A 2-D Coordination Polymer Incorporating Cobalt(II), 2-Sulfoterepthalate and the Flexible Bridging Ligand 1,3-di(4-pyridyl)propane: Preparation, Gas Adsorption, and EPR Studies†

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Supplementary Information

Additional information on Physical techniques

Fluorescence

The fluorescence quantum yield of the complexes was determined using anthracene as a reference with known Φ_R of 0.27 in ethanol. The complex and the reference dye were excited at same wavelength, maintaining nearly equal absorbance (~0.1), and the emission spectra were recorded. The area of the emission spectrum was integrated using the software available in the instrument and the quantum yield is calculated according to the following equation:

$$\phi_s / \phi_R = \left[A_S / A_R \right] \times \left[(Abs)_R / (Abs)_S \right] \times \left[{\eta_S}^2 / {\eta_R}^2 \right]$$

Here, Φ_S and Φ_R are the fluorescence quantum yield of the sample and reference, respectively. A_S and A_R are the area under the fluorescence spectra of the sample and the reference, respectively, $(Abs)_S$ and $(Abs)_R$ are the respective optical densities of the sample and the reference solution at the wavelength of excitation, and η_S and η_R are the values of refractive index for the respective solvent used for the sample and reference.

EPR

EPR spectra were recorded from 0 to 10000 Gauss in the temperature range 77-298 K with an X-band (9.15 GHz) Varian E-9 spectrometer. EPR parameters reported in the text for the solid polycrystalline compound were obtained by simulating the spectra with the computer program Bruker WinEPR SimFonia.[S1] In all the simulations, second-order effects were taken into account and the ratio Lorentzian/Gaussian, affecting the line shape, was set to 1. To increase the signal to noise ratio, in these systems, signal averaging was used. Signal averaging involves repeatedly acquiring the spectrum and adding each spectrum together. Actually, this is not an average in the strict mathematical sense but is the sum of the individual spectra. As a result, the signal increases proportionally to *N*, where *N* is the number of scans, and the noise to √N, owing to its random nature; therefore, the resultant enhancement of the signal to noise ratio is proportional to √N.

Additional Figures

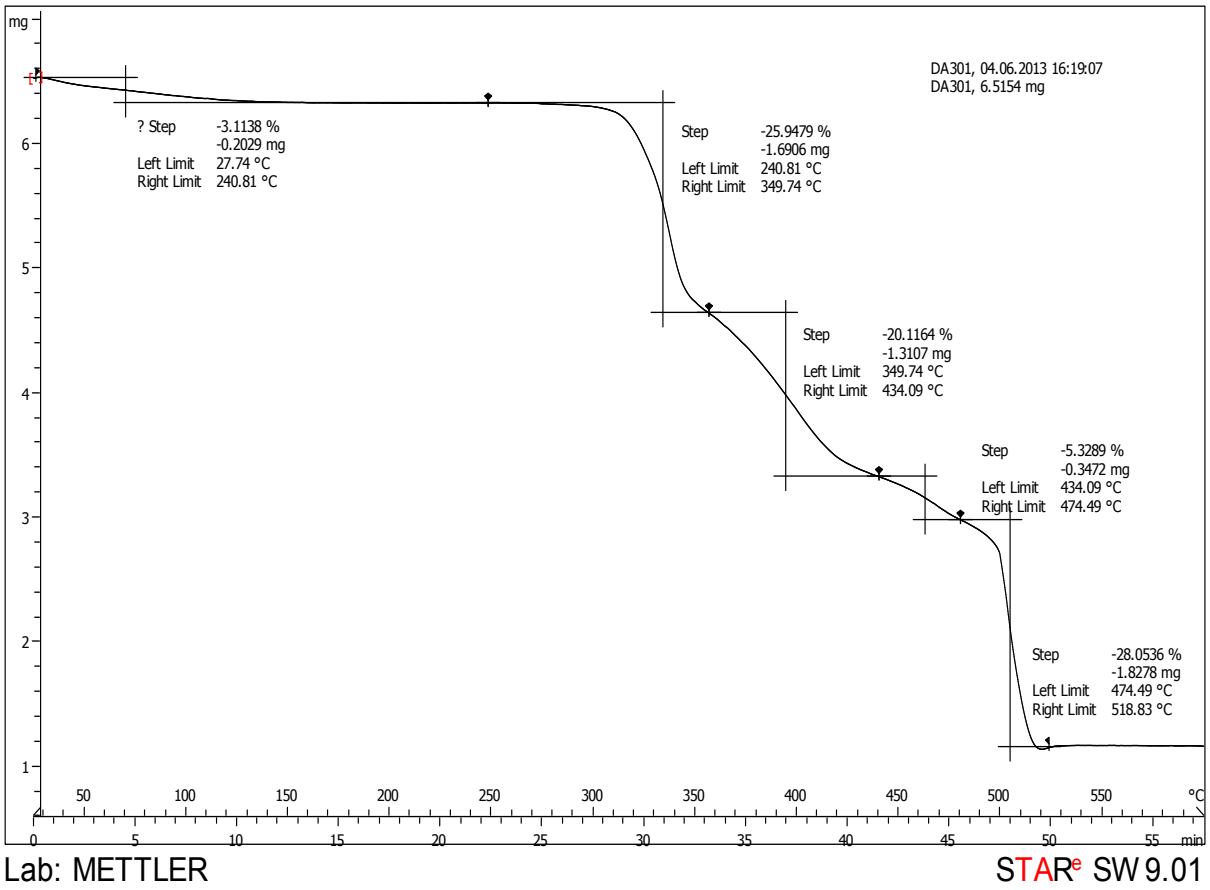

Fig. S1 Thermogravimetric analysis plot for **1**.

