Supporting Information

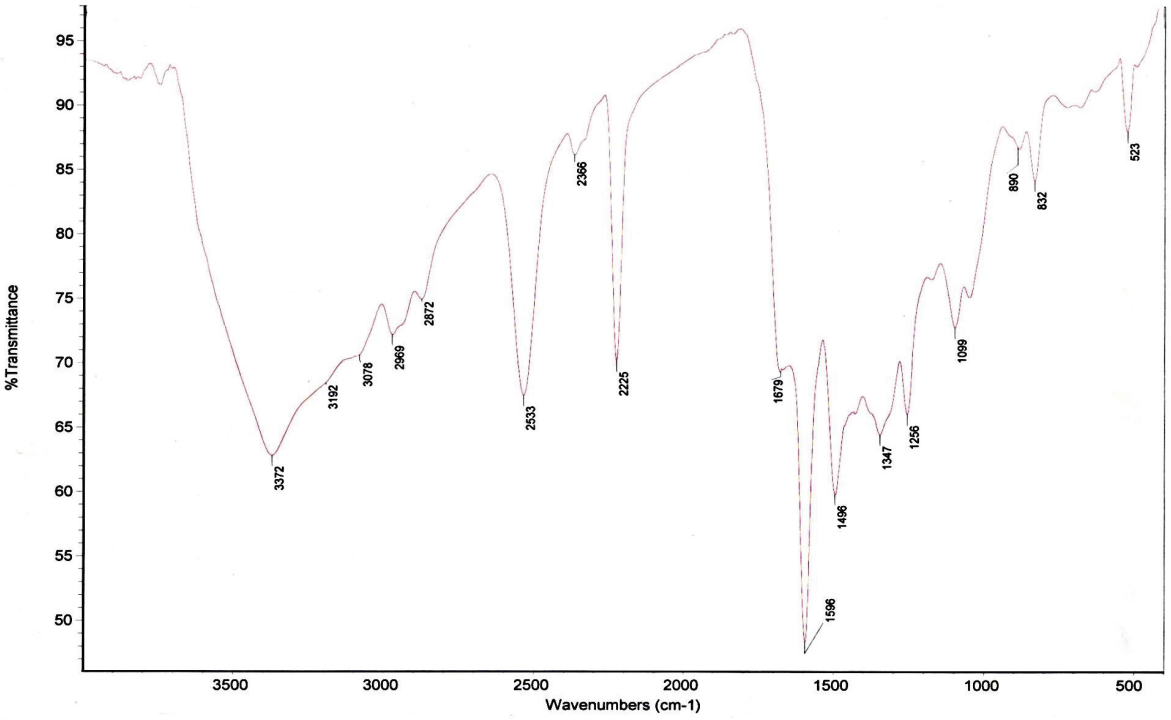


Figure S1 FT-IR Spectrum of **3**.

