Supplementary Material (ESI) for Dalton Transactions

Electronic supplementary information (ESI)

(8 pages)

Intermediate (S=1) spin state in five-coordinate cobalt(III) : Magnetic properties of N-*o*-hydroxy-benzamido-*meso*-tetraphenylporphyrin cobalt(III), Co(N-NCO(*o*-O)C_6H_4-tpp)

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Contents

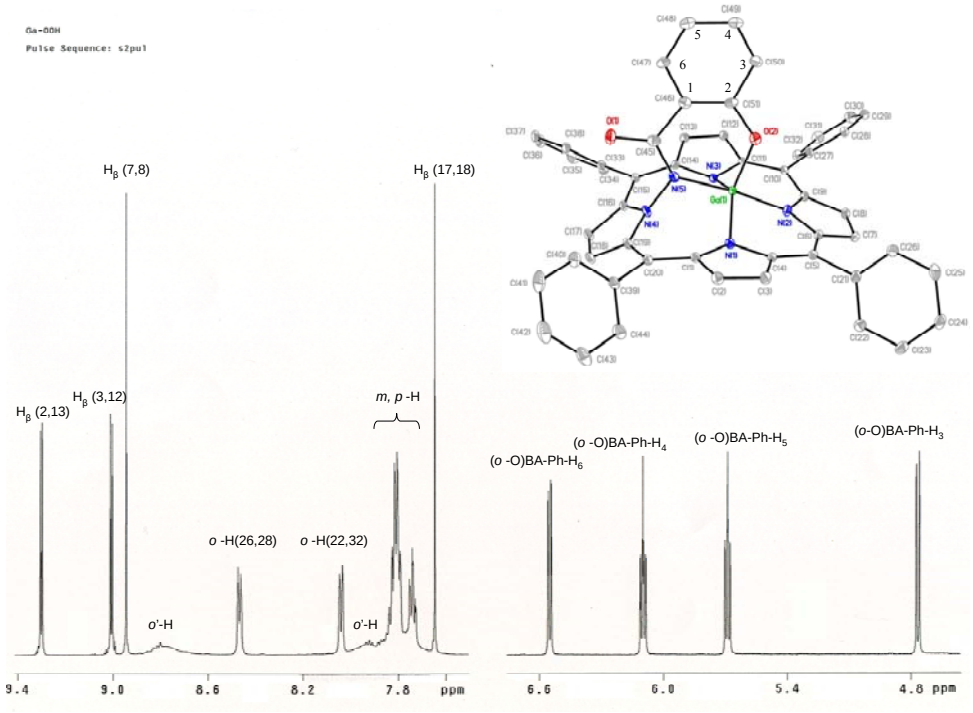


Figure S1(a) 20°C

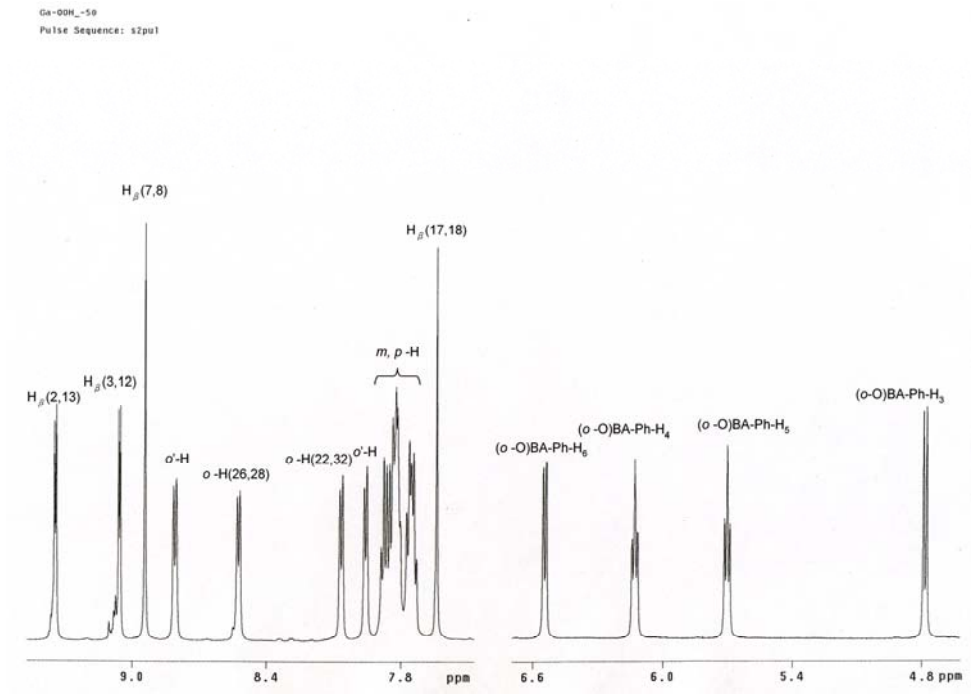
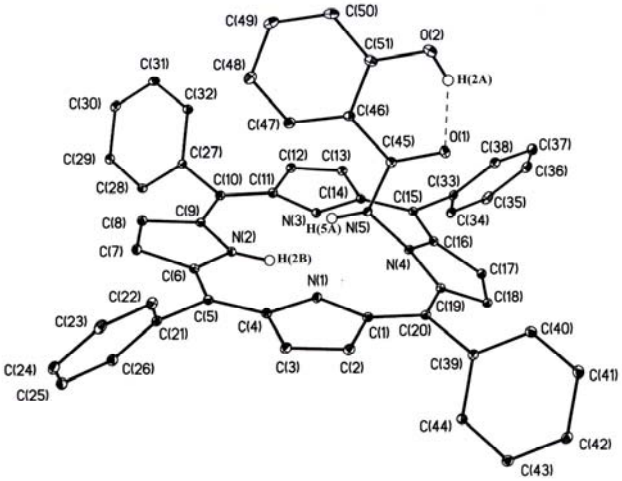


Figure S1(b) -50°C

Figure S1. ^{1}H NMR spectra for **3** at 599.95 MHz in $CDCl_3$ showing four different β-pyrrole protons H_β, phenyl protons (*o*-H, *m*, *p*-H) and (*o*-O)BA-Ph protons: (a) 20°C and (b) -50°C.