

Synthesis and Structure of Copper Complexes of a N₆O₄ Macrocyclic Ligand and Catalytic Application in Alcohol Oxidation

Table S1. Decomposition processes in TG-DTA of the complexes 1-3, 5 and 6.

Complex	T range (°C)	Weight loss (%)	Assignment of the released fragment
1	T _i – 200	1.9	solvents
	200 – 430	52.3	Two N(C ₂ H ₄) ₂ and four SO ₃ CF ₃ groups
	430 – 575	33.7	CH ₂ PhO fragments
2	T _i – 150	17.7	solvents
	250 – 450	32.1	Two N(C ₂ H ₄) ₂ and four SO ₃ and CH ₃ groups
	450 – 720	39.6	CH ₂ PhO fragments
3	T _i – 175	19.6	solvents
	210 – 270	34.5	NO ₃ and all CH ₂ fragments
	375 – 548	28.4	PhO fragments
5	T _i – 162	7.1	Solvents
	189 – 375	38.8	Four phenyl groups, two CH ₂ CH ₂ and two C ₄ H ₁₁ N ₃ groups
	375 – 380	9.5	Four CO ₂ groups
	380 – 444	8.6	Four CH ₂ and O- groups of the ligand
	444 – 600	22.9	Four aryl groups of the ligand
6	T _i – 110	6.9	Solvents
	165 – 230	22.4	Two CH ₂ CH ₂ and two C ₄ H ₁₁ N ₃ of the ligand
	230 – 470	23.2	Four O ₂ CMe ligands
	470 – 800	33.1	CH ₂ PhO fragments

^a T_i = initial temperature.

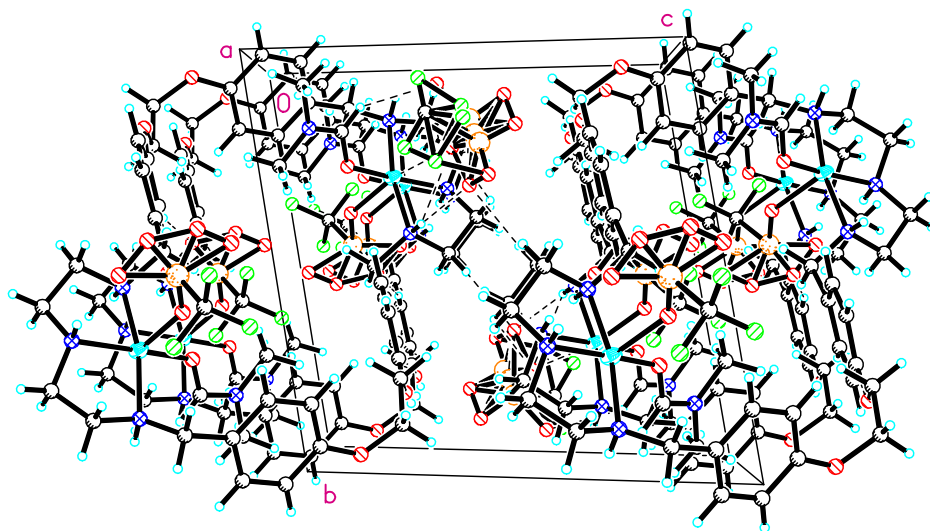


Figure S1-1. A view of the crystal packing of compound 1 along the *a* axis.

