109.5
H(13C)-C(22)-H(13D)	109.5
C(21)-C(22)-H(13E)	109.5
H(13C)-C(22)-H(13E)	109.5
H(13D)-C(22)-H(13E)	109.5
C(2)-C(3)-C(4)	105.6(5)
C(2)-C(3)-C(31)	124.1(6)
C(4)-C(3)-C(31)	129.4(6)
C(32)-C(31)-C(3)	112.9(8)
C(32)-C(31)-H(14A)	109.0
C(3)-C(31)-H(14A)	109.0
C(32)-C(31)-H(14B)	109.0
C(3)-C(31)-H(14B)	109.0
H(14A)-C(31)-H(14B)	107.8
C(31)-C(32)-H(14C)	109.5
C(31)-C(32)-H(14D)	109.5
H(14C)-C(32)-H(14D)	109.5
C(31)-C(32)-H(14E)	109.5
H(14C)-C(32)-H(14E)	109.5
H(14D)-C(32)-H(14E)	109.5
N(1)-C(4)-C(5)	121.3(5)
N(1)-C(4)-C(3)	110.2(5)
C(5)-C(4)-C(3)	128.1(5)
C(6)-C(5)-C(4)	121.7(5)
C(6)-C(5)-C(5AA)	120.8(10)
C(4)-C(5)-C(5AA)	115.4(10)
C(6)-C(5)-C(51)	117.3(8)
C(4)-C(5)-C(51)	120.9(8)
C(5AA)-C(5)-C(51)	17.7(10)
C(6)-N(2)-C(9)	103.7(5)
C(6)-N(2)-Fe(1)	127.0(4)
C(9)-N(2)-Fe(1)	123.9(4)
N(2)-C(6)-C(5)	121.1(5)
N(2)-C(6)-C(7)	111.6(5)
C(5)-C(6)-C(7)	127.2(5)
C(8)-C(7)-C(6)	107.0(5)
C(8)-C(7)-C(71)	123.5(6)
C(6)-C(7)-C(71)	129.1(5)
C(7)-C(71)-C(72)	109.0(5)
C(7)-C(71)-H(23A)	109.9
C(72)-C(71)-H(23A)	109.9
C(7)-C(71)-H(23B)	109.9
C(72)-C(71)-H(23B)	109.9
H(23A)-C(71)-H(23B)	108.3
C(71)-C(72)-H(23C)	109.5
C(71)-C(72)-H(23D)	109.5
H(23C)-C(72)-H(23D)	109.5
C(71)-C(72)-H(23E)	109.5
H(23C)-C(72)-H(23E)	109.5
H(23D)-C(72)-H(23E)	109.5
C(7)-C(8)-C(9)	105.6(5)
C(7)-C(8)-C(81)	125.2(6)
C(9)-C(8)-C(81)	128.4(5)
C(8)-C(81)-C(82)	108.8(6)
C(8)-C(81)-H(24F)	109.9
C(82)-C(81)-H(24F)	109.9
C(8)-C(81)-H(24G)	109.9
C(82)-C(81)-H(24G)	109.9
H(24F)-C(81)-H(24G)	108.3
C(81)-C(82)-H(24H)	109.5
C(81)-C(82)-H(24I)	109.5
H(24H)-C(82)-H(24I)	109.5
C(81)-C(82)-H(24J)	109.5
H(24H)-C(82)-H(24J)	109.5
H(24I)-C(82)-H(24J)	109.5
C(10)-C(9)-N(2)	120.1(6)
C(10)-C(9)-C(8)	128.5(6)
N(2)-C(9)-C(8)	111.2(5)
C(9)-C(10)-C(11)	123.6(6)
C(9)-C(10)-C(10A)	114.2(7)
C(11)-C(10)-C(10A)	121.3(6)
C(9)-C(10)-C(101)	116.5(8)
C(11)-C(10)-C(101)	116.5(9)
C(10A)-C(10)-C(101)	29.2(7)
C(52)-C(51)-C(56)	118.0(13)
C(52)-C(51)-C(5)	117.8(11)
C(56)-C(51)-C(5)	123.8(11)
C(51)-C(52)-C(53)	120.7(14)

C(51)-C(52)-H(162)	119.7
C(53)-C(52)-H(162)	119.7
C(54)-C(53)-C(52)	118.7(14)
C(54)-C(53)-H(163)	120.6
C(52)-C(53)-H(163)	120.6
C(53)-C(54)-C(55)	122.0(14)
C(53)-C(54)-H(164)	119.0
C(55)-C(54)-H(164)	119.0
C(54)-C(55)-C(56)	117.7(14)
C(54)-C(55)-H(165)	121.2
C(56)-C(55)-H(165)	121.2
C(55)-C(56)-C(51)	122.4(14)
C(55)-C(56)-H(166)	118.8
C(51)-C(56)-H(166)	118.8
C(5BB)-C(5AA)-C(5FF)	121.7(17)
C(5BB)-C(5AA)-C(5)	123.5(13)
C(5FF)-C(5AA)-C(5)	113.7(13)
C(5AA)-C(5BB)-C(5CC)	116.5(17)
C(5AA)-C(5BB)-H(172)	121.7
C(5CC)-C(5BB)-H(172)	121.7
C(5DD)-C(5CC)-C(5BB)	120.1(16)
C(5DD)-C(5CC)-H(173)	119.9
C(5BB)-C(5CC)-H(173)	119.9
C(5CC)-C(5DD)-C(5EE)	122.4(16)
C(5CC)-C(5DD)-H(174)	118.8
C(5EE)-C(5DD)-H(174)	118.8
C(5DD)-C(5EE)-C(5FF)	116.7(15)
C(5DD)-C(5EE)-H(175)	121.6
C(5FF)-C(5EE)-H(175)	121.6
C(5AA)-C(5FF)-C(5EE)	120.8(16)
C(5AA)-C(5FF)-H(176)	119.6
C(5EE)-C(5FF)-H(176)	119.6
C(106)-C(101)-C(102)	117.8(18)
C(106)-C(101)-C(10)	116.6(14)
C(102)-C(101)-C(10)	125.3(13)
C(103)-C(102)-C(101)	120.9(18)
C(103)-C(102)-H(262)	119.6
C(101)-C(102)-H(262)	119.6
C(104)-C(103)-C(102)	115(2)
C(104)-C(103)-H(263)	122.4
C(102)-C(103)-H(263)	122.4
C(105)-C(104)-C(103)	128(2)
C(105)-C(104)-H(264)	115.9
C(103)-C(104)-H(264)	115.9
C(104)-C(105)-C(106)	112(2)
C(104)-C(105)-H(265)	124.2
C(106)-C(105)-H(265)	124.2
C(101)-C(106)-C(105)	125.4(19)
C(101)-C(106)-H(266)	117.3
C(105)-C(106)-H(266)	117.3
C(10B)-C(10A)-C(10F)	118.1(12)
C(10B)-C(10A)-C(10)	127.0(9)
C(10F)-C(10A)-C(10)	114.8(9)
C(10A)-C(10B)-C(10C)	118.4(13)
C(10A)-C(10B)-H(272)	120.8
C(10C)-C(10B)-H(272)	120.8
C(10B)-C(10C)-C(10D)	117.9(15)
C(10B)-C(10C)-H(273)	121.0
C(10D)-C(10C)-H(273)	121.0
C(10E)-C(10D)-C(10C)	126.4(17)
C(10E)-C(10D)-H(274)	116.8
C(10C)-C(10D)-H(274)	116.8
C(10F)-C(10E)-C(10D)	110.4(16)
C(10F)-C(10E)-H(275)	124.8
C(10D)-C(10E)-H(275)	124.8
C(10E)-C(10F)-C(10A)	128.5(14)
C(10E)-C(10F)-H(276)	115.7
C(10A)-C(10F)-H(276)	115.7
C(11)-N(3)-C(14)	105.3(5)
C(11)-N(3)-Fe(1)	123.4(4)
C(14)-N(3)-Fe(1)	124.3(4)
N(3)-C(11)-C(10)	121.1(6)
N(3)-C(11)-C(12)	111.4(5)
C(10)-C(11)-C(12)	127.3(6)
C(13)-C(12)-C(11)	107.0(5)
C(13)-C(12)-C(121)	124.1(7)
C(11)-C(12)-C(121)	127.9(6)
C(122)-C(121)-C(12)	109.5(7)
C(122)-C(121)-H(33A)	109.8
C(12)-C(121)-H(33A)	109.8
C(122)-C(121)-H(33B)	109.8
C(12)-C(121)-H(33B)	109.8
H(33A)-C(121)-H(33B)	108.2
C(121)-C(122)-H(33C)	109.5
C(121)-C(122)-H(33D)	109.5
H(33C)-C(122)-H(33D)	109.5
C(121)-C(122)-H(33E)	109.5
H(33C)-C(122)-H(33E)	109.5
H(33D)-C(122)-H(33E)	109.5
C(12)-C(13)-C(14)	106.8(5)
C(12)-C(13)-C(131)	124.5(7)
C(14)-C(13)-C(131)	128.7(6)
C(132)-C(131)-C(13)	112.5(9)
C(132)-C(131)-H(34A)	109.1
C(13)-C(131)-H(34A)	109.1
C(132)-C(131)-H(34B)	109.1
C(13)-C(131)-H(34B)	109.1
H(34A)-C(131)-H(34B)	107.8
C(131)-C(132)-H(34C)	109.5
C(131)-C(132)-H(34D)	109.5
H(34C)-C(132)-H(34D)	109.5
C(131)-C(132)-H(34E)	109.5
H(34C)-C(132)-H(34E)	109.5
H(34D)-C(132)-H(34E)	109.5
C(15)-C(14)-N(3)	121.8(5)
C(15)-C(14)-C(13)	129.1(5)
N(3)-C(14)-C(13)	109.0(5)
C(14)-C(15)-C(16)	123.0(5)
C(14)-C(15)-C(151)	117.1(10)
C(16)-C(15)-C(151)	118.4(10)
C(14)-C(15)-C(15A)	120.2(9)
C(16)-C(15)-C(15A)	116.6(9)
C(151)-C(15)-C(15A)	17.3(9)
C(19)-N(4)-C(16)	105.7(5)
C(19)-N(4)-Fe(1)	123.5(4)
C(16)-N(4)-Fe(1)	125.9(4)

C(15)-C(16)-N(4)	121.5(5)
C(15)-C(16)-C(17)	128.0(5)
N(4)-C(16)-C(17)	110.4(5)
C(18)-C(17)-C(16)	106.0(5)
C(18)-C(17)-C(171)	124.8(6)
C(16)-C(17)-C(171)	128.9(5)
C(17)-C(171)-C(172)	110.9(5)
C(17)-C(171)-H(43A)	109.5
C(172)-C(171)-H(43A)	109.5
C(17)-C(171)-H(43B)	109.5
C(172)-C(171)-H(43B)	109.5
H(43A)-C(171)-H(43B)	108.0
C(171)-C(172)-H(43C)	109.5
C(171)-C(172)-H(43D)	109.5
H(43C)-C(172)-H(43D)	109.5
C(171)-C(172)-H(43E)	109.5
H(43C)-C(172)-H(43E)	109.5
H(43D)-C(172)-H(43E)	109.5
C(17)-C(18)-C(19)	105.8(5)
C(17)-C(18)-C(181)	125.1(6)
C(19)-C(18)-C(181)	127.8(5)
C(18)-C(181)-C(182)	110.1(6)
C(18)-C(181)-H(44A)	109.6
C(182)-C(181)-H(44A)	109.6
C(18)-C(181)-H(44B)	109.6
C(182)-C(181)-H(44B)	109.6
H(44A)-C(181)-H(44B)	108.2
C(181)-C(182)-H(44C)	109.5
C(181)-C(182)-H(44D)	109.5
H(44C)-C(182)-H(44D)	109.5
C(181)-C(182)-H(44E)	109.5
H(44C)-C(182)-H(44E)	109.5
H(44D)-C(182)-H(44E)	109.5
N(4)-C(19)-C(20)	121.2(6)
N(4)-C(19)-C(18)	111.4(5)
C(20)-C(19)-C(18)	126.5(6)
C(1)-C(20)-C(19)	122.1(6)
C(1)-C(20)-C(20A)	116.4(10)
C(19)-C(20)-C(20A)	120.2(10)
C(1)-C(20)-C(201)	120.8(7)
C(19)-C(20)-C(201)	114.2(7)
C(20A)-C(20)-C(201)	29.2(8)
C(156)-C(151)-C(152)	118.3(13)
C(156)-C(151)-C(15)	117.0(11)
C(152)-C(151)-C(15)	124.5(11)
C(153)-C(152)-C(151)	120.4(13)
C(153)-C(152)-H(362)	119.8
C(151)-C(152)-H(362)	119.8
C(154)-C(153)-C(152)	117.5(13)
C(154)-C(153)-H(363)	121.3
C(152)-C(153)-H(363)	121.3
C(153)-C(154)-C(155)	125.2(13)
C(153)-C(154)-H(364)	117.4
C(155)-C(154)-H(364)	117.4
C(154)-C(155)-C(156)	114.1(12)
C(154)-C(155)-H(365)	122.9
C(156)-C(155)-H(365)	122.9
C(151)-C(156)-C(155)	124.4(13)
C(151)-C(156)-H(366)	117.8
C(155)-C(156)-H(366)	117.8
C(15F)-C(15A)-C(15B)	119.0(12)
C(15F)-C(15A)-C(15)	125.0(10)
C(15B)-C(15A)-C(15)	115.9(9)
C(15A)-C(15B)-C(15C)	121.5(12)
C(15A)-C(15B)-H(372)	119.3
C(15C)-C(15B)-H(372)	119.3
C(15D)-C(15C)-C(15B)	115.8(12)
C(15D)-C(15C)-H(373)	122.1
C(15B)-C(15C)-H(373)	122.1
C(15C)-C(15D)-C(15E)	125.8(12)
C(15C)-C(15D)-H(374)	117.1
C(15E)-C(15D)-H(374)	117.1
C(15F)-C(15E)-C(15D)	114.7(12)
C(15F)-C(15E)-H(375)	122.7
C(15D)-C(15E)-H(375)	122.7
C(15A)-C(15F)-C(15E)	123.1(13)
C(15A)-C(15F)-H(376)	118.5
C(15E)-C(15F)-H(376)	118.5
C(202)-C(201)-C(206)	117.6(12)
C(202)-C(201)-C(20)	131.2(10)
C(206)-C(201)-C(20)	110.7(10)
C(201)-C(202)-C(203)	117.3(12)
C(201)-C(202)-H(462)	121.3
C(203)-C(202)-H(462)	121.3
C(202)-C(203)-C(204)	123.2(14)
C(202)-C(203)-H(463)	118.4
C(204)-C(203)-H(463)	118.4
C(205)-C(204)-C(203)	120.5(15)
C(205)-C(204)-H(464)	119.7
C(203)-C(204)-H(464)	119.7
C(204)-C(205)-C(206)	114.0(15)
C(204)-C(205)-H(465)	123.0
C(206)-C(205)-H(465)	123.0
C(205)-C(206)-C(201)	127.1(15)
C(205)-C(206)-H(466)	116.5
C(201)-C(206)-H(466)	116.5
C(20F)-C(20A)-C(20B)	110.5(18)
C(20F)-C(20A)-C(20)	128.8(16)
C(20B)-C(20A)-C(20)	119.1(14)
C(20A)-C(20B)-C(20C)	115(2)
C(20A)-C(20B)-H(472)	122.6
C(20C)-C(20B)-H(472)	122.6
C(20D)-C(20C)-C(20B)	121(2)
C(20D)-C(20C)-H(473)	119.5
C(20B)-C(20C)-H(473)	119.5
C(20C)-C(20D)-C(20E)	131(2)
C(20C)-C(20D)-H(474)	114.5
C(20E)-C(20D)-H(474)	114.5
C(20F)-C(20E)-C(20D)	95.9(18)
C(20F)-C(20E)-H(475)	132.1
C(20D)-C(20E)-H(475)	132.1
C(20A)-C(20F)-C(20E)	145.2(16)
C(20A)-C(20F)-H(476)	107.4
C(20E)-C(20F)-H(476)	107.4
C(2C)-N(1A)-C(2A)	106.8(10)
C(2C)-N(1A)-C(5A)	26.1(8)

