Supporting Informations

Formation and characterization of six-coordinate iron(III) complex with the most ruffled porphyrin ring

Akira Ikezaki[ab] and Mikio Nakamura[*abc]

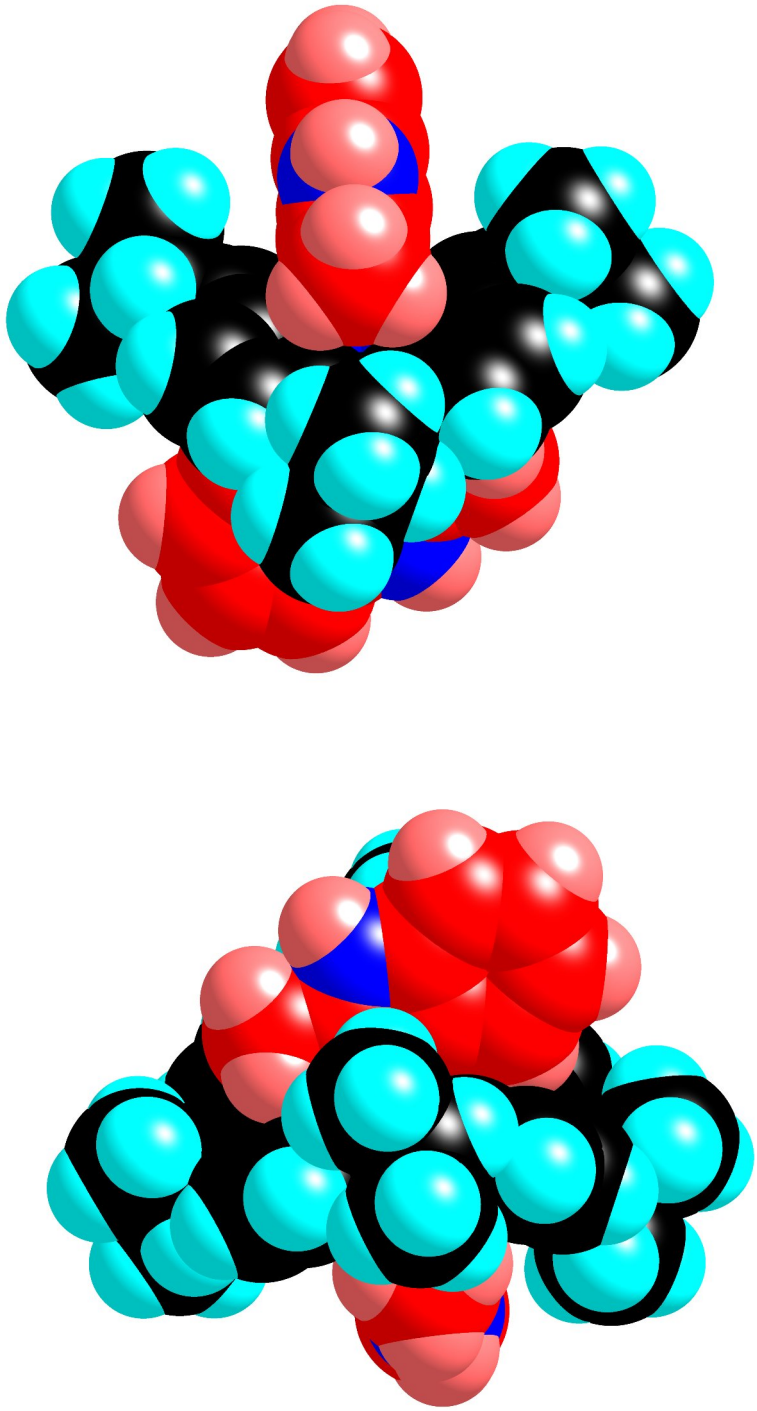

Fig. S1. Molecular structure of $[Fe(T^{i}PrP)(2\text{-MeBzIm})_2]^+$(**1**) presented by CPK model, where C, H, N atoms in the porphyrin core are expressed by black, cyan, and blue, respectively, and C, H, N atoms in the coordinating 2-MeBzIm ligands are expressed by red, pink, and blue, respectively.