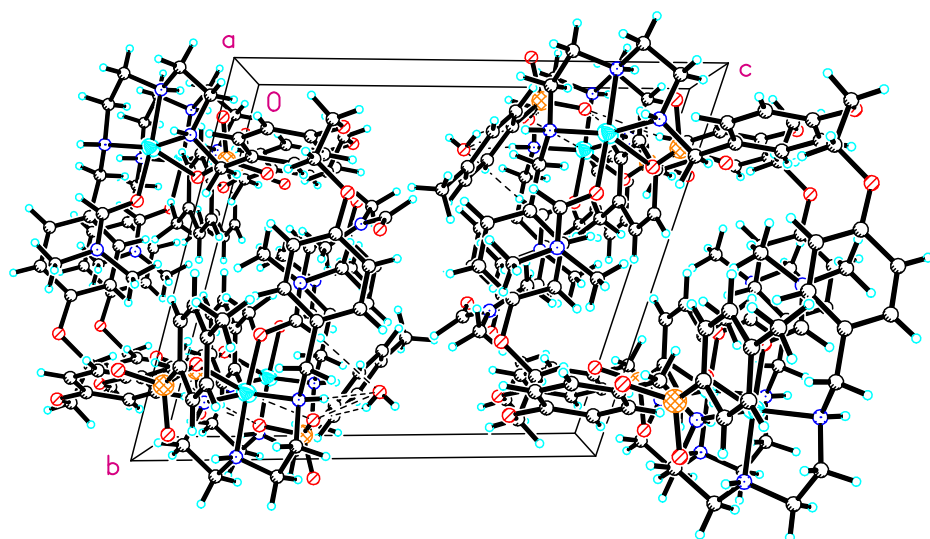


Figure S1-2. A view of the crystal packing of compound 2 along the *a* axis.

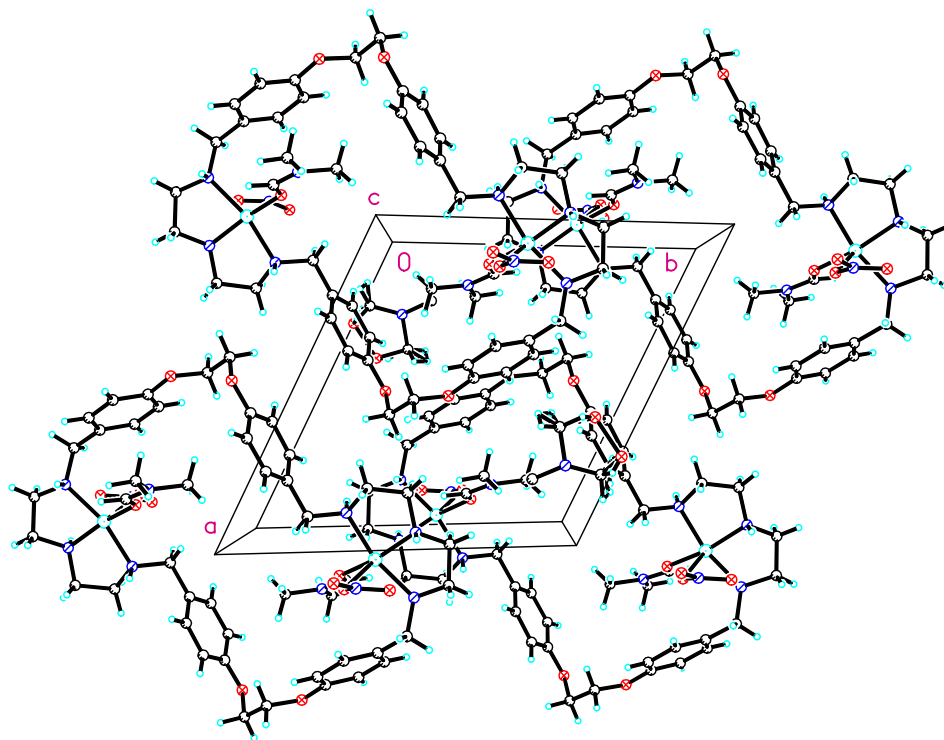


Figure S1-3. A view of the crystal packing of compound **3** along the *c* axis.

