

Supporting Information for:

NMR and EPR Studies of Fe(III) Tetraphenylchlorin Complexes

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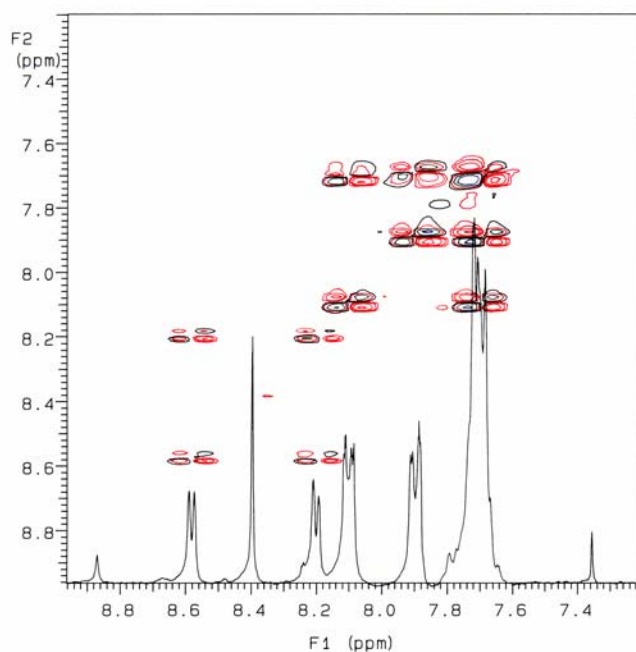


Figure S1. DQF-COSY spectrum of the aromatic region of H₂TPC recorded at 30 °C in CD₂Cl₂, showing the cross peaks between 7,18-H and 8,17-H and between each *o*-H and the overlapping *m,p*-H of the two types of phenyl rings.

