

## Supporting Information

### Coordination-driven self-assembly of a series of dinuclear $M_2L_2$ mesocate with bis-bidentate pyridylimine ligand

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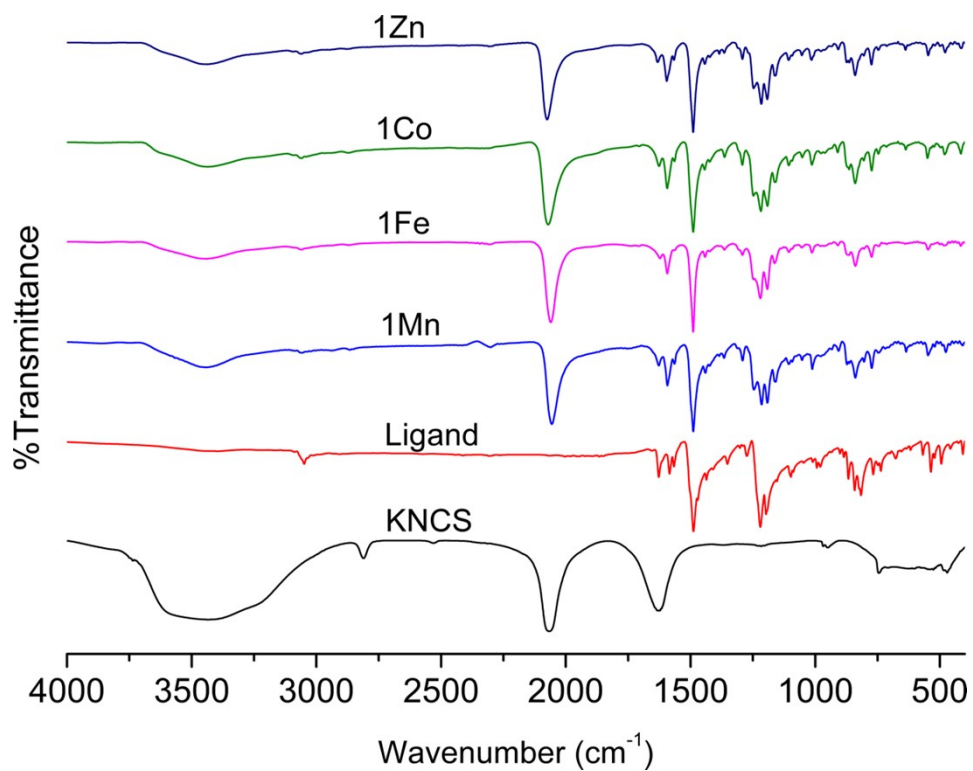
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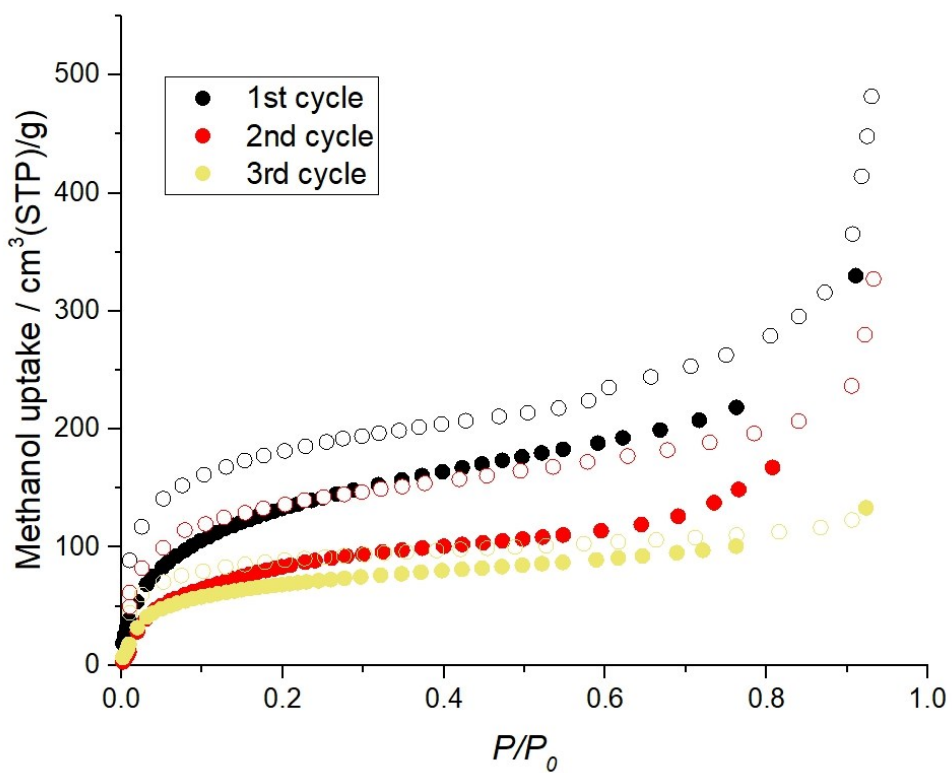
**Table S1.** Selected bond lengths (Å) and bond angles (°) around the metal(II) ions for **1<sub>M</sub>**.