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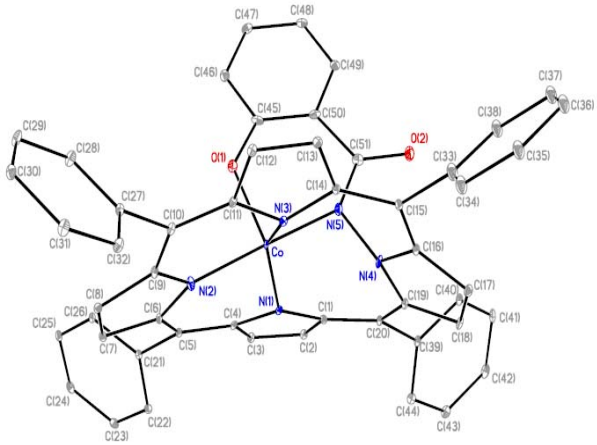
(a) **1**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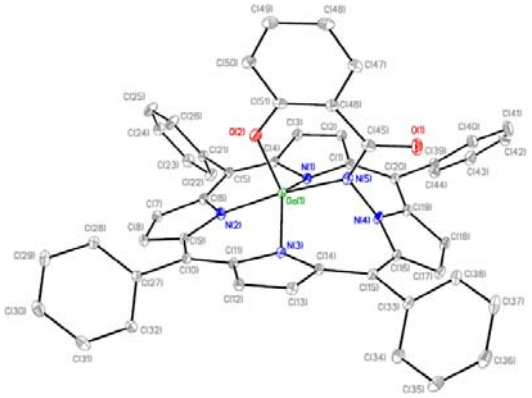
C(23)

(b) **2**



(c) **3**

Figure S2. Molecular configuration and atom-labeling scheme for (a) **1** and (b) Co(N-NCO((*o*-O)C_6H_4-tpp)) (**2)** and (c) [Ga(N-NCO(*o*-O)C_6H_4-tpp) ·0.5$CHCl_3$·MeOH; **3**·0.5$CHCl_3$·MeOH], with 30% thermal ellipsoids. Hydrogen atoms, solvent $CHCl_3$ and MeOH for **3**·0.5$CHCl_3$·MeOH are omitted for clarity.