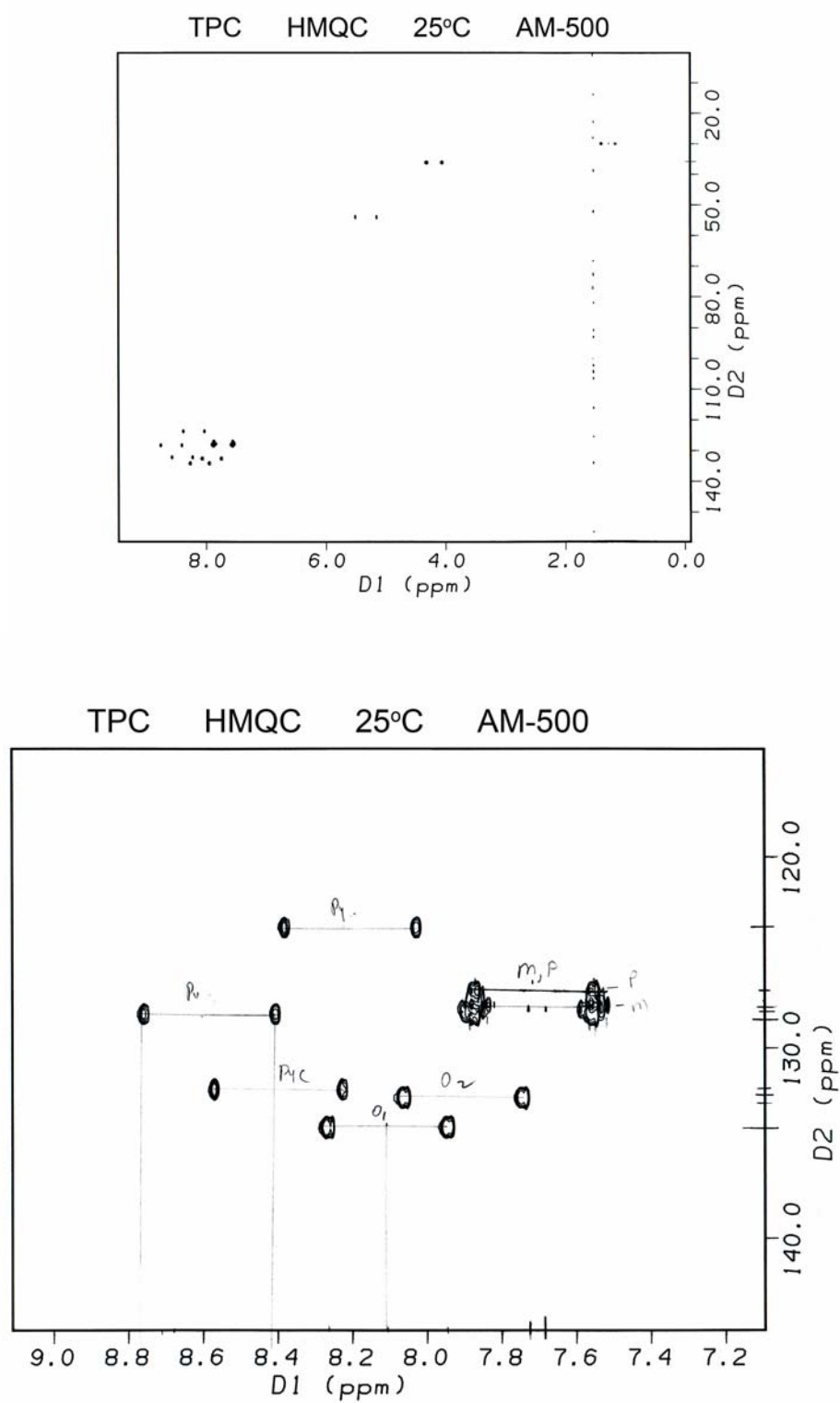


Figure S2. HMQC spectra of H₂TPC

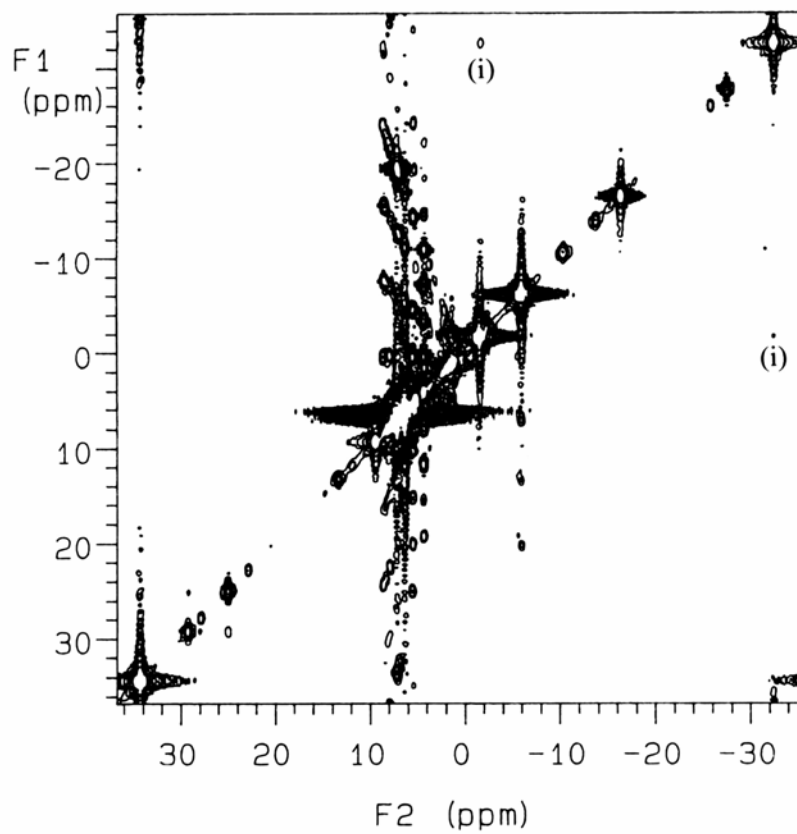


Figure S3. COSY spectrum of $[\text{TPCFE}(\text{Im-}d_4)_2]\text{Cl}$ in CD_2Cl_2 at 30 °C. The cross peaks marked with (i) denote the coupling between pyrrole-7,18 and pyrrole-8,17 protons.