C(2A)-N(1A)-C(5A)	112.2(8)	C(2D)-N(1B)-C(5D)	110.1(16)
C(2C)-N(1A)-C(5C)	101.5(9)	C(2B)-N(1B)-C(5D)	27.3(16)
C(2A)-N(1A)-C(5C)	24.8(9)	C(2D)-N(1B)-C(5B)	35.6(15)
C(5A)-N(1A)-C(5C)	96.5(9)	C(2B)-N(1B)-C(5B)	107.3(8)
C(2C)-N(1A)-Fe(1)	126.4(8)	C(5D)-N(1B)-C(5B)	104.5(15)
C(2A)-N(1A)-Fe(1)	122.1(6)	C(2D)-N(1B)-Fe(1)	125.1(11)
C(5A)-N(1A)-Fe(1)	125.5(6)	C(2B)-N(1B)-Fe(1)	127.1(6)
C(5C)-N(1A)-Fe(1)	132.0(7)	C(5D)-N(1B)-Fe(1)	123.8(12)
N(1A)-C(2A)-N(3A)	105.4(9)	C(5B)-N(1B)-Fe(1)	125.6(6)
N(1A)-C(2A)-H(2A)	127.3	N(1B)-C(2B)-N(3B)	110.3(9)
N(3A)-C(2A)-H(2A)	127.3	N(1B)-C(2B)-H(2B)	124.9
C(4A)-N(3A)-C(2A)	105.1(11)	N(3B)-C(2B)-H(2B)	124.9
C(4A)-N(3A)-C(3A)	120.0(12)	C(2B)-N(3B)-C(4B)	105.8(10)
C(2A)-N(3A)-C(3A)	134.0(10)	C(2B)-N(3B)-C(3B)	125.1(11)
N(3A)-C(3A)-H(3A1)	109.5	C(4B)-N(3B)-C(3B)	128.9(12)
N(3A)-C(3A)-H(3A2)	109.5	N(3B)-C(3B)-H(3B1)	109.5
H(3A1)-C(3A)-H(3A2)	109.5	N(3B)-C(3B)-H(3B2)	109.5
N(3A)-C(3A)-H(3A3)	109.5	H(3B1)-C(3B)-H(3B2)	109.5
H(3A1)-C(3A)-H(3A3)	109.5	N(3B)-C(3B)-H(3B3)	109.5
H(3A2)-C(3A)-H(3A3)	109.5	H(3B1)-C(3B)-H(3B3)	109.5
C(5A)-C(4A)-N(3A)	109.9(12)	H(3B2)-C(3B)-H(3B3)	109.5
C(5A)-C(4A)-H(4A)	125.0	C(5B)-C(4B)-N(3B)	107.6(11)
N(3A)-C(4A)-H(4A)	125.0	C(5B)-C(4B)-H(4B)	126.2
C(4A)-C(5A)-N(1A)	104.6(10)	N(3B)-C(4B)-H(4B)	126.2
C(4A)-C(5A)-H(5A)	127.7	C(4B)-C(5B)-N(1B)	108.8(9)
N(1A)-C(5A)-H(5A)	127.7	C(4B)-C(5B)-H(5B)	125.6
N(1A)-C(2C)-N(3C)	112.2(11)	N(1B)-C(5B)-H(5B)	125.6
N(1A)-C(2C)-H(2C)	123.9	N(1B)-C(2D)-N(3D)	105.9(16)
N(3C)-C(2C)-H(2C)	123.9	N(1B)-C(2D)-H(2D)	127.0
C(4C)-N(3C)-C(3C)	124.5(17)	N(3D)-C(2D)-H(2D)	127.0
C(4C)-N(3C)-C(2C)	107.4(13)	C(4D)-N(3D)-C(2D)	108.0(18)
C(3C)-N(3C)-C(2C)	127.3(14)	C(4D)-N(3D)-C(3D)	124(2)
N(3C)-C(3C)-H(3C1)	109.5	C(2D)-N(3D)-C(3D)	128(2)
N(3C)-C(3C)-H(3C2)	109.5	N(3D)-C(3D)-H(3D1)	109.5
H(3C1)-C(3C)-H(3C2)	109.5	N(3D)-C(3D)-H(3D2)	109.5
N(3C)-C(3C)-H(3C3)	109.5	H(3D1)-C(3D)-H(3D2)	109.5
H(3C1)-C(3C)-H(3C3)	109.5	N(3D)-C(3D)-H(3D3)	109.5
H(3C2)-C(3C)-H(3C3)	109.5	H(3D1)-C(3D)-H(3D3)	109.5
N(3C)-C(4C)-C(5C)	102.7(14)	H(3D2)-C(3D)-H(3D3)	109.5
N(3C)-C(4C)-H(4C)	128.6	C(5D)-C(4D)-N(3D)	105.7(19)
C(5C)-C(4C)-H(4C)	128.6	C(5D)-C(4D)-H(4D)	127.1
C(4C)-C(5C)-N(1A)	114.7(11)	N(3D)-C(4D)-H(4D)	127.1
C(4C)-C(5C)-H(5C)	122.7	C(4D)-C(5D)-N(1B)	107.0(19)
N(1A)-C(5C)-H(5C)	122.7	C(4D)-C(5D)-H(5D)	126.5
C(2D)-N(1B)-C(2B)	96.2(15)	N(1B)-C(5D)-H(5D)	126.5

Table S8. Anisotropic displacement parameters ($Å^2 \times 10^3$) for [(OETPP)Fe(N-MeIm)$_2$]Cl. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2 a^{*2} U^{11} + ... + 2 h k a^* b^* U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	38(1)	71(1)	26(1)	2(1)	4(1)	19(1)
N(1)	52(3)	72(3)	25(2)	9(2)	8(2)	30(3)
C(1)	32(3)	102(5)	31(3)	8(3)	1(3)	8(4)
C(2)	55(4)	89(5)	44(4)	3(3)	0(3)	7(3)
C(21)	79(4)	94(5)	61(4)	-6(4)	8(4)	-3(4)
C(22)	120(6)	106(6)	113(6)	-29(5)	4(5)	2(5)
C(3)	58(4)	68(4)	38(3)	8(3)	4(3)	19(3)
C(31)	96(5)	96(5)	69(4)	28(4)	-5(4)	11(4)
C(32)	169(8)	119(7)	130(7)	17(6)	-4(6)	58(6)
C(4)	49(4)	88(5)	33(3)	11(3)	1(3)	26(4)
C(5)	46(4)	82(5)	40(4)	14(3)	11(3)	27(4)
N(2)	38(3)	70(3)	39(3)	10(2)	4(2)	20(3)
C(6)	50(4)	72(4)	25(3)	9(3)	0(3)	28(3)
C(7)	47(3)	73(4)	30(3)	10(3)	8(3)	30(3)
C(71)	59(3)	75(4)	39(3)	2(3)	5(3)	31(3)
C(72)	87(5)	107(5)	73(5)	-10(4)	-4(4)	56(4)
C(8)	41(3)	97(4)	30(3)	4(3)	4(2)	31(3)
C(81)	49(3)	109(5)	45(3)	1(3)	11(3)	11(3)
C(82)	115(6)	102(5)	67(5)	13(4)	11(5)	-9(5)
C(9)	45(4)	105(6)	26(3)	3(3)	9(3)	22(4)
C(10)	46(4)	142(7)	31(3)	-6(4)	1(3)	41(4)
C(51)	31(6)	38(8)	25(5)	-1(5)	3(4)	12(5)
C(52)	56(8)	59(8)	31(6)	5(5)	-7(5)	28(6)
C(53)	63(8)	63(8)	42(6)	0(6)	6(6)	27(6)
C(54)	60(8)	63(8)	43(6)	5(6)	14(6)	10(6)
C(55)	52(7)	70(9)	54(7)	-5(6)	14(5)	25(6)
C(56)	37(6)	45(8)	48(6)	0(5)	18(5)	16(6)
C(5AA)	56(7)	56(10)	44(7)	4(6)	2(5)	30(7)
C(5BB)	73(9)	74(9)	38(7)	10(6)	2(5)	38(7)
C(5CC)	86(8)	77(9)	59(7)	19(7)	17(6)	40(6)
C(5DD)	63(8)	73(9)	49(7)	10(6)	13(6)	28(7)
C(5EE)	65(8)	68(9)	46(7)	1(6)	5(6)	25(6)
C(5FF)	56(8)	62(9)	54(6)	14(6)	17(6)	25(7)
C(101)	77(6)	106(7)	63(6)	-15(5)	1(5)	42(5)
C(102)	86(6)	117(7)	68(6)	-14(5)	-9(5)	52(5)
C(103)	99(6)	128(7)	80(6)	-18(5)	-15(5)	52(5)
C(104)	105(6)	135(7)	95(7)	-26(6)	-7(6)	45(5)
C(105)	85(6)	124(7)	89(7)	-27(6)	3(6)	35(5)
C(106)	81(6)	110(7)	69(6)	-27(5)	6(5)	30(5)
C(10A)	23(5)	77(7)	42(6)	-6(5)	6(4)	22(5)
C(10B)	40(5)	79(6)	48(6)	-26(5)	10(4)	18(5)
C(10C)	33(5)	101(8)	84(7)	-16(6)	7(5)	29(5)
C(10D)	86(7)	115(8)	83(8)	-16(7)	-11(6)	44(6)
C(10E)	53(6)	122(8)	49(6)	-21(6)	-10(5)	40(6)
C(10F)	53(6)	107(8)	47(6)	-14(5)	-10(5)	56(5)
N(3)	39(3)	73(4)	30(3)	-6(2)	7(2)	20(3)
C(11)	41(4)	97(5)	43(4)	-7(4)	2(3)	23(4)
C(12)	42(3)	134(6)	47(4)	9(4)	3(3)	38(4)
C(121)	63(4)	144(6)	75(4)	14(4)	4(3)	53(4)
C(122)	103(6)	185(7)	133(7)	21(6)	-5(5)	107(5)
C(13)	58(4)	129(6)	42(4)	-13(4)	8(3)	42(4)