	<b>1<sub>Mn</sub></b>	<b>1<sub>Fe</sub></b>	<b>1<sub>Co</sub></b>	<b>1<sub>Zn</sub></b>
M1–N1	2.130 (3)	2.062 (4)	2.049 (3)	2.051 (3)
M1–N2	2.173 (3)	2.176 (4)	2.079 (3)	2.125 (3)
M1–N3	2.260 (3)	2.141 (3)	2.137 (3)	2.144 (2)
M1–N4	2.355 (3)	2.222 (3)	2.202 (3)	2.315 (2)
M1–N5 <sup>i</sup>	2.334 (3)	2.206 (3)	2.194 (2)	2.282 (2)
M1–N6 <sup>i</sup>	2.277 (3)	2.153 (3)	2.159 (3)	2.171 (2)
M···M <sup>i</sup>	15.0929 (11)	14.7201 (11)	14.8104 (9)	15.0433 (9)
N1–M1–N2	100.80 (13)	96.91 (12)	98.10 (11)	98.99 (10)
N1–M1–N3	97.66 (12)	96.56 (12)	93.57 (10)	96.27 (10)
N1–M1–N4	93.97 (12)	94.27 (12)	93.61 (11)	93.61 (10)
N1–M1–N5 <sup>i</sup>	161.13 (12)	164.96 (12)	165.72 (11)	164.19 (10)
N1–M1–N6 <sup>i</sup>	92.37 (12)	92.18 (12)	92.80 (10)	93.24 (10)
N2–M1–N3	95.75 (11)	93.32 (10)	94.67 (10)	95.93 (9)
N2–M1–N4	162.18 (11)	165.40 (11)	165.53 (10)	165.04 (9)
N2–M1–N5 <sup>i</sup>	92.65 (10)	94.06 (11)	91.89 (10)	92.89 (9)
N2–M1–N6 <sup>i</sup>	98.38 (11)	93.67 (10)	94.31 (10)	97.11 (9)
N3–M1–N4	72.26 (10)	75.31 (10)	76.05 (10)	74.57 (9)
N3–M1–N5 <sup>i</sup>	94.06 (10)	97.38 (11)	95.76 (9)	92.82 (9)
N3–M1–N6 <sup>i</sup>	160.82 (10)	164.66 (11)	168.15 (10)	162.45 (9)
N4–M1–N5 <sup>i</sup>	75.56 (10)	77.68 (10)	78.24 (9)	76.36 (8)
N4–M1–N6 <sup>i</sup>	90.83 (10)	91.53 (10)	93.58 (10)	90.16 (9)

Symmetry code: (i)  $-x+1, -y+1, -z+1$ .