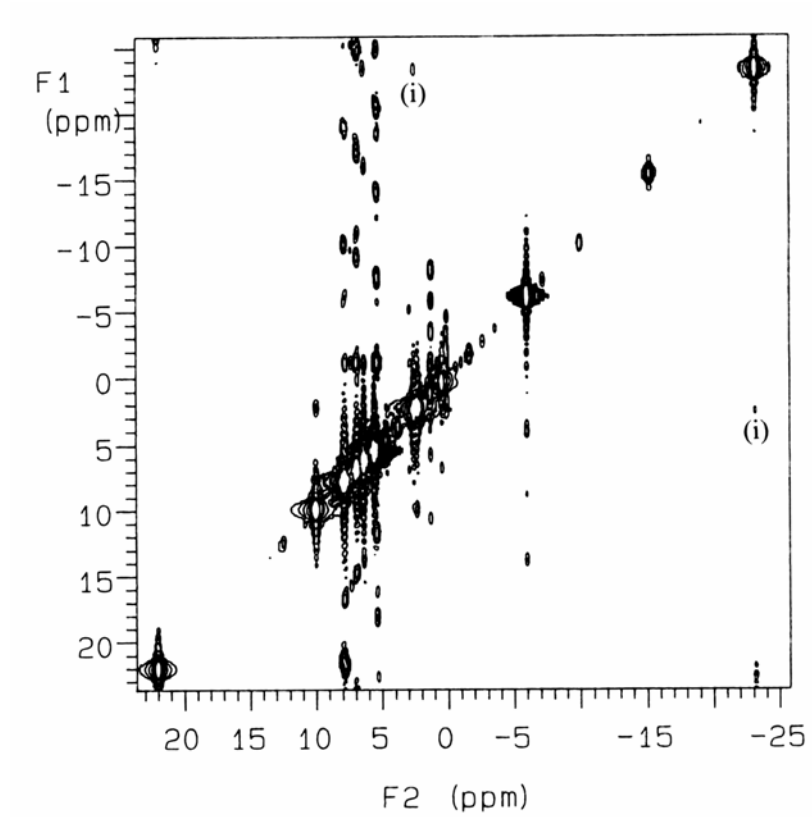


Figure S4. COSY spectrum of $[\text{TPCFE}(\text{2-MeIm})_2]\text{Cl}$ at $0\text{ }^\circ\text{C}$. The cross peaks mark with (i) denote the coupling between pyrrole-7,18 and pyrrole-8,17 protons.

