Electronic Supporting Information

Assessment of the Intramolecular Magnetic Interactions in the Highly Iron(III) Porphyrin π- Radical Cations: Change From Planar to saddled conformations

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Table S1. Crystal data and structure refinement for [Fe(OETPP•)Cl][$SbCl_6$].

Identification code	feoetppsbcl6	
Empirical formula	C61 H62 Cl9 Fe N4 Sb	
Formula weight	1347.79	
Temperature	150(2) K	
Wavelength	0.71076 Å	
Crystal system	Monoclinic	
Space group	$P2_1/n$	
Unit cell dimensions	a = 17.4501(8) Å	α= 90°.
	b = 18.5354(10) Å	β= 106.174(2)°.
	c = 21.6356(12) Å	γ = 90°.
Volume	6720.9(6) $Å^3$	
Z	4	
Density (calculated)	1.332 Mg/m^3	
Absorption coefficient	1.014 mm^{-1}	
F(000)	2744	
Crystal size	0.21 x 0.18 x 0.095 mm^3	
Theta range for data collection	2.852 to 25.999°.	
Index ranges	-21<=h<=21, -22<=k<=22, -26<=l<=26	
Reflections collected	216615	
Independent reflections	13176 [R(int) = 0.0427]	
Completeness to theta = 25.243°	99.7 %	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	13176 / 299 / 637	
Goodness-of-fit on F^2	1.075	
Final R indices [I>2sigma(I)]	R1 = 0.0799, wR2 = 0.2894	
R indices (all data)	R1 = 0.0950, wR2 = 0.3407	
Extinction coefficient	n/a	
Largest diff. peak and hole	4.181 and -1.790 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for [Fe(OMTPP•)Cl][$SbCl_6$].

Identification code	[Fe(OMTPP)Cl][SbCl6]	
Empirical formula	C52 H44 Cl7 Fe N4 Sb	
Formula weight	1150.66	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	$Cmc2_1$	
Unit cell dimensions	a = 16.944(2) Å	α= 90°.
	b = 34.231(5) Å	β= 90°.
	c = 9.7978(11) Å	γ = 90°.
Volume	5682.8(12) $Å^3$	
Z	4	
Density (calculated)	1.345 Mg/m^3	
Absorption coefficient	1.095 mm^{-1}	
F(000)	2320	
Crystal size	0.4 x 0.4 x 0.4 mm^3	
Theta range for data collection	2.992 to 26.000°.	
Index ranges	-20<=h<=20, -42<=k<=42, -12<=l<=12	
Reflections collected	76685	
Independent reflections	5780 [R(int) = 0.0390]	
Completeness to theta = 25.242°	99.7 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	26.403 and 2.9615	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	5780 / 1 / 309	
Goodness-of-fit on F^2	1.045	
Final R indices [I>2sigma(I)]	R1 = 0.0368, wR2 = 0.1213	
R indices (all data)	R1 = 0.0390, wR2 = 0.1244	
Absolute structure parameter	0.01(2)	
Extinction coefficient	n/a	
Largest diff. peak and hole	2.639 and -1.062 e.$Å^{-3}$	

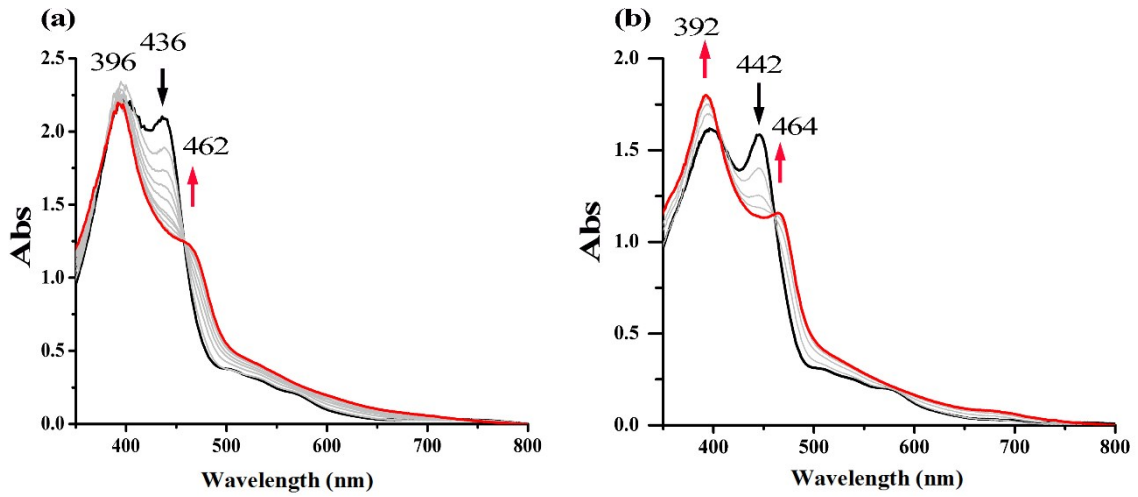

Fig. S1. Absorption spectral changes of (a) Fe(OMTPP)Cl and (b) Fe(OETPP)Cl upon one-electron oxidation with 1.2 equiv of (Phox+•)$SbCl_6$ in a solution of dichloromethane at room temperature.

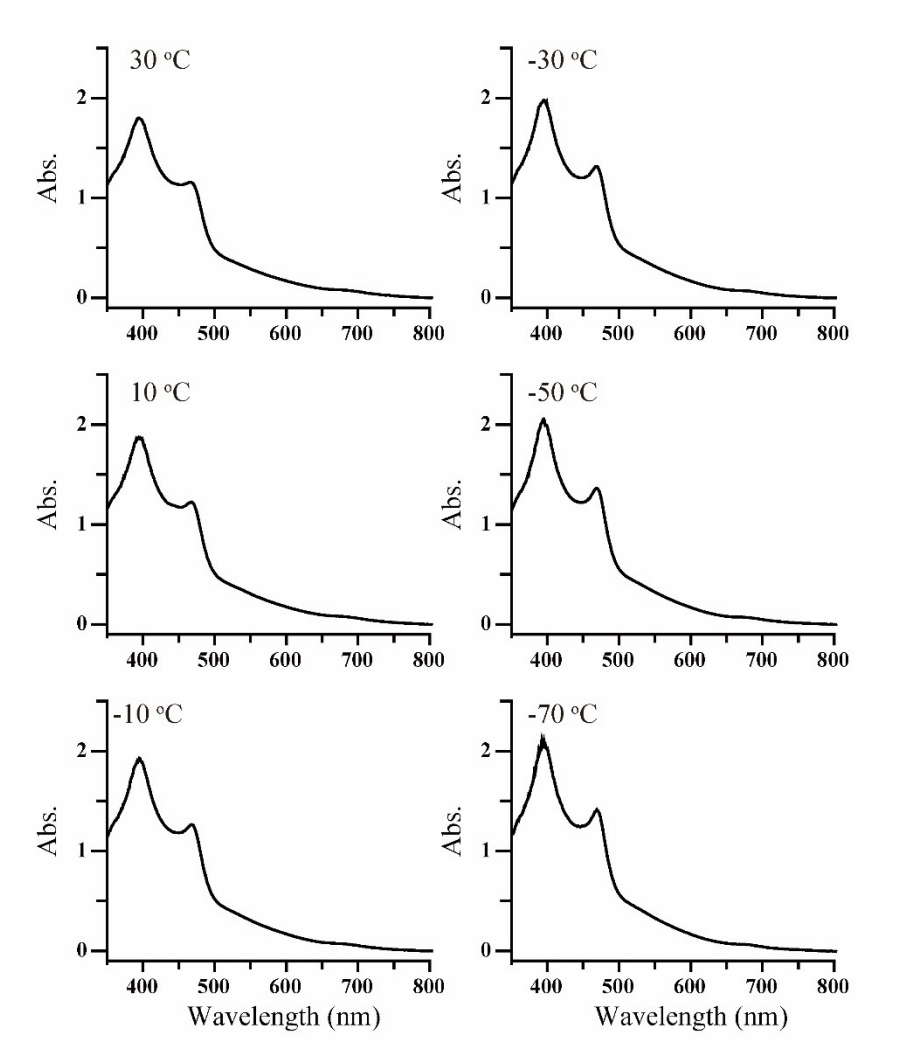

Fig. S2. Variable-Temperature visible spectra of [Fe(OETPP)Cl][$SbCl_6$] at 30 ˚C - -70

˚C in CH_2Cl_2.

