

## Supplementary Materials

### Structure, DFT Calculations and Magnetic Characterization of Coordination Polymers of Bridged Dicyanamido-metal(II) Complexes

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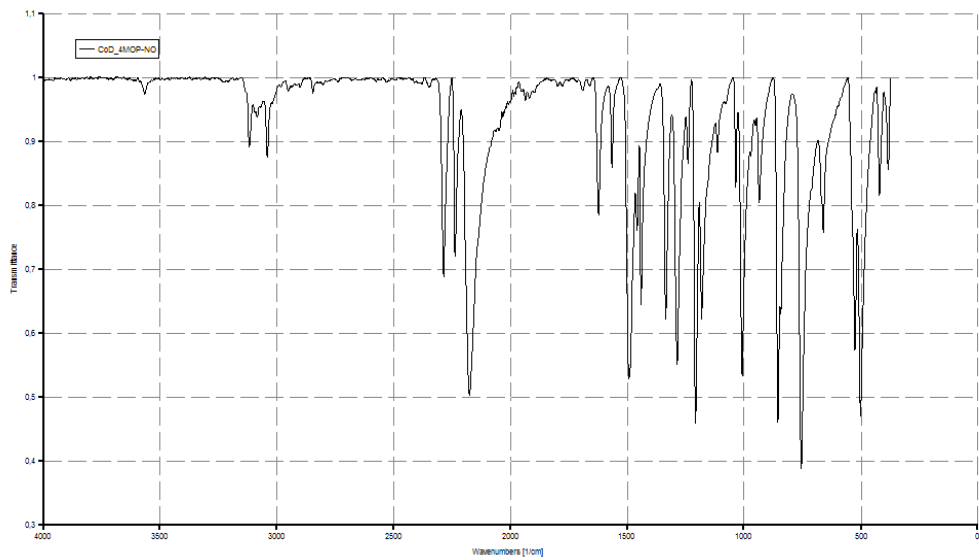
**Fig. S1 - S4.** IR spectra of **1** – **4** compounds, respectively..

**Fig. S5 - S7.** UV-VIS-NIR spectra of **1**, **2** and **4** compounds, respectively.

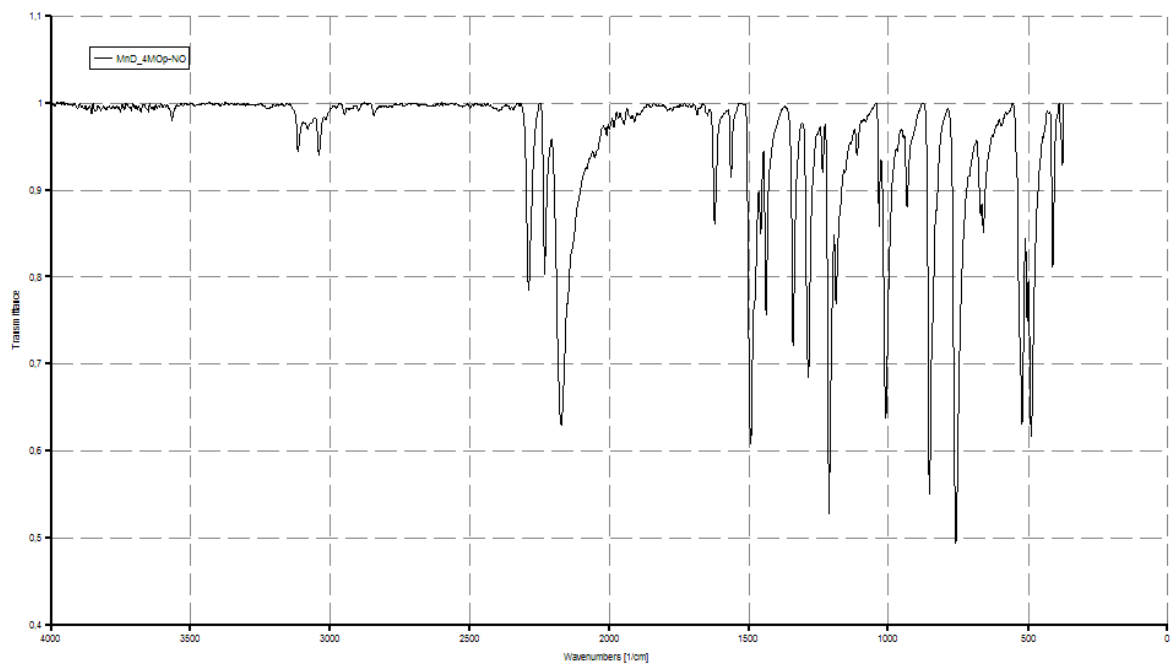
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**Table S1.** The ground state minimum energy of Co(II) or Mn(II) centers of **1** and **2**, respectively in their high-spin and low-spin configurations.