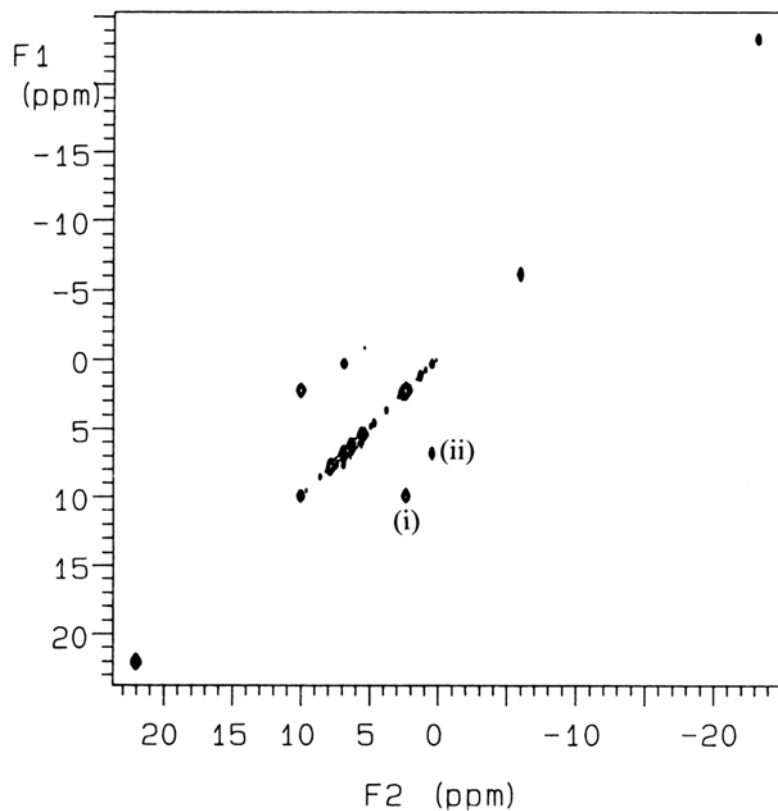


Figure S5. NOESY spectrum of $[\text{TPCFE}(\text{2-MeIm})_2]\text{Cl}$ at $0\text{ }^\circ\text{C}$. All cross peaks arise from chemical exchange between free and bound axial ligands. The cross peak with mark (i) results from the 2-Me group of the axial ligand, the cross peak with (ii) from 4/5-H.

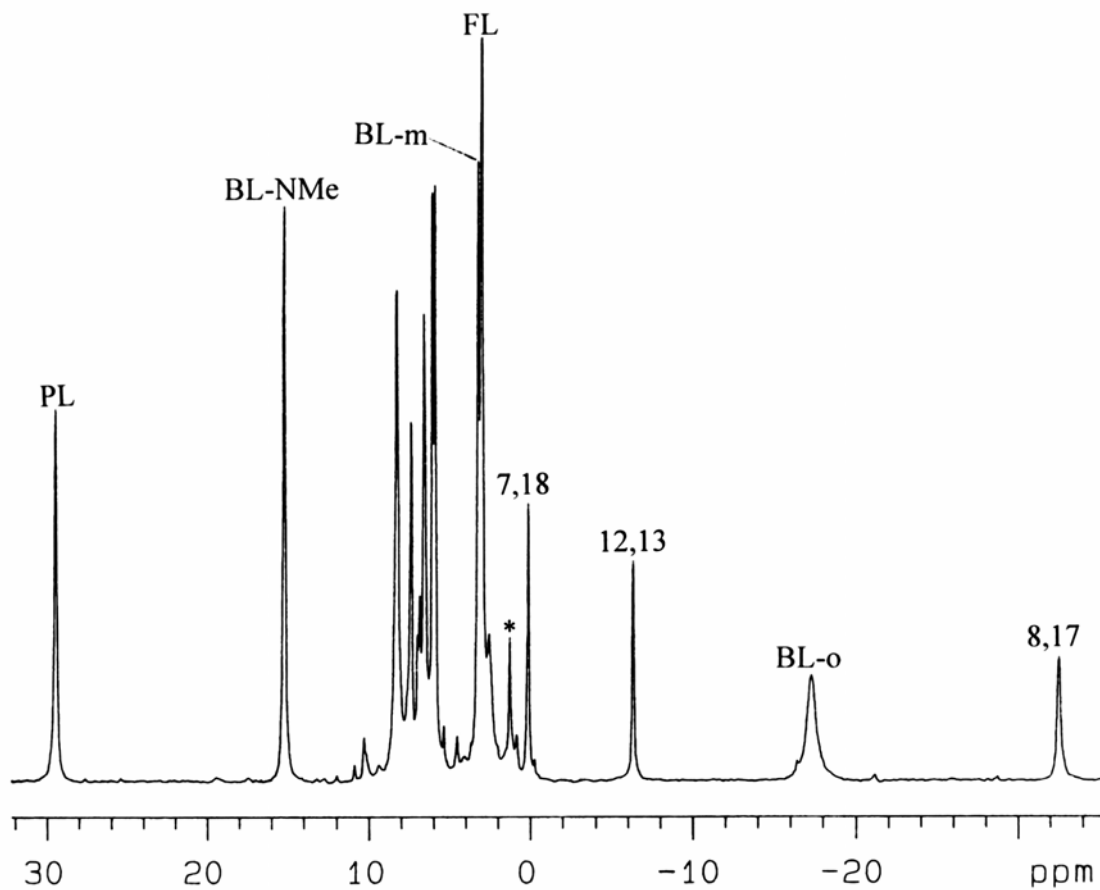


Figure S6. ^1H spectrum of low-spin $[\text{TPCFE}(4\text{-Me}_2\text{NPy})_2]\text{Cl}$ in CD_2Cl_2 at $0\text{ }^\circ\text{C}$. The peak labeled with an asterisk is from an impurity.