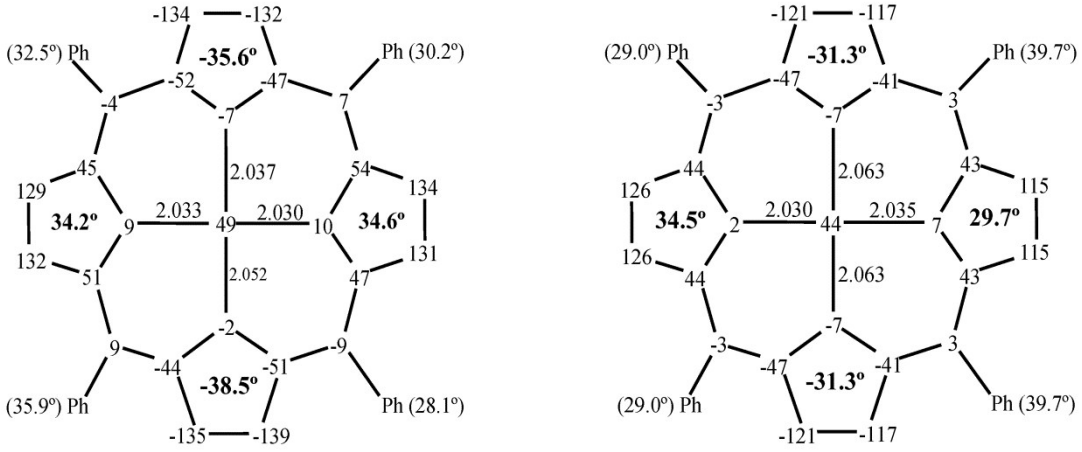

Fig. S3. Deviations of the core atoms from the average plane of 24 porphyrin atoms in unit of 10^{-2} Å together with the Fe-N_p bond length (Å) for [Fe(OETPP•)Cl][$SbCl_6$] **1** and [Fe(OETPP•)Cl][$SbCl_6$] **2**. The angle (°) described in each pyrrole ring is the dihedral angle between the pyrrole and the mean porphyrin plane.

Table 3. Selected Molecular orbital energies (eV) and compositions (α-set and β-set) for [Fe(OETPP•)Cl]$^+$ ($S = 2$).

Orb Energy(eV)	Orb.	Occ	Primary Contributors SFO (percent)
Symmetry Representation for Spin-α-A1 symmetry			
-8.140	$a_{2u}+d_{x^2-y^2}(\alpha)$	1	C15(1P:z)(16.36) Cl2(1P:z)(14.12) C15(1P:x)(13.39) Fe1(1D:z2)(12.66) C23(1P:z)(7.94)
-7.669	$d_{z^2}(\alpha)$	1	N4(1P:z)(18.32) Fe1(1D:x2-y2)(17.76) C23(1P:z)(10.46) Cl2(1P:z)(8.07) Fe1(1D:z2)(7.52)
-6.734	$d_{x^2-y^2}-a_{2u}(\alpha)$	0	C23(1P:z)(21.81) Fe1(1D:x2-y2)(20.67) N3(1P:x)(15.91) N4(1P:y)(12.01)
Symmetry Representation for Spin-β-A1 symmetry			
-7.754	$a_{2u}+ d_{x^2-y^2} (\beta)$	1	C23(1P:z)(33.33) C15(1P:z)(5.96) N4(1P:z)(5.64)
-6.042	$d_{z^2} (\beta)$	0	Fe1(1D:z2)(59.79) Cl2(1P:z)(15.38) C23(1P:z)(5.10)
-5.275	$d_{x^2-y^2} (\beta)$	0	Fe1(1D:x2-y2)(59.55) N4(1P:y)(8.71) N3(1P:x)(7.65)
Symmetry Representation for Spin-α-A2 symmetry			
-10.856	$d_{xy}(\alpha)$	1	Fe1(1D:xy)(53.91)
Symmetry Representation for Spin-β-A2 symmetry			
-7.319	$d_{xy}(\beta)$	0	Fe1(1D:xy)(66.68) C9(1P:y)(5.93) C7(1P:z)(5.86)
Symmetry Representation for Spin-α-B1 symmetry			
-9.995	$d_{xz}(\alpha)$	1	Cl2(1P:x)(15.08) N3(1P:x)(13.83) Fe1(1D:xz)(8.62) C23(1P:z)(8.56)
Symmetry Representation for Spin-β-B1 symmetry			
-6.559	$d_{xz}(\beta)$	0	Fe1(1D:xz)(75.44) Cl2(1P:x)(10.43)
Symmetry Representation for Spin-α-B2 symmetry			
-10.635	$d_{yz}(\alpha)$	1	Fe1(1D:yz)(20.36) Cl2(1P:y)(7.64) H71(1S)(6.47) H91(1S)(5.05)
Symmetry Representation for Spin-β-B2 symmetry			

-6.750	$d_{yz}(\beta)$	0	Fe1(1D:yz)(63.98) Cl2(1P:y)(12.67)

Table S4 Calculated effective α-set orbital interactions between P^{1-} and $FeCl^{2+}$ fragments for $[Fe(TPP•)Cl]^+$, $[Fe(OMTPP•)Cl]^+$ and $[Fe(OETPP•)Cl]^+$

	$[Fe(TPP•)Cl]^+$ (S = 2)	**$[Fe(OMTPP•)Cl]^+$ (S = 2)**	**$[Fe(OETPP•)Cl]^+$ (S = 2)**
$\langle d_{x^2-y^2} \mid P_\sigma \rangle$	-0.0754	-0.0497	-0.0454
$\langle d_{x^2-y^2} \mid a_{2u} \rangle$	-0.0271	-0.0456	-0.0494
$\langle d_{z^2} \mid P_\sigma \rangle$	-0.0051	-0.0093	-0.0125
$\langle d_{z^2} \mid a_{2u} \rangle$	-0.0094	-0.0071	-0.0066
$\langle d_{xz} \mid P_\pi \rangle$	-0.0107	-0.0032	-0.0050
$\langle d_{yz} \mid P_\pi \rangle$	-0.0088	-0.0015	-0.0018
$\langle d_{xy} \mid a_{1u} \rangle$	-0.0003	-0.0002	-0.0022

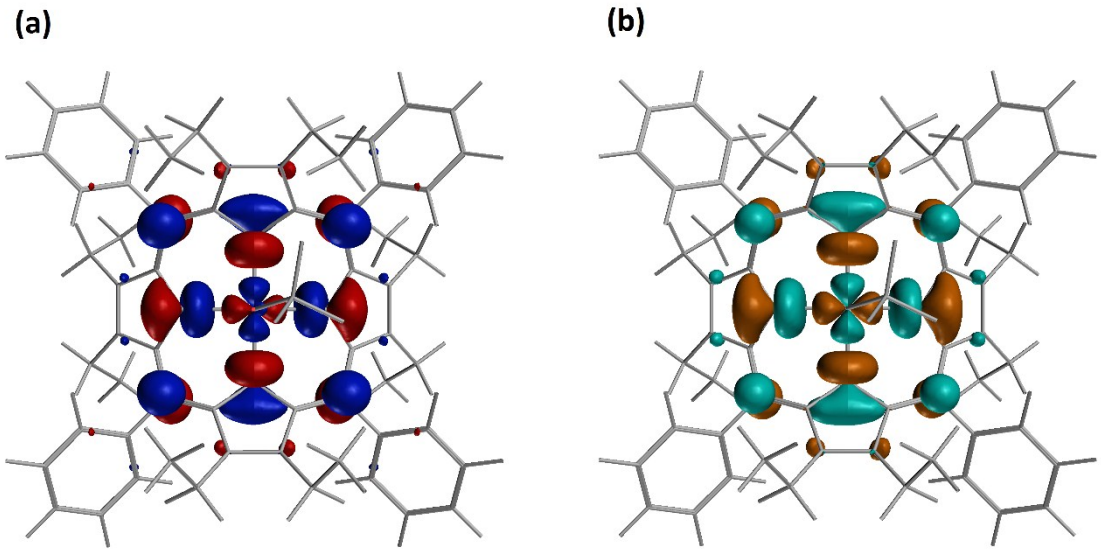

Fig. S4. (a) The occupied α-set $d_{x^2-y^2}$-a_{2u} MO, and (b) the unoccupied β-set $d_{x^2-y^2}$-a_{2u} MO in the ferromagnetic spin state (S = 1) calculation.