C(131)	87(5)	160(6)	84(5)	-39(5)	2(4)	71(4)
C(132)	150(7)	158(7)	134(7)	-16(6)	6(6)	78(6)
C(14)	36(3)	79(4)	35(3)	-3(3)	8(3)	19(3)
C(15)	47(4)	74(4)	39(3)	-11(3)	6(3)	26(3)
N(4)	25(3)	66(3)	35(3)	-5(2)	0(2)	6(2)
C(16)	46(4)	73(4)	23(3)	-9(3)	1(2)	26(3)
C(17)	51(3)	68(4)	35(3)	-6(3)	10(3)	24(3)
C(171)	50(3)	69(3)	40(3)	-1(3)	2(3)	20(3)
C(172)	101(5)	81(4)	82(5)	10(4)	-18(4)	20(4)
C(18)	42(3)	98(5)	18(3)	1(3)	5(2)	22(3)
C(181)	60(4)	134(5)	37(3)	9(3)	8(3)	41(4)
C(182)	100(5)	182(7)	78(5)	9(5)	16(4)	96(5)
C(19)	49(4)	110(6)	30(3)	9(3)	15(3)	31(4)
C(20)	44(4)	103(6)	47(4)	12(4)	-2(3)	-7(4)
C(151)	51(6)	62(6)	41(5)	-5(5)	2(4)	27(5)
C(152)	64(6)	64(6)	38(5)	-6(5)	2(4)	20(5)
C(153)	69(6)	68(6)	41(5)	-12(5)	0(5)	23(5)
C(154)	59(6)	66(6)	40(5)	-4(5)	-1(5)	22(5)
C(155)	51(6)	65(6)	45(5)	-10(5)	-4(4)	29(5)
C(156)	50(6)	57(6)	41(5)	-3(5)	-4(4)	23(5)
C(15A)	40(5)	49(5)	38(5)	3(4)	10(4)	21(5)
C(15B)	49(6)	57(5)	36(5)	1(4)	3(4)	20(5)
C(15C)	55(6)	65(5)	38(5)	1(5)	6(4)	20(5)
C(15D)	47(5)	70(5)	45(5)	0(4)	14(4)	27(4)
C(15E)	39(5)	62(5)	46(5)	7(4)	14(4)	23(4)
C(15F)	40(5)	56(5)	36(4)	6(4)	8(4)	20(5)
C(201)	25(5)	72(7)	40(5)	22(5)	-2(4)	-1(5)
C(202)	43(5)	60(6)	39(5)	18(5)	2(4)	0(5)
C(203)	37(5)	93(8)	89(7)	25(6)	8(5)	15(5)
C(204)	64(6)	97(8)	83(8)	7(6)	-20(6)	15(6)
C(205)	82(7)	75(8)	70(7)	-9(6)	-14(6)	7(6)
C(206)	62(6)	72(8)	55(7)	1(6)	-12(5)	7(6)
C(20A)	97(5)	117(6)	81(5)	17(4)	-13(4)	38(4)
C(20B)	95(5)	121(6)	85(5)	19(4)	-13(4)	39(4)
C(20C)	98(5)	125(6)	95(5)	14(5)	-11(4)	35(4)
C(20D)	105(5)	125(6)	96(5)	12(4)	-13(4)	34(4)
C(20E)	107(5)	124(6)	91(5)	9(4)	-11(4)	32(4)
C(20F)	102(5)	117(6)	84(5)	12(4)	-11(4)	33(4)
N(1A)	84(3)	81(3)	33(2)	5(2)	10(2)	42(2)
C(2A)	87(3)	83(3)	38(2)	6(2)	12(2)	44(3)
N(3A)	93(3)	83(3)	44(2)	6(2)	13(2)	46(3)
C(3A)	110(5)	89(4)	65(4)	2(4)	21(4)	52(4)
C(4A)	93(3)	82(3)	41(3)	6(2)	10(2)	43(3)
C(5A)	88(3)	82(3)	37(2)	5(2)	11(2)	41(3)
C(2C)	99(5)	83(4)	38(4)	5(3)	13(4)	35(4)
N(3C)	110(6)	81(4)	43(4)	11(4)	6(4)	39(4)
C(3C)	150(11)	83(8)	76(8)	27(6)	9(9)	36(8)
C(4C)	106(6)	79(5)	47(4)	10(4)	15(5)	47(4)
C(5C)	97(5)	81(5)	38(4)	11(3)	15(4)	49(4)
N(1B)	77(3)	99(3)	56(3)	-7(2)	-6(2)	44(3)
C(2B)	99(5)	106(4)	74(3)	-4(3)	-14(4)	52(4)
N(3B)	116(5)	105(4)	87(4)	-3(3)	-7(4)	57(4)
C(3B)	151(9)	115(7)	130(7)	18(6)	-8(7)	61(7)
C(4B)	115(5)	99(4)	87(4)	-6(4)	8(4)	50(4)
C(5B)	105(5)	99(4)	74(3)	-10(3)	-1(4)	46(4)
C(2D)	79(6)	102(5)	62(5)	-9(4)	-7(4)	44(5)
N(3D)	82(6)	101(5)	70(6)	-10(5)	-5(5)	46(5)
C(3D)	98(11)	102(7)	90(11)	-18(9)	-8(10)	45(9)

C(4D)	79(6)	101(6)	66(6)	-3(5)	-5(5)	45(5)
C(5D)	77(6)	101(5)	61(5)	-4(5)	-6(4)	43(5)
Cl(1)	329(7)	297(7)	231(6)	39(5)	-3(5)	130(6)

Table S9. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [(OETPP)Fe(N-MeIm)$_2$]Cl.

	x	y	z	U(eq)
H(13A)	-2964	1589	9569	119
H(13B)	-2913	1943	8535	119
H(13C)	-2718	976	8375	206
H(13D)	-2061	1348	9103	206
H(13E)	-2019	1694	8068	206
H(14A)	-2133	2416	11739	124
H(14B)	-2641	1825	10980	124
H(14C)	-2022	1424	11849	218
H(14D)	-1287	2093	11518	218
H(14E)	-1784	1511	10741	218
H(23A)	624	5333	12999	71
H(23B)	-137	4623	12955	71
H(23C)	-313	5633	12915	129
H(23D)	-566	5226	11903	129
H(23E)	189	5937	11986	129
H(24F)	2112	5830	11716	96
H(24G)	1553	5953	12319	96
H(24H)	2216	6906	11187	185
H(24I)	1381	6527	10989	185
H(24J)	1872	6348	10322	185
H(162)	-520	3152	12592	59
H(163)	-925	3024	14204	70
H(164)	-1853	3232	14553	78
H(165)	-2221	3785	13430	73
H(166)	-1728	4009	11879	54
H(172)	-256	3206	12514	73
H(173)	-853	2709	14003	89
H(174)	-1619	3066	14596	77
H(175)	-2103	3578	13582	76
H(176)	-1782	3712	11933	72
H(262)	1838	4133	11275	108
H(263)	2872	4462	12203	125
H(264)	3870	5534	11834	142
H(265)	3943	6293	10604	128
H(266)	2947	5809	9564	113
H(272)	2785	6232	9391	73
H(273)	3920	6739	10129	90
H(274)	4035	6230	11544	117
H(275)	3169	5109	12107	92
H(276)	2099	4637	11286	74
H(33A)	2954	4539	8068	112
H(33B)	2932	4868	9096	112
H(33C)	2757	3717	9266	187
H(33D)	2062	3417	8606	187
H(33E)	2079	3753	9640	187
H(34A)	2091	4539	5934	128
H(34B)	2646	4511	6665	128
H(34C)	2071	3473	5815	220
H(34D)	1319	3349	6175	220
H(34E)	1858	3316	6930	220
H(43A)	-604	4703	4665	69

H(43B)	168	4786	4748	69
H(43C)	281	5940	4738	148
H(43D)	547	5818	5759	148
H(43E)	-223	5737	5665	148
H(44A)	-2122	3731	6019	96
H(44B)	-1573	4381	5361	96
H(44C)	-2153	4776	6443	163
H(44D)	-1323	5172	6691	163
H(44E)	-1875	4522	7344	163
H(362)	325	3431	5225	73
H(363)	744	3543	3628	77
H(364)	1620	4645	3104	71
H(365)	2118	5657	4081	64
H(366)	1742	5485	5701	61
H(372)	451	3691	5053	60
H(373)	993	3910	3505	68
H(374)	1847	5072	3146	67
H(375)	2262	6007	4263	60
H(376)	1680	5745	5776	55
H(462)	-2815	3456	8280	71
H(463)	-3911	2853	7483	97
H(464)	-4119	2061	6228	111
H(465)	-3159	1989	5541	108
H(466)	-2098	2556	6397	90
H(472)	-2942	3040	8007	128
H(473)	-3970	2107	7216	139
H(474)	-3836	1660	5820	143
H(475)	-2773	1642	5326	143
H(476)	-1910	2389	6405	133
H(2A)	-765	4830	9852	83
H(3A1)	-237	6769	9326	130
H(3A2)	-189	6489	10376	130
H(3A3)	-918	6101	9785	130
H(4A)	358	6507	8137	87
H(5A)	811	5674	7883	83
H(2C)	296	5397	7475	93
H(3C1)	230	7016	8104	169
H(3C2)	-170	6467	7244	169
H(3C3)	667	6801	7383	169
H(4C)	19	6427	9694	92
H(5C)	-298	5200	10176	84
H(2B)	95	3031	10257	111
H(3B1)	-44	1336	9577	202
H(3B2)	-357	1595	10432	202
H(3B3)	483	1966	10276	202
H(4B)	-31	1889	7911	123
H(5B)	-95	2945	7394	113
H(2D)	-769	2615	7876	98
H(3D1)	-493	1144	8735	149
H(3D2)	-413	1416	7644	149
H(3D3)	-1114	1226	8245	149
H(4D)	580	2231	9413	99
H(5D)	630	3333	10032	96

Table S10. Torsion angles [°] for [(OETPP)Fe(N-MeIm)$_2$]Cl.

N(2)-Fe(1)-N(1)-C(1)	-165.2(5)
N(1B)-Fe(1)-N(1)-C(1)	-72.7(5)
N(3)-Fe(1)-N(1)-C(1)	-74(3)
N(4)-Fe(1)-N(1)-C(1)	20.4(6)
N(1A)-Fe(1)-N(1)-C(1)	107.4(5)
N(2)-Fe(1)-N(1)-C(4)	-20.1(5)
N(1B)-Fe(1)-N(1)-C(4)	72.4(5)
N(3)-Fe(1)-N(1)-C(4)	71(3)
N(4)-Fe(1)-N(1)-C(4)	165.5(5)
N(1A)-Fe(1)-N(1)-C(4)	-107.5(5)
C(4)-N(1)-C(1)-C(20)	171.1(8)
Fe(1)-N(1)-C(1)-C(20)	-38.4(10)
C(4)-N(1)-C(1)-C(2)	-5.8(8)
Fe(1)-N(1)-C(1)-C(2)	144.6(5)
N(1)-C(1)-C(2)-C(3)	5.4(9)
C(20)-C(1)-C(2)-C(3)	-171.3(9)
N(1)-C(1)-C(2)-C(21)	-163.7(8)
C(20)-C(1)-C(2)-C(21)	19.5(15)
C(3)-C(2)-C(21)-C(22)	-95.5(11)
C(1)-C(2)-C(21)-C(22)	72.0(12)
C(1)-C(2)-C(3)-C(4)	-2.6(9)
C(21)-C(2)-C(3)-C(4)	166.6(8)
C(1)-C(2)-C(3)-C(31)	-172.7(8)
C(21)-C(2)-C(3)-C(31)	-3.5(14)
C(2)-C(3)-C(31)-C(32)	96.2(11)
C(4)-C(3)-C(31)-C(32)	-71.4(12)
C(1)-N(1)-C(4)-C(5)	-169.3(7)
Fe(1)-N(1)-C(4)-C(5)	41.1(9)
C(1)-N(1)-C(4)-C(3)	4.4(8)
Fe(1)-N(1)-C(4)-C(3)	-145.2(5)
C(2)-C(3)-C(4)-N(1)	-1.1(8)
C(31)-C(3)-C(4)-N(1)	168.3(8)
C(2)-C(3)-C(4)-C(5)	172.1(8)
C(31)-C(3)-C(4)-C(5)	-18.5(13)
N(1)-C(4)-C(5)-C(6)	-22.1(10)
C(3)-C(4)-C(5)-C(6)	165.4(7)
N(1)-C(4)-C(5)-C(5AA)	173.9(9)
C(3)-C(4)-C(5)-C(5AA)	1.4(12)
N(1)-C(4)-C(5)-C(51)	154.8(8)
C(3)-C(4)-C(5)-C(51)	-17.7(13)
N(1B)-Fe(1)-N(2)-C(6)	-105.4(6)
N(3)-Fe(1)-N(2)-C(6)	167.3(6)
N(1)-Fe(1)-N(2)-C(6)	-16.9(5)
N(4)-Fe(1)-N(2)-C(6)	70(2)
N(1A)-Fe(1)-N(2)-C(6)	75.0(6)
N(1B)-Fe(1)-N(2)-C(9)	104.6(6)
N(3)-Fe(1)-N(2)-C(9)	17.4(6)
N(1)-Fe(1)-N(2)-C(9)	-166.9(6)
N(4)-Fe(1)-N(2)-C(9)	-80(2)
N(1A)-Fe(1)-N(2)-C(9)	-75.0(6)
C(9)-N(2)-C(6)-C(5)	-168.4(6)
Fe(1)-N(2)-C(6)-C(5)	36.9(9)
C(9)-N(2)-C(6)-C(7)	7.6(7)
Fe(1)-N(2)-C(6)-C(7)	-147.1(5)
C(4)-C(5)-C(6)-N(2)	-17.3(10)
C(5AA)-C(5)-C(6)-N(2)	145.8(9)
C(51)-C(5)-C(6)-N(2)	165.7(8)
C(4)-C(5)-C(6)-C(7)	167.4(7)