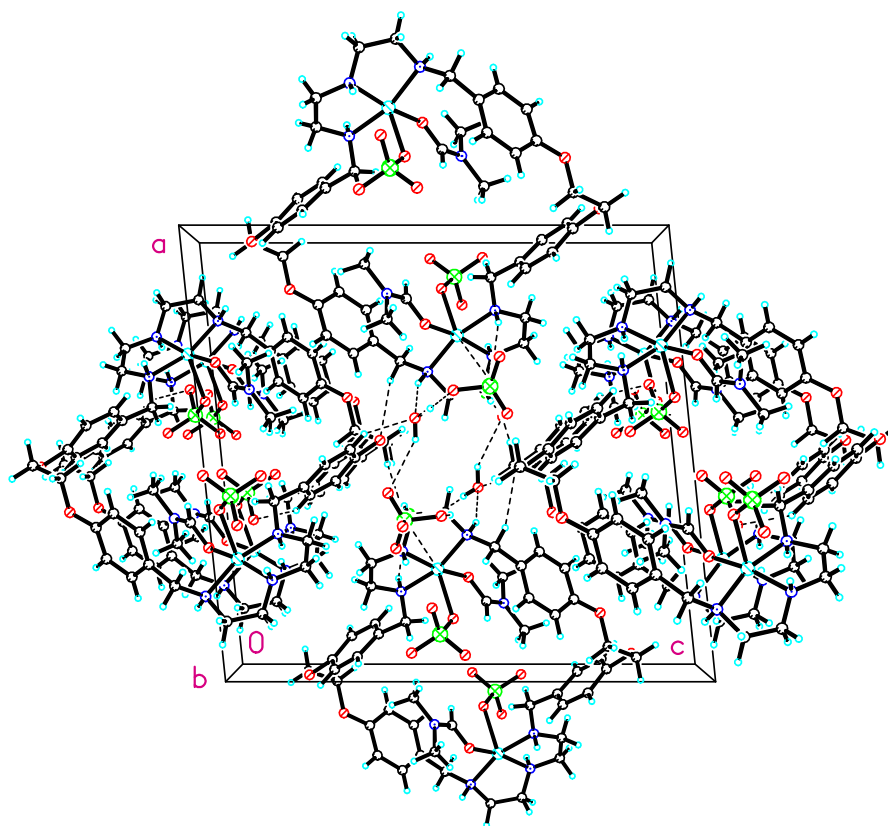


Figure S1-4. A view of the crystal packing of compound **4** along the *a* axis.

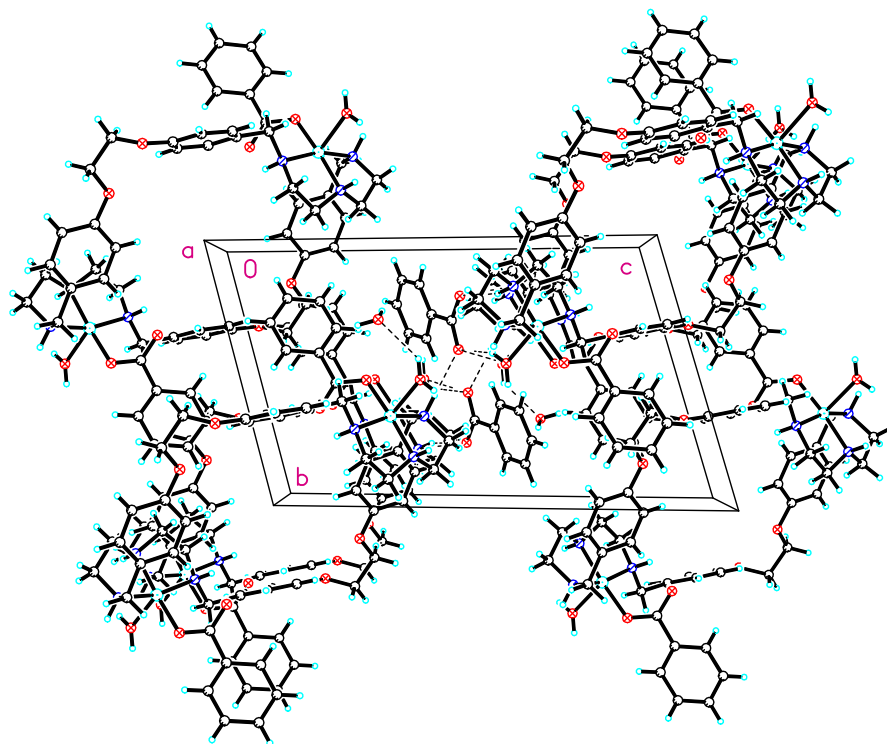


Figure S1-5. A view of the crystal packing of compound 5 along the *a* axis.

