

Supported material

Second ligands-assisted structural variation of entangled coordination polymers with polycatenated or polythreaded features

Feilong Hu*^a, Huahong Zou^b, Xuebo Zhao^c, Yan Mi^a, Caili Luo^a, Yunxiao Wang^a

^aCollege of chemistry and materials, Yulin normal university, Yulin, 537000, PR China

^bSchool of chemistry & chemical engineering of Guangxi Normal University, Guilin, PR. China

^cQindao Institute of Bioenergy and Bioprocess Technology, Chinese academy of Sciences.

Magnetic:

It is well known that magnetic research for the high spin Co system is complicated and difficult because the strong spin-orbital coupling. And from a magnetic point of view, the long oba cannot favor any noticeable magnetic coupling. Thus, the whole system for **5** can be considered magnetically as one-dimensional. The 1D infinite metal chain consists of repeated linear Co^{II}₃ unit ([Fig. S6](#)). Co1 and Co2 (intratrimer) are bridged by two $\mu_2\text{-}\eta^2$ and one *syn-syn* $\text{-}\mu_2\text{-}\eta^1\text{:}\eta^1$ mode of carboxylate groups. Co1 and Co1 (intertrimer) are bridged by two *syn-syn* $\text{-}\mu_2\text{-}\eta^1\text{:}\eta^2$ mode of carboxylate groups and one $\mu_2\text{-}\eta^2$ water molecule. To get a reasonable estimate of the spin-orbit coupling, a simple phenomenological equation is introduced as shown below. [\[1\]](#)

$$\chi_m T = A \exp(-E_1/kT) + B \exp(-E_2/kT) \quad (1)$$

In equation (1), $A + B$ equals the Curie constant, and E_1 and E_2 represent the activation energies corresponding to the spin-orbit coupling and antiferromagnetic exchange interactions, respectively. The best fit of the experimental data gives $A + B = 16.02 \text{ cm}^3 \text{Kmol}^{-1}$, $E_1/k = +57.35 \text{ K}$, $E_2/k = -9.6 \text{ K}$ ([Fig. S7](#)). The values for $E_1/k = +57.35 \text{ K}$ is small than those given in the literature for both the effects of spin-orbit coupling and site distortion. [\[2\]](#) The negative values of E_2 indicate that dominant antiferromagnetic interactions between Co^{II} ions exist in **5**.

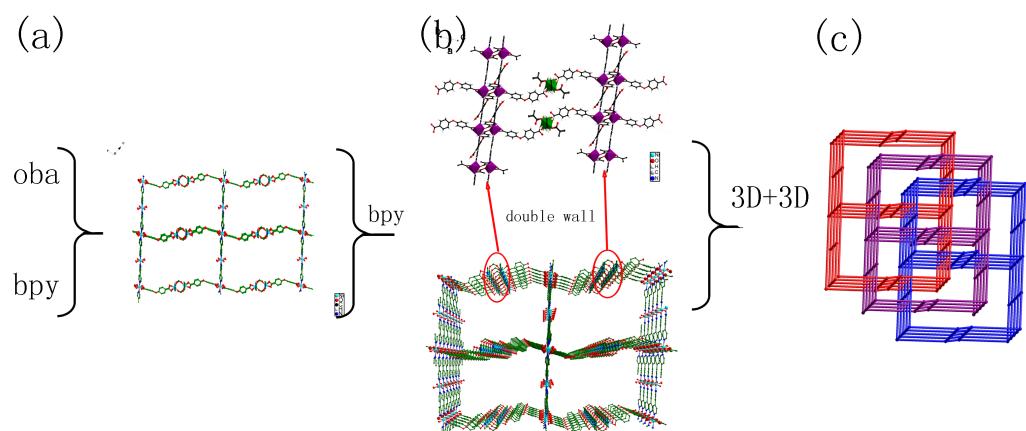


Figure s1. the sql layer of 2.