C(5AA)-C(5)-C(6)-C(7)	-29.5(13)
C(51)-C(5)-C(6)-C(7)	-9.6(11)
N(2)-C(6)-C(7)-C(8)	-3.0(8)
C(5)-C(6)-C(7)-C(8)	172.7(7)
N(2)-C(6)-C(7)-C(71)	170.2(6)
C(5)-C(6)-C(7)-C(71)	-14.1(11)
C(8)-C(7)-C(71)-C(72)	96.9(8)
C(6)-C(7)-C(71)-C(72)	-75.2(9)
C(6)-C(7)-C(8)-C(9)	-2.9(7)
C(71)-C(7)-C(8)-C(9)	-176.5(6)
C(6)-C(7)-C(8)-C(81)	168.0(7)
C(71)-C(7)-C(8)-C(81)	-5.6(10)
C(7)-C(8)-C(81)-C(82)	-106.2(8)
C(9)-C(8)-C(81)-C(82)	62.7(10)
C(6)-N(2)-C(9)-C(10)	165.3(7)
Fe(1)-N(2)-C(9)-C(10)	-39.0(10)
C(6)-N(2)-C(9)-C(8)	-9.5(8)
Fe(1)-N(2)-C(9)-C(8)	146.2(5)
C(7)-C(8)-C(9)-C(10)	-166.3(8)
C(81)-C(8)-C(9)-C(10)	23.1(13)
C(7)-C(8)-C(9)-N(2)	7.9(8)
C(81)-C(8)-C(9)-N(2)	-162.6(7)
N(2)-C(9)-C(10)-C(11)	21.7(13)
C(8)-C(9)-C(10)-C(11)	-164.5(8)
N(2)-C(9)-C(10)-C(10A)	-168.9(8)
C(8)-C(9)-C(10)-C(10A)	4.8(13)
N(2)-C(9)-C(10)-C(101)	-136.7(9)
C(8)-C(9)-C(10)-C(101)	37.1(14)
C(6)-C(5)-C(51)-C(52)	-76.1(17)
C(4)-C(5)-C(51)-C(52)	106.9(16)
C(5AA)-C(5)-C(51)-C(52)	30(4)
C(6)-C(5)-C(51)-C(56)	111.0(15)
C(4)-C(5)-C(51)-C(56)	-66.0(18)
C(5AA)-C(5)-C(51)-C(56)	-143(6)
C(56)-C(51)-C(52)-C(53)	-7(3)
C(5)-C(51)-C(52)-C(53)	179.4(16)
C(51)-C(52)-C(53)-C(54)	8(3)
C(52)-C(53)-C(54)-C(55)	-6(3)
C(53)-C(54)-C(55)-C(56)	3(3)
C(54)-C(55)-C(56)-C(51)	-2(3)
C(52)-C(51)-C(56)-C(55)	4(3)
C(5)-C(51)-C(56)-C(55)	176.8(16)
C(6)-C(5)-C(5AA)-C(5BB)	-51(2)
C(4)-C(5)-C(5AA)-C(5BB)	114(2)
C(51)-C(5)-C(5AA)-C(5BB)	-134(6)
C(6)-C(5)-C(5AA)-C(5FF)	117.3(16)
C(4)-C(5)-C(5AA)-C(5FF)	-78.6(18)
C(51)-C(5)-C(5AA)-C(5FF)	34(3)
C(5FF)-C(5AA)-C(5BB)-C(5CC)	9(3)
C(5)-C(5AA)-C(5BB)-C(5CC)	176.3(19)
C(5AA)-C(5BB)-C(5CC)-C(5DD)	-15(3)
C(5BB)-C(5CC)-C(5DD)-C(5EE)	11(3)
C(5CC)-C(5DD)-C(5EE)-C(5FF)	1(3)
C(5BB)-C(5AA)-C(5FF)-C(5EE)	2(3)
C(5)-C(5AA)-C(5FF)-C(5EE)	-166.0(17)
C(5DD)-C(5EE)-C(5FF)-C(5AA)	-8(3)
C(9)-C(10)-C(101)-C(106)	-124.3(15)
C(11)-C(10)-C(101)-C(106)	75.8(18)

C(10A)-C(10)-C(101)-C(106)	-31.6(14)
C(9)-C(10)-C(101)-C(102)	49(2)
C(11)-C(10)-C(101)-C(102)	-110.9(18)
C(10A)-C(10)-C(101)-C(102)	142(3)
C(106)-C(101)-C(102)-C(103)	5(3)
C(10)-C(101)-C(102)-C(103)	-168.4(16)
C(101)-C(102)-C(103)-C(104)	1(3)
C(102)-C(103)-C(104)-C(105)	-2(4)
C(103)-C(104)-C(105)-C(106)	-4(4)
C(102)-C(101)-C(106)-C(105)	-12(3)
C(10)-C(101)-C(106)-C(105)	162.1(18)
C(104)-C(105)-C(106)-C(101)	11(3)
C(9)-C(10)-C(10A)-C(10B)	-113.8(13)
C(11)-C(10)-C(10A)-C(10B)	55.8(16)
C(101)-C(10)-C(10A)-C(10B)	145(3)
C(9)-C(10)-C(10A)-C(10F)	69.6(13)
C(11)-C(10)-C(10A)-C(10F)	-120.8(11)
C(101)-C(10)-C(10A)-C(10F)	-31.8(16)
C(10F)-C(10A)-C(10B)-C(10C)	2.9(18)
C(10)-C(10A)-C(10B)-C(10C)	-173.6(12)
C(10A)-C(10B)-C(10C)-C(10D)	-5(2)
C(10B)-C(10C)-C(10D)-C(10E)	7(3)
C(10C)-C(10D)-C(10E)-C(10F)	-5(3)
C(10D)-C(10E)-C(10F)-C(10A)	2(2)
C(10B)-C(10A)-C(10F)-C(10E)	-1(2)
C(10)-C(10A)-C(10F)-C(10E)	175.4(13)
N(2)-Fe(1)-N(3)-C(11)	20.5(6)
N(1B)-Fe(1)-N(3)-C(11)	-71.9(6)
N(1)-Fe(1)-N(3)-C(11)	-70(3)
N(4)-Fe(1)-N(3)-C(11)	-165.0(6)
N(1A)-Fe(1)-N(3)-C(11)	108.0(6)
N(2)-Fe(1)-N(3)-C(14)	167.0(5)
N(1B)-Fe(1)-N(3)-C(14)	74.6(5)
N(1)-Fe(1)-N(3)-C(14)	76(3)
N(4)-Fe(1)-N(3)-C(14)	-18.5(5)
N(1A)-Fe(1)-N(3)-C(14)	-105.5(5)
C(14)-N(3)-C(11)-C(10)	167.7(7)
Fe(1)-N(3)-C(11)-C(10)	-40.5(10)
C(14)-N(3)-C(11)-C(12)	-6.8(8)
Fe(1)-N(3)-C(11)-C(12)	145.0(5)
C(9)-C(10)-C(11)-N(3)	19.7(13)
C(10A)-C(10)-C(11)-N(3)	-148.9(9)
C(101)-C(10)-C(11)-N(3)	178.1(9)
C(9)-C(10)-C(11)-C(12)	-166.7(9)
C(10A)-C(10)-C(11)-C(12)	24.7(14)
C(101)-C(10)-C(11)-C(12)	-8.3(14)
N(3)-C(11)-C(12)-C(13)	4.0(10)
C(10)-C(11)-C(12)-C(13)	-170.2(9)
N(3)-C(11)-C(12)-C(121)	-164.8(8)
C(10)-C(11)-C(12)-C(121)	21.1(14)
C(13)-C(12)-C(121)-C(122)	-96.7(11)
C(11)-C(12)-C(121)-C(122)	70.3(13)
C(11)-C(12)-C(13)-C(14)	0.7(10)
C(121)-C(12)-C(13)-C(14)	170.0(8)
C(11)-C(12)-C(13)-C(131)	-176.5(8)
C(121)-C(12)-C(13)-C(131)	-7.2(14)
C(12)-C(13)-C(131)-C(132)	95.7(12)
C(14)-C(13)-C(131)-C(132)	-80.9(13)

C(11)-N(3)-C(14)-C(15)	-170.3(7)
Fe(1)-N(3)-C(14)-C(15)	38.3(9)
C(11)-N(3)-C(14)-C(13)	7.1(8)
Fe(1)-N(3)-C(14)-C(13)	-144.3(5)
C(12)-C(13)-C(14)-C(15)	172.3(8)
C(131)-C(13)-C(14)-C(15)	-10.6(14)
C(12)-C(13)-C(14)-N(3)	-4.9(9)
C(131)-C(13)-C(14)-N(3)	172.2(8)
N(3)-C(14)-C(15)-C(16)	-20.3(10)
C(13)-C(14)-C(15)-C(16)	162.8(8)
N(3)-C(14)-C(15)-C(151)	173.8(8)
C(13)-C(14)-C(15)-C(151)	-3.1(12)
N(3)-C(14)-C(15)-C(15A)	154.4(8)
C(13)-C(14)-C(15)-C(15A)	-22.5(12)
N(2)-Fe(1)-N(4)-C(19)	-69(2)
N(1B)-Fe(1)-N(4)-C(19)	105.6(6)
N(3)-Fe(1)-N(4)-C(19)	-167.2(6)
N(1)-Fe(1)-N(4)-C(19)	17.0(6)
N(1A)-Fe(1)-N(4)-C(19)	-74.8(6)
N(2)-Fe(1)-N(4)-C(16)	82(2)
N(1B)-Fe(1)-N(4)-C(16)	-102.7(6)
N(3)-Fe(1)-N(4)-C(16)	-15.5(5)
N(1)-Fe(1)-N(4)-C(16)	168.8(5)
N(1A)-Fe(1)-N(4)-C(16)	76.9(5)
C(14)-C(15)-C(16)-N(4)	-16.8(10)
C(151)-C(15)-C(16)-N(4)	148.9(9)
C(15A)-C(15)-C(16)-N(4)	168.3(7)
C(14)-C(15)-C(16)-C(17)	165.6(7)
C(151)-C(15)-C(16)-C(17)	-28.6(12)
C(15A)-C(15)-C(16)-C(17)	-9.2(11)
C(19)-N(4)-C(16)-C(15)	-169.7(6)
Fe(1)-N(4)-C(16)-C(15)	34.6(9)
C(19)-N(4)-C(16)-C(17)	8.3(7)
Fe(1)-N(4)-C(16)-C(17)	-147.5(5)
C(15)-C(16)-C(17)-C(18)	173.0(7)
N(4)-C(16)-C(17)-C(18)	-4.8(7)
C(15)-C(16)-C(17)-C(171)	-13.7(11)
N(4)-C(16)-C(17)-C(171)	168.5(6)
C(18)-C(17)-C(171)-C(172)	93.6(8)
C(16)-C(17)-C(171)-C(172)	-78.6(9)
C(16)-C(17)-C(18)-C(19)	-0.4(7)
C(171)-C(17)-C(18)-C(19)	-174.1(6)
C(16)-C(17)-C(18)-C(181)	167.1(7)
C(171)-C(17)-C(18)-C(181)	-6.5(11)
C(17)-C(18)-C(181)-C(182)	-101.5(8)
C(19)-C(18)-C(181)-C(182)	63.2(10)
C(16)-N(4)-C(19)-C(20)	161.5(7)
Fe(1)-N(4)-C(19)-C(20)	-42.0(10)
C(16)-N(4)-C(19)-C(18)	-8.5(8)
Fe(1)-N(4)-C(19)-C(18)	148.0(5)
C(17)-C(18)-C(19)-N(4)	5.7(8)
C(181)-C(18)-C(19)-N(4)	-161.3(7)
C(17)-C(18)-C(19)-C(20)	-163.6(8)
C(181)-C(18)-C(19)-C(20)	29.3(13)
N(1)-C(1)-C(20)-C(19)	15.2(14)
C(2)-C(1)-C(20)-C(19)	-168.4(9)
N(1)-C(1)-C(20)-C(20A)	-177.5(10)
C(2)-C(1)-C(20)-C(20A)	-1.2(16)

N(1)-C(1)-C(20)-C(201)	-144.5(9)
C(2)-C(1)-C(20)-C(201)	31.9(15)
N(4)-C(19)-C(20)-C(1)	27.7(14)
C(18)-C(19)-C(20)-C(1)	-163.9(8)
N(4)-C(19)-C(20)-C(20A)	-139.1(11)
C(18)-C(19)-C(20)-C(20A)	29.3(16)
N(4)-C(19)-C(20)-C(201)	-171.4(8)
C(18)-C(19)-C(20)-C(201)	-2.9(13)
C(14)-C(15)-C(151)-C(156)	-77.1(19)
C(16)-C(15)-C(151)-C(156)	116.3(16)
C(15A)-C(15)-C(151)-C(156)	28(4)
C(14)-C(15)-C(151)-C(152)	108(2)
C(16)-C(15)-C(151)-C(152)	-58(2)
C(15A)-C(15)-C(151)-C(152)	-147(7)
C(156)-C(151)-C(152)-C(153)	-1(3)
C(15)-C(151)-C(152)-C(153)	173.5(18)
C(151)-C(152)-C(153)-C(154)	-1(3)
C(152)-C(153)-C(154)-C(155)	1(3)
C(153)-C(154)-C(155)-C(156)	2(3)
C(152)-C(151)-C(156)-C(155)	4(3)
C(15)-C(151)-C(156)-C(155)	-170.9(17)
C(154)-C(155)-C(156)-C(151)	-5(3)
C(14)-C(15)-C(15A)-C(15F)	-67(2)
C(16)-C(15)-C(15A)-C(15F)	108.0(18)
C(151)-C(15)-C(15A)-C(15F)	-151(6)
C(14)-C(15)-C(15A)-C(15B)	110.8(15)
C(16)-C(15)-C(15A)-C(15B)	-74.2(17)
C(151)-C(15)-C(15A)-C(15B)	26(4)
C(15F)-C(15A)-C(15B)-C(15C)	4(3)
C(15)-C(15A)-C(15B)-C(15C)	-174.0(16)
C(15A)-C(15B)-C(15C)-C(15D)	-3(2)
C(15B)-C(15C)-C(15D)-C(15E)	2(2)
C(15C)-C(15D)-C(15E)-C(15F)	-3(2)
C(15B)-C(15A)-C(15F)-C(15E)	-5(3)
C(15)-C(15A)-C(15F)-C(15E)	173.1(16)
C(15D)-C(15E)-C(15F)-C(15A)	4(2)
C(1)-C(20)-C(201)-C(202)	47.9(17)
C(19)-C(20)-C(201)-C(202)	-113.4(13)
C(20A)-C(20)-C(201)-C(202)	138(3)
C(1)-C(20)-C(201)-C(206)	-123.8(11)
C(19)-C(20)-C(201)-C(206)	75.0(13)
C(20A)-C(20)-C(201)-C(206)	-34.1(19)
C(206)-C(201)-C(202)-C(203)	1.3(18)
C(20)-C(201)-C(202)-C(203)	-169.8(12)
C(201)-C(202)-C(203)-C(204)	1(2)
C(202)-C(203)-C(204)-C(205)	-5(3)
C(203)-C(204)-C(205)-C(206)	6(3)
C(204)-C(205)-C(206)-C(201)	-4(3)
C(202)-C(201)-C(206)-C(205)	0(2)
C(20)-C(201)-C(206)-C(205)	173.2(15)
C(1)-C(20)-C(20A)-C(20F)	-121(2)
C(19)-C(20)-C(20A)-C(20F)	47(3)
C(201)-C(20)-C(20A)-C(20F)	133(4)
C(1)-C(20)-C(20A)-C(20B)	75(2)
C(19)-C(20)-C(20A)-C(20B)	-117.5(18)
C(201)-C(20)-C(20A)-C(20B)	-31.4(16)
C(20F)-C(20A)-C(20B)-C(20C)	10(3)
C(20)-C(20A)-C(20B)-C(20C)	177.5(18)