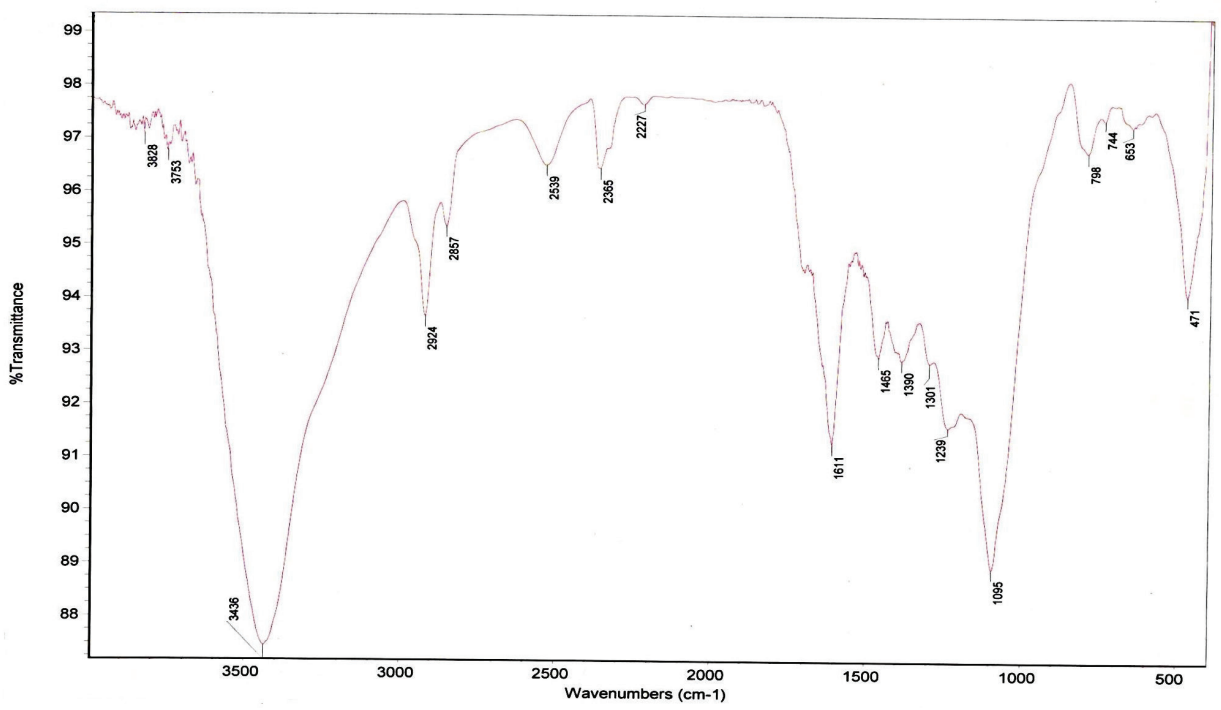


Figure S2 FT-IR Spectrum of **4**.

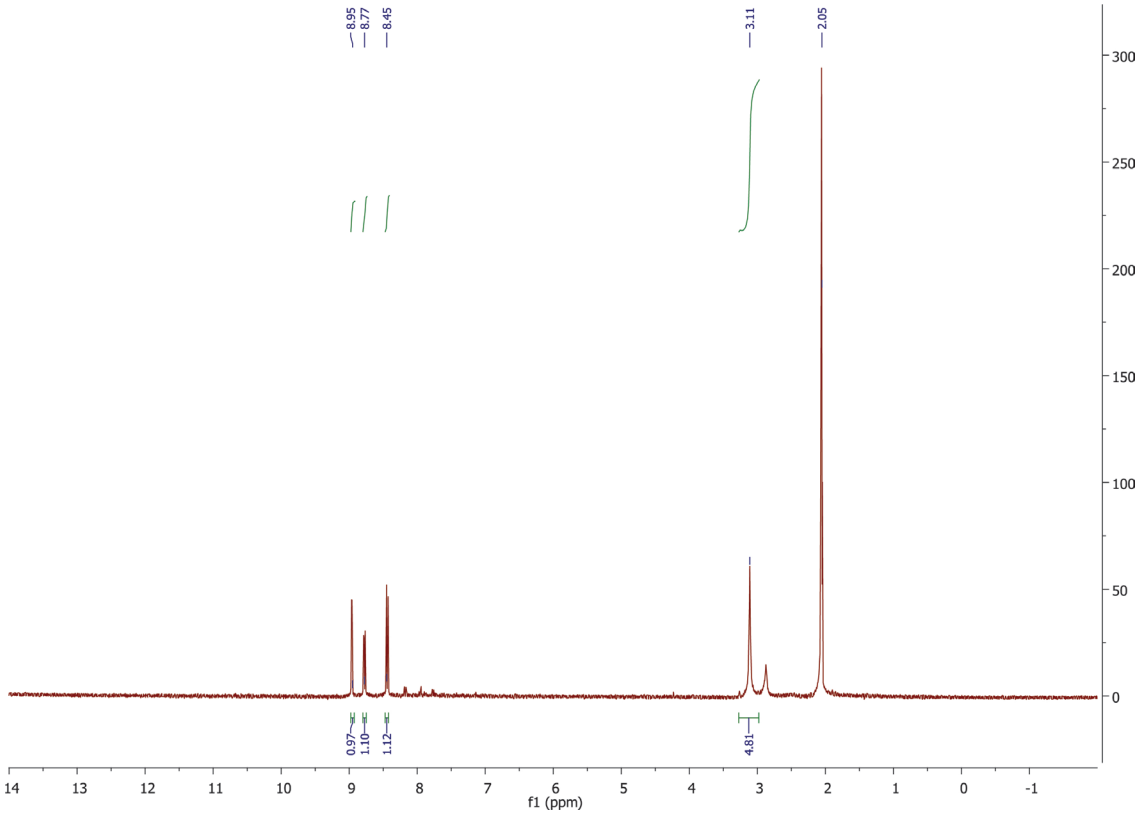


Figure S3 [1] H-NMR of **3** in d_6-acetone.

