Supporting Information for:

Design and construction of coordination polymers based on 2,2'-dinitro-4,4'-biphenyldicarboxylate and three semi-rigid N-donor ligands: diverse structural topology, and magnetic properties

Baiyan Li, Fen Yang, Yiming Zhang, Guanghua Li, Qi Zhou, Jia Hua, Zhan Shi and Shouhua Feng*

State Key Laboratory of Inorganic Synthesis and Preparative Chemistry, College of Chemistry, Jilin University, Changchun, 130012, People's Republic of China

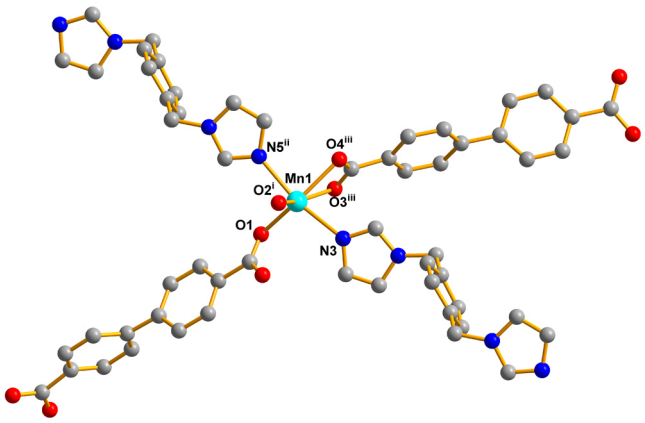

Figure S1. The coordination configuration of Mn(II) atom in crystal **1** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) -x+2, -y, -z+1; (ii) x-1, y, z; (iii) x+1/2, -y+1/2, z+1/2.

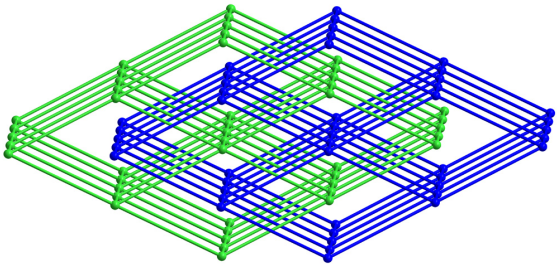

Figure S2. Two-fold interpenetrating pcu topology of crystal 1.