C(20A)-C(20B)-C(20C)-C(20D)	-15(3)
C(20B)-C(20C)-C(20D)-C(20E)	13(4)
C(20C)-C(20D)-C(20E)-C(20F)	-5(4)
C(20B)-C(20A)-C(20F)-C(20E)	-4(5)
C(20)-C(20A)-C(20F)-C(20E)	-170(3)
C(20D)-C(20E)-C(20F)-C(20A)	1(5)
N(2)-Fe(1)-N(1A)-C(2C)	143.8(10)
N(1B)-Fe(1)-N(1A)-C(2C)	66(34)
N(3)-Fe(1)-N(1A)-C(2C)	52.8(10)
N(1)-Fe(1)-N(1A)-C(2C)	-127.3(10)
N(4)-Fe(1)-N(1A)-C(2C)	-36.8(10)
N(2)-Fe(1)-N(1A)-C(2A)	-63.5(8)
N(1B)-Fe(1)-N(1A)-C(2A)	-141(34)
N(3)-Fe(1)-N(1A)-C(2A)	-154.4(7)
N(1)-Fe(1)-N(1A)-C(2A)	25.5(8)
N(4)-Fe(1)-N(1A)-C(2A)	116.0(8)
N(2)-Fe(1)-N(1A)-C(5A)	111.4(8)
N(1B)-Fe(1)-N(1A)-C(5A)	34(34)
N(3)-Fe(1)-N(1A)-C(5A)	20.4(8)
N(1)-Fe(1)-N(1A)-C(5A)	-159.7(8)
N(4)-Fe(1)-N(1A)-C(5A)	-69.1(8)
N(2)-Fe(1)-N(1A)-C(5C)	-34.7(13)
N(1B)-Fe(1)-N(1A)-C(5C)	-112(34)
N(3)-Fe(1)-N(1A)-C(5C)	-125.6(13)
N(1)-Fe(1)-N(1A)-C(5C)	54.3(13)
N(4)-Fe(1)-N(1A)-C(5C)	144.8(13)
C(2C)-N(1A)-C(2A)-N(3A)	-30.2(11)
C(5A)-N(1A)-C(2A)-N(3A)	-3.0(11)
C(5C)-N(1A)-C(2A)-N(3A)	51(2)
Fe(1)-N(1A)-C(2A)-N(3A)	172.4(6)
N(1A)-C(2A)-N(3A)-C(4A)	11.9(11)
N(1A)-C(2A)-N(3A)-C(3A)	-178.9(3)
C(2A)-N(3A)-C(4A)-C(5A)	-17.1(14)
C(3A)-N(3A)-C(4A)-C(5A)	171.9(9)
N(3A)-C(4A)-C(5A)-N(1A)	15.1(14)
C(2C)-N(1A)-C(5A)-C(4A)	76(2)
C(2A)-N(1A)-C(5A)-C(4A)	-7.2(13)
C(5C)-N(1A)-C(5A)-C(4A)	-27.2(13)
Fe(1)-N(1A)-C(5A)-C(4A)	177.5(8)
C(2A)-N(1A)-C(2C)-N(3C)	22.4(15)
C(5A)-N(1A)-C(2C)-N(3C)	-84(2)
C(5C)-N(1A)-C(2C)-N(3C)	-2.6(15)
Fe(1)-N(1A)-C(2C)-N(3C)	178.6(9)
N(1A)-C(2C)-N(3C)-C(4C)	9.7(17)
N(1A)-C(2C)-N(3C)-C(3C)	-180.0(3)
C(3C)-N(3C)-C(4C)-C(5C)	177.5(12)
C(2C)-N(3C)-C(4C)-C(5C)	-11.8(19)
N(3C)-C(4C)-C(5C)-N(1A)	11(2)
C(2C)-N(1A)-C(5C)-C(4C)	-5.4(19)
C(2A)-N(1A)-C(5C)-C(4C)	-111(3)
C(5A)-N(1A)-C(5C)-C(4C)	20.5(18)
Fe(1)-N(1A)-C(5C)-C(4C)	173.3(12)
N(2)-Fe(1)-N(1B)-C(2D)	151(2)
N(3)-Fe(1)-N(1B)-C(2D)	-118(2)
N(1)-Fe(1)-N(1B)-C(2D)	62(2)
N(4)-Fe(1)-N(1B)-C(2D)	-28(2)
N(1A)-Fe(1)-N(1B)-C(2D)	-131(34)
N(2)-Fe(1)-N(1B)-C(2B)	16.7(8)

N(3)-Fe(1)-N(1B)-C(2B)	107.7(8)
N(1)-Fe(1)-N(1B)-C(2B)	-72.2(8)
N(4)-Fe(1)-N(1B)-C(2B)	-162.8(8)
N(1A)-Fe(1)-N(1B)-C(2B)	94(34)
N(2)-Fe(1)-N(1B)-C(5D)	-17(2)
N(3)-Fe(1)-N(1B)-C(5D)	74(2)
N(1)-Fe(1)-N(1B)-C(5D)	-106(2)
N(4)-Fe(1)-N(1B)-C(5D)	164(2)
N(1A)-Fe(1)-N(1B)-C(5D)	61(34)
N(2)-Fe(1)-N(1B)-C(5B)	-164.9(9)
N(3)-Fe(1)-N(1B)-C(5B)	-74.0(9)
N(1)-Fe(1)-N(1B)-C(5B)	106.1(9)
N(4)-Fe(1)-N(1B)-C(5B)	15.6(9)
N(1A)-Fe(1)-N(1B)-C(5B)	-87(34)
C(2D)-N(1B)-C(2B)-N(3B)	33.1(19)
C(5D)-N(1B)-C(2B)-N(3B)	-90(3)
C(5B)-N(1B)-C(2B)-N(3B)	-1.5(13)
Fe(1)-N(1B)-C(2B)-N(3B)	177.1(7)
N(1B)-C(2B)-N(3B)-C(4B)	3.6(13)
N(1B)-C(2B)-N(3B)-C(3B)	179.9(3)
C(2B)-N(3B)-C(4B)-C(5B)	-4.3(14)
C(3B)-N(3B)-C(4B)-C(5B)	179.6(9)
N(3B)-C(4B)-C(5B)-N(1B)	3.5(15)
C(2D)-N(1B)-C(5B)-C(4B)	-77(2)
C(2B)-N(1B)-C(5B)-C(4B)	-1.3(14)
C(5D)-N(1B)-C(5B)-C(4B)	27(2)
Fe(1)-N(1B)-C(5B)-C(4B)	-179.9(8)
C(2B)-N(1B)-C(2D)-N(3D)	-30(3)
C(5D)-N(1B)-C(2D)-N(3D)	-6(4)
C(5B)-N(1B)-C(2D)-N(3D)	81(3)
Fe(1)-N(1B)-C(2D)-N(3D)	-175.0(16)
N(1B)-C(2D)-N(3D)-C(4D)	-6(4)
N(1B)-C(2D)-N(3D)-C(3D)	179.9(3)
C(2D)-N(3D)-C(4D)-C(5D)	15(4)
C(3D)-N(3D)-C(4D)-C(5D)	-170(2)
N(3D)-C(4D)-C(5D)-N(1B)	-18(4)
C(2D)-N(1B)-C(5D)-C(4D)	15(4)
C(2B)-N(1B)-C(5D)-C(4D)	78(4)
C(5B)-N(1B)-C(5D)-C(4D)	-21(3)
Fe(1)-N(1B)-C(5D)-C(4D)	-175(2)

Symmetry transformations used to generate equivalent atoms:

Table S11. Atomic coordinates (x 10^4) and equivalent isotropic displacement parameters ($Å^2$x 10^3) for [(OETPP)Fe(N-BzIm)$_2$]Cl. U(eq) is defined as one third of the trace of the orthogonalized U^{ij} tensor.

	x	y	z	U(eq)
Fe(1)	5896(1)	5896(1)	5000	38(1)
N(1)	5659(3)	6028(3)	3679(3)	38(1)
C(1)	5163(4)	6224(4)	3476(4)	47(2)
C(2)	4836(4)	5919(4)	2544(4)	43(2)
C(21)	4167(4)	5847(5)	2155(6)	65(2)
C(22)	3536(6)	5346(7)	2707(9)	109(4)
C(3)	5198(3)	5620(3)	2181(4)	37(1)
C(31)	4990(4)	5168(3)	1270(4)	41(2)
C(32)	4548(5)	4401(4)	1489(6)	71(2)
C(4)	5728(3)	5712(3)	2860(4)	37(2)
C(5)	6273(4)	5559(4)	2752(5)	48(2)
C(51)	6394(11)	5353(8)	1743(13)	28(3)
C(52)	6737(9)	5886(8)	1087(10)	32(3)
C(53)	6914(9)	5817(9)	154(10)	34(3)
C(54)	6752(8)	5131(8)	-85(11)	36(3)
C(55)	6444(9)	4551(8)	575(10)	38(3)
C(56)	6246(9)	4671(8)	1473(11)	29(3)
C(5AA)	6517(11)	5570(8)	1779(13)	31(4)
C(5BB)	6791(12)	6140(9)	1177(12)	48(4)
C(5CC)	7003(10)	6124(9)	237(11)	50(4)
C(5DD)	6864(10)	5455(10)	-53(12)	49(4)
C(5EE)	6574(11)	4851(9)	502(13)	55(4)
C(5FF)	6407(10)	4925(9)	1441(12)	42(4)
N(2)	6423(3)	5442(3)	4468(3)	45(1)
C(6)	6681(4)	5544(4)	3542(5)	45(2)
C(7)	7340(4)	5551(4)	3551(5)	53(2)
C(71)	7871(6)	5785(7)	2736(6)	93(4)
C(72)	8271(9)	6562(9)	2591(11)	190(9)
C(8)	7473(5)	5441(5)	4469(5)	67(2)
C(81)	8169(5)	5519(7)	4814(7)	89(3)
C(82)	8622(6)	6245(9)	5277(9)	123(4)
C(9)	6888(4)	5336(4)	5036(5)	51(2)
C(10)	6718(5)	5093(5)	5982(5)	66(2)
C(101)	6963(8)	4597(9)	6397(10)	41(3)
C(102)	6849(8)	3950(8)	6061(12)	52(3)
C(103)	7225(9)	3688(9)	6577(11)	59(3)
C(104)	7669(9)	4056(9)	7357(12)	62(3)
C(105)	7792(9)	4700(10)	7704(13)	59(3)
C(106)	7431(8)	4936(9)	7154(12)	51(3)
C(1AA)	7196(9)	4913(9)	6554(12)	50(4)
C(1BB)	7150(11)	4271(10)	6319(14)	72(4)
C(1CC)	7488(13)	3966(12)	6823(17)	94(5)
C(1DD)	7885(15)	4430(14)	7549(18)	103(6)
C(1EE)	8084(13)	5113(14)	7866(17)	102(6)
C(1FF)	7637(10)	5278(12)	7316(12)	67(4)
N(1A)	6810(4)	6810(4)	5000	55(2)
C(2A)	7079(6)	7288(5)	4316(7)	93(3)
N(3A)	7685(5)	7829(5)	4567(6)	110(3)
C(4A)	8109(13)	8455(15)	4140(20)	115(8)
C(5A)	8840(30)	8650(70)	3790(60)	440(30)

C(6A)	9350(70)	9250(50)	4270(60)	440(30)
C(7A)	10010(60)	9320(40)	4460(40)	440(30)
C(8A)	10160(30)	8790(70)	4180(60)	440(30)
C(9A)	9640(70)	8200(50)	3700(50)	440(30)
C(10A)	8990(50)	8120(40)	3510(50)	440(30)
N(1B)	4980(4)	4980(4)	5000	43(2)
C(2B)	4793(6)	4478(5)	4364(7)	84(3)
N(3B)	4119(5)	3925(4)	4615(7)	112(3)
C(4B)	3814(10)	3211(10)	4261(13)	73(5)
C(5B)	3094(9)	3004(10)	3853(14)	137(9)
C(6B)	2538(11)	2314(9)	3724(13)	105(7)
C(7B)	1905(9)	2195(8)	3314(16)	163(11)
C(8B)	1828(9)	2766(11)	3033(15)	218(17)
C(9B)	2384(11)	3456(9)	3161(12)	102(6)
C(10B)	3017(9)	3575(8)	3571(14)	143(10)
Cl(1)	7929(6)	6935(7)	-2070(8)	201(4)

Table S12. Bond lengths [Å] and angles [°] for [(OETPP)Fe(N-BzIm)$_2$]Cl.

