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### **Supporting Information**

# Diverse cobalt (II) coordination polymers for water/ethanol separation and luminescence water sensing applications

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#### **1-Physical measurements**

Elemental analyses (C, H, N) were carried out with a Perkin-Elmer 240C elemental analyzer. FT-IR spectra were recorded from KBr pellets in the range of 4000-400 cm<sup>-1</sup> on a VECTOR 22 spectrometer. UV-Visible absorption spectra were recorded on a UV-2501PC UV-Visible Spectrophotometer. The powder X-ray diffraction (PRXD) was recorded on a Bruker D8 ADVANCE diffractometer (CuK $\alpha$ , 1.5418 Å) at 40 kV and 40 mA. Thermal analyses and DSC were performed on a TGA V5.1A Dupont 2100 instrument from room temperature to 800 °C with a heating rate of 10 °C min<sup>-1</sup> in the air, and the data are consistent with the structures. The adsorption isotherms of CO<sub>2</sub> (at 195 K), N<sub>2</sub> and H<sub>2</sub> (at 77 K) were measured by using BELmax 00027 adsorption equipment (BEL Japan). The methanol (298 K), alcohol (298 K) and toluene (298 K) vapor were measured with a BELSORP-max automatic volumetric sorption apparatus. An exactly measured amount of the sample was introduced into the gas sorption instrument after the sample was pre-desolvated in a Schlenk tube at 120 °C under vacuum for 24 h. The adsorbate was placed into the sample tube, then the change of the pressure was monitored and the degree of adsorption was determined by the decrease of the pressure at the equilibrium state. The sorption properties were analyzed using Autosorb 1 for Windows 1.24 software.

### 2-X-ray crystallography

The diffraction data were collected on a Oxford Gemini S Ultra diffractometer equipped with Cu-K $\alpha$  radiation ( $\lambda$  = 1.54178 Å) for complex **1**, or on the same diffractometer equipped with Mo-K $\alpha$  radiation ( $\lambda$  = 0.71073 Å) for complexes **2**, **3** at 150 K by using  $\phi$ and  $\omega$  scans. Multiscan adsorption corrections were applied for all complexes. The structures were solved by the direct methods (SHELXS) and refined by the full matrix least-squares method against  $F_0^2$  using the SHELXTL software.<sup>1,2</sup> The coordinates of the non-hydrogen atoms were refined anisotropically. Most of hydrogen atoms were introduced in calculated positions and refined with fixed geometry with respect to their carrier atoms, and the guest methanol hydrogen atoms have not been added. Details of the crystal parameters, data collections and refinement for complexes **1**, **2**, **3** are summarized in Table 1. Further details are provided in Supporting Information. CCDC numbers 1833839, 1833841, 1833841 are for three complexes **1**, **2**, **3** respectively.

- 1 G.M. Sheldrick, SHELXS-97, Program for the Solution of Crystal Structures, University of Göttingen, Germany 1997.
- 2 G.M. Sheldrick, SHELXL-97, Program for the Refinement of Crystal Structures From Diffraction Data, Univ. of Göttingen, Göttingen (Germany), 1997.

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**Scheme S1**. Four conformations of the 3-pmpmd ligand (N, N´-bis(3-pyridylmethyl) pyromellitic diimide).





Fig. S2. Emission spectra of complex 1 with different time.



Fig. S3. A color change photograph of complex 1 in DMF upon increasing F<sup>-</sup> anion concentration



**Fig. S4.** UV-visible spectra of complex **1** in DMF upon increasing F<sup>-</sup> anion concentration.



Fig. S5. The XRPD of 3 simulated and desolvated 3 dispersing in different solvents.



**Fig. S6.** The  $\pi \cdots \pi$  interactions between the adjacent chains in **1** along *b* axis.



Fig. S7. UV-visible absorption spectra of 3-pmpmd and compounds 1, 2 and 3 in DMF.



Fig. S8. PXRD pattern of compound 3 after thermal-treatment at 110 °C.



Fig. S9. PXRD pattern of compound 3 after water vapour adsorption experiments.



Fig. S10. PXRD pattern of compound 3 after soaking into organic solvents.



Fig. S11. Calculated and measured PXRD for compound 1.



Fig. S12. Calculated and measured PXRD for compound 2.



Fig. S13. Calculated and measured PXRD for compound 3.



Fig. S14. Calculated and measured PXRD for compound 4.



Fig. S15. Water and ethanol sorption isotherms at 298 K for compound 2.

Table S1. Select	ed bond ler	ngths (A) and ang	les (deg) fo
Complex 1			
N(1)-Co(1)	2.252(4)	N(4)-Co(1)	2.225(4)
Cl(1)-Co(1)	2.4465(13)	N(4)-Co(1)-N(1)	90.15(14)
N(4)-Co(1)-Cl(1)	90.28(10)	N(1)-Co(1)-Cl(1)	90.75(11)
Complex 2			
N(1)-Co(1)	2.173(7)	N(4)-Co(1)	2.190(7)
N(9)-Co(1)	2.086(10)	N(10)-Co(1)	2.063(9)
N(10)-Co(1)-	179.2(3)	N(10)-Co(1)-	90.0(3)
N(9)		N(1)	
N(10)-Co(1)-	90.7(3)	N(10)-Co(1)-	90.1(3)
N(5)		N(4)	
N(1)-Co(1)-N(4)	92.1(3)	N(5)-Co(1)-N(4)	177.7(3)
Complex <b>3</b>			
Co(1)-N(1)	2.140(2)	Co(1)-N(4)	2.153(2)
Co(1)-N(5)	2.160(2)	Co(1)-O(8)	2.127(2)
Co(1)-O(10)	2.159(2)	Co(1)-O(11)	2.254(2)
N(1)-Co(1)-N(4)	92.92(9)	N(1)-Co(1)-N(4)	93.70(9)
N(5)-Co(1)-N(4)	173.37(10)	N(1)-Co(1)- O(10)	141.01(9)

Table S1. Selected bond lengths (Å) and angles (deg) for 1, 2 and 3.							
Complex <b>1</b>							
N(1)-Co(1)	2.252(4)	N(4)-Co(1)	2.225(4)				
Cl(1)-Co(1)	2.4465(13)	N(4)-Co(1)-N(1)	90.15(14)				

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