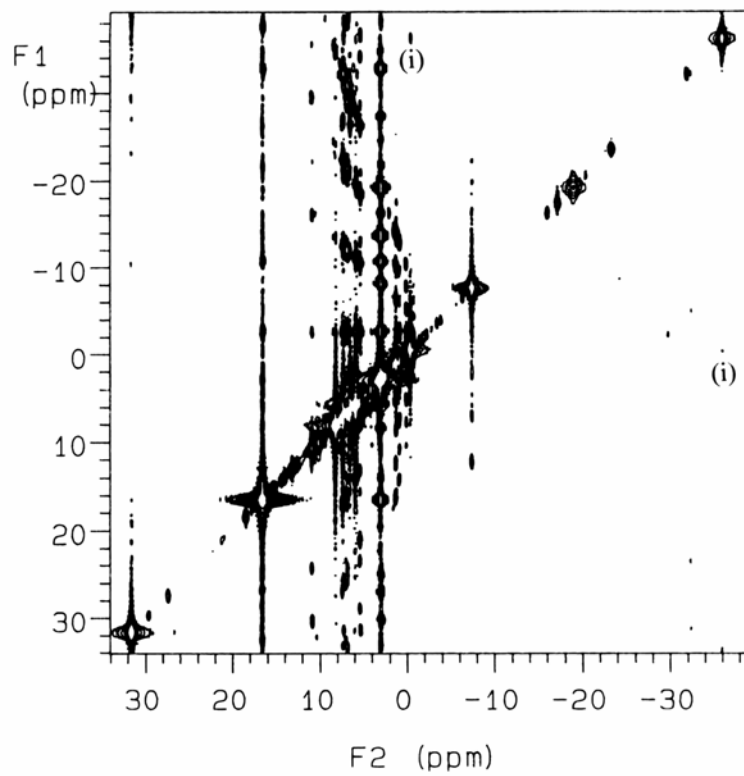


Figure S7. COSY spectrum of $[\text{TPCFE}(4\text{-Me}_2\text{NPy})_2]\text{Cl}$ at $-20\text{ }^\circ\text{C}$. The cross peaks marked with (i) result from the coupling between pyrrole-7,18 and pyrrole-8,17 protons.