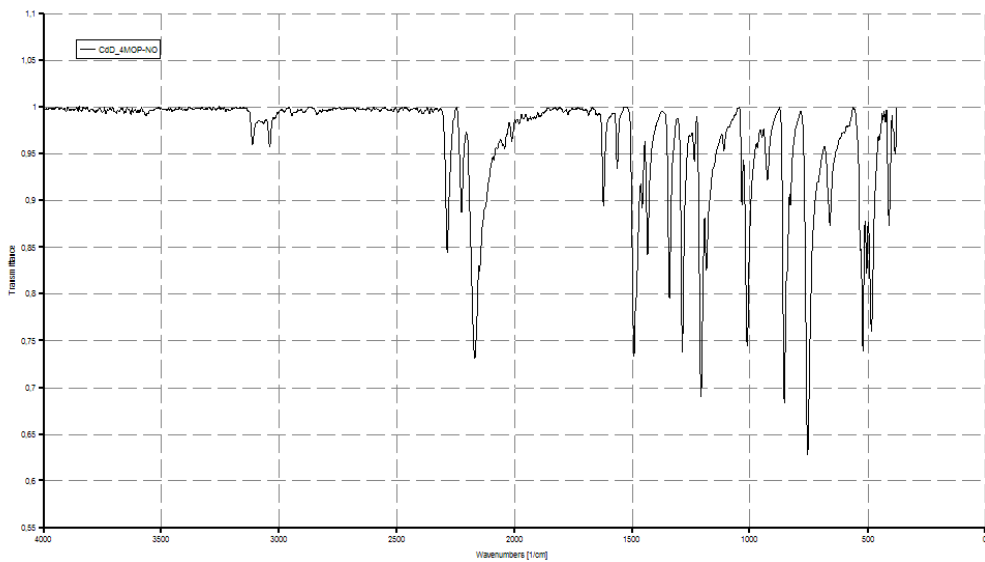
Spin Multiplicity	Absolute Energy / Hartree
Co(II) – quartet ( <b>1</b> )	-2975.5856
Co(II) - singlet	-2975.4610
Mn(II) – sextet ( <b>2</b> )	-2893.3463
Mn(II) - singlet	-2893.2149