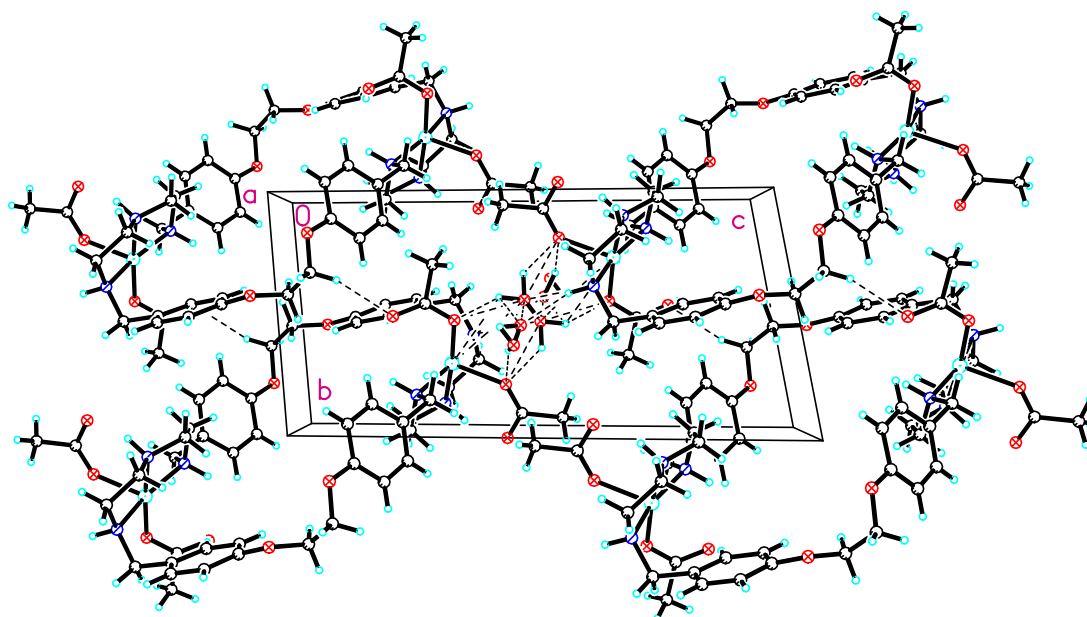


Figure S1-6. A view of the crystal packing of compound 6 along the *a* axis.

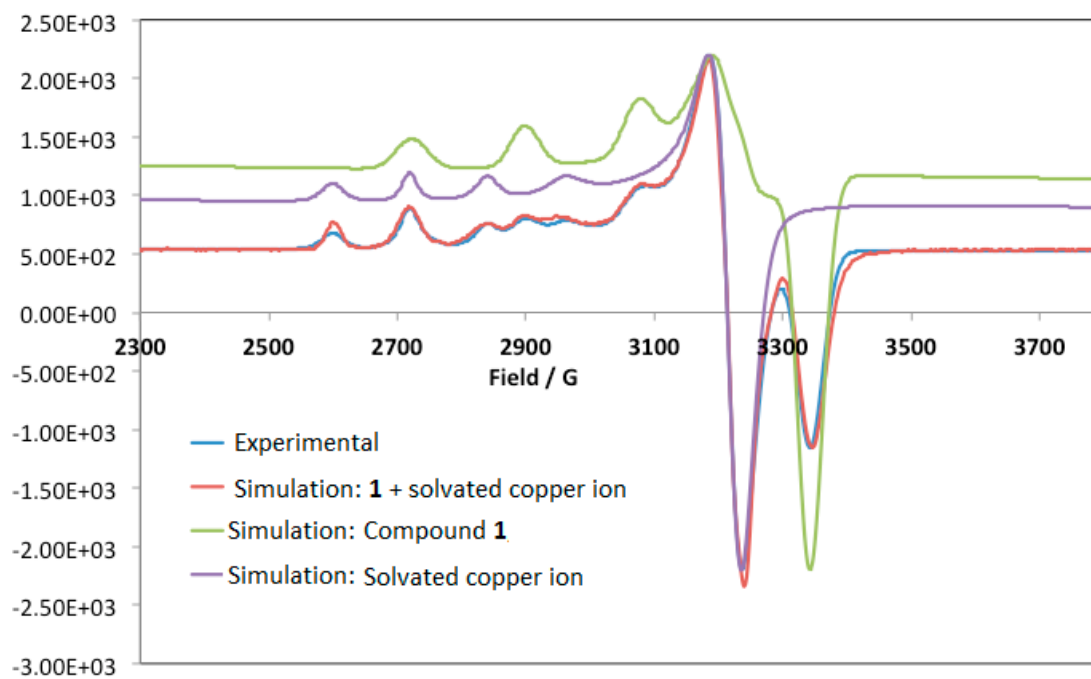


Figure S2-1. Experimental and simulated EPR spectra of a DMF solution of 1.