Fe(1)-N(1)#1	1.970(5)	C(7)-C(71)	1.515(11)
Fe(1)-N(1)	1.970(5)	C(71)-C(72)	1.479(15)
Fe(1)-N(1A)	1.988(10)	C(71)-H(14A)	0.9900
Fe(1)-N(1B)	1.992(8)	C(71)-H(14B)	0.9900
Fe(1)-N(2)#1	1.993(4)	C(72)-H(14C)	0.9800
Fe(1)-N(2)	1.993(4)	C(72)-H(14D)	0.9800
N(1)-C(1)	1.373(8)	C(72)-H(14E)	0.9800
N(1)-C(4)	1.379(7)	C(8)-C(9)	1.417(10)
C(1)-C(10)#1	1.382(9)	C(8)-C(81)	1.515(11)
C(1)-C(2)	1.469(9)	C(81)-C(82)	1.526(18)
C(2)-C(3)	1.344(9)	C(81)-H(13A)	0.9900
C(2)-C(21)	1.486(10)	C(81)-H(13B)	0.9900
C(21)-C(22)	1.472(14)	C(82)-H(13C)	0.9800
C(21)-H(23A)	0.9900	C(82)-H(13D)	0.9800
C(21)-H(23B)	0.9900	C(82)-H(13E)	0.9800
C(22)-H(23C)	0.9800	C(9)-C(10)	1.400(9)
C(22)-H(23D)	0.9800	C(10)-C(1)#1	1.382(9)
C(22)-H(23E)	0.9800	C(10)-C(1AA)	1.511(18)
C(3)-C(4)	1.427(8)	C(10)-C(101)	1.536(16)
C(3)-C(31)	1.529(8)	C(101)-C(102)	1.384(16)
C(31)-C(32)	1.483(11)	C(101)-C(106)	1.393(16)
C(31)-H(24A)	0.9900	C(102)-C(103)	1.405(14)
C(31)-H(24B)	0.9900	C(102)-H(123)	0.9500
C(32)-H(24C)	0.9800	C(103)-C(104)	1.409(10)
C(32)-H(24D)	0.9800	C(103)-H(124)	0.9500
C(32)-H(24E)	0.9800	C(104)-C(105)	1.375(17)
C(4)-C(5)	1.389(9)	C(104)-H(125)	0.9500
C(5)-C(6)	1.423(10)	C(105)-C(106)	1.366(15)
C(5)-C(5AA)	1.451(18)	C(105)-H(126)	0.9500
C(5)-C(51)	1.537(19)	C(106)-H(127)	0.9500
C(51)-C(52)	1.367(15)	C(1AA)-C(1BB)	1.388(16)
C(51)-C(56)	1.403(15)	C(1AA)-C(1FF)	1.383(16)
C(52)-C(53)	1.385(15)	C(1BB)-C(1CC)	1.399(10)
C(52)-H(262)	0.9500	C(1BB)-H(2Z)	0.9500
C(53)-C(54)	1.393(15)	C(1CC)-C(1DD)	1.385(18)
C(53)-H(263)	0.9500	C(1CC)-H(3Z)	0.9500
C(54)-C(55)	1.428(15)	C(1DD)-C(1EE)	1.394(18)
C(54)-H(264)	0.9500	C(1DD)-H(4Z)	0.9500
C(55)-C(56)	1.390(14)	C(1EE)-C(1FF)	1.418(17)
C(55)-H(265)	0.9500	C(1EE)-H(5Z)	0.9500
C(56)-H(266)	0.9500	C(1FF)-H(6Z)	0.9500
C(5AA)-C(5BB)	1.362(15)	N(1A)-C(2A)#1	1.313(11)
C(5AA)-C(5FF)	1.383(15)	N(1A)-C(2A)	1.313(11)
C(5BB)-C(5CC)	1.395(15)	C(2A)-N(3A)	1.302(13)
C(5BB)-H(272)	0.9500	C(2A)-H(2A)	0.9500
C(5CC)-C(5DD)	1.389(16)	N(3A)-N(3A)#1	1.324(16)
C(5CC)-H(192)	0.9500	N(3A)-C(4A)	1.34(3)
C(5DD)-C(5EE)	1.375(16)	C(4A)-C(5A)	1.51(2)
C(5DD)-H(193)	0.9500	C(4A)-H(4A1)	0.9900
C(5EE)-C(5FF)	1.388(16)	C(4A)-H(4A2)	0.9900
C(5EE)-H(194)	0.9500	C(5A)-C(6A)	1.3900(14)
C(5FF)-H(195)	0.9500	C(5A)-C(10A)	1.3900
N(2)-C(6)	1.379(8)	C(6A)-C(7A)	1.3900
N(2)-C(9)	1.389(8)	C(6A)-H(6A)	0.9500
C(6)-C(7)	1.426(10)	C(7A)-C(8A)	1.3900
C(7)-C(8)	1.359(10)	C(7A)-H(7A)	0.9500

C(8A)-C(9A)	1.3900
C(8A)-H(8A)	0.9500
C(9A)-C(10A)	1.3900
C(9A)-H(9A)	0.9500
C(10A)-H(10A)	0.9500
N(1B)-C(2B)	1.304(10)
N(1B)-C(2B)#1	1.304(10)
C(2B)-N(3B)	1.398(13)
C(2B)-H(2B)	0.9500
N(3B)-N(3B)#1	1.297(16)
N(3B)-C(4B)	1.44(2)
C(4B)-C(5B)	1.51(2)
C(5B)-C(6B)	1.3900
C(5B)-C(10B)	1.3900
C(6B)-C(7B)	1.3900
C(6B)-H(6B)	0.9500
C(7B)-C(8B)	1.3900
C(7B)-H(7B)	0.9500
C(8B)-C(9B)	1.3900
C(8B)-H(8B)	0.9500
C(9B)-C(10B)	1.3900
C(9B)-H(9B)	0.9500
C(10B)-H(10B)	0.9500

N(1)#1-Fe(1)-N(1)	173.3(3)
N(1)#1-Fe(1)-N(1A)	93.34(16)
N(1)-Fe(1)-N(1A)	93.34(16)
N(1)#1-Fe(1)-N(1B)	86.66(16)
N(1)-Fe(1)-N(1B)	86.66(16)
N(1A)-Fe(1)-N(1B)	180.000(1)
N(1)#1-Fe(1)-N(2)#1	89.0(2)
N(1)-Fe(1)-N(2)#1	91.27(19)
N(1A)-Fe(1)-N(2)#1	87.69(18)
N(1B)-Fe(1)-N(2)#1	92.31(18)
N(1)#1-Fe(1)-N(2)	91.27(19)
N(1)-Fe(1)-N(2)	89.0(2)
N(1A)-Fe(1)-N(2)	87.69(18)
N(1B)-Fe(1)-N(2)	92.31(18)
N(2)#1-Fe(1)-N(2)	175.4(4)
C(1)-N(1)-C(4)	106.4(5)
C(1)-N(1)-Fe(1)	122.8(4)
C(4)-N(1)-Fe(1)	126.7(4)
N(1)-C(1)-C(10)#1	122.5(6)
N(1)-C(1)-C(2)	108.6(5)
C(10)#1-C(1)-C(2)	128.2(6)
C(3)-C(2)-C(1)	106.4(5)
C(3)-C(2)-C(21)	126.2(6)
C(1)-C(2)-C(21)	126.7(6)
C(22)-C(21)-C(2)	112.9(8)
C(22)-C(21)-H(23A)	109.0
C(2)-C(21)-H(23A)	109.0
C(22)-C(21)-H(23B)	109.0
C(2)-C(21)-H(23B)	109.0
H(23A)-C(21)-H(23B)	107.8
C(21)-C(22)-H(23C)	109.5
C(21)-C(22)-H(23D)	109.5
H(23C)-C(22)-H(23D)	109.5
C(21)-C(22)-H(23E)	109.5
H(23C)-C(22)-H(23E)	109.5
H(23D)-C(22)-H(23E)	109.5
C(2)-C(3)-C(4)	108.1(5)
C(2)-C(3)-C(31)	124.5(6)
C(4)-C(3)-C(31)	126.8(5)
C(32)-C(31)-C(3)	111.7(6)
C(32)-C(31)-H(24A)	109.3
C(3)-C(31)-H(24A)	109.3
C(32)-C(31)-H(24B)	109.3
C(3)-C(31)-H(24B)	109.3
H(24A)-C(31)-H(24B)	107.9
C(31)-C(32)-H(24C)	109.5
C(31)-C(32)-H(24D)	109.5
H(24C)-C(32)-H(24D)	109.5
C(31)-C(32)-H(24E)	109.5
H(24C)-C(32)-H(24E)	109.5
H(24D)-C(32)-H(24E)	109.5
N(1)-C(4)-C(5)	121.9(6)
N(1)-C(4)-C(3)	109.6(5)
C(5)-C(4)-C(3)	128.5(5)
C(4)-C(5)-C(6)	122.5(6)
C(4)-C(5)-C(5AA)	116.4(10)
C(6)-C(5)-C(5AA)	119.7(10)
C(4)-C(5)-C(51)	117.3(10)
C(6)-C(5)-C(51)	120.1(10)
C(5AA)-C(5)-C(51)	15.6(8)
C(52)-C(51)-C(56)	117.2(14)
C(52)-C(51)-C(5)	117.7(12)
C(56)-C(51)-C(5)	124.7(12)
C(51)-C(52)-C(53)	126.8(14)
C(51)-C(52)-H(262)	116.6
C(53)-C(52)-H(262)	116.6
C(52)-C(53)-C(54)	113.9(13)
C(52)-C(53)-H(263)	123.1
C(54)-C(53)-H(263)	123.1
C(53)-C(54)-C(55)	123.3(12)
C(53)-C(54)-H(264)	118.4
C(55)-C(54)-H(264)	118.4
C(56)-C(55)-C(54)	117.8(13)
C(56)-C(55)-H(265)	121.1
C(54)-C(55)-H(265)	121.1
C(55)-C(56)-C(51)	120.8(14)
C(55)-C(56)-H(266)	119.6
C(51)-C(56)-H(266)	119.6
C(5BB)-C(5AA)-C(5FF)	119.2(14)
C(5BB)-C(5AA)-C(5)	125.5(13)
C(5FF)-C(5AA)-C(5)	115.1(12)
C(5AA)-C(5BB)-C(5CC)	123.7(15)
C(5AA)-C(5BB)-H(272)	118.1
C(5CC)-C(5BB)-H(272)	118.1
C(5DD)-C(5CC)-C(5BB)	113.4(15)
C(5DD)-C(5CC)-H(192)	123.3
C(5BB)-C(5CC)-H(192)	123.3
C(5EE)-C(5DD)-C(5CC)	126.4(16)
C(5EE)-C(5DD)-H(193)	116.8
C(5CC)-C(5DD)-H(193)	116.8
C(5DD)-C(5EE)-C(5FF)	116.0(14)
C(5DD)-C(5EE)-H(194)	122.0