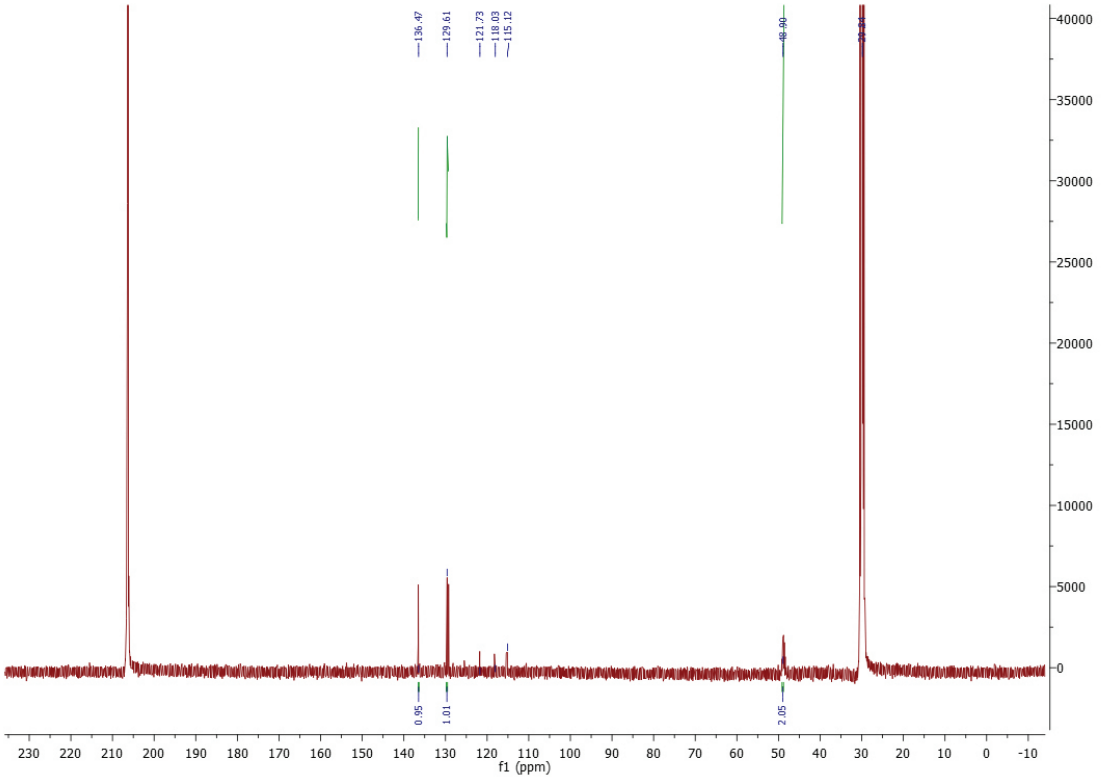


Figure S4 [13] C-NMR of **3** in d_6-acetone.