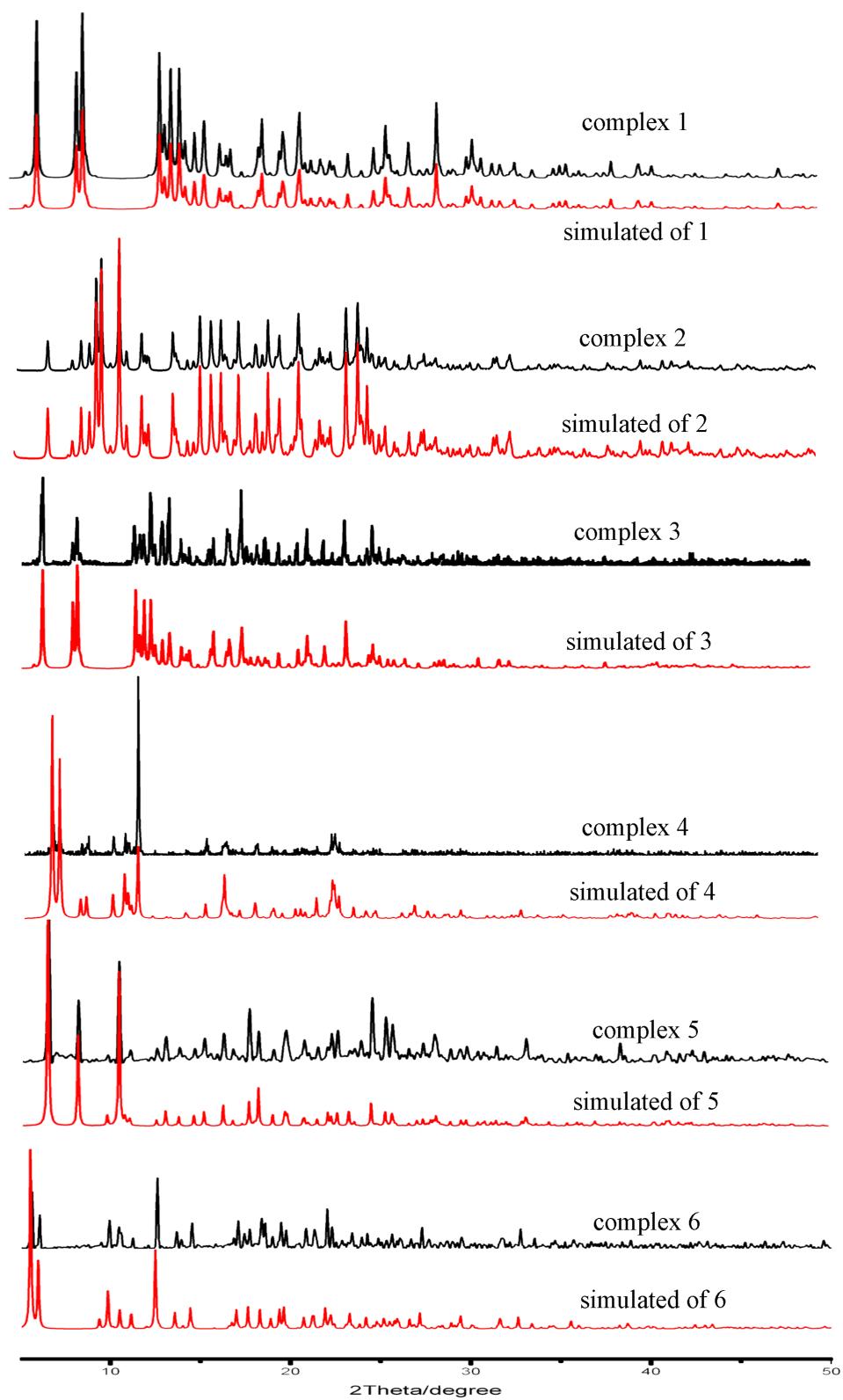


Fig. S1. The xrd pattern of **1-6**.