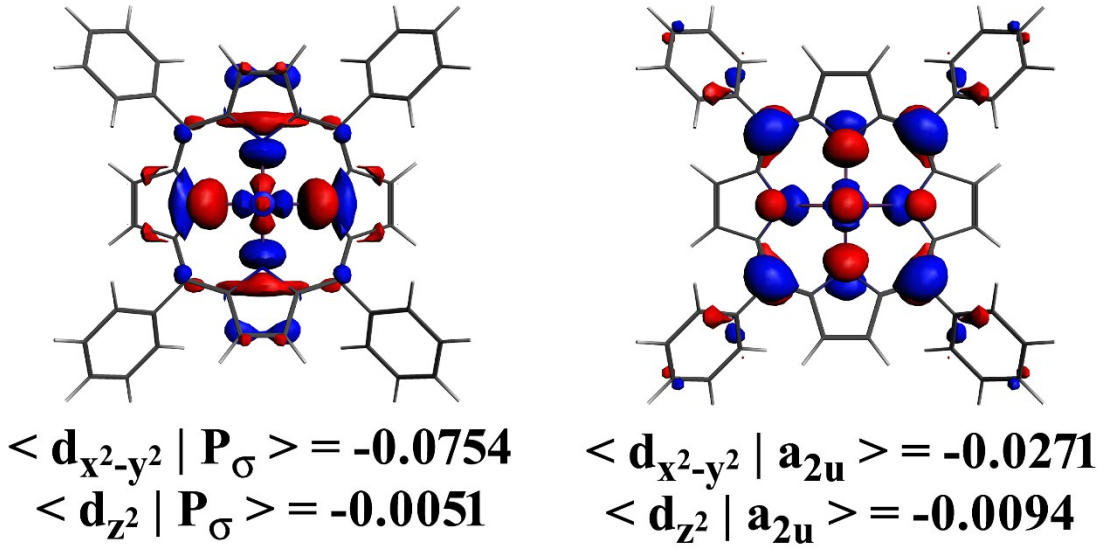

Fig. S5. Selected α-set molecular orbitals based on spin-unrestricted calculations show the distinct orbital interactions between the iron $d_{x^2-y^2}$/d_{z^2} and porphyrin a_{2u}/σ orbital for $[Fe(TPP•)Cl]^+$.

Equations for paramagnetic ^{1}H NMR shifts[1-5]

$$\delta_{obs} = \delta_{dia} + \delta_{iso} \quad \text{(S4)}$$

$$\delta_{iso} = \delta_{con} + \delta_{dip} = \delta_{con} + \delta_{dip}^{M.C.} \quad \text{(S5)}$$

$$\delta_{con} = \frac{\mu_0 \mu_\beta^2 g_e^2 (\mathrm{S}+1)}{9 k_B T} \rho_{\alpha\beta} \quad \text{(S6)}$$

$$\delta_{dip}^{M.C.} = -\frac{\mu_0}{4\pi}\left(\frac{1}{3N}\right)(\chi_{\parallel} - \chi_{\perp})\left[\frac{(3cos^2\theta - 1)}{r^3}\right] = -\frac{\mu_0}{4\pi}\left(\frac{1}{3N}\right)(\chi_{\parallel} - \chi_{\perp}) \times G \quad \text{(S7)}$$

In order to estimate the dipolar contribution of paramagnetic shift, the magnetic susceptibility should be estimated by the Van Vleck equation:

$$\chi = \frac{N\sum_n \left(\frac{E_n^{(1)2}}{kT} - 2E_n^{(2)}\right) exp\left(-\frac{E_n^{(0)}}{kT}\right)}{\sum_n exp\left(-E_n^{(0)}/kT\right)}$$

Where the total spin Hamiltonian operator is:

$$\hat{H} = g_u \mu_\beta S_u H_u + D[\hat{S}_z^2 - S(S+1)/3] + E(\hat{S}_x^2 - \hat{S}_y^2), \quad u = x, y, z$$

For S = 2 systems with axial symmetry and external magnetic field (B) parallel to molecular z axis:

$\hat{H}_z$	|2>	|-2>	|1>	|-1>	|0>
<2|	$4D+2g_z\mu_\beta H_z$	0	0	0	0
<-2|	0	$4D-2g_z\mu_\beta H_z$	0	0	0
<1|	0	0	$D+g_z\mu_\beta H_z$	0	0
<-1|	0	0	0	$D-g_z\mu_\beta H_z$	0
<0|	0	0	0	0	0

$$\chi_z = \frac{N\sum_n E_n^{(1)2} exp(-\frac{E_n^{(0)}}{kT})}{kT\sum_n exp(-E_n^{(0)}/kT)} = \frac{N[2\times g_z^2\mu_\beta^2 \times \exp\left(-\frac{D}{kT}\right) + 2\times 4g_z^2\mu_\beta^2}{kT[\exp(0) + 2\times \exp\left(-\frac{D}{kT}\right) + 2\times}$$

$$= \frac{2Ng_z^2\mu_\beta^2[\exp\left(-\frac{D}{kT}\right) + 4\times \exp\left(-\frac{4D}{kT}\right)]}{kT[1 + 2\exp\left(-\frac{D}{kT}\right) + 2\exp\left(-\frac{4D}{kT}\right)]} = \frac{2Ng_z^2\mu_\beta^2(e^{-x} + 4e^{-4x})}{kT(1 + 2e^{-x} + 2e^{-4x})} \quad , where\ x = \frac{D}{kT} \quad \text{(S8)}$$

Equation S8 is then expanded by Taylor series:

$$\chi_z = \frac{2Ng_z^2\mu_\beta^2}{kT} - \frac{14Ng_z^2\mu_\beta^2 D}{5(kT)^2} \quad \text{(S9)}$$

When external magnetic field (B) perpendicular to molecular z axis:

$\hat{H}_x$	|2>	|−2>	|1>	|-1>	|0>
<2|	**4D**	**0**	$\mathbf{g_x\mu_\beta H_x}$	**0**	**0**
<-2|	**0**	**4D**	**0**	$\mathbf{g_x\mu_\beta H_x}$	**0**
<1|	$\mathbf{g_x\mu_\beta H_x}$	**0**	**D**	**0**	$\sqrt{\frac{3}{2}}\,\mathbf{g_x\mu_\beta H_x}$
<-1|	**0**	$\mathbf{g_x\mu_\beta H_x}$	**0**	**D**	$\sqrt{\frac{3}{2}}\,\mathbf{g_x\mu_\beta H_x}$
<0|	**0**	**0**	$\sqrt{\frac{3}{2}}\,\mathbf{g_x\mu_\beta H_x}$	$\sqrt{\frac{3}{2}}\,\mathbf{g_x\mu_\beta H_x}$	**0**

The eigenvalues can be obtained by using of Mathematica program:

$$E_1 = 4D + \frac{g_\perp^2\mu_\beta^2 H_x^2}{3D} \quad E_2 = 4D + \frac{g_\perp^2\mu_\beta^2 H_x^2}{3D}$$

$$E_3 = D + \frac{8g_\perp^2\mu_\beta^2 H_x^2}{3D} \quad E_4 = D - \frac{g_\perp^2\mu_\beta^2 H_x^2}{3D} \quad E_5 = -\frac{3g_\perp^2\mu_\beta^2 H_x^2}{D}$$

The energy values for each energy level are listed as follow:

n	$E^{(0)}$	$E^{(1)}$	$E^{(2)}$
1	4D	0	$\frac{g_x^2\mu_\beta^2}{3D}$

2	4D	0	$\frac{g_x^2\mu_\beta^2}{3D}$
3	D	0	$\frac{8g_x^2\mu_\beta^2}{3D}$
4	D	0	$-\frac{g_x^2\mu_\beta^2}{3D}$
5	0	0	$-\frac{3g_x^2\mu_\beta^2}{D}$

$$\chi_x = \frac{N\sum_n\left(\frac{E_n^{(1)2}}{kT} - 2E_n^{(2)}\right)exp\left(-\frac{E_n^{(0)}}{kT}\right)}{\sum_n exp(-E_n^{(0)}/kT)} = \frac{N(-\frac{4g_\perp^2\mu_\beta^2}{3D}exp\left(-\frac{4D}{kT}\right) - \frac{14g_\perp^2\mu_\beta^2}{3D}exp\left(-\frac{D}{kT}\right) + \frac{6g_\perp^2\mu_\beta^2}{D})}{1 + 2exp\left(-\frac{D}{kT}\right) + 2exp\left(-\frac{4D}{kT}\right)}$$

$$= \frac{2Ng_\perp^2\mu_\beta^2(9 - 7exp\left(-\frac{D}{kT}\right) - 2exp\left(-\frac{4D}{kT}\right))}{3D(1 + 2exp\left(-\frac{D}{kT}\right) + 2exp\left(-\frac{4D}{kT}\right))}$$

$$= \frac{2Ng_\perp^2\mu_\beta^2(9 - 7e^{-x} - 2e^{-4x})}{3kTx(1 + 2e^{-x} + 2e^{-4x})},\ where\ x = \frac{D}{kT} \quad \text{(S10)}$$