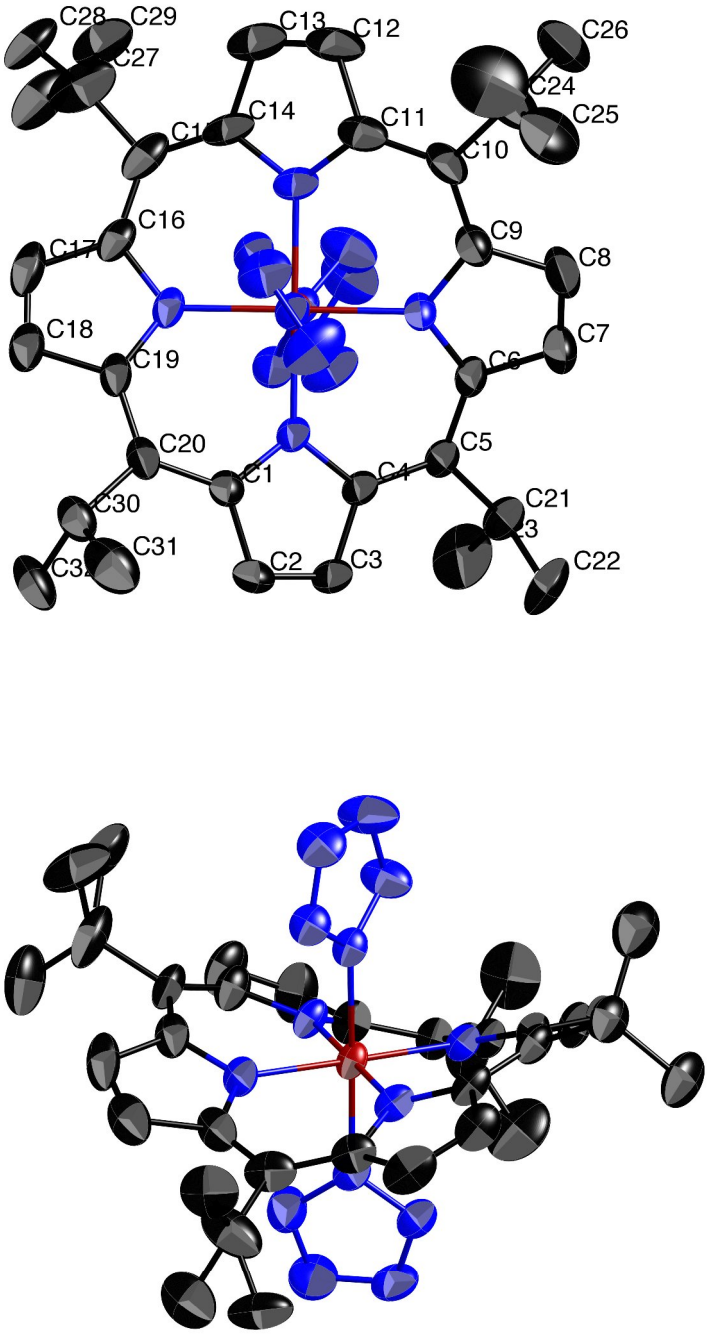

Fig. S2. Molecular structure of $[Fe(T^{i}PrP)(HIm)_2]^{+}$(2). Thermal ellipsoids are drawn to enclose 50 % probability.