C(5FF)-C(5EE)-H(194)	122.0
C(5AA)-C(5FF)-C(5EE)	121.1(14)
C(5AA)-C(5FF)-H(195)	119.4
C(5EE)-C(5FF)-H(195)	119.4
C(6)-N(2)-C(9)	106.8(5)
C(6)-N(2)-Fe(1)	123.7(4)
C(9)-N(2)-Fe(1)	121.1(4)
N(2)-C(6)-C(5)	121.3(6)
N(2)-C(6)-C(7)	108.6(6)
C(5)-C(6)-C(7)	129.8(6)
C(8)-C(7)-C(6)	107.9(6)
C(8)-C(7)-C(71)	124.7(7)
C(6)-C(7)-C(71)	126.3(7)
C(72)-C(71)-C(7)	113.5(10)
C(72)-C(71)-H(14A)	108.9
C(7)-C(71)-H(14A)	108.9
C(72)-C(71)-H(14B)	108.9
C(7)-C(71)-H(14B)	108.9
H(14A)-C(71)-H(14B)	107.7
C(71)-C(72)-H(14C)	109.5
C(71)-C(72)-H(14D)	109.5
H(14C)-C(72)-H(14D)	109.5
C(71)-C(72)-H(14E)	109.5
H(14C)-C(72)-H(14E)	109.5
H(14D)-C(72)-H(14E)	109.5
C(7)-C(8)-C(9)	107.4(6)
C(7)-C(8)-C(81)	124.6(7)
C(9)-C(8)-C(81)	127.5(7)
C(8)-C(81)-C(82)	109.9(8)
C(8)-C(81)-H(13A)	109.7
C(82)-C(81)-H(13A)	109.7
C(8)-C(81)-H(13B)	109.7
C(82)-C(81)-H(13B)	109.7
H(13A)-C(81)-H(13B)	108.2
C(81)-C(82)-H(13C)	109.5
C(81)-C(82)-H(13D)	109.5
H(13C)-C(82)-H(13D)	109.5
C(81)-C(82)-H(13E)	109.5
H(13C)-C(82)-H(13E)	109.5
H(13D)-C(82)-H(13E)	109.5
N(2)-C(9)-C(10)	121.5(6)
N(2)-C(9)-C(8)	109.0(5)
C(10)-C(9)-C(8)	129.2(6)
C(1)#1-C(10)-C(9)	123.1(5)
C(1)#1-C(10)-C(1AA)	114.5(8)
C(9)-C(10)-C(1AA)	120.6(8)
C(1)#1-C(10)-C(101)	115.7(8)
C(9)-C(10)-C(101)	120.1(7)
C(1AA)-C(10)-C(101)	24.8(6)
C(102)-C(101)-C(106)	120.3(14)
C(102)-C(101)-C(10)	129.8(12)
C(106)-C(101)-C(10)	109.4(12)
C(101)-C(102)-C(103)	113.3(15)
C(101)-C(102)-H(123)	123.3
C(103)-C(102)-H(123)	123.3
C(102)-C(103)-C(104)	122.4(15)
C(102)-C(103)-H(124)	118.8
C(104)-C(103)-H(124)	118.8
C(105)-C(104)-C(103)	125.4(14)
C(105)-C(104)-H(125)	117.3
C(103)-C(104)-H(125)	117.3
C(106)-C(105)-C(104)	109.3(15)
C(106)-C(105)-H(126)	125.4
C(104)-C(105)-H(126)	125.4
C(105)-C(106)-C(101)	129.1(16)
C(105)-C(106)-H(127)	115.4
C(101)-C(106)-H(127)	115.4
C(1BB)-C(1AA)-C(1FF)	116.1(16)
C(1BB)-C(1AA)-C(10)	115.1(14)
C(1FF)-C(1AA)-C(10)	128.6(13)
C(1AA)-C(1BB)-C(1CC)	124.6(18)
C(1AA)-C(1BB)-H(2Z)	117.7
C(1CC)-C(1BB)-H(2Z)	117.7
C(1DD)-C(1CC)-C(1BB)	108(2)
C(1DD)-C(1CC)-H(3Z)	126.1
C(1BB)-C(1CC)-H(3Z)	126.1
C(1CC)-C(1DD)-C(1EE)	139(2)
C(1CC)-C(1DD)-H(4Z)	110.5
C(1EE)-C(1DD)-H(4Z)	110.5
C(1DD)-C(1EE)-C(1FF)	102(2)
C(1DD)-C(1EE)-H(5Z)	128.8
C(1FF)-C(1EE)-H(5Z)	128.8
C(1AA)-C(1FF)-C(1EE)	129.3(19)
C(1AA)-C(1FF)-H(6Z)	115.3
C(1EE)-C(1FF)-H(6Z)	115.3
C(2A)#1-N(1A)-C(2A)	103.5(11)
C(2A)#1-N(1A)-Fe(1)	128.3(5)
C(2A)-N(1A)-Fe(1)	128.3(5)
N(3A)-C(2A)-N(1A)	111.8(9)
N(3A)-C(2A)-H(2A)	124.1
N(1A)-C(2A)-H(2A)	124.1
C(2A)-N(3A)-N(3A)#1	106.4(5)
C(2A)-N(3A)-C(4A)	132.2(14)
N(3A)#1-N(3A)-C(4A)	121.3(13)
N(3A)-C(4A)-C(5A)	121(5)
N(3A)-C(4A)-H(4A1)	107.0
C(5A)-C(4A)-H(4A1)	107.0
N(3A)-C(4A)-H(4A2)	107.0
C(5A)-C(4A)-H(4A2)	107.0
H(4A1)-C(4A)-H(4A2)	106.7
C(6A)-C(5A)-C(10A)	120.0
C(6A)-C(5A)-C(4A)	111(10)
C(10A)-C(5A)-C(4A)	120(10)
C(7A)-C(6A)-C(5A)	120.0
C(7A)-C(6A)-H(6A)	120.0
C(5A)-C(6A)-H(6A)	120.0
C(6A)-C(7A)-C(8A)	120.00(9)
C(6A)-C(7A)-H(7A)	120.0
C(8A)-C(7A)-H(7A)	120.0
C(9A)-C(8A)-C(7A)	120.0
C(9A)-C(8A)-H(8A)	120.0
C(7A)-C(8A)-H(8A)	120.0
C(8A)-C(9A)-C(10A)	120.0
C(8A)-C(9A)-H(9A)	120.0
C(10A)-C(9A)-H(9A)	120.0
C(9A)-C(10A)-C(5A)	120.00(8)

C(9A)-C(10A)-H(10A)	120.0	C(5B)-C(6B)-C(7B)	120.0
C(5A)-C(10A)-H(10A)	120.0	C(5B)-C(6B)-H(6B)	120.0
C(2B)-N(1B)-C(2B)#1	109.8(11)	C(7B)-C(6B)-H(6B)	120.0
C(2B)-N(1B)-Fe(1)	125.1(5)	C(8B)-C(7B)-C(6B)	120.0
C(2B)#1-N(1B)-Fe(1)	125.1(5)	C(8B)-C(7B)-H(7B)	120.0
N(1B)-C(2B)-N(3B)	107.7(8)	C(6B)-C(7B)-H(7B)	120.0
N(1B)-C(2B)-H(2B)	126.1	C(9B)-C(8B)-C(7B)	120.0
N(3B)-C(2B)-H(2B)	126.1	C(9B)-C(8B)-H(8B)	120.0
N(3B)#1-N(3B)-C(2B)	107.4(5)	C(7B)-C(8B)-H(8B)	120.0
N(3B)#1-N(3B)-C(4B)	125.8(9)	C(8B)-C(9B)-C(10B)	120.0
C(2B)-N(3B)-C(4B)	124.2(10)	C(8B)-C(9B)-H(9B)	120.0
N(3B)-C(4B)-C(5B)	107.5(15)	C(10B)-C(9B)-H(9B)	120.0
C(6B)-C(5B)-C(10B)	120.0	C(9B)-C(10B)-C(5B)	120.0
C(6B)-C(5B)-C(4B)	125.8(14)	C(9B)-C(10B)-H(10B)	120.0
C(10B)-C(5B)-C(4B)	114.2(14)	C(5B)-C(10B)-H(10B)	120.0

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z+1

Table S13. Anisotropic displacement parameters ($Å^2 x\ 10^3$) for [(OETPP)Fe(N-BzIm)$_2$]Cl. The anisotropic displacement factor exponent takes the form: $-2\pi^2[h^2\ a^{*2}U^{11} + ... + 2\ h\ k\ a^*\ b^*\ U^{12}]$

	U^{11}	U^{22}	U^{33}	U^{23}	U^{13}	U^{12}
Fe(1)	55(1)	55(1)	26(1)	1(1)	-1(1)	45(1)
N(1)	48(3)	43(3)	32(3)	1(2)	-6(2)	29(3)
C(1)	75(5)	62(4)	30(3)	-10(3)	-14(3)	55(4)
C(2)	64(4)	57(4)	27(3)	-4(3)	-4(3)	46(4)
C(21)	72(5)	95(6)	58(5)	-16(4)	-5(4)	65(5)
C(22)	69(6)	151(11)	116(9)	4(8)	18(6)	61(7)
C(3)	51(4)	40(4)	25(3)	9(3)	0(3)	27(3)
C(31)	54(4)	48(4)	28(3)	-7(3)	-4(3)	33(3)
C(32)	98(7)	53(5)	66(5)	-7(4)	-2(5)	40(5)
C(4)	61(4)	32(3)	28(3)	11(2)	14(3)	31(3)
C(5)	61(5)	69(5)	36(4)	8(3)	10(3)	49(4)
C(51)	27(6)	32(5)	26(5)	-6(4)	-7(4)	15(5)
C(52)	35(5)	32(5)	26(5)	-3(4)	-14(4)	15(5)
C(53)	34(5)	39(5)	28(4)	-3(5)	-10(4)	18(5)
C(54)	33(5)	45(5)	31(4)	-5(4)	4(4)	19(4)
C(55)	35(5)	38(5)	37(5)	-8(4)	2(4)	16(4)
C(56)	24(5)	34(5)	32(4)	-4(4)	1(4)	18(4)
C(5AA)	31(8)	45(7)	22(6)	5(5)	6(5)	23(6)
C(5BB)	60(8)	49(7)	37(6)	3(5)	3(6)	29(7)
C(5CC)	47(7)	61(6)	43(6)	2(6)	12(5)	28(6)
C(5DD)	54(8)	50(7)	44(6)	1(6)	2(6)	28(7)
C(5EE)	63(8)	52(7)	53(7)	-3(6)	-1(6)	31(7)
C(5FF)	48(8)	45(7)	36(6)	2(6)	-5(5)	26(6)
N(2)	65(4)	69(4)	30(3)	4(3)	13(3)	55(3)
C(6)	59(4)	52(4)	39(4)	2(3)	12(3)	40(3)
C(7)	55(4)	78(5)	46(4)	5(4)	6(3)	49(4)
C(71)	100(7)	189(12)	45(5)	28(6)	27(5)	113(9)
C(72)	141(13)	193(18)	125(12)	77(12)	30(10)	0(12)
C(8)	80(5)	128(6)	45(4)	10(4)	6(3)	90(5)
C(81)	89(5)	168(7)	57(5)	14(4)	7(4)	99(5)
C(82)	94(7)	212(10)	86(7)	-18(7)	-25(5)	94(7)
C(9)	59(4)	89(5)	42(4)	12(3)	7(3)	66(4)
C(10)	100(6)	117(7)	37(4)	15(4)	10(4)	96(6)
C(101)	35(5)	63(5)	47(5)	16(4)	11(4)	40(4)
C(102)	46(5)	65(5)	65(5)	11(4)	4(4)	44(4)
C(103)	54(6)	65(5)	77(6)	16(4)	1(4)	43(4)
C(104)	51(5)	74(5)	74(6)	21(5)	-2(4)	42(4)
C(105)	53(6)	72(5)	58(5)	21(4)	-1(4)	34(5)
C(106)	42(5)	67(5)	53(5)	14(4)	6(4)	34(4)
C(1AA)	53(7)	67(7)	42(6)	15(6)	9(5)	40(6)
C(1BB)	81(8)	74(7)	77(8)	-6(6)	6(6)	51(7)
C(1CC)	103(10)	102(8)	100(9)	6(7)	5(7)	69(7)
C(1DD)	116(10)	109(8)	101(9)	9(7)	-6(7)	68(7)
C(1EE)	97(9)	114(8)	96(9)	3(7)	-24(7)	53(7)
C(1FF)	61(8)	92(8)	58(7)	-8(6)	5(5)	45(6)
N(1A)	68(3)	68(3)	44(4)	2(2)	-2(2)	45(4)
C(2A)	102(5)	71(5)	75(5)	20(4)	-28(4)	20(4)
N(3A)	109(6)	83(5)	97(5)	14(4)	-27(4)	17(4)
N(1B)	57(4)	57(4)	33(4)	-2(2)	2(2)	42(4)
C(2B)	105(7)	62(5)	72(6)	-10(4)	30(5)	32(5)
N(3B)	110(6)	65(5)	127(8)	-10(5)	41(6)	19(4)

Cl(1)	188(7)	242(8)	164(6)	10(6)	-12(6)	101(6)

Table S14. Hydrogen coordinates (x 10^4) and isotropic displacement parameters (Å^2 x 10^3) for [(OETPP)Fe(N-BzIm)$_2$]Cl..

	x	y	z	U(eq)
H(23A)	4202	6318	2156	77
H(23B)	4110	5683	1481	77
H(23C)	3113	5326	2427	164
H(23D)	3589	5506	3375	164
H(23E)	3487	4873	2685	164
H(24A)	4722	5313	840	49
H(24B)	5425	5254	929	49
H(24C)	4422	4128	889	107
H(24D)	4115	4314	1821	107
H(24E)	4816	4253	1901	107
H(262)	6867	6352	1293	38
H(263)	7127	6204	-284	40
H(264)	6852	5043	-718	44
H(265)	6376	4098	406	45
H(266)	6008	4288	1910	34
H(272)	6841	6573	1411	58
H(192)	7222	6530	-166	60
H(193)	6980	5411	-697	59
H(194)	6492	4409	256	66
H(195)	6214	4526	1858	51
H(14A)	8212	5619	2868	112
H(14B)	7616	5554	2135	112
H(14C)	8606	6678	2059	285
H(14D)	8532	6795	3178	285
H(14E)	7939	6730	2439	285
H(13A)	8428	5466	4265	107
H(13B)	8075	5141	5286	107
H(13C)	9072	6293	5494	185
H(13D)	8368	6292	5828	185
H(13E)	8716	6617	4807	185
H(123)	6547	3707	5534	62
H(124)	7177	3245	6393	71
H(125)	7903	3843	7670	74
H(126)	8081	4942	8241	71
H(127)	7512	5396	7309	61
H(2Z)	6870	4021	5779	86
H(3Z)	7451	3520	6689	112
H(4Z)	8081	4220	7954	124
H(5Z)	8430	5395	8331	123
H(6Z)	7641	5701	7496	81
H(2A)	6859	7244	3711	112
H(4A1)	8167	8829	4599	138
H(4A2)	7845	8488	3583	138
H(6A)	9255	9609	4463	527
H(7A)	10366	9730	4787	527
H(8A)	10611	8843	4307	527
H(9A)	9744	7836	3505	527
H(10A)	8633	7715	3181	527
H(2B)	5066	4486	3827	101
H(6B)	2590	1924	3916	126
H(7B)	1525	1724	3226	195

H(8B)	1396	2685	2753	262
H(9B)	2332	3847	2969	123
H(10B)	3397	4047	3659	172

Table S15. Torsion angles [°] for [(OETPP)Fe(N-BzIm)$_2$]Cl..