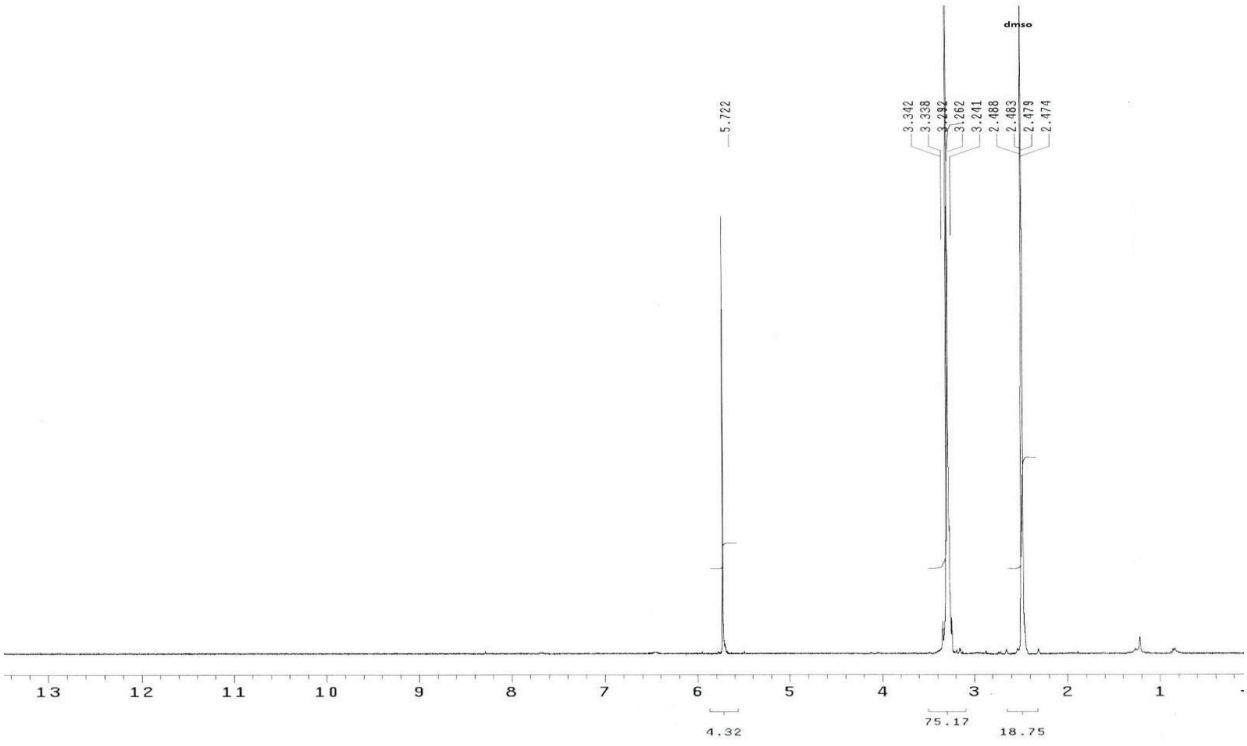


Figure S5 [1] H-NMR of **4** in d_6-DMSO.

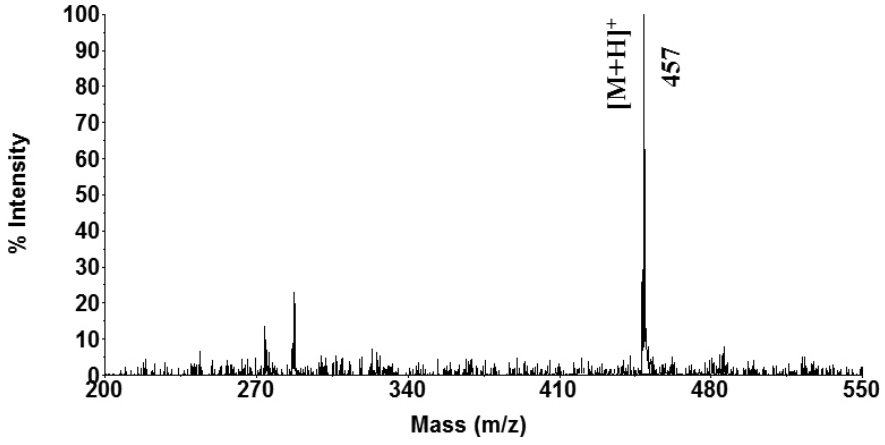


Figure S6 Positive ion and linear mode MALDI mass spectrum of **3** obtained from nitrogen laser (at 337 nm wavelength) ablation of a 2,5-dihydroxybenzoic acid MALDI matrix. Accumulation from 100 laser shots.