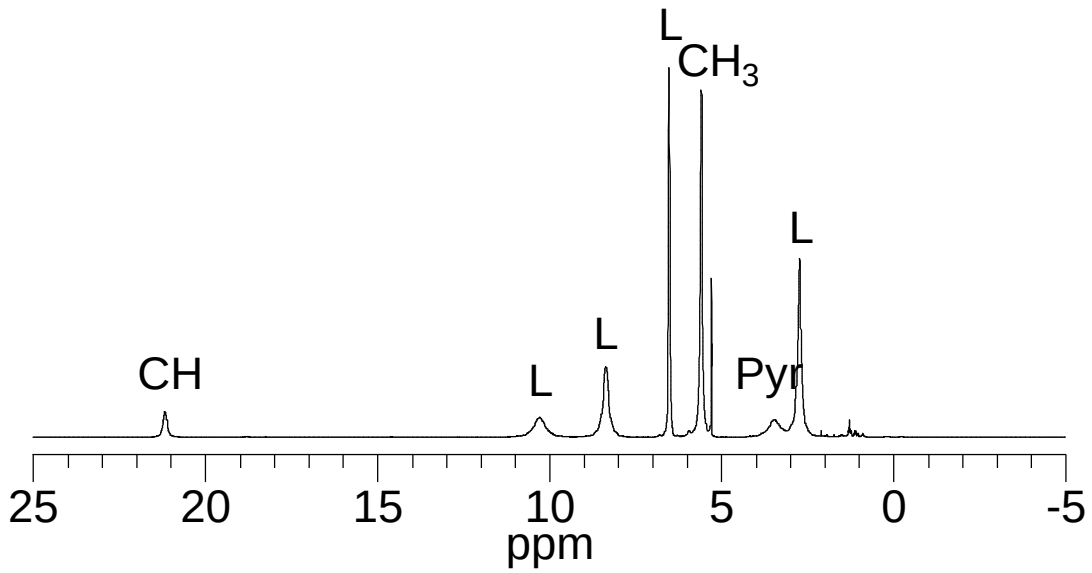

Fig. S3. ^{1}H NMR spectrum of **1** taken in CD_2Cl_2 at 298 K.

Table S1. Crystal data and structure refinement for $[Fe(T^{i}PrP)(2\text{-}MeBzIm)_2]ClO_4$ (**1**).

Empirical formula	C50 H54 Cl7 Fe N8 O4	
Formula weight	1135.01	
Temperature	223 K	
Wavelength	0.71073 Å	
Crystal system	Orthorhombic	
Space group	Pca2(1)	
Unit cell dimensions	a = 43.200(9) Å	α= 90°.
	b = 11.700(2) Å	β= 90°.
	c = 10.682(2) Å	γ = 90°.
Volume	5399.1(18) $Å^3$	
Z	4	
Density (calculated)	1.396 Mg/m^3	
Absorption coefficient	0.677 mm^{-1}	
F(000)	2348	
Crystal size	0.48 x 0.14 x 0.06 mm^3	
Theta range for data collection	0.94 to 25.17°.	
Index ranges	-51<=h<=45, -13<=k<=12, -12<=l<=12	
Reflections collected	27760	
Independent reflections	9301 [R(int) = 0.1792]	
Completeness to theta = 25.17°	99.6 %	
Absorption correction	Analytical	
Max. and min. transmission	0.9605 and 0.7372	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9301 / 1 / 641	
Goodness-of-fit on F^2	0.916	
Final R indices [I>2sigma(I)]	R1 = 0.0641, wR2 = 0.1307	
R indices (all data)	R1 = 0.1042, wR2 = 0.1487	
Absolute structure parameter	-0.01(3)	
Largest diff. peak and hole	0.645 and -0.608 $e.Å^{-3}$	

Table S2. Crystal data and structure refinement for $[Fe(T^{i}PrP)(HIm)_2]ClO_4$ (**2**).

Empirical formula	C45 H57 Cl4 Fe N8 O4	
Formula weight	971.64	
Temperature	223 K	
Wavelength	0.71073 Å	
Crystal system	Monoclinic	
Space group	P2(1)/c	
Unit cell dimensions	a = 9.4670(19) Å	α= 90°.
	b = 40.940(8) Å	β= 98.23(3)°.
	c = 12.708(3) Å	γ = 90°.
Volume	4874.7(17) $Å^3$	
Z	4	
Density (calculated)	1.324 Mg/m^3	
Absorption coefficient	0.578 mm^{-1}	
F(000)	2036	
Crystal size	0.49 x 0.27 x 0.09 mm^3	
Theta range for data collection	1.69 to 25.69°.	
Index ranges	-11<=h<=11, -41<=k<=49, -15<=l<=10	
Reflections collected	27016	
Independent reflections	9256 [R(int) = 0.1470]	
Completeness to theta = 25.69°	99.8 %	
Absorption correction	Analytical	
Max. and min. transmission	0.9498 and 0.7649	
Refinement method	Full-matrix least-squares on F^2	
Data / restraints / parameters	9256 / 0 / 589	
Goodness-of-fit on F^2	1.042	
Final R indices [I>2sigma(I)]	R1 = 0.0742, wR2 = 0.1952	
R indices (all data)	R1 = 0.1143, wR2 = 0.2139	
Largest diff. peak and hole	0.767 and -0.717 e.$Å^{-3}$	