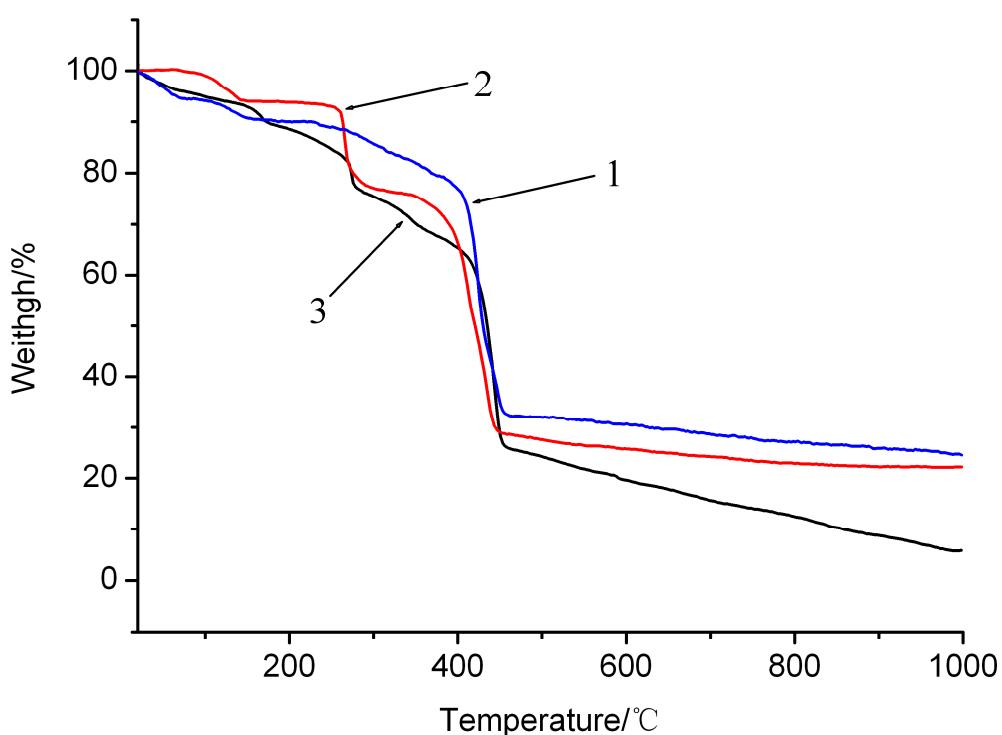


Fig. S2. The TG curves of **1-3**.

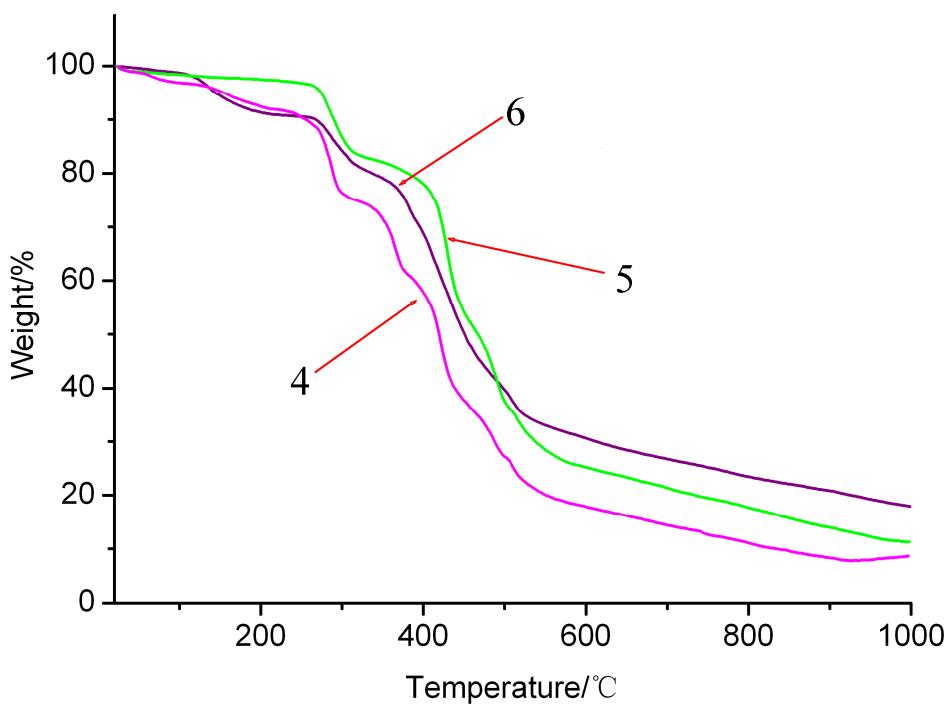


Fig. S3. The TG curves of **4-6**.