Equation S10 was then expanded by Taylor series:

$$\chi_x = \frac{2Ng_x^2\mu_\beta^2}{kT} - \frac{7Ng_x^2\mu_\beta^2 D}{5(kT)^2} \quad \text{(S11)}$$

$$\chi_\parallel - \chi_\perp = \frac{2Ng_z^2\mu_\beta^2}{kT} - \frac{14Ng_z^2\mu_\beta^2 D}{5(kT)^2} - \frac{2Ng_x^2\mu_\beta^2}{kT} - \frac{7Ng_x^2\mu_\beta^2 D}{5(kT)^2}$$

$$= \frac{2N\mu_\beta^2(g_\parallel^2 - g_\perp^2)}{kT} - \frac{14N\mu_\beta^2(g_\parallel^2 + \frac{1}{2}g_\perp^2)D}{5(kT)^2} = \frac{21N\mu_\beta^2 g_e^2 D}{5(kT)^2} \quad \text{(S12)}$$

Based on equation S12, dipolar contribution can be calculated as follow:

$$\delta_{dip}^{M.C.} = -\frac{\mu_0(\chi_\parallel - \chi_\perp)}{4\pi\ \ 3N} \times G = -\frac{\mu_0 9\mu_\beta^2 g_e^2 GD}{4\pi\ 5(k_BT)^2} = -0.0567(\frac{ppm}{cm^{-1}}cm^3) \times G \times D \quad \text{(S13)}$$

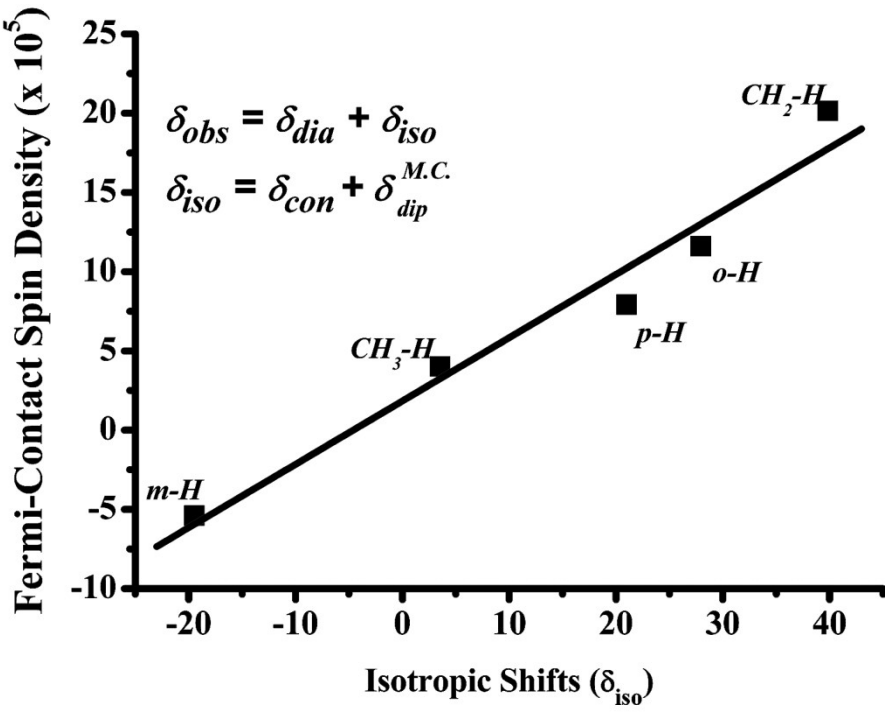

Fig. 6. Correlation between the calculated Fermi contact spin densities at each symmetry-distinct hydrogen atom and the experimental isotropic shifts of [Fe(OETPP•)Cl][$SbCl_6$] with a slope of 4.00×10^{-6} au ppm^{-1}, $R^2 = 0.948$.

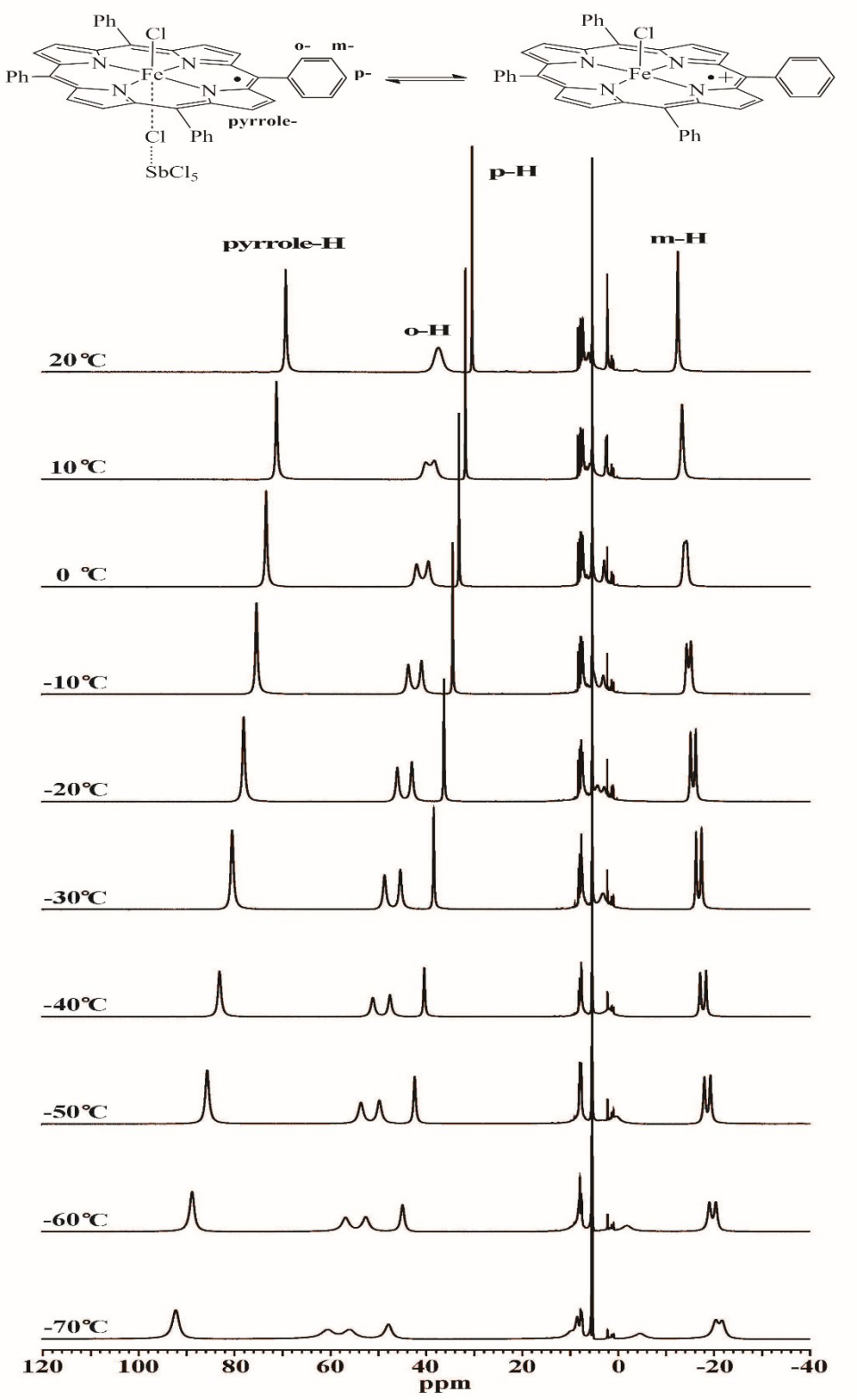

Fig. S7. Observed Variable-Temperature ^{1}H NMR (600 MHz) spectra of [Fe(TPP•)Cl][$SbCl_6$] in CD_2Cl_2.