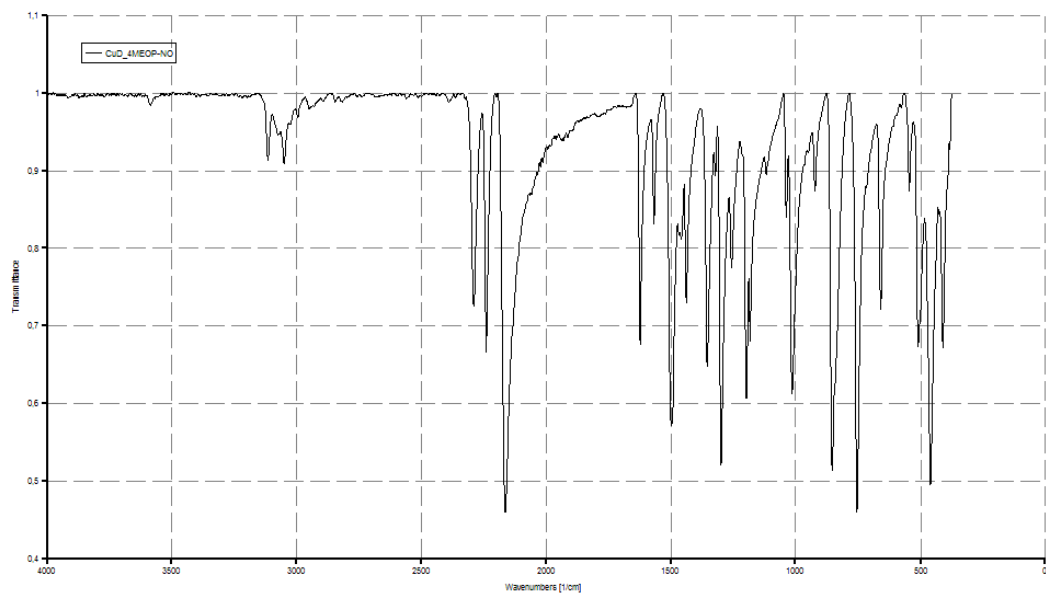
**Figure S1.** IR spectrum of *catena*-[Co( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**1**)



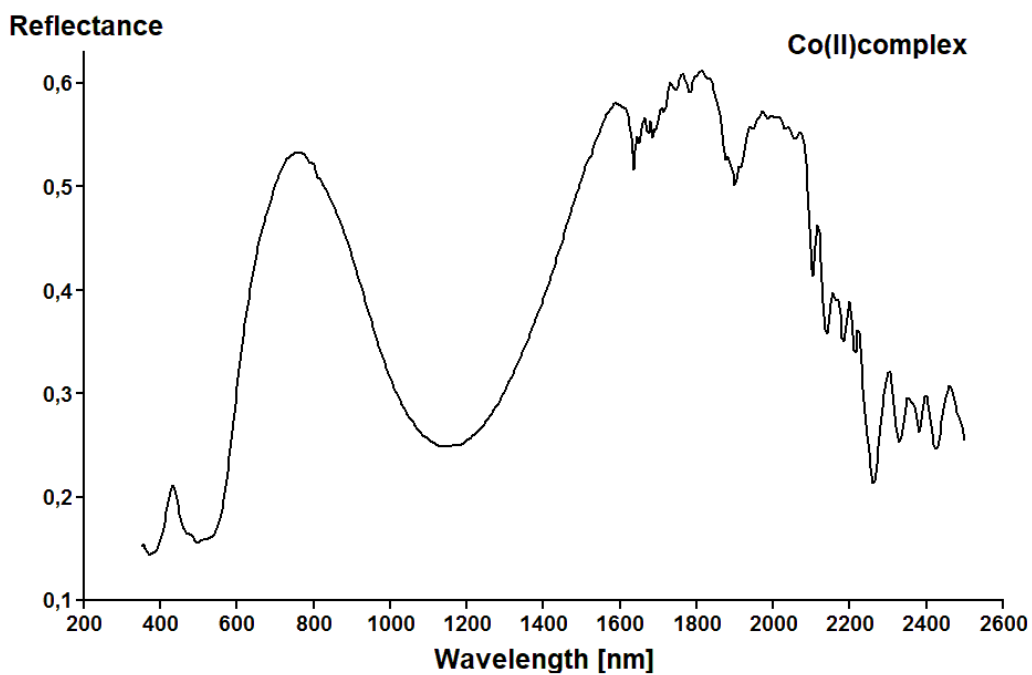
**Figure S2.** IR spectrum of *catena*-[Mn( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**2**)