N(1)#1-Fe(1)-N(1)-C(1)	75.8(5)	C(51)-C(5)-C(5AA)-C(5BB)	156(8)
N(1A)-Fe(1)-N(1)-C(1)	-104.2(5)	C(4)-C(5)-C(5AA)-C(5FF)	-116.0(16)
N(1B)-Fe(1)-N(1)-C(1)	75.8(5)	C(6)-C(5)-C(5AA)-C(5FF)	77.1(18)
N(2)#1-Fe(1)-N(1)-C(1)	-16.4(6)	C(51)-C(5)-C(5AA)-C(5FF)	-19(5)
N(2)-Fe(1)-N(1)-C(1)	168.2(6)	C(5FF)-C(5AA)-C(5BB)-C(5CC)	-3(3)
N(1)#1-Fe(1)-N(1)-C(4)	-78.5(5)	C(5)-C(5AA)-C(5BB)-C(5CC)	-178.3(19)
N(1A)-Fe(1)-N(1)-C(4)	101.5(5)	C(5AA)-C(5BB)-C(5CC)-C(5DD)	4(3)
N(1B)-Fe(1)-N(1)-C(4)	-78.5(5)	C(5BB)-C(5CC)-C(5DD)-C(5EE)	-3(3)
N(2)#1-Fe(1)-N(1)-C(4)	-170.8(5)	C(5CC)-C(5DD)-C(5EE)-C(5FF)	0(3)
N(2)-Fe(1)-N(1)-C(4)	13.8(6)	C(5BB)-C(5AA)-C(5FF)-C(5EE)	0(3)
C(4)-N(1)-C(1)-C(10)#1	-162.0(7)	C(5)-C(5AA)-C(5FF)-C(5EE)	175.9(17)
Fe(1)-N(1)-C(1)-C(10)#1	39.2(10)	C(5DD)-C(5EE)-C(5FF)-C(5AA)	1(3)
C(4)-N(1)-C(1)-C(2)	8.9(7)	N(1)#1-Fe(1)-N(2)-C(6)	-165.0(6)
Fe(1)-N(1)-C(1)-C(2)	-149.9(5)	N(1)-Fe(1)-N(2)-C(6)	21.7(6)
N(1)-C(1)-C(2)-C(3)	-6.4(8)	N(1A)-Fe(1)-N(2)-C(6)	-71.7(6)
C(10)#1-C(1)-C(2)-C(3)	163.8(8)	N(1B)-Fe(1)-N(2)-C(6)	108.3(6)
N(1)-C(1)-C(2)-C(21)	164.2(7)	N(2)#1-Fe(1)-N(2)-C(6)	-71.7(6)
C(10)#1-C(1)-C(2)-C(21)	-25.6(13)	N(1)#1-Fe(1)-N(2)-C(9)	-21.0(6)
C(3)-C(2)-C(21)-C(22)	102.7(9)	N(1)-Fe(1)-N(2)-C(9)	165.7(6)
C(1)-C(2)-C(21)-C(22)	-66.2(11)	N(1A)-Fe(1)-N(2)-C(9)	72.3(5)
C(1)-C(2)-C(3)-C(4)	1.3(7)	N(1B)-Fe(1)-N(2)-C(9)	-107.7(5)
C(21)-C(2)-C(3)-C(4)	-169.4(7)	N(2)#1-Fe(1)-N(2)-C(9)	72.3(5)
C(1)-C(2)-C(3)-C(31)	173.0(6)	C(9)-N(2)-C(6)-C(5)	170.1(7)
C(21)-C(2)-C(3)-C(31)	2.3(11)	Fe(1)-N(2)-C(6)-C(5)	-41.6(9)
C(2)-C(3)-C(31)-C(32)	-93.9(8)	C(9)-N(2)-C(6)-C(7)	-4.1(8)
C(4)-C(3)-C(31)-C(32)	76.2(9)	Fe(1)-N(2)-C(6)-C(7)	144.2(5)
C(1)-N(1)-C(4)-C(5)	168.7(6)	C(4)-C(5)-C(6)-N(2)	22.3(11)
Fe(1)-N(1)-C(4)-C(5)	-33.6(8)	C(5AA)-C(5)-C(6)-N(2)	-171.6(9)
C(1)-N(1)-C(4)-C(3)	-8.2(7)	C(51)-C(5)-C(6)-N(2)	-153.7(9)
Fe(1)-N(1)-C(4)-C(3)	149.5(4)	C(4)-C(5)-C(6)-C(7)	-164.9(7)
C(2)-C(3)-C(4)-N(1)	4.2(7)	C(5AA)-C(5)-C(6)-C(7)	1.2(13)
C(31)-C(3)-C(4)-N(1)	-167.2(6)	C(51)-C(5)-C(6)-C(7)	19.1(13)
C(2)-C(3)-C(4)-C(5)	-172.4(7)	N(2)-C(6)-C(7)-C(8)	1.1(9)
C(31)-C(3)-C(4)-C(5)	16.2(10)	C(5)-C(6)-C(7)-C(8)	-172.5(8)
N(1)-C(4)-C(5)-C(6)	16.4(10)	N(2)-C(6)-C(7)-C(71)	-167.6(8)
C(3)-C(4)-C(5)-C(6)	-167.4(6)	C(5)-C(6)-C(7)-C(71)	18.9(14)
N(1)-C(4)-C(5)-C(5AA)	-150.2(8)	C(8)-C(7)-C(71)-C(72)	-93.6(12)
C(3)-C(4)-C(5)-C(5AA)	26.1(12)	C(6)-C(7)-C(71)-C(72)	73.3(14)
N(1)-C(4)-C(5)-C(51)	-167.6(8)	C(6)-C(7)-C(8)-C(9)	2.3(10)
C(3)-C(4)-C(5)-C(51)	8.7(12)	C(71)-C(7)-C(8)-C(9)	171.2(8)
C(4)-C(5)-C(51)-C(52)	77.2(19)	C(6)-C(7)-C(8)-C(81)	-170.4(9)
C(6)-C(5)-C(51)-C(52)	-106.6(17)	C(71)-C(7)-C(8)-C(81)	-1.5(15)
C(5AA)-C(5)-C(51)-C(52)	-14(5)	C(7)-C(8)-C(81)-C(82)	97.9(11)
C(4)-C(5)-C(51)-C(56)	-109.9(18)	C(9)-C(8)-C(81)-C(82)	-73.4(13)
C(6)-C(5)-C(51)-C(56)	66(2)	C(6)-N(2)-C(9)-C(10)	-168.6(7)
C(5AA)-C(5)-C(51)-C(56)	159(8)	Fe(1)-N(2)-C(9)-C(10)	42.1(10)
C(56)-C(51)-C(52)-C(53)	5(3)	C(6)-N(2)-C(9)-C(8)	5.5(8)
C(5)-C(51)-C(52)-C(53)	178.2(16)	Fe(1)-N(2)-C(9)-C(8)	-143.8(6)
C(51)-C(52)-C(53)-C(54)	-4(3)	C(7)-C(8)-C(9)-N(2)	-4.9(10)
C(52)-C(53)-C(54)-C(55)	-1(2)	C(81)-C(8)-C(9)-N(2)	167.6(9)
C(53)-C(54)-C(55)-C(56)	5(2)	C(7)-C(8)-C(9)-C(10)	168.6(9)
C(54)-C(55)-C(56)-C(51)	-5(2)	C(81)-C(8)-C(9)-C(10)	-18.9(16)
C(52)-C(51)-C(56)-C(55)	0(3)	N(2)-C(9)-C(10)-C(1)#1	-22.1(13)
C(5)-C(51)-C(56)-C(55)	-172.9(17)	C(8)-C(9)-C(10)-C(1)#1	165.1(9)
C(4)-C(5)-C(5AA)-C(5BB)	59(2)	N(2)-C(9)-C(10)-C(1AA)	173.9(10)
C(6)-C(5)-C(5AA)-C(5BB)	-108(2)	C(8)-C(9)-C(10)-C(1AA)	1.1(16)

N(2)-C(9)-C(10)-C(101)	145.1(10)
C(8)-C(9)-C(10)-C(101)	-27.7(15)
C(1)#1-C(10)-C(101)-C(102)	112.6(16)
C(9)-C(10)-C(101)-C(102)	-55.6(19)
C(1AA)-C(10)-C(101)-C(102)	-154(3)
C(1)#1-C(10)-C(101)-C(106)	-75.6(14)
C(9)-C(10)-C(101)-C(106)	116.3(13)
C(1AA)-C(10)-C(101)-C(106)	17.7(19)
C(106)-C(101)-C(102)-C(103)	2(2)
C(10)-C(101)-C(102)-C(103)	173.3(14)
C(101)-C(102)-C(103)-C(104)	0(2)
C(102)-C(103)-C(104)-C(105)	0(3)
C(103)-C(104)-C(105)-C(106)	-2(3)
C(104)-C(105)-C(106)-C(101)	4(3)
C(102)-C(101)-C(106)-C(105)	-5(3)
C(10)-C(101)-C(106)-C(105)	-177.8(16)
C(1)#1-C(10)-C(1AA)-C(1BB)	118.5(15)
C(9)-C(10)-C(1AA)-C(1BB)	-76.2(18)
C(101)-C(10)-C(1AA)-C(1BB)	20.0(18)
C(1)#1-C(10)-C(1AA)-C(1FF)	-57(2)
C(9)-C(10)-C(1AA)-C(1FF)	108.3(18)
C(101)-C(10)-C(1AA)-C(1FF)	-155(4)
C(1FF)-C(1AA)-C(1BB)-C(1CC)	3(3)
C(10)-C(1AA)-C(1BB)-C(1CC)	-173.0(18)
C(1AA)-C(1BB)-C(1CC)-C(1DD)	-2(3)
C(1BB)-C(1CC)-C(1DD)-C(1EE)	-7(5)
C(1CC)-C(1DD)-C(1EE)-C(1FF)	11(5)
C(1BB)-C(1AA)-C(1FF)-C(1EE)	4(3)
C(10)-C(1AA)-C(1FF)-C(1EE)	179(2)
C(1DD)-C(1EE)-C(1FF)-C(1AA)	-9(3)
N(1)#1-Fe(1)-N(1A)-C(2A)#1	1.7(7)
N(1)-Fe(1)-N(1A)-C(2A)#1	-178.3(7)
N(1B)-Fe(1)-N(1A)-C(2A)#1	-68(100)
N(2)#1-Fe(1)-N(1A)-C(2A)#1	90.5(7)
N(2)-Fe(1)-N(1A)-C(2A)#1	-89.5(7)
N(1)#1-Fe(1)-N(1A)-C(2A)	-178.3(7)
N(1)-Fe(1)-N(1A)-C(2A)	1.7(7)
N(1B)-Fe(1)-N(1A)-C(2A)	112(100)
N(2)#1-Fe(1)-N(1A)-C(2A)	-89.5(7)
N(2)-Fe(1)-N(1A)-C(2A)	90.5(7)
C(2A)#1-N(1A)-C(2A)-N(3A)	-1.0(7)
Fe(1)-N(1A)-C(2A)-N(3A)	179.0(7)
N(1A)-C(2A)-N(3A)-N(3A)#1	2.5(17)
N(1A)-C(2A)-N(3A)-C(4A)	-173.1(18)
C(2A)-N(3A)-C(4A)-C(5A)	-115(6)
N(3A)#1-N(3A)-C(4A)-C(5A)	70(6)
N(3A)-C(4A)-C(5A)-C(6A)	-118(7)
N(3A)-C(4A)-C(5A)-C(10A)	28(8)
C(10A)-C(5A)-C(6A)-C(7A)	0.0
C(4A)-C(5A)-C(6A)-C(7A)	147(6)
C(5A)-C(6A)-C(7A)-C(8A)	0.0
C(6A)-C(7A)-C(8A)-C(9A)	0.0
C(7A)-C(8A)-C(9A)-C(10A)	0.0
C(8A)-C(9A)-C(10A)-C(5A)	0.0
C(6A)-C(5A)-C(10A)-C(9A)	0.0
C(4A)-C(5A)-C(10A)-C(9A)	-144(6)
N(1)#1-Fe(1)-N(1B)-C(2B)	-125.4(6)
N(1)-Fe(1)-N(1B)-C(2B)	54.6(6)
N(1A)-Fe(1)-N(1B)-C(2B)	-56(100)
N(2)#1-Fe(1)-N(1B)-C(2B)	145.7(6)
N(2)-Fe(1)-N(1B)-C(2B)	-34.3(6)
N(1)#1-Fe(1)-N(1B)-C(2B)#1	54.6(6)
N(1)-Fe(1)-N(1B)-C(2B)#1	-125.4(6)
N(1A)-Fe(1)-N(1B)-C(2B)#1	124(100)
N(2)#1-Fe(1)-N(1B)-C(2B)#1	-34.3(6)
N(2)-Fe(1)-N(1B)-C(2B)#1	145.7(6)
C(2B)#1-N(1B)-C(2B)-N(3B)	-0.1(6)
Fe(1)-N(1B)-C(2B)-N(3B)	179.9(6)
N(1B)-C(2B)-N(3B)-N(3B)#1	0.4(16)
N(1B)-C(2B)-N(3B)-C(4B)	-162.1(12)
N(3B)#1-N(3B)-C(4B)-C(5B)	73(2)
C(2B)-N(3B)-C(4B)-C(5B)	-127.5(15)
N(3B)-C(4B)-C(5B)-C(6B)	-157.9(13)
N(3B)-C(4B)-C(5B)-C(10B)	23.7(16)
C(10B)-C(5B)-C(6B)-C(7B)	0.0
C(4B)-C(5B)-C(6B)-C(7B)	-178(2)
C(5B)-C(6B)-C(7B)-C(8B)	0.0
C(6B)-C(7B)-C(8B)-C(9B)	0.0
C(7B)-C(8B)-C(9B)-C(10B)	0.0
C(8B)-C(9B)-C(10B)-C(5B)	0.0
C(6B)-C(5B)-C(10B)-C(9B)	0.0
C(4B)-C(5B)-C(10B)-C(9B)	178.4(17)

Symmetry transformations used to generate equivalent atoms:
#1 y,x,-z+1