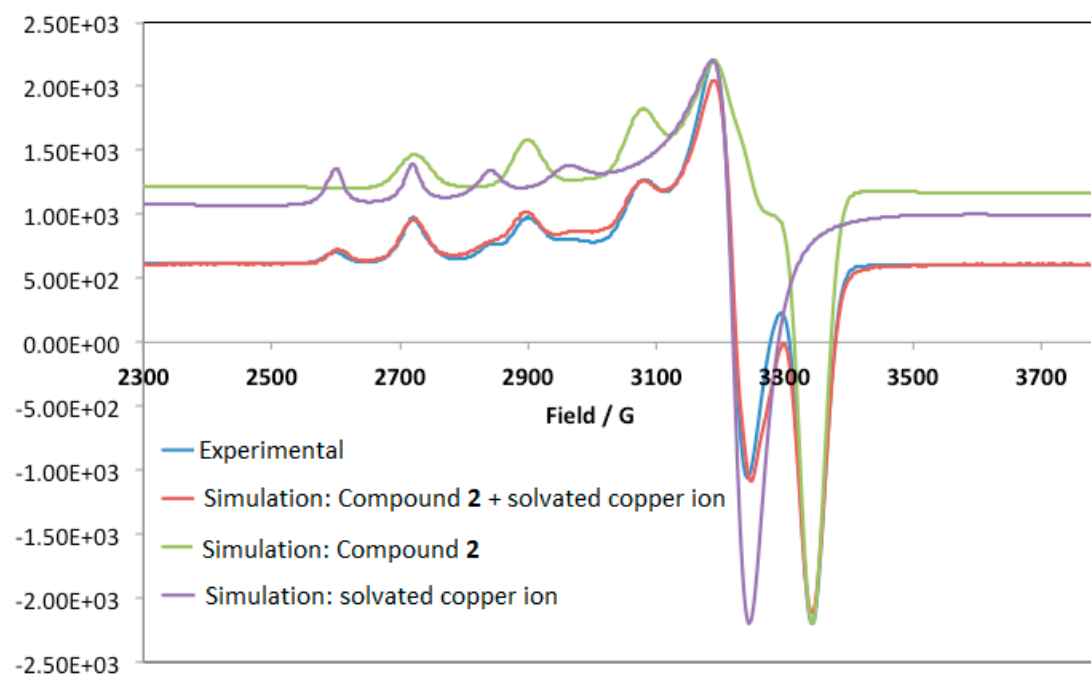


Figure S2-2. Experimental and simulated EPR spectra of a DMF solution of 2.