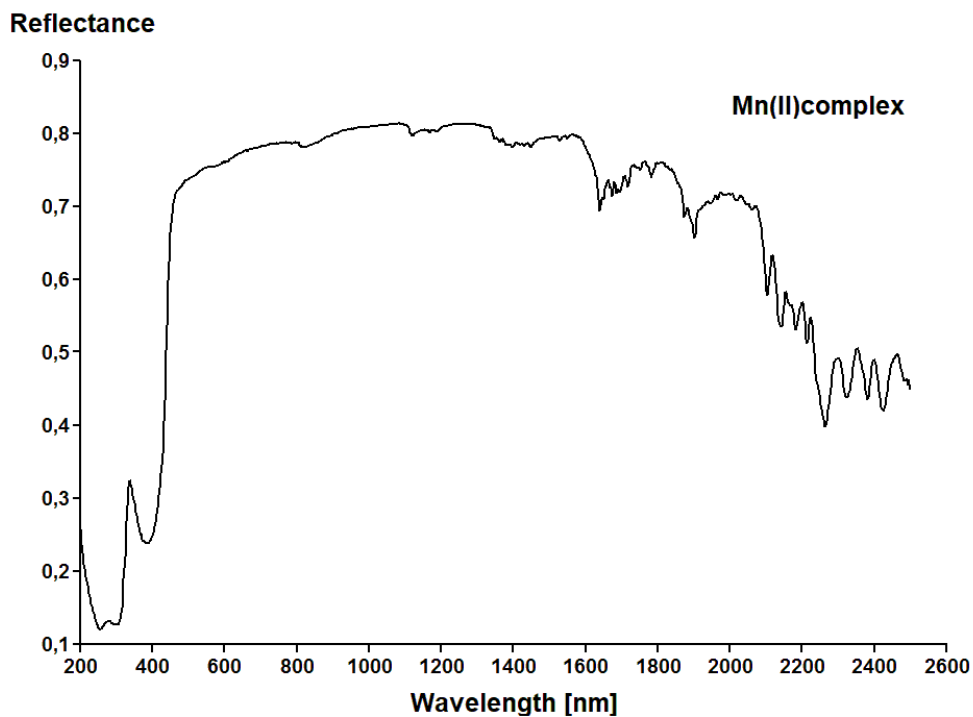
**Figure S3.** IR spectrum of *catena*-[Cd( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**3**)



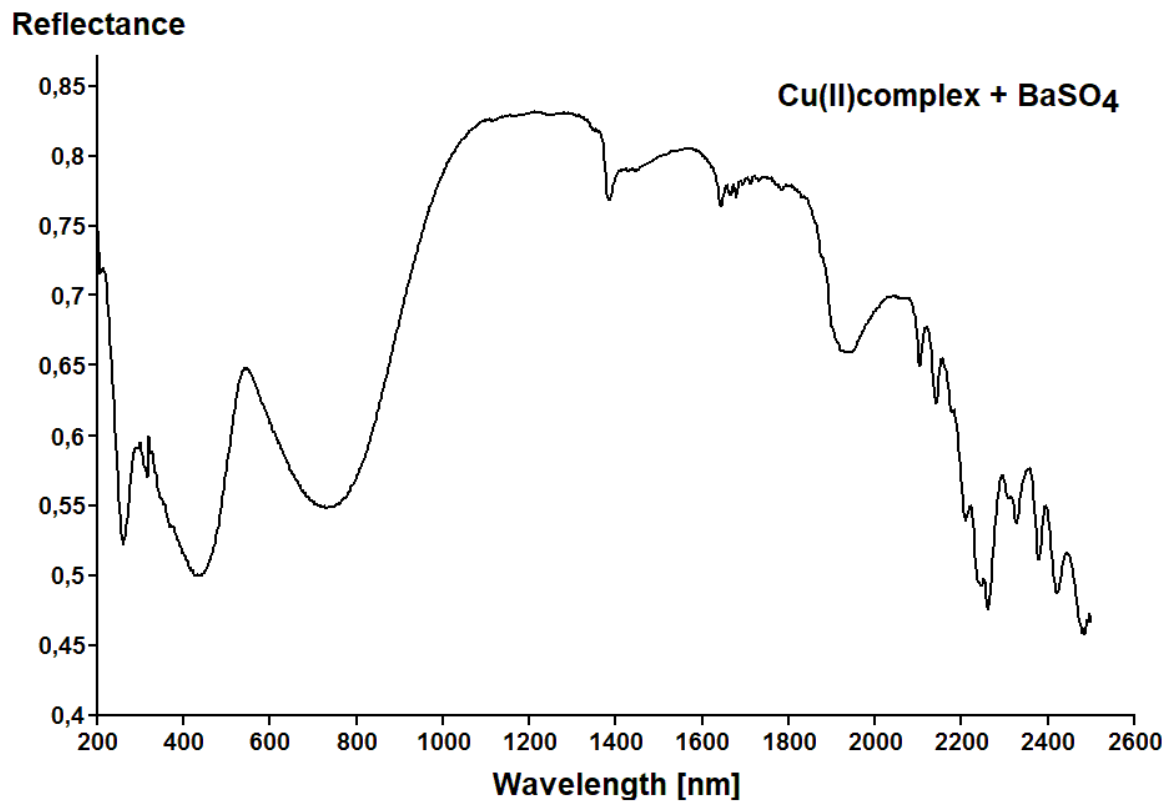
**Figure S4.** IR spectrum of [Cu( $\kappa^1$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**4**)