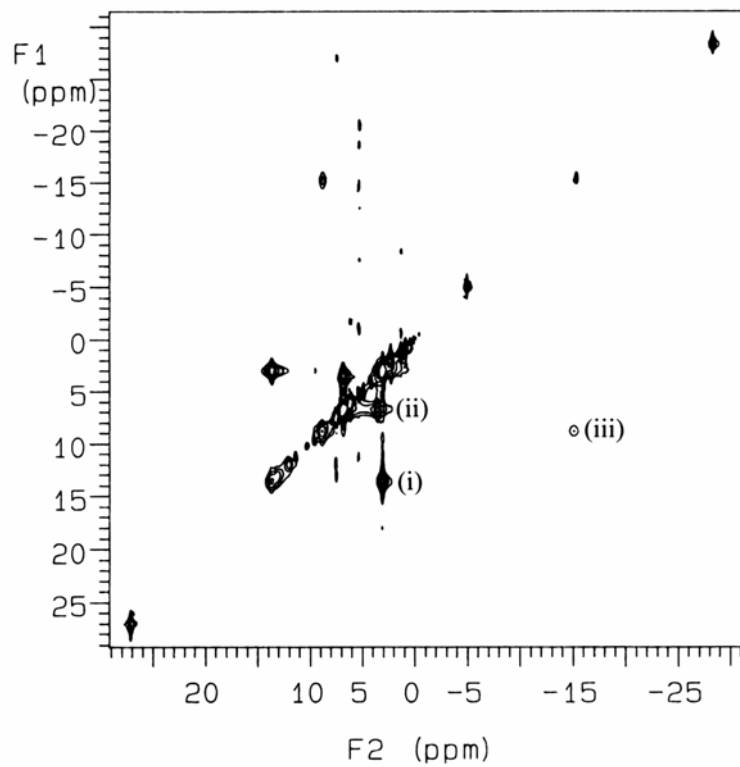


Figure S8. NOESY spectrum of $[\text{TPCFE}(4\text{-Me}_2\text{NPy})_2]\text{Cl}$ at 30 °C. There are three pairs of cross peaks from the chemical exchange between (i) N-Me, (ii) meta, and (iii) ortho protons of the free and bound axial ligands.

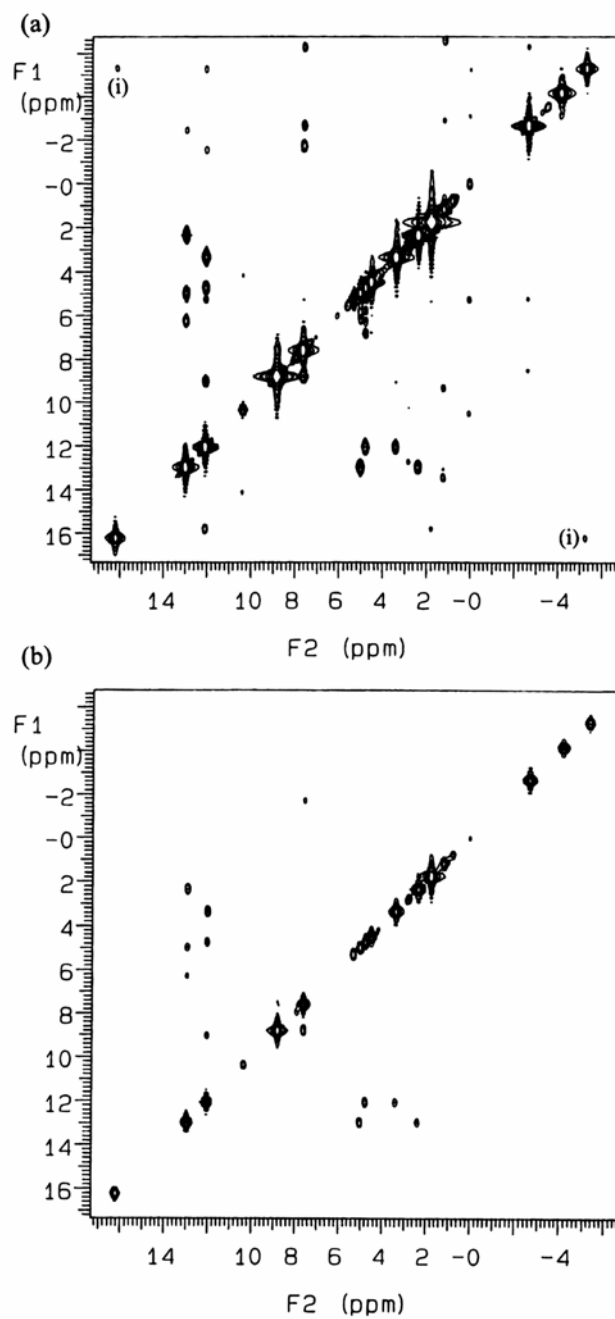


Figure S9. (a) COSY spectrum of $[\text{TPCFE}(\text{Py})_2]\text{Cl}$ at $30\text{ }^\circ\text{C}$. The cross peaks from the coupling between pyrrole-7,18 and pyrrole-8,17 protons (marked (i)) and the cross peaks from the *meso* phenyl groups were observed. (b) The same spectrum with a half vertical intensity. Only four pairs of cross peaks from the *meso* phenyl groups are shown.