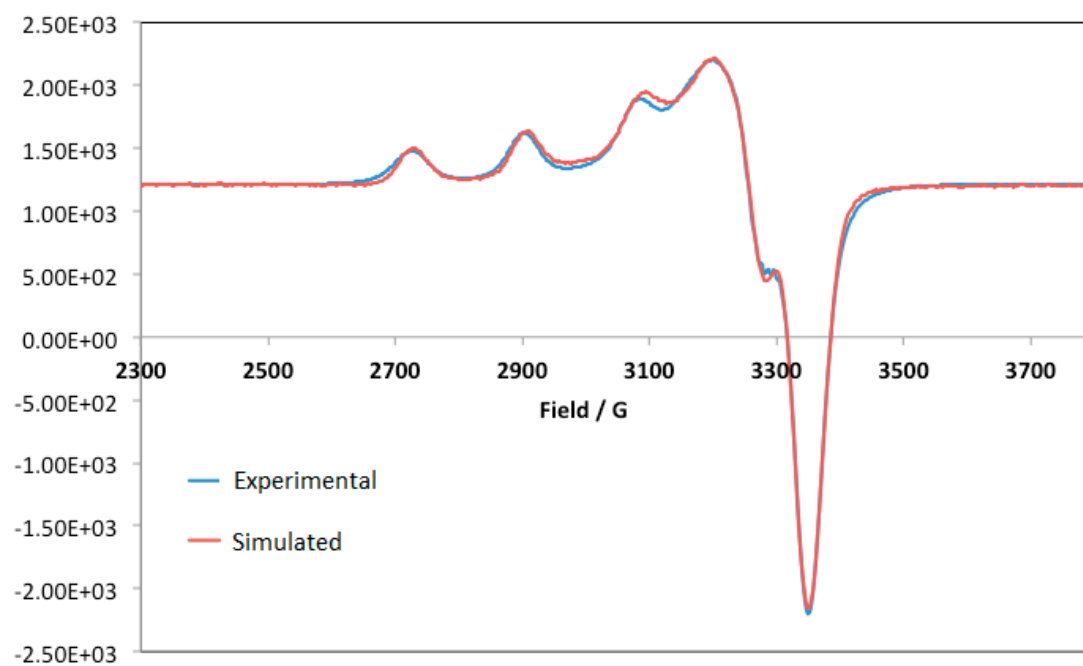


Figure S2-3. Experimental and simulated EPR spectra of a DMF solution of **3**.

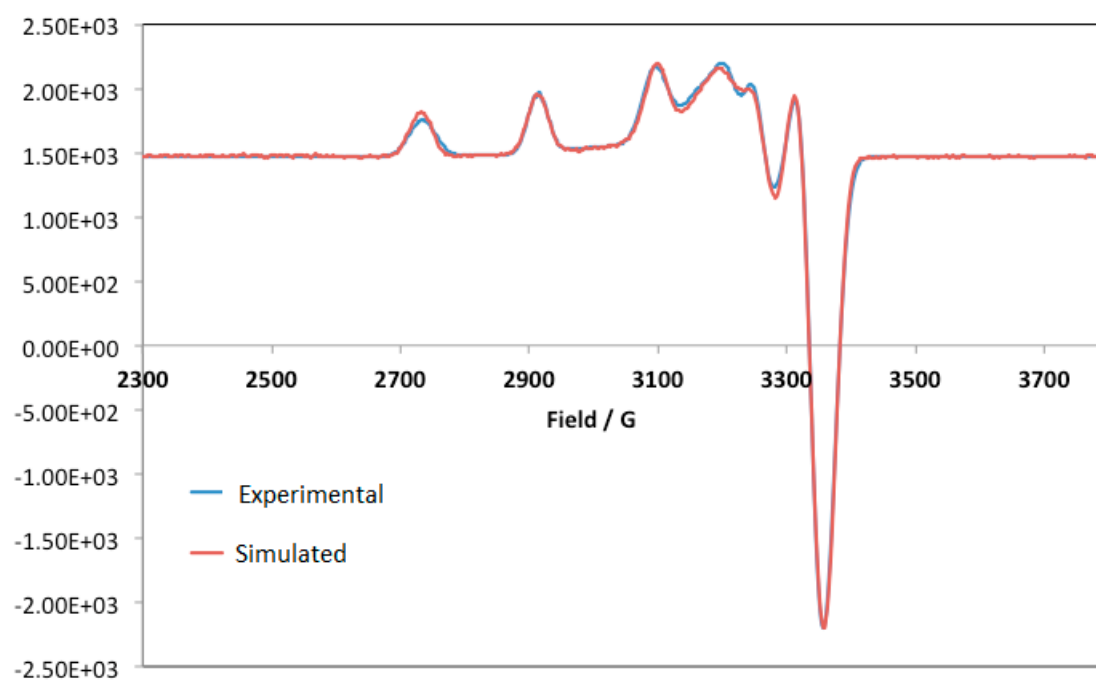


Figure S2-4. Experimental and simulated EPR spectra of a dichloromethane:methanol (0.85:0.15) solution of **5**.