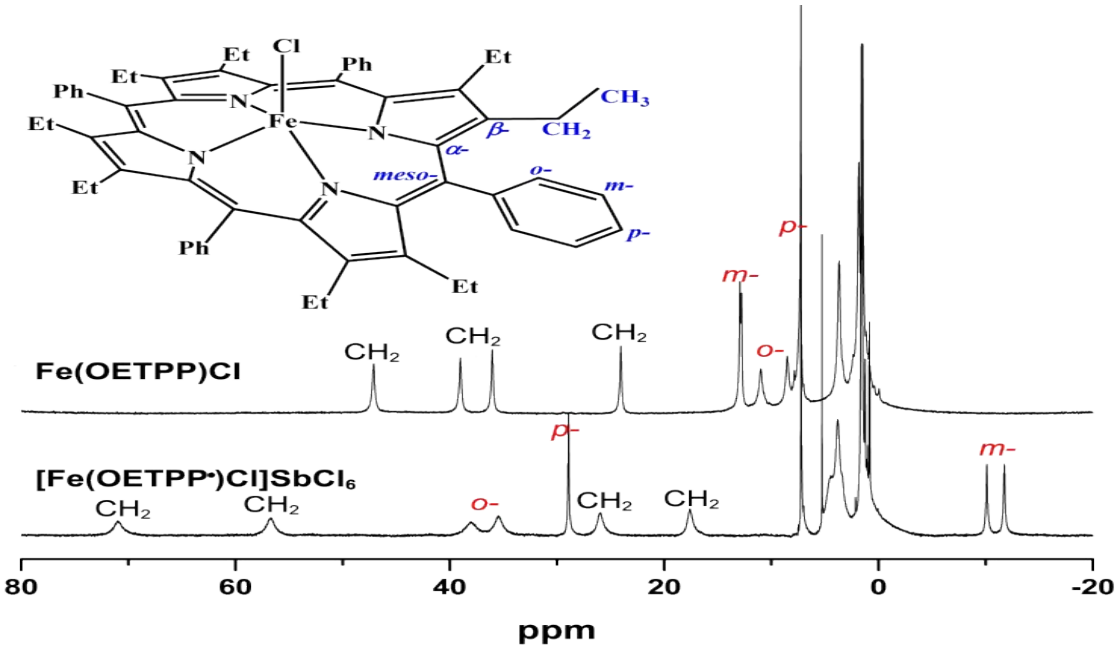

Fig. S8. NMR spectra of Fe(OETPP)Cl and [Fe(OETPP•)Cl][$SbCl_6$] in $CDCl_3$.

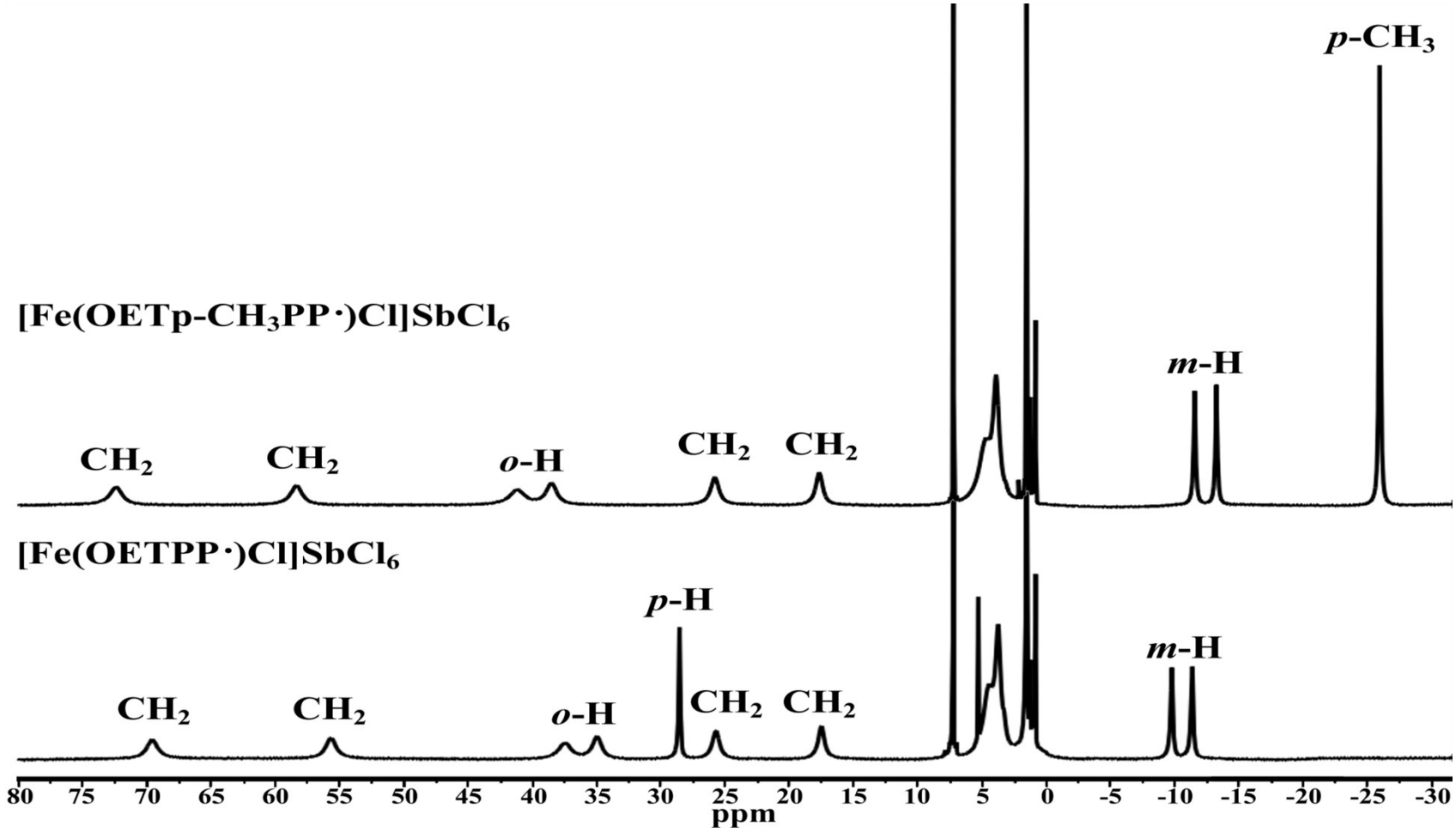

Fig. S9. ^{1}H NMR of [Fe(OETPP)Cl][$SbCl_6$] and [Fe(OETp-CH_3PP)Cl][$SbCl_6$] in $CDCl_3$

Table S5. Theoretically calculated paramagnetic shift of [Fe(OETPP•)Cl][$SbCl_6$].[a]

	Fermi contact spin density, ρ	δ_{con} (ppm)	Geometric factor, G ($\times 10^{21}$ cm^{-3})	$\delta_{dip}^{M.C.}$ (ppm)	δ_{iso} (ppm)	averaged δ_{iso} (ppm)	$\delta_{calc.}$ (DFT)[b]	δ_{obs} (exp. data)[b]
o-H	0.000096626	22.89	-6.365211194	1.62	24.52	28.87	37.18	36.3
o-H	0.000135605	32.13	-4.308080504	1.10	33.22	-		
m-H	-0.000062796	-14.88	-1.854117305	0.47	-14.40	-12.27	-4.60	-10.8
m-H	-0.000045130	-10.69	-2.203983332	0.56	-10.13	-		
p-H	0.000079223	18.77	-1.565047604	0.40	19.17	19.17	26.96	28.8
CH_2-H	0.000173232	41.04	-4.896048401	1.25	42.29	48.55	50.86	42.2
CH_2-H	0.000180293	42.71	-4.896048401	1.25	43.96	-		
CH_2-H	0.000478239	113.30	-2.377718371	0.61	113.90	-		
CH_2-H	-0.000025895	-6.13	-0.650611801	0.17	-5.97	-		
CH_3-H	0.000122465	29.01	0.933128859	-0.24	28.77	9.29	9.75	4.0
CH_3-H	-0.000001597	-0.38	0.933128859	-0.24	-0.62			
CH_3-H	-0.000017765	-4.21	0.933128859	-0.24	-4.45			
CH_3-H	-0.000047236	-11.19	0.773139824	-0.20	-11.39			
CH_3-H	0.000235195	55.72	0.773139824	-0.20	55.52			
CH_3-H	-0.000050289	-11.91	0.773139824	-0.20	-12.11			

[a] Chemical shifts are in unit of ppm. [b] $\delta_{calc.}(DFT) = \delta_{iso} + \delta_{dia}$; ^{1}H NMR resonances of Zn(OETPP) are employed as diamagnetic reference (δ_{dia}), in which the chemical shifts are 8.31ppm for o-H, 7.67 ppm for m-H, 7.79 ppm for p-H, 2.31 ppm for CH_2-H, and 0.46 ppm for CH_3-H.