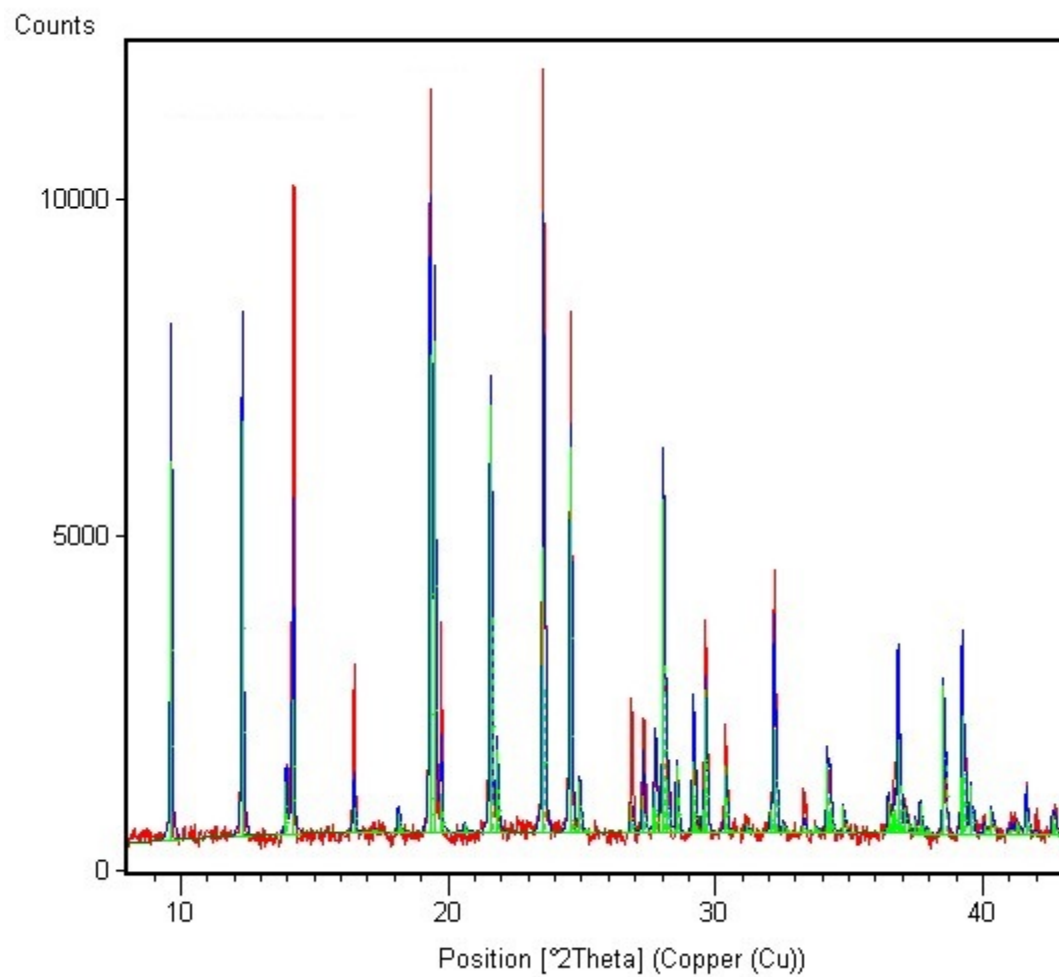
**Figure S5.** The solid state UV-VIS-NIR spectrum of *catena*-[Co( $\mu_{1,5}$ -dca) $_2$ (4-MOP-NO) $_2$ ] (**1**)