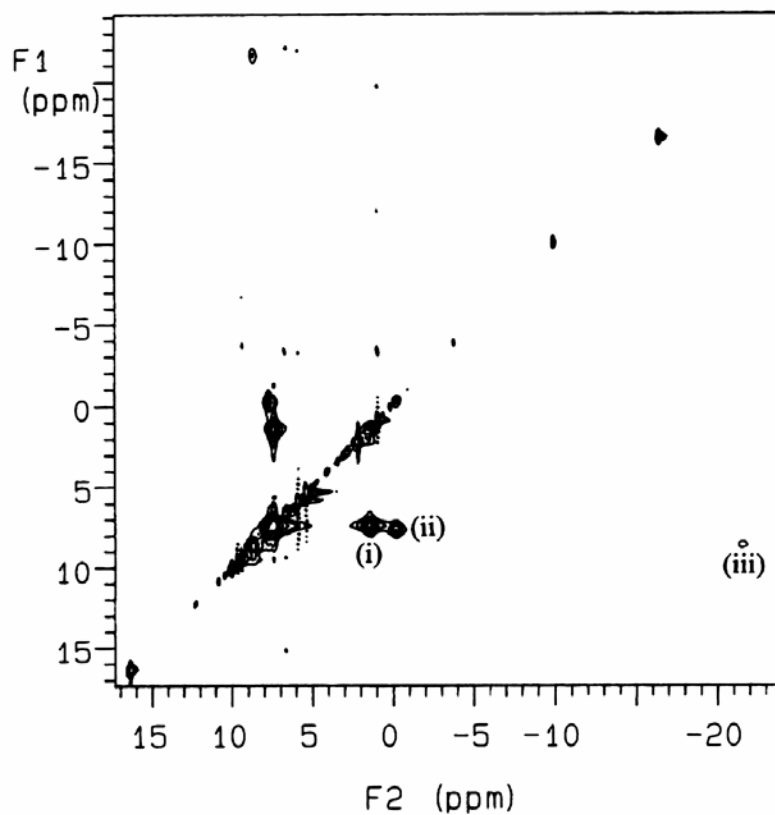


Figure S10. NOESY spectrum of $[\text{TPCFE}(\text{Py})_2]\text{Cl}$ at $30\text{ }^\circ\text{C}$. There are three pairs of cross peaks from the chemical exchange between (i) meta, (ii) para, (iii) ortho protons of the free and bound axial ligands.