Table S6. Crystal data and structure refinement for [Fe(OET(*p*-CH_3)PP•)Cl][$SbCl_6$].

Identification code	fesbcl6	
Empirical formula	C70 H82 Cl7 Fe N4 Sb	
Formula weight	1405.15	
Temperature	150(2) K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P 21/n	
Unit cell dimensions	a = 17.8349(9) Å	α= 90°.
	b = 22.2509(12) Å	β= 94.594(5)°.
	c = 18.1681(11) Å	γ = 90°.
Volume	7186.7(7) $Å^3$	
Z	4	
Density (calculated)	1.299 Mg/m^3	
Absorption coefficient	0.879 mm^{-1}	
F(000)	2904	
Crystal size	0.37 x 0.18 x 0.12 mm^3	
Theta range for data collection	2.76 to 29.19°.	
Index ranges	-21<=h<=24, -30<=k<=30, -20<=l<=24	
Reflections collected	37056	
Independent reflections	16651 [R(int) = 0.1025]	
Completeness to theta = 26.00°	99.8 %	
Absorption correction	Semi-empirical from equivalents	
Max. and min. transmission	1.00000 and 0.92974	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	16651 / 0 / 748	
Goodness-of-fit on F^2	0.996	
Final R indices [I>2sigma(I)]	R1 = 0.1086, wR2 = 0.2472	
R indices (all data)	R1 = 0.2139, wR2 = 0.3000	
Largest diff. peak and hole	1.731 and -1.301 $e.Å^{-3}$	

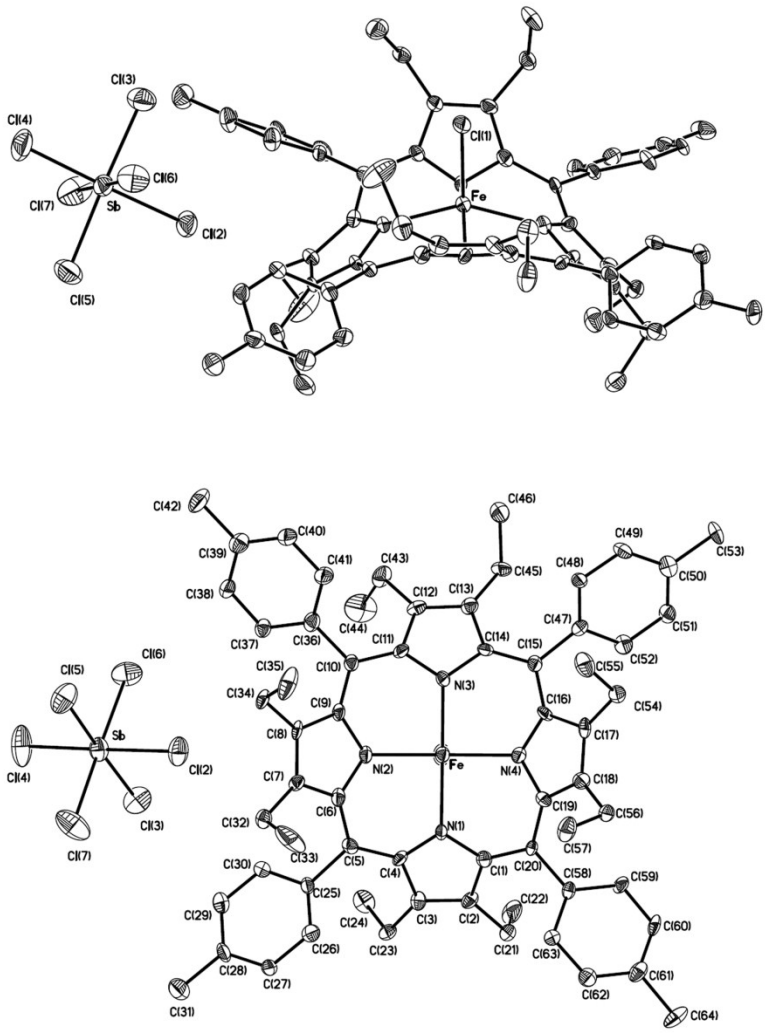

Fig. S10. ORTEP diagram of [Fe(OET(p-CH_3)PP•)Cl][$SbCl_6$] with 30% probability ellipsoids. Hydrogen atoms are omitted for clarity.

Cartesian coordinates of [Fe(TPP•)Cl]$^+$ for calculation[9]

Fe	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	2.168000
N	-2.019000	0.000000	-0.461000
N	0.000000	2.024000	-0.407000
N	2.019000	0.000000	-0.461000
N	0.000000	-2.024000	-0.407000
C	-2.824000	-1.104000	-0.594000
C	-2.824000	1.104000	-0.594000
C	-1.103000	2.821000	-0.170000
C	1.103000	2.821000	-0.170000
C	2.824000	1.104000	-0.594000
C	2.824000	-1.104000	-0.594000
C	1.103000	-2.821000	-0.170000
C	-1.103000	-2.821000	-0.170000
C	-4.164000	-0.683000	-0.919000
C	-4.164000	0.683000	-0.919000
C	-0.692000	4.119000	0.254000
C	0.692000	4.119000	0.254000
C	4.164000	0.683000	-0.919000
C	4.164000	-0.683000	-0.919000
C	0.692000	-4.119000	0.254000
C	-0.692000	-4.119000	0.254000
C	-2.419000	2.419000	-0.358000
C	2.419000	2.419000	-0.358000
C	2.419000	-2.419000	-0.358000
C	-2.419000	-2.419000	-0.358000
C	-3.469000	3.469000	-0.241000
C	3.469000	3.469000	-0.241000
C	3.469000	-3.469000	-0.241000
C	-3.469000	-3.469000	-0.241000
C	-4.537000	3.273000	0.660000
C	4.537000	3.273000	0.660000
C	4.537000	-3.273000	0.660000
C	-4.537000	-3.273000	0.660000
C	-3.418000	4.620000	-1.006000
C	3.418000	4.620000	-1.006000
C	3.418000	-4.620000	-1.006000
C	-3.418000	-4.620000	-1.006000
C	-5.509000	4.256000	0.808000
C	5.509000	4.256000	0.808000
C	5.509000	-4.256000	0.808000
C	-5.509000	-4.256000	0.808000
C	-4.400000	5.600000	-0.868000
C	4.400000	5.600000	-0.868000
C	4.400000	-5.600000	-0.868000
C	-4.400000	-5.600000	-0.868000
C	-5.437000	5.437000	0.031000
C	5.437000	5.437000	0.031000
C	5.437000	-5.437000	0.031000
C	-5.437000	-5.437000	0.031000
H	-5.008000	-1.326000	-1.124000
H	-5.008000	1.326000	-1.124000
H	-1.336000	4.943000	0.523000
H	1.336000	4.943000	0.523000
H	5.008000	1.326000	-1.124000
H	5.008000	-1.326000	-1.124000

H	1.336000	-4.943000	0.523000
H	-1.336000	-4.943000	0.523000
H	-4.600000	2.360000	1.234000
H	4.600000	2.360000	1.234000
H	4.600000	-2.360000	1.234000
H	-4.600000	-2.360000	1.234000
H	-2.614000	4.760000	-1.713000
H	2.614000	4.760000	-1.713000
H	2.614000	-4.760000	-1.713000
H	-2.614000	-4.760000	-1.713000
H	-6.316000	4.119000	1.513000
H	6.316000	4.119000	1.513000
H	6.316000	-4.119000	1.513000
H	-6.316000	-4.119000	1.513000
H	-4.350000	6.495000	-1.470000
H	4.350000	6.495000	-1.470000
H	4.350000	-6.495000	-1.470000
H	-4.350000	-6.495000	-1.470000
H	6.179000	-6.179000	0.285000
H	-6.179000	-6.179000	0.285000
H	-6.179000	6.179000	0.285000
H	6.179000	6.179000	0.285000

Cartesian coordinates of Fe(OETPP)Cl for calculation[10]

