Supporting information

Syntheses, Structures, Photoluminescent and Magnetic Studies of Metal-Organic Frameworks Assembled with 5-Sulfosalicylic Acid and 1,4-Bis(imidazol-1-ylmethyl)-Benzene

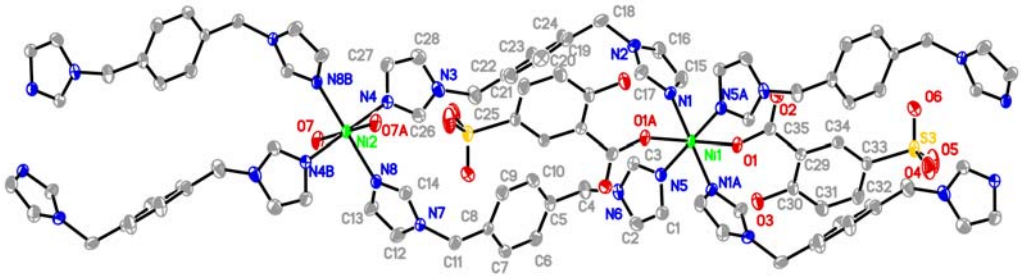
Zhenda Lu, Lili Wen, Zhaoping Ni, Yizhi Li, Huizhen Zhu, and Qingjin Meng*

Coordination Chemistry Institute, State Key Laboratory of Coordination Chemistry

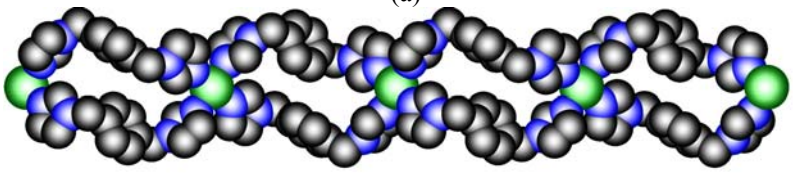
School of Chemistry and Chemical Engineering, Nanjing University

Nanjing 210093(P.R. China)

E-mail: mengqj@nju.edu.cn



(a)



(b)

Figure S1. (a) Perspective view of the coordination environments of the Ni ions (b) Space-filling representation of the double-stranded chain in compound 3 (coordination Sulfosalicylic acid and water have been omitted for clarity.)