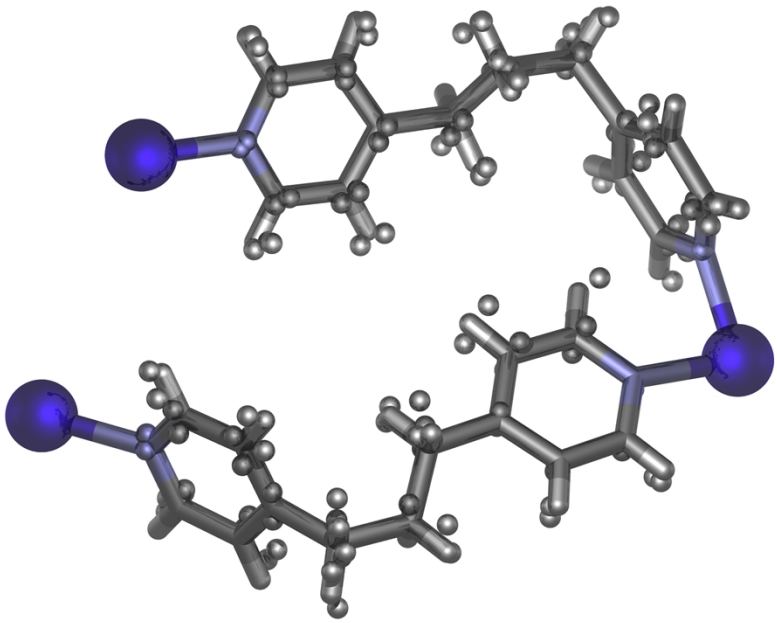

Fig. S2. Diagram showing the disorder present in the **dpp** ligands in the desolvated structure $\{[Co_3(\mathbf{2\text{-}stp})_2(\mathbf{dpp})_4]\}_n$.

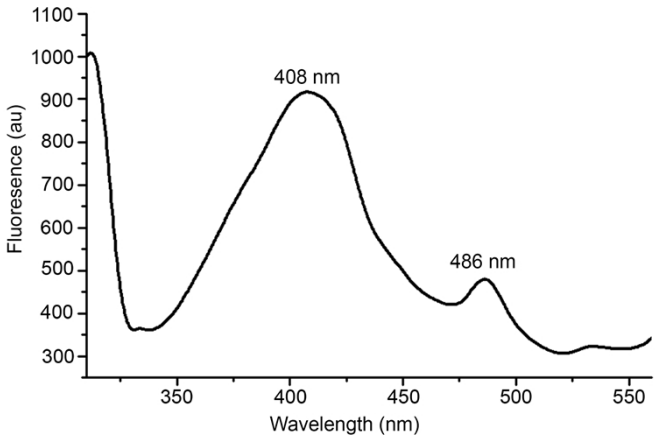

Fig. S3. Emission spectrum of complex **1** in the solid state.

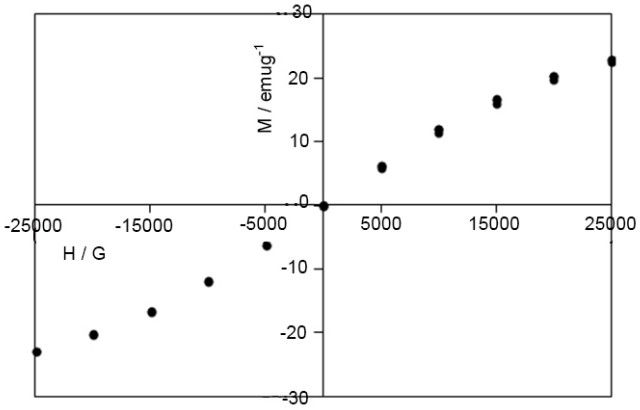

Fig. S4. The M vs H plot for the complex at 5 K for **1**.