Fe	0.000000	0.000000	0.000000
Cl	0.000000	0.000000	2.242000
N	-1.968000	0.000000	-0.571000
N	0.000000	1.980000	-0.362000
N	1.968000	0.000000	-0.571000
N	0.000000	-1.980000	-0.362000
C	-2.731000	-1.108000	-0.878000
C	-2.731000	1.108000	-0.878000
C	-1.097000	2.738000	0.000000
C	1.097000	2.738000	0.000000
C	2.731000	1.108000	-0.878000
C	2.731000	-1.108000	-0.878000
C	1.097000	-2.738000	0.000000
C	-1.097000	-2.738000	0.000000
C	-3.942000	-0.673000	-1.565000
C	-3.942000	0.673000	-1.565000
C	-0.678000	3.894000	0.741000
C	0.678000	3.894000	0.741000
C	3.942000	0.673000	-1.565000
C	3.942000	-0.673000	-1.565000
C	0.678000	-3.894000	0.741000
C	-0.678000	-3.894000	0.741000
C	-2.389000	2.389000	-0.434000
C	2.389000	2.389000	-0.434000
C	2.389000	-2.389000	-0.434000
C	-2.389000	-2.389000	-0.434000
C	-4.946000	-1.541000	-2.268000
C	-4.946000	1.541000	-2.268000
C	-1.522000	4.794000	1.580000
C	1.522000	4.794000	1.580000
C	4.946000	1.541000	-2.268000
C	4.946000	-1.541000	-2.268000

C	1.522000	-4.794000	1.580000
C	-1.522000	-4.794000	1.580000
C	-3.435000	3.435000	-0.376000
C	3.435000	3.435000	-0.376000
C	3.435000	-3.435000	-0.376000
C	-3.435000	-3.435000	-0.376000
C	-4.514000	3.292000	0.482000
C	4.514000	3.292000	0.482000
C	4.514000	-3.292000	0.482000
C	-4.514000	-3.292000	0.482000
C	-3.365000	4.541000	-1.165000
C	3.365000	4.541000	-1.165000
C	3.365000	-4.541000	-1.165000
C	-3.365000	-4.541000	-1.165000
C	-5.478000	4.278000	0.541000
C	5.478000	4.278000	0.541000
C	5.478000	-4.278000	0.541000
C	-5.478000	-4.278000	0.541000
C	-4.327000	5.506000	-1.105000
C	4.327000	5.506000	-1.105000
C	4.327000	-5.506000	-1.105000
C	-4.327000	-5.506000	-1.105000
C	-5.360000	5.359000	-0.253000
C	5.360000	5.359000	-0.253000
C	5.360000	-5.359000	-0.253000
C	-5.360000	-5.359000	-0.253000
H	6.115000	6.130000	-0.205000
H	4.261000	6.381000	-1.735000
H	2.536000	4.656000	-1.848000
H	4.600000	2.412000	1.102000
H	6.316000	4.184000	1.215000
H	4.600000	-2.412000	1.102000
H	6.316000	-4.184000	1.215000
H	6.115000	-6.130000	-0.205000
H	4.261000	-6.381000	-1.735000
H	2.536000	-4.656000	-1.848000
H	-2.536000	-4.656000	-1.848000
H	-4.261000	-6.381000	-1.735000
H	-6.115000	-6.130000	-0.205000
H	-6.316000	-4.184000	1.215000
H	-4.600000	-2.412000	1.102000
H	-4.600000	2.412000	1.102000
H	-6.316000	4.184000	1.215000
H	-6.115000	6.130000	-0.205000
H	-4.261000	6.381000	-1.735000
H	-2.536000	4.656000	-1.848000
C	4.408000	-2.100000	-3.588000
C	4.408000	2.100000	-3.588000
C	1.931000	-4.093000	2.878000
C	-1.931000	-4.093000	2.878000
C	1.931000	4.093000	2.878000
C	-1.931000	4.093000	2.878000
C	-4.408000	-2.100000	-3.588000
C	-4.408000	2.100000	-3.588000
H	2.550000	-4.769000	3.479000
H	2.504000	-3.189000	2.640000
H	0.953000	-5.698000	1.823000
H	1.034000	-3.818000	3.444000
H	2.423000	-5.069000	1.020000
H	-1.034000	-3.818000	3.444000

H	-2.550000	-4.769000	3.479000
H	-0.953000	-5.698000	1.823000
H	-2.504000	-3.189000	2.640000
H	-2.423000	-5.069000	1.020000
H	-1.034000	3.818000	3.444000
H	-2.504000	3.189000	2.640000
H	-2.550000	4.769000	3.479000
H	-0.953000	5.698000	1.823000
H	-2.423000	5.069000	1.020000
H	-5.209000	-2.378000	-1.612000
H	-3.515000	-2.705000	-3.392000
H	-4.149000	-1.272000	-4.257000
H	-5.176000	-2.724000	-4.060000
H	-5.842000	-0.945000	-2.477000
H	-5.209000	2.378000	-1.612000
H	-3.515000	2.705000	-3.392000
H	-4.149000	1.272000	-4.257000
H	-5.842000	0.945000	-2.477000
H	-5.176000	2.724000	-4.060000
H	1.034000	3.818000	3.444000
H	2.504000	3.189000	2.640000
H	2.423000	5.069000	1.020000
H	0.953000	5.698000	1.823000
H	2.550000	4.769000	3.479000
H	4.149000	-1.272000	-4.257000
H	5.176000	-2.724000	-4.060000
H	3.515000	-2.705000	-3.392000
H	5.209000	-2.378000	-1.612000
H	5.842000	-0.945000	-2.477000
H	5.842000	0.945000	-2.477000
H	5.209000	2.378000	-1.612000
H	4.149000	1.272000	-4.257000
H	3.515000	2.705000	-3.392000
H	5.176000	2.724000	-4.060000

Cartesian coordinates of [Fe(OETPP•)Cl]$^{+}$ for calculation

Fe	0.000000	0.000000	0.000000
Cl	0.000000	-0.000000	-2.217000
N	-1.991000	-0.000000	0.403000
N	1.991000	0.000000	0.403000
N	-0.000100	-1.972000	0.541000
N	-0.000100	1.972000	0.541000
C	-2.717000	1.097000	0.001000
C	-2.717000	-1.097000	0.001000
C	2.717000	-1.097000	0.001000
C	2.717000	1.097000	0.001000
C	-1.093000	-2.669000	0.974000
C	1.093000	-2.669000	0.974000
C	1.093000	2.669000	0.974000
C	-1.093000	2.669000	0.974000
C	-2.391000	2.376000	0.486000
C	-2.391000	-2.376000	0.486000
C	2.391000	-2.376000	0.486000
C	2.391000	2.376000	0.486000

C	-3.833000	0.681000	-0.821000
C	-3.833000	-0.681000	-0.821000
C	3.833000	-0.681000	-0.821000
C	3.833000	0.681000	-0.821000
C	-0.682000	-3.748000	1.842000
C	0.682000	-3.748000	1.842000
C	0.682000	3.748000	1.842000
C	-0.682000	3.748000	1.842000
C	-4.722000	1.546000	-1.666000
C	-4.722000	-1.546000	-1.666000
C	4.722000	-1.546000	-1.666000
C	4.722000	1.546000	-1.666000
C	-1.558000	-4.569000	2.750000
C	1.558000	-4.569000	2.750000
C	1.558000	4.569000	2.750000
C	-1.558000	4.569000	2.750000
C	-4.028000	2.018000	-2.916000
C	-4.028000	-2.018000	-2.916000
C	4.028000	-2.018000	-2.916000
C	4.028000	2.018000	-2.916000
C	-1.918000	-3.766000	3.972000
C	1.918000	-3.766000	3.972000
C	1.918000	3.766000	3.972000
C	-1.918000	3.766000	3.972000
C	-3.382000	-3.463000	0.440000
C	3.382000	-3.463000	0.440000
C	3.382000	3.463000	0.440000
C	-3.382000	3.463000	0.440000
C	-3.057000	-4.633000	-0.210000
C	3.057000	-4.633000	-0.210000
C	3.057000	4.633000	-0.210000
C	-3.057000	4.633000	-0.210000
C	-3.973000	-5.661000	-0.275000
C	3.973000	-5.661000	-0.275000
C	3.973000	5.661000	-0.275000
C	-3.973000	5.661000	-0.275000
C	-5.216000	-5.518000	0.311000
C	5.216000	-5.518000	0.311000
C	5.216000	5.518000	0.311000
C	-5.216000	5.518000	0.311000
C	-5.542000	-4.348000	0.961000
C	5.542000	-4.348000	0.961000
C	5.542000	4.348000	0.961000
C	-5.542000	4.348000	0.961000
C	-4.625000	-3.320000	1.025000
C	4.625000	-3.320000	1.025000
C	4.625000	3.320000	1.025000
C	-4.625000	3.320000	1.025000
H	-5.597000	0.977100	-1.945200
H	-5.597000	-0.977100	-1.945200
H	5.597000	-0.977100	-1.945000
H	5.597000	0.977100	-1.945000
H	-5.022000	2.406500	-1.086400
H	-5.022000	-2.406500	-1.086400
H	5.022000	-2.406500	-1.086400
H	5.022000	2.406500	-1.086400
H	-1.028000	-5.460800	3.049900
H	1.028000	-5.460800	3.049900
H	1.028000	5.460800	3.049900
H	-1.028000	5.460800	3.049900