XRPD

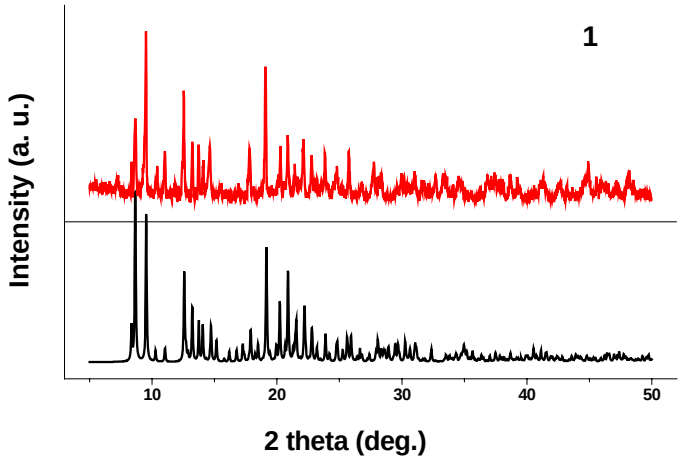


Figure S2. Simulated (black) and experimental (red) XRD spectra for **1**

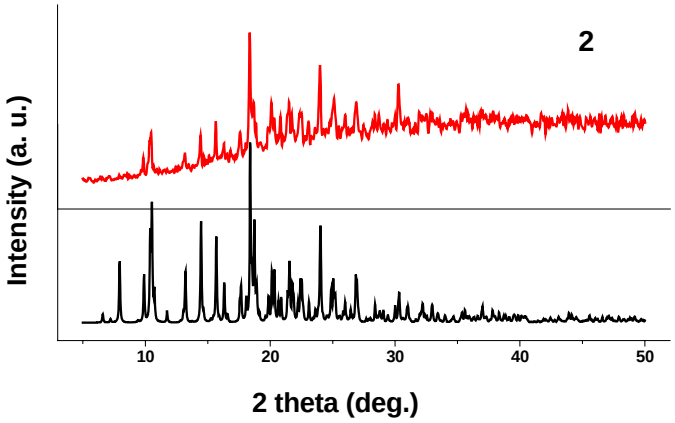


Figure S3. Simulated (black) and experimental (red) XRD spectra for **2**

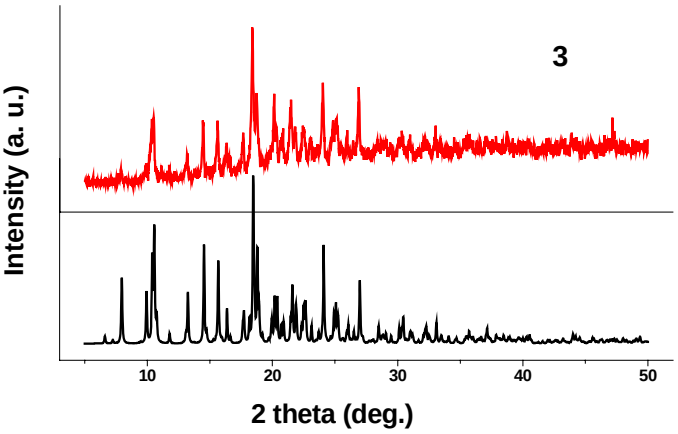


Figure S4. Simulated (black) and experimental (red) XRD spectra for **3**

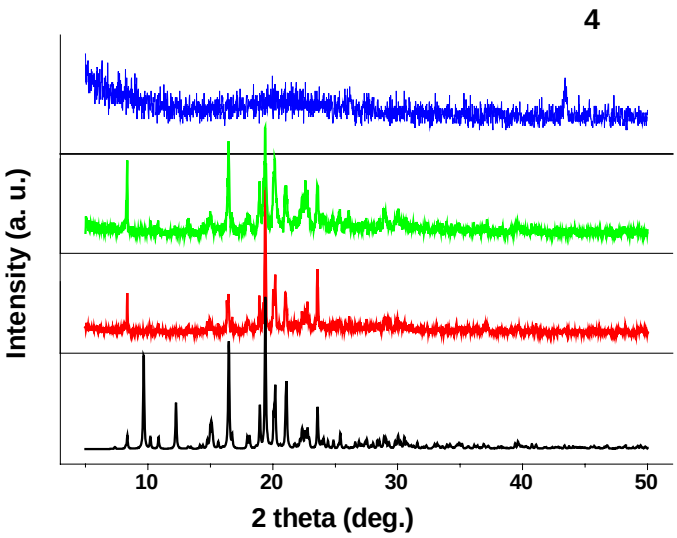


Figure S5. XRD spectra for **4**, black: Simulated; red: taken at room temperature; green: after heating to 190 °C for 1h; blue: after heating to 230 °C for 1h.

Magnetic

Equations

$$\chi_{mono} = \frac{1}{T} \times \frac{\frac{7(3-A)^2 x}{5} + \frac{12(2+A)^2}{25A} + \left(\frac{2(11-2A)^2 x}{45} + \frac{176(2+A)^2}{675A}\right)\exp\left(\frac{-5Ax}{2}\right) + \left(\frac{(5+A)^2 x}{9} - \frac{20(2+A)^2}{27A}\right)\exp(-4Ax)}{\frac{8x}{3}\left[3 + 2\exp\left(\frac{-5Ax}{2}\right) + \exp(-4Ax)\right]} \quad \textbf{(S1)}$$

$$x = \lambda / k_B T \quad \textbf{(S2)}$$

$$\chi = \frac{\chi_{mono}}{1 - \left(2zj / Ng^2\beta^2\right)\chi_{mono}} \quad \textbf{(S3)}$$