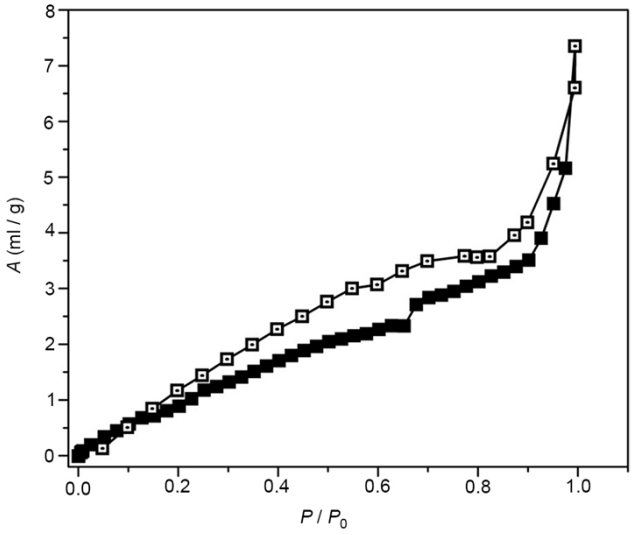

Fig. S5. N_2 adsorption isotherm of desolvated **1** measured at 77 K. P_0 = 690 mm of Hg. Closed symbols and open symbols correspond to adsorption and desorption, respectively.

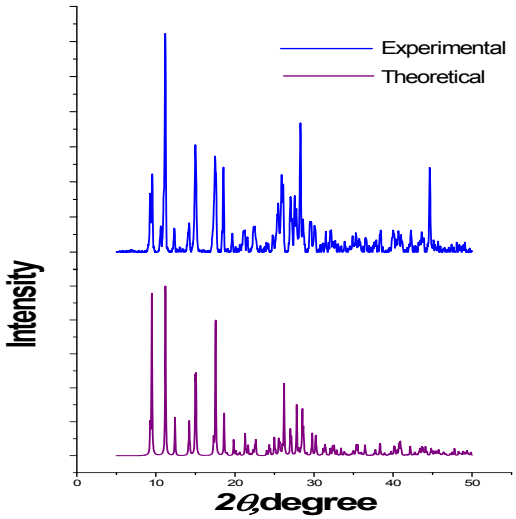

Fig. S6. PXRD patterns for $\{[Co_3(\mathbf{2\text{-}stp})_2(\mathbf{dpp})_4]\cdot 2H_2O\}_n$ as prepared (top) and predicted from the single crystal structure (bottom).

Additional discussion regarding topology of 1

While we have chosen to assign the topology of **1** as (3,4,5)-c trinodal net with point symbol $\{4.6^2\}_2\{4^2.6^3.8\}\{4^2.6^6.8^2\}_2$ by defining Co1 as a 5-connected node, Co2 as a 4-c node, the **2-stp** ligand as 3-c node and the **dpp** ligand as linear connector, it is possible to describe the topology differently using the cluster simplification approach.[S2] For example, if the trimeric unit $[Co_3(\mathbf{2\text{-}stp})_2]$ isconsidered as a cluster node and **dpp** as a simple connector, **1** can be described as as a sql/Shubnikov tetragonal plane net $\{4^4.6^2\}$ with vertex symbol [4.4.4.4.*.*][S322] (Fig. S6) or as a hxl/Shubnikov 6-c plane net $\{3^6.4^6.5^3\}$ with vertex symbol [3.3.3.3.3.3.*.*.*.*.*.*.*.*.*.*] (Fig. S7).

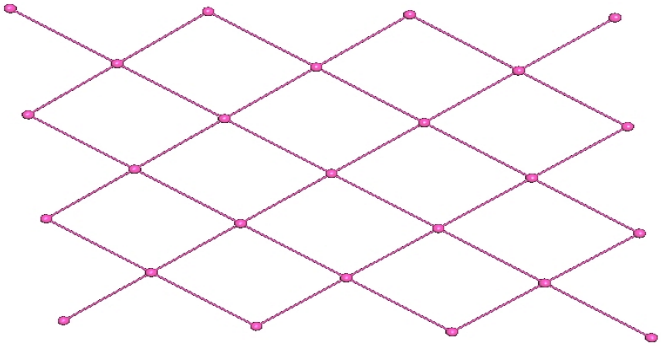

Fig. S6. View of the **sql** tetragonal plane net.

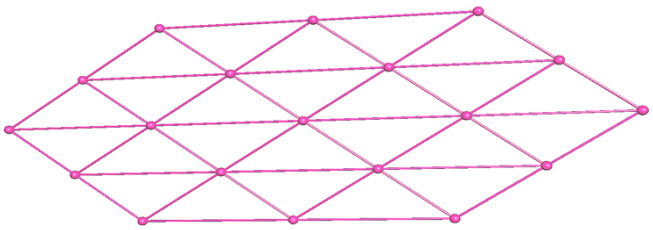

Fig. S7. View of the **hxl** 6-c plane net.

References

S1. Bruker WINEPR System 2.11 (shareware), Bruker-Franzen Analytic GmbH, Bremen, Germany, 1996

S2. E. V. Alexandrov, V. A. Blatov, A. V. Kochetkov and D. M. Proserpio, *CrystEngComm*, 2011, **13**, 3947-3958.

S3. V. A. Blatov, M. O'Keeffe and D. M. Proserpio, *CrystEngComm*, 2010, **12**, 44-48.