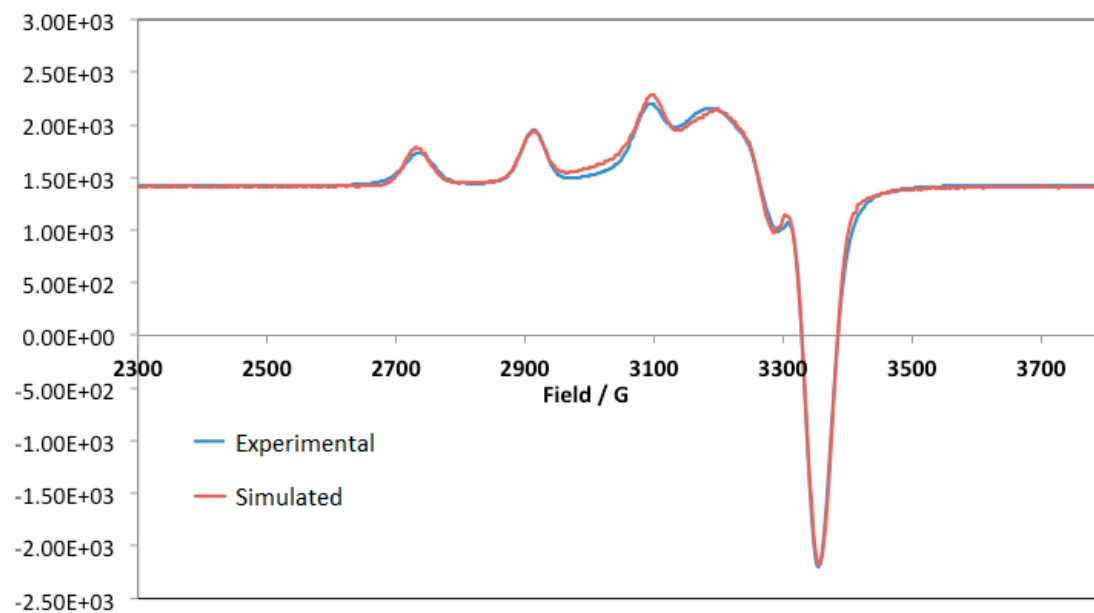


Figure S2-5. Experimental and simulated EPR spectra of a dichloromethane:methanol (0.85:0.15) solution of **6**.

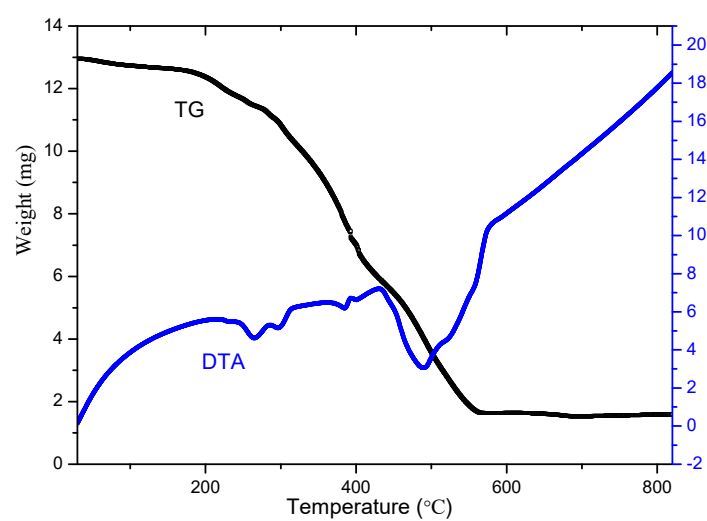


Figure S3-1. TG-DTA curves of compound **1**.

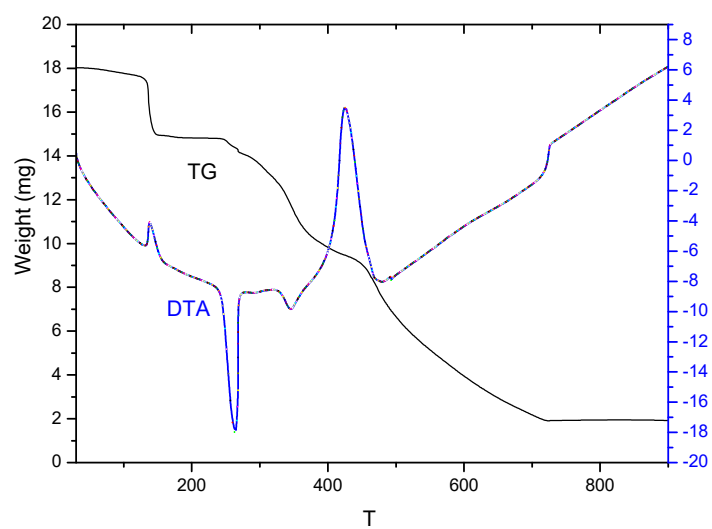


Figure S3-2. TG-DTA curves of compound 2.