H	-2.459700	-4.846100	2.224100
H	2.459700	-4.846100	2.224100
H	2.459700	4.846100	2.224100
H	-2.459700	4.846100	2.224100
H	-4.041000	1.327000	-3.746000
H	-4.041000	-1.327000	-3.746000
H	4.041000	-1.327000	-3.746000
H	4.041000	1.327000	-3.746000
H	-2.972000	2.131000	-2.721000
H	-2.972000	-2.131000	-2.721000
H	2.972000	-2.131000	-2.721000
H	2.972000	2.131000	-2.721000
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H	-4.310000	-3.002000	-3.262000
H	4.310000	-3.002000	-3.262000
H	4.310000	3.002000	-3.262000
H	-2.294000	2.772000	3.782000
H	2.294000	2.772000	3.782000
H	2.294000	-2.772000	3.782000
H	-2.294000	-2.772000	3.782000
H	-2.560000	4.263000	4.684000
H	2.560000	4.263000	4.684000
H	2.560000	-4.263000	4.684000
H	-2.560000	-4.263000	4.684000
H	-1.027000	3.574000	4.552000
H	1.027000	3.574000	4.552000
H	1.027000	-3.574000	4.552000
H	-1.027000	-3.574000	4.552000
H	2.085300	4.744200	-0.668100
H	-2.085300	4.744200	-0.668100
H	-2.085300	-4.744200	-0.668100
H	2.085300	-4.744200	-0.668100
H	3.717000	6.578000	-0.784800
H	-3.717000	6.578000	-0.784800
H	-3.717000	-6.578000	-0.784800
H	3.717000	-6.578000	-0.784800
H	5.935000	6.322700	0.261000
H	-5.935000	6.322700	0.261000
H	-5.935000	-6.322700	0.261000
H	5.935000	-6.322700	0.261000
H	6.513700	4.237000	1.419000
H	-6.513700	4.237000	1.419000
H	-6.513700	-4.237000	1.419000
H	6.513700	-4.237000	1.419000
H	4.880500	2.402200	1.534000
H	-4.880500	2.402200	1.534000
H	-4.880500	-2.402200	1.534000
H	4.880500	-2.402200	1.534000

Cartesian coordinates of Cu(OETPP•)ClO_4 for calculation[11]

Cu	0.000000	0.000000	0.000000
O	0.000000	0.000000	2.443000
N	-1.968000	0.000000	-0.137000
N	0.000000	1.971000	-0.050000
N	1.968000	0.000000	-0.137000

N	0.000000	-1.971000	-0.050000
C	-2.683000	-1.093000	-0.571000
C	-2.683000	1.093000	-0.571000
C	-1.094000	2.670000	0.418000
C	1.094000	2.670000	0.418000
C	2.683000	1.093000	-0.571000
C	2.683000	-1.093000	-0.571000
C	1.094000	-2.670000	0.418000
C	-1.094000	-2.670000	0.418000
C	-3.793000	-0.679000	-1.396000
C	-3.793000	0.679000	-1.396000
C	-0.680000	3.727000	1.303000
C	0.680000	3.727000	1.303000
C	3.793000	0.679000	-1.396000
C	3.793000	-0.679000	-1.396000
C	0.680000	-3.727000	1.303000
C	-0.680000	-3.727000	1.303000
C	-2.375000	2.364000	-0.062000
C	2.375000	2.364000	-0.062000
C	2.375000	-2.364000	-0.062000
C	-2.375000	-2.364000	-0.062000
C	-1.474000	4.529000	2.223000
C	1.474000	4.529000	2.223000
C	4.652000	1.556000	-2.254000
C	4.652000	-1.556000	-2.254000
C	1.474000	-4.529000	2.223000
C	-1.474000	-4.529000	2.223000
C	-4.652000	-1.556000	-2.254000
C	-4.652000	1.556000	-2.254000
C	-3.422000	3.404000	-0.016000
C	3.422000	3.404000	-0.016000
C	3.422000	-3.404000	-0.016000
C	-3.422000	-3.404000	-0.016000
C	-3.216000	4.618000	-0.618000
C	3.216000	4.618000	-0.618000
C	3.216000	-4.618000	-0.618000
C	-3.216000	-4.618000	-0.618000
C	-4.602000	3.171000	0.632000
C	4.602000	3.171000	0.632000
C	4.602000	-3.171000	0.632000
C	-4.602000	-3.171000	0.632000
C	-4.193000	5.587000	-0.551000
C	4.193000	5.587000	-0.551000
C	4.193000	-5.587000	-0.551000
C	-4.193000	-5.587000	-0.551000
C	-5.555000	-4.144000	0.700000
C	-5.555000	4.144000	0.700000
C	5.555000	4.144000	0.700000
C	5.555000	-4.144000	0.700000
C	-5.341000	5.338000	0.103000
C	5.341000	5.338000	0.103000
C	5.341000	-5.338000	0.103000
C	-5.341000	-5.338000	0.103000
H	5.007000	2.397000	-1.648000
H	5.509000	0.970000	-2.604000
H	5.509000	-0.970000	-2.604000
H	5.007000	-2.397000	-1.648000
C	3.911000	-2.112000	-3.473000
H	4.591000	-2.743000	-4.057000
H	3.557000	-1.282000	-4.095000

H	3.055000	-2.709000	-3.139000
C	3.911000	2.112000	-3.473000
H	4.591000	2.743000	-4.057000
H	3.055000	2.709000	-3.139000
H	3.557000	1.282000	-4.095000
H	-5.509000	0.970000	-2.604000
H	-5.007000	2.397000	-1.648000
C	-3.911000	2.112000	-3.473000
H	-3.055000	2.709000	-3.139000
H	-4.591000	2.743000	-4.057000
H	-3.557000	1.282000	-4.095000
H	-5.007000	-2.397000	-1.648000
H	-5.509000	-0.970000	-2.604000
C	-3.911000	-2.112000	-3.473000
H	-3.055000	-2.709000	-3.139000
H	-3.557000	-1.282000	-4.095000
H	-4.591000	-2.743000	-4.057000
H	-2.295000	-4.985000	1.659000
H	-0.831000	-5.316000	2.633000
H	0.831000	-5.316000	2.633000
H	2.295000	-4.985000	1.659000
C	-2.074000	-3.743000	3.392000
H	-1.268000	-3.289000	3.979000
H	-2.653000	-4.422000	4.030000
H	-2.732000	-2.957000	3.004000
C	2.074000	-3.743000	3.392000
H	2.732000	-2.957000	3.004000
H	2.653000	-4.422000	4.030000
H	1.268000	-3.289000	3.979000
H	2.295000	4.985000	1.659000
H	0.831000	5.316000	2.633000
C	2.074000	3.743000	3.392000
H	2.732000	2.957000	3.004000
H	1.268000	3.289000	3.979000
H	2.653000	4.422000	4.030000
H	-0.831000	5.316000	2.633000
H	-2.295000	4.985000	1.659000
C	-2.074000	3.743000	3.392000
H	-1.268000	3.289000	3.979000
H	-2.732000	2.957000	3.004000
H	-2.653000	4.422000	4.030000
H	-4.035000	-6.560000	-1.030000
H	-6.114000	-6.114000	0.153000
H	-6.492000	-3.959000	1.237000
H	-4.784000	-2.197000	1.100000
H	-2.279000	-4.817000	-1.150000
H	-2.279000	4.817000	-1.150000
H	-4.035000	6.560000	-1.030000
H	-4.784000	2.197000	1.100000
H	-6.492000	3.959000	1.237000
H	-6.114000	6.114000	0.153000
H	4.784000	2.197000	1.100000
H	6.492000	3.959000	1.237000
H	6.114000	6.114000	0.153000
H	4.035000	6.560000	-1.030000
H	2.279000	4.817000	-1.150000
H	4.784000	-2.197000	1.100000
H	6.492000	-3.959000	1.237000
H	6.114000	-6.114000	0.153000
H	4.035000	-6.560000	-1.030000

H	2.279000	-4.817000	-1.150000
O	1.147000	1.667000	3.608000
O	0.483000	-0.288000	4.691000
O	2.189000	-0.308000	3.105000
Cl	0.919000	0.288000	3.487000

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