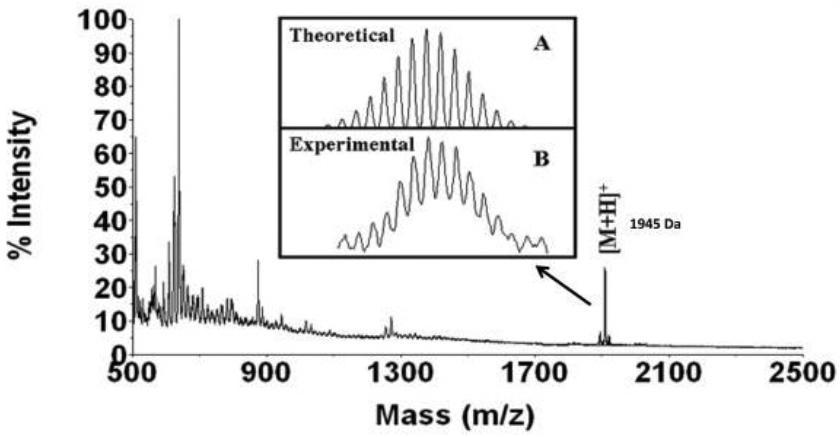


Figure S7 Positive ion MALDI-TOF-MS spectrum of **4** obtained from a Dithranol MALDI matrix using nitrogen laser (at 337 nm wavelength) ablation. Accumulation from 100 laser shots. Inset is an expansion of the molecular ion peak region with the theoretical isotopic pattern.

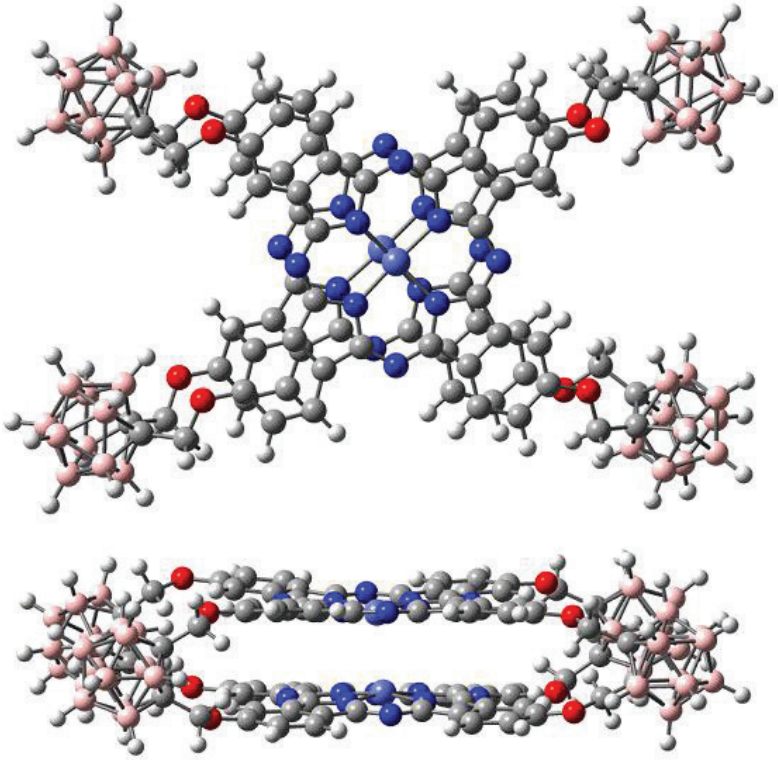
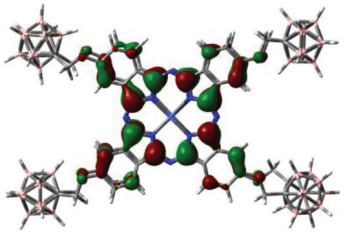
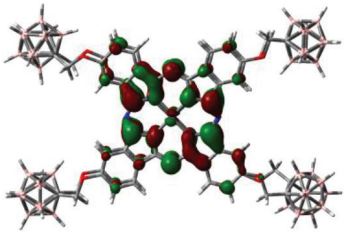
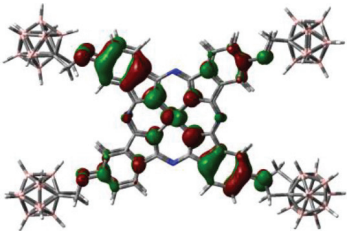
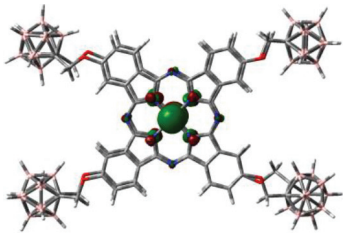
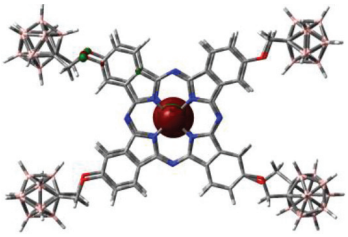
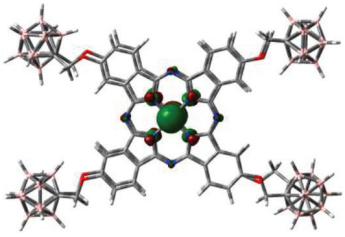
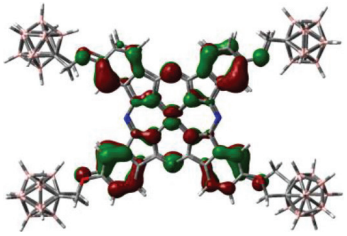
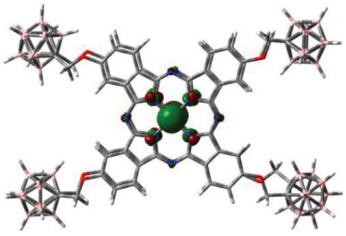
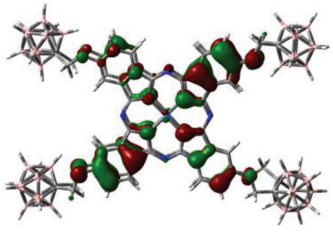
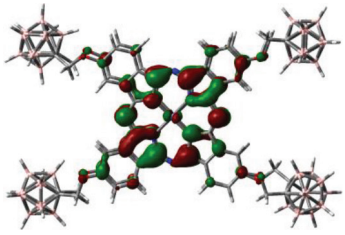