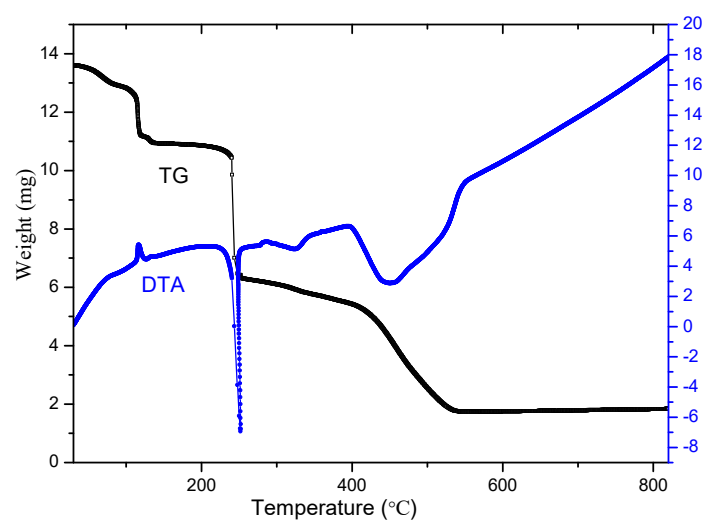


Figure S3-3. TG-DTA curves of compound 3.

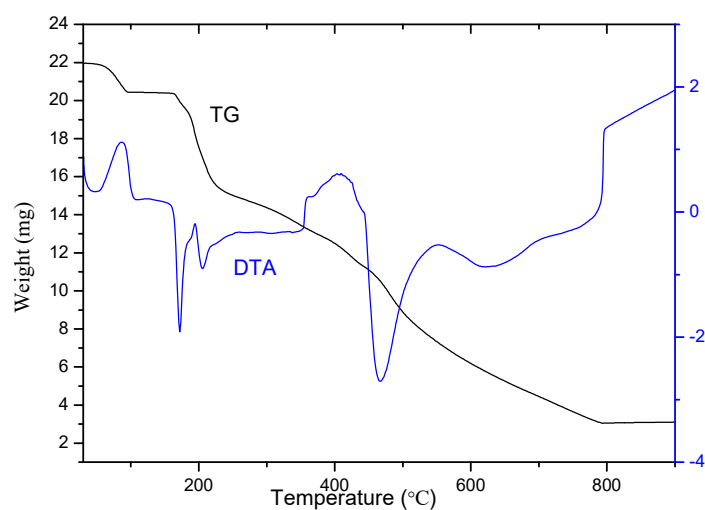


Figure S3-4. TG-DTA curves of compound 5.

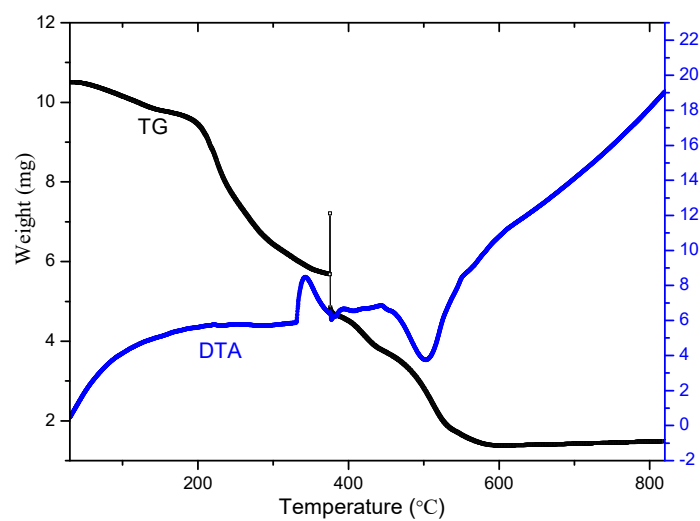


Figure S3-5. TG-DTA curves of compound 6.