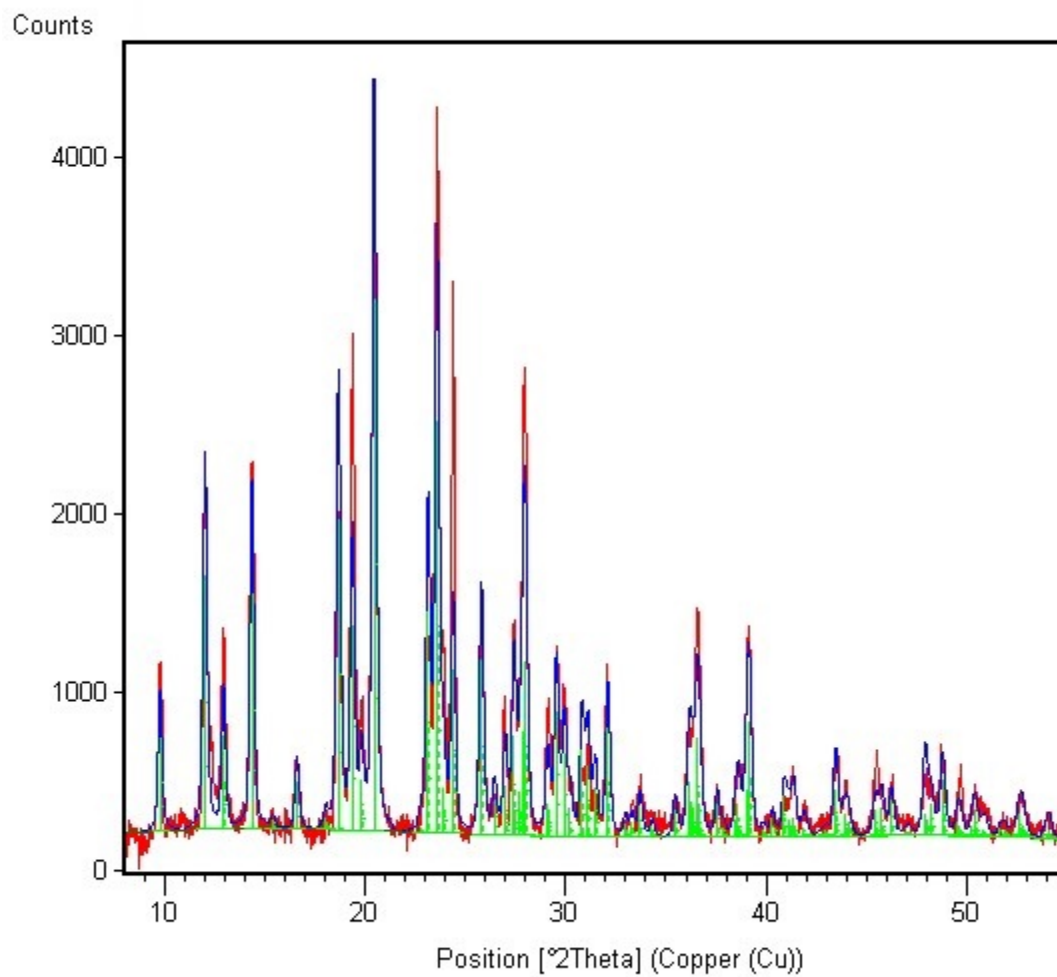
**Figure S6.** The solid state UV-VIS-NIR spectrum of *catena*-[Mn( $\mu_{1,5}$ -dca) $_2$ (4-MOP-NO) $_2$ ] (**2**). (Uncorrected spectrum, offset at approx. 810 nm is caused by detector change)