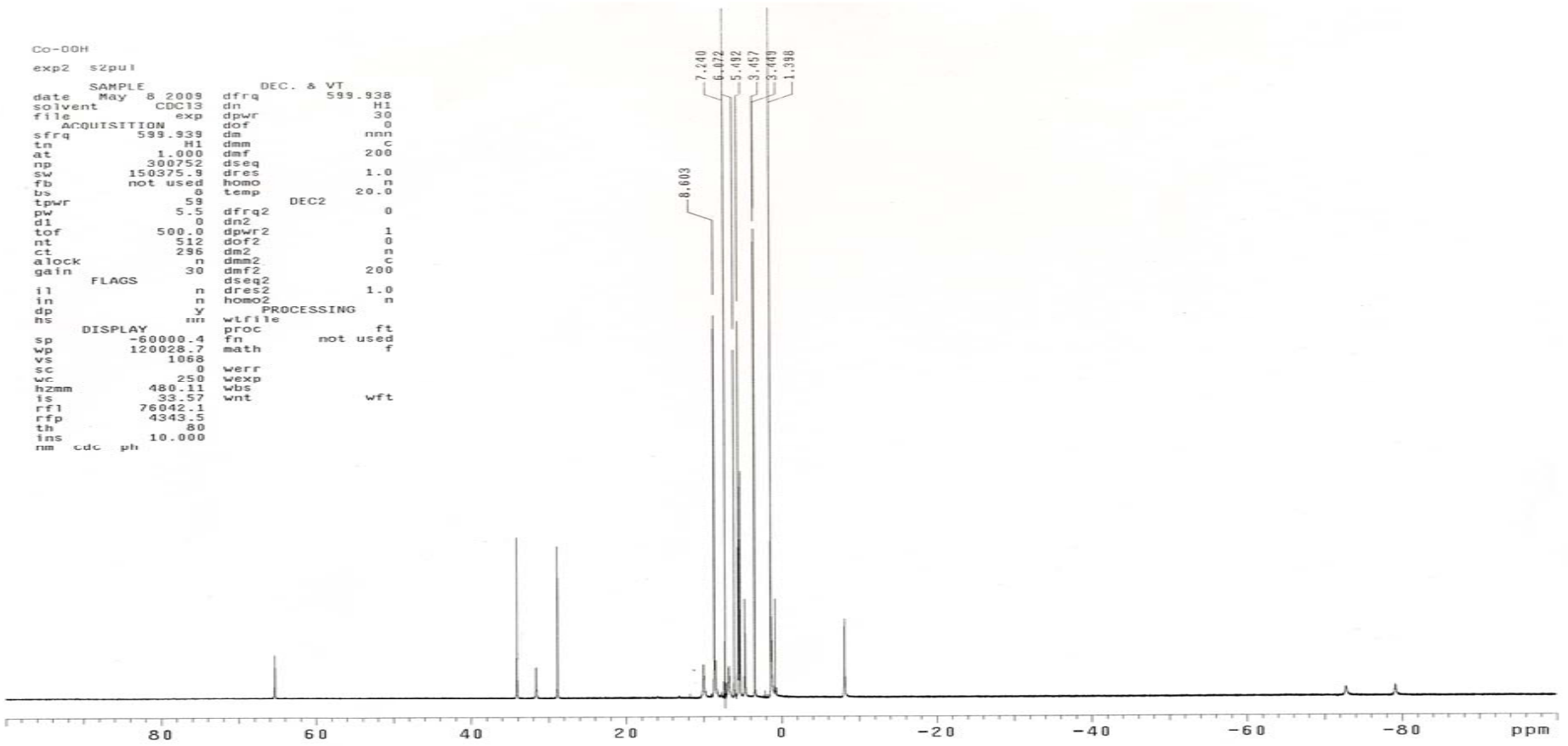
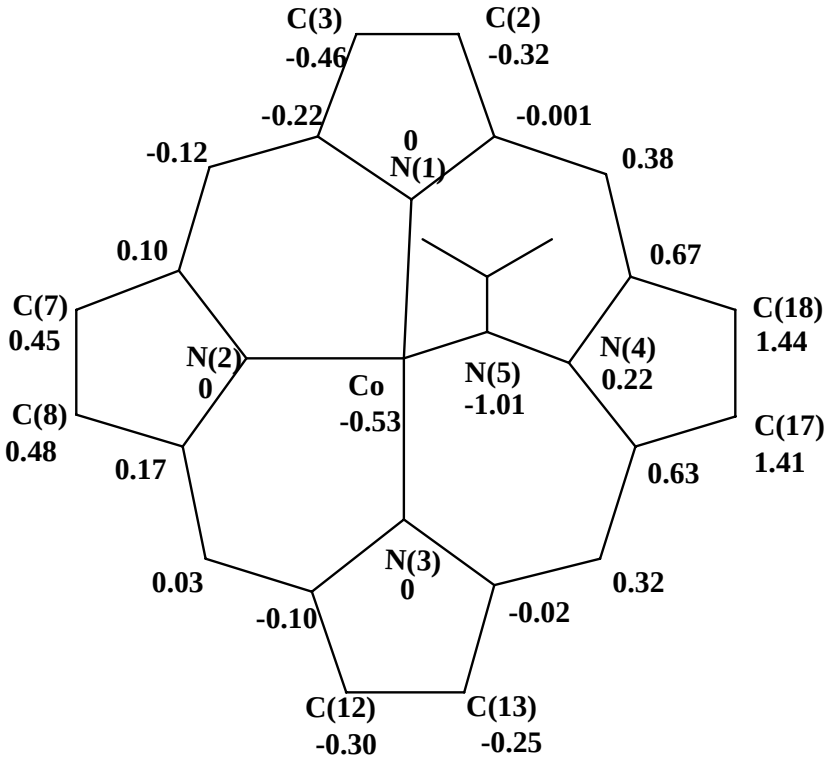
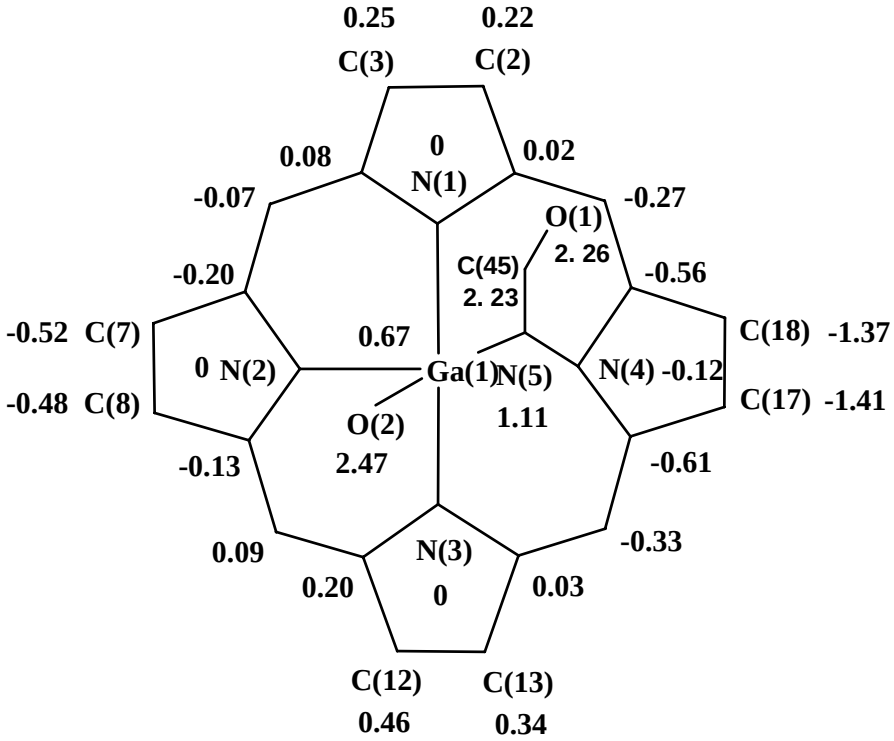


Figure S3. ^{1}H NMR spectra for **2** at 599.95 MHz at 20°C in $CDCl_3$.



(a) **2**



(b) **3**

Figure S4. Diagram of the porphyrinato core ($C_{20}N_4$, M, and BA) of (a) compound **2** and (b) compound **3**. The values represent the displacement (in angstroms) of the atoms from the mean 3N plane [i.e. N(1)-N(3) for **2** and **3**].

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