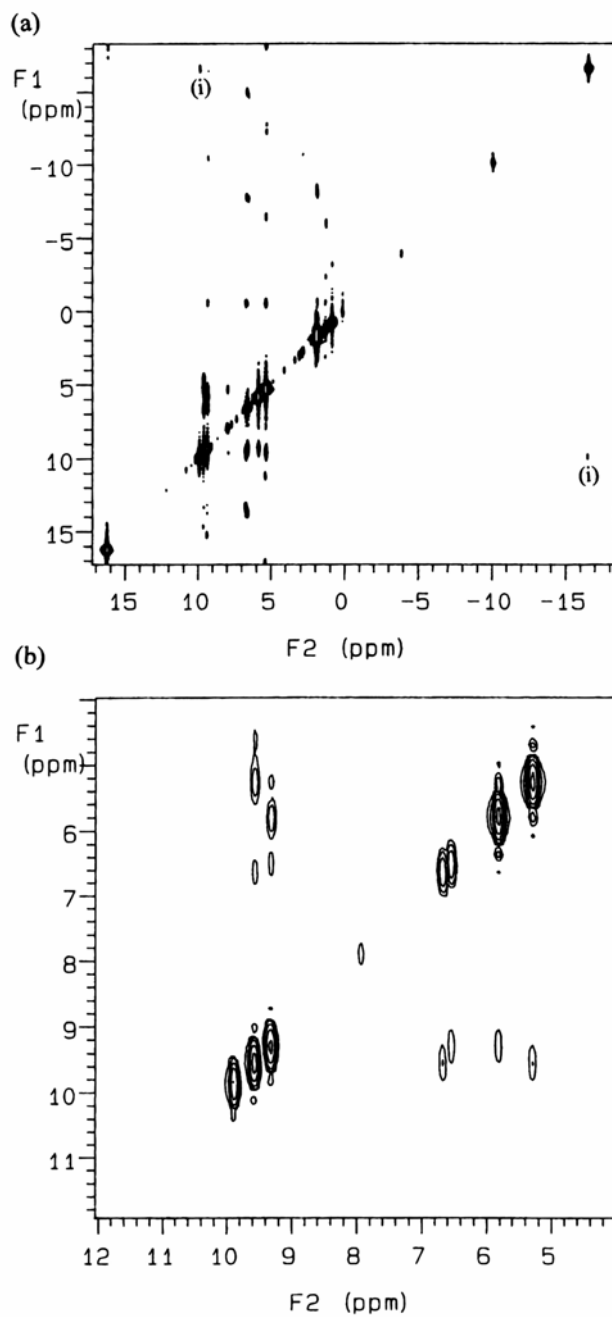


Figure S11. (a) COSY spectrum of $[\text{TPCFE}(4\text{-CNPY})_2]\text{Cl}$ at $-30\text{ }^\circ\text{C}$. The cross peaks from the coupling between pyrrole-7,18 and pyrrole-8,17 protons (marked (i)) and the cross peaks from the *meso* phenyl groups were observed. (b) Expanded region showing the four pairs of cross peaks from the *meso* phenyl groups.

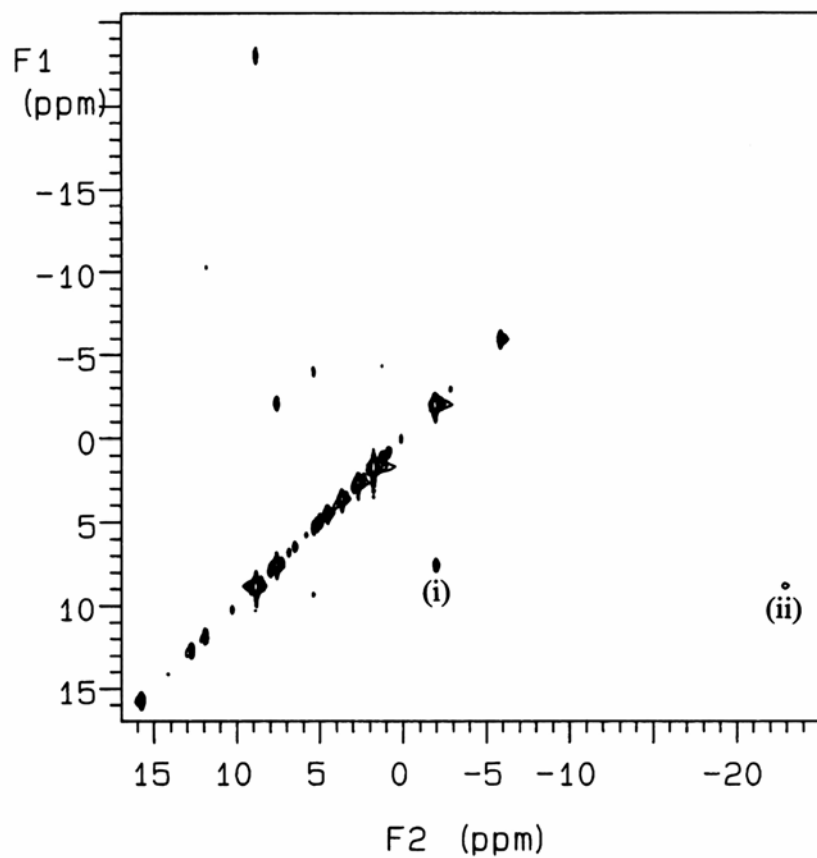


Figure S12. NOESY spectrum of $[\text{TPCFE}(4\text{-CNPy})_2]\text{Cl}$ at $-20\text{ }^\circ\text{C}$. There are two pairs of cross peaks from the chemical exchange between (i) meta and (ii) ortho protons of the free and bound axial ligands.