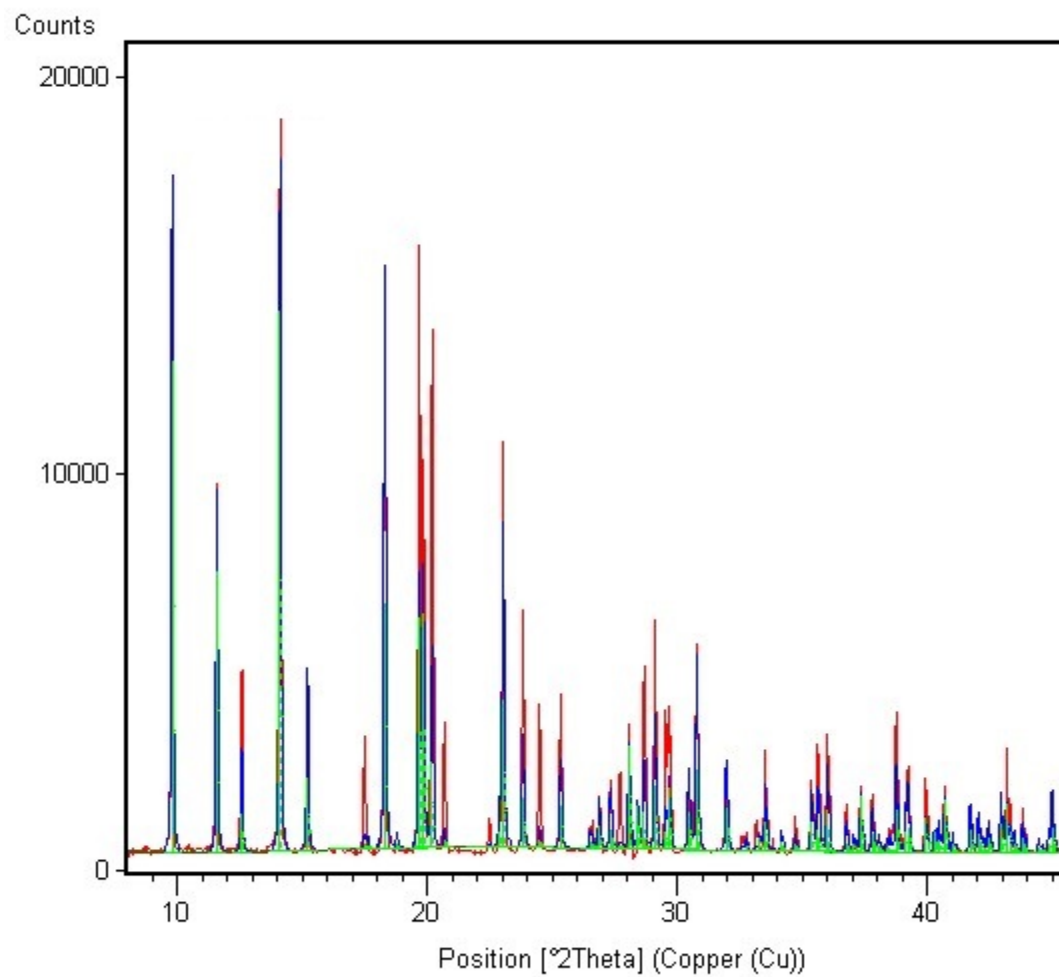
**Figure S7.** The solid state UV-VIS-NIR spectrum of mixture of  $[\text{Cu}(\kappa^1\text{-dca})_2(4\text{-MOP-NO})_2]$  (4) with  $\text{BaSO}_4$  (1:5 w:w) (uncorrected spectrum; the spike at approx. 315 nm is caused by change of UV lamp)