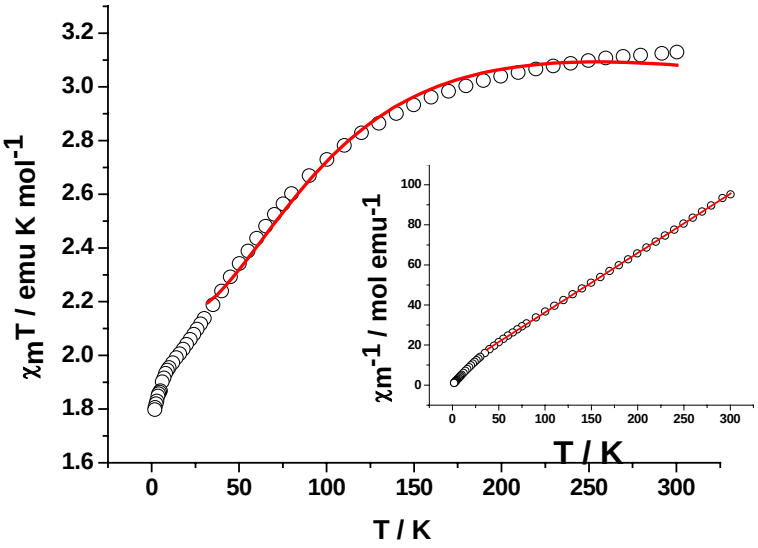


Figure S6. Magnetic behavior of the complex **2** in the form of $\chi_m T$ vs T and χ^{-1} vs T (inset) plots. Solid line shows the best fit to the model.

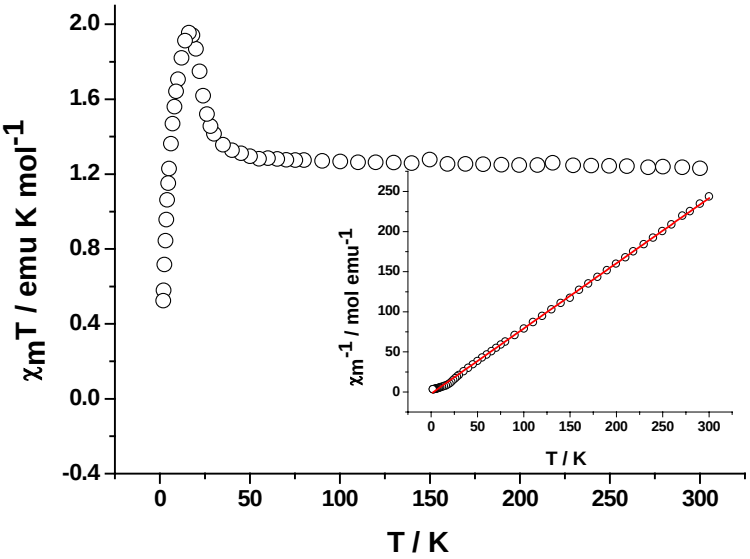


Figure S7. Magnetic behavior of the complex **3** in the form of $\chi_m T$ vs T and χ^{-1} vs T (inset) plots. Solid line shows the best fit to the model.

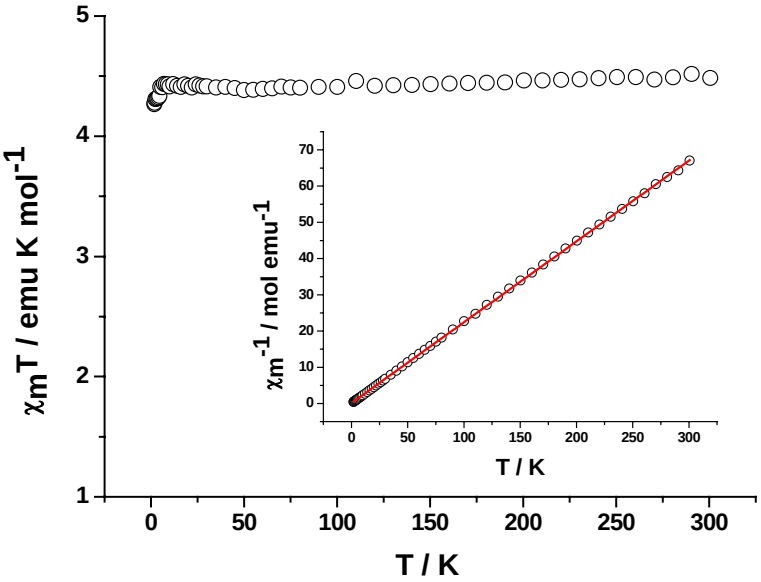


Figure S8. Magnetic behavior of the complex **4** in the form of $\chi_m T$ vs T and χ^{-1} vs T (inset) plots. Solid line shows the best fit to the model.