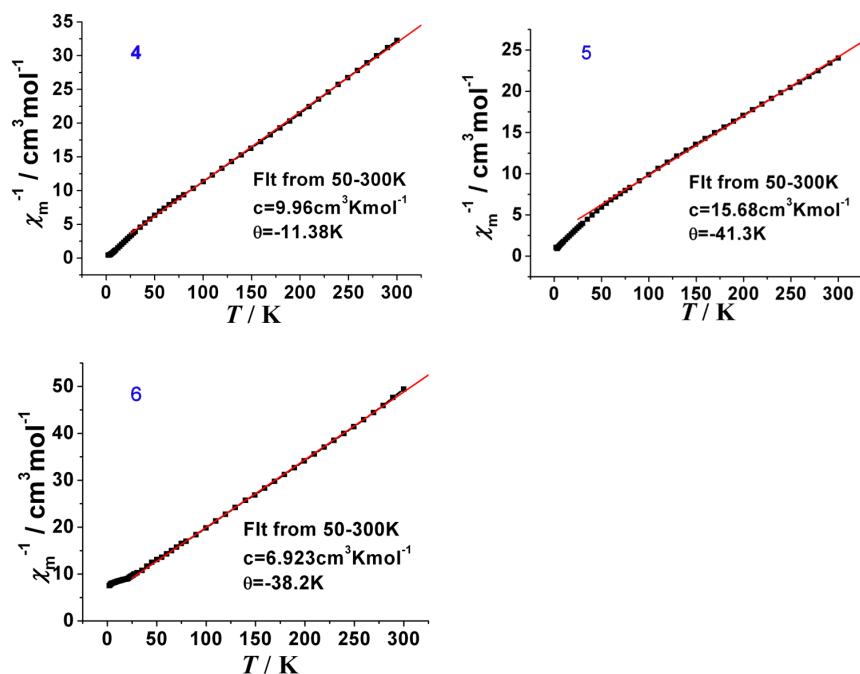


Fig S4. Plots of χ^{-1} vs. T and the fit of Curie-Weiss law (red curve) of 4-6.

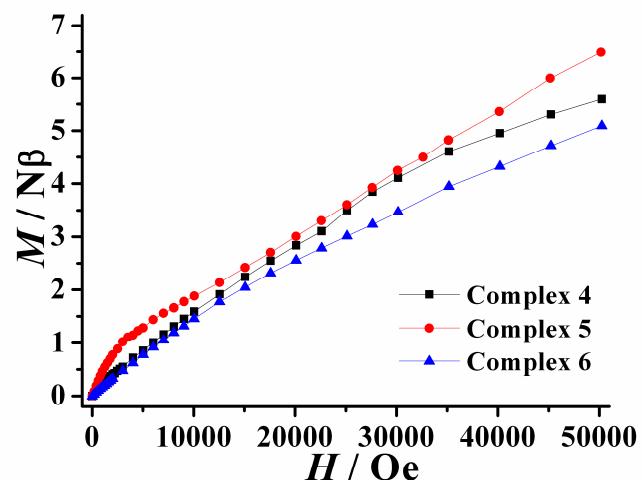


Fig S5. Field dependence of the magnetization of 4-6 at 2 K.