**Figure S8.** Observed and simulated X-ray powder pattern of *catena*-[Co( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**1**)

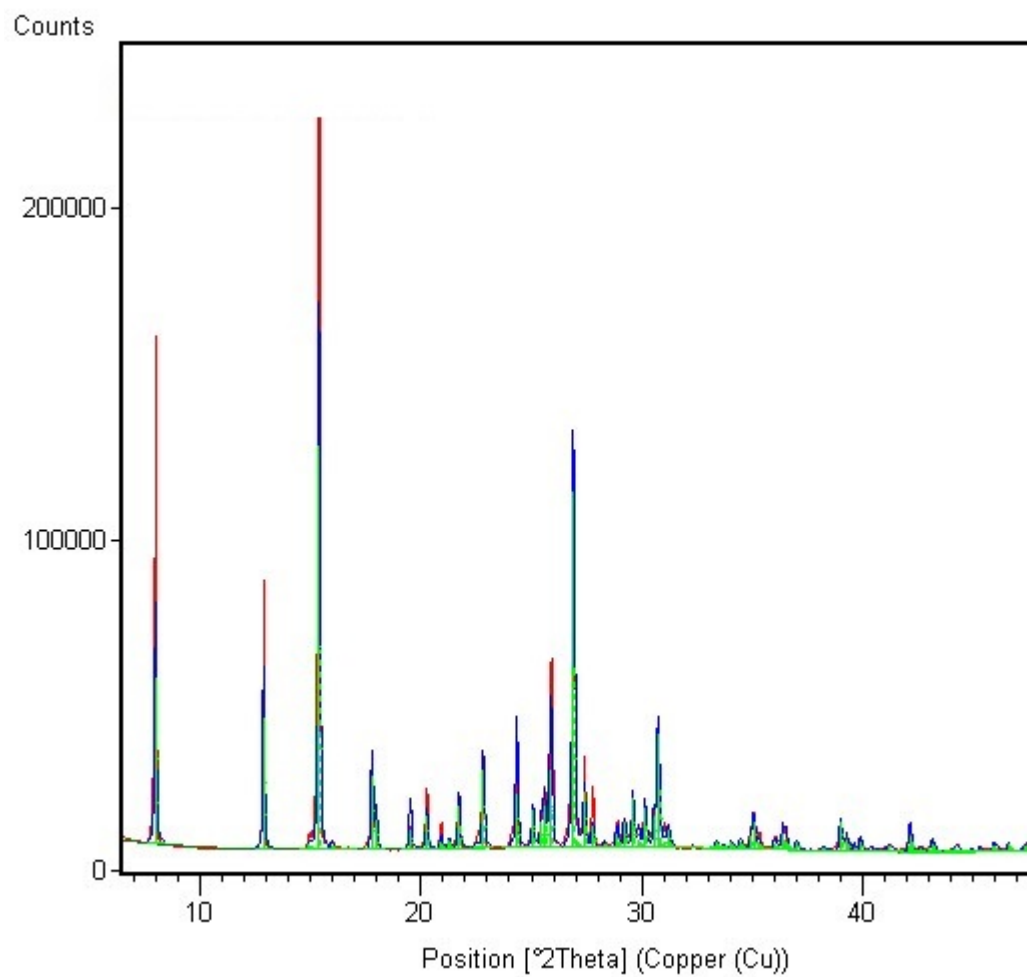


**Figure S9.** Observed and simulated X-ray powder pattern of *catena*-[Mn( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**2**)



**Figure S10.** Observed and simulated X-ray powder pattern of *catena*-[Cd( $\mu_{1,5}$ -dca)<sub>2</sub>(4-MOP-NO)<sub>2</sub>] (**3**)





**Figure S11.** Observed and simulated X-ray powder pattern of  $[\text{Cu}(\kappa^1\text{-dca})_2(4\text{-MOP-NO})_2]$  (**4**)