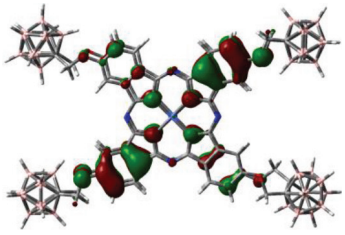
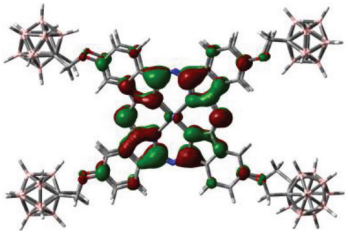
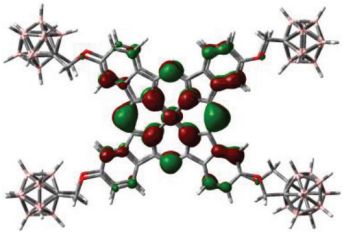
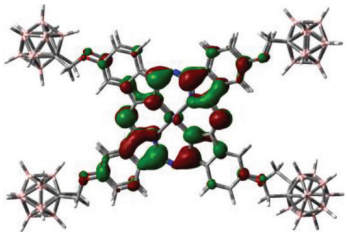
Figure S8 Optimized ground-state structure of **4** (top and side views) at the B3LYP/6-31G(d,p)/LANL2DZ level of theory in DMSO.

Table S1 Selected excitation wavelengths (λex), oscillator strengths (f), molecular orbitals and excitation characters of compound **4** in DMSO calculated at B3LYP/6-31G**/LANL2DZ level

	λex (nm) (f)	Orbitals		Character
S_{12}	680.1 (1.376)			LE1
		HOMO-1	LUMO+1	
S_{18}	616.5 (0.284)			LMCT, LE2
		HOMO-2	LUMO	
S_{20}	572.3 (0.204)			LE2
		HOMO-5	LUMO	
S_{31}	499.3 (0.007)			LMCT, LE2
		HOMO-10	LUMO	
S_{77}	395.8 (0.510)			LE1, ICT1
		HOMO-11	LUMO+2	

(*Continued*)

Table S1 Continued

	λex (nm) (f)	Orbitals		Character
S_{88}	381.0 (0.341)			LE1, ICT1
		HOMO-6	LUMO+4	
S_{91}	376.0 (0.008)			LE1, LE2
		HOMO-12	LUMO+2	

LE1: local excitation of Pc; LE2: local excitation of Co; ICT1: intramolecular charge transfer from oxygen atom to Pc; LMCT: metal-to-ligand charge transfer.