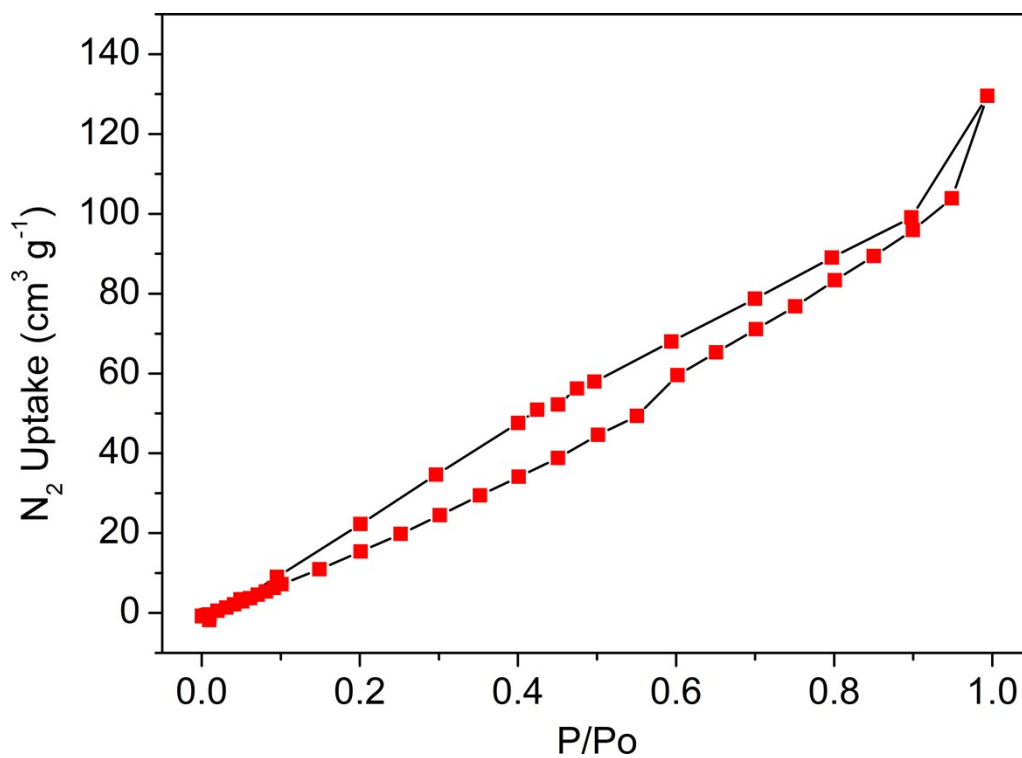


**Figure S1.** IR spectra of ligand L, KNCS·xH<sub>2</sub>O, and compounds **1<sub>M</sub>**.

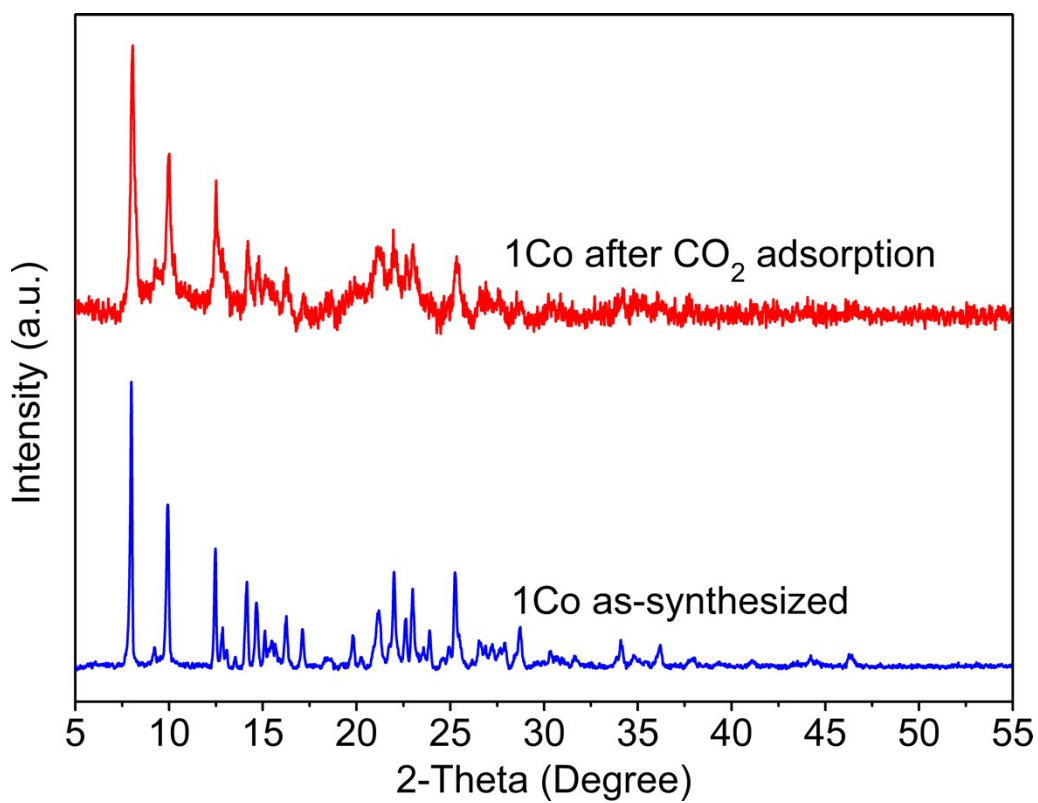


**Figure S2.** Three cycles of MeOH vapor adsorption-desorption of **1<sub>Co</sub>** at STP.

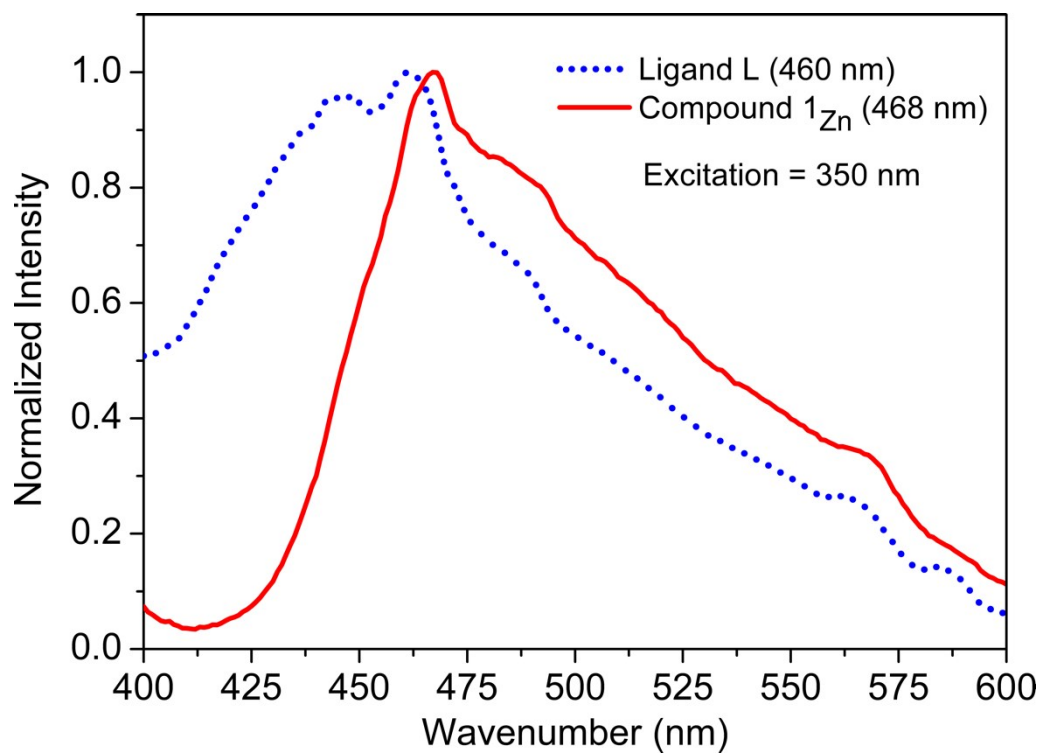




**Figure S3.** N<sub>2</sub> adsorption isotherm at 77 K for **1Co**.



**Figure S4.** PXRD patterns of **1Co**: as-synthesized and after CO<sub>2</sub> adsorption.



**Figure S5.** The photoluminescent spectra in the solid state at room temperature of ligand L and compound  $1_{Zn}$ .