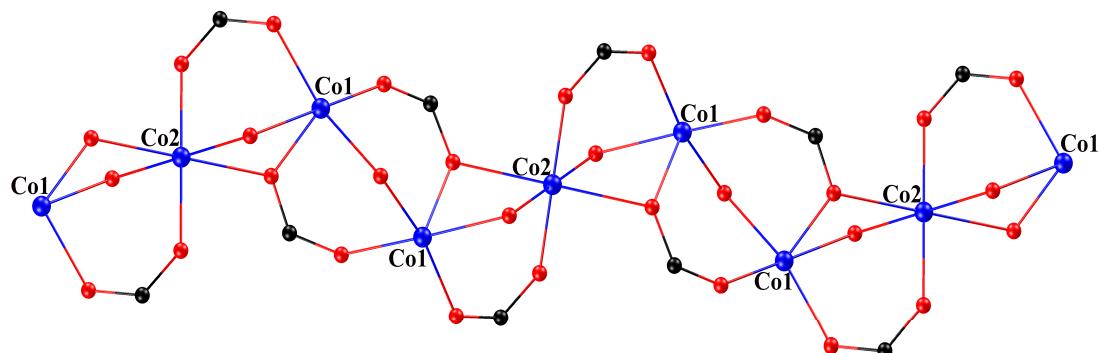


Fig S6. 1D metal chain of **5**.

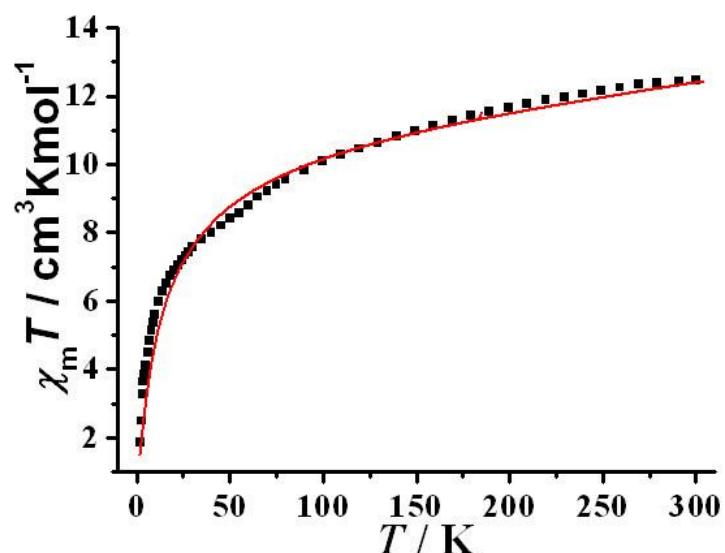


Fig S7. Temperature dependence of magnetic susceptibilities in the forms of $\chi_m T$ at an applied field of 1 kOe and red solid line shows the best fit at 2–300 K.

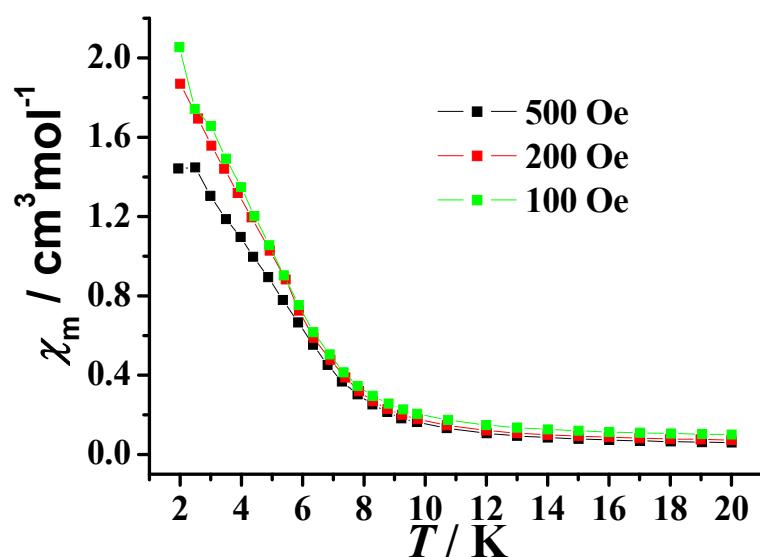


Fig. S8. Temperature dependence of χ_m at different fields of **4**.

- [1] S.J. Liu, L. Xue, T.L. Hu, X.H. Bu, *Dalton Trans.*, 2012, 41, 6813.
- [2] J.M. Rueff, C. Paulsen, J. Souletie, M. Drillon, P. Rabu, *J. Solid State Chem.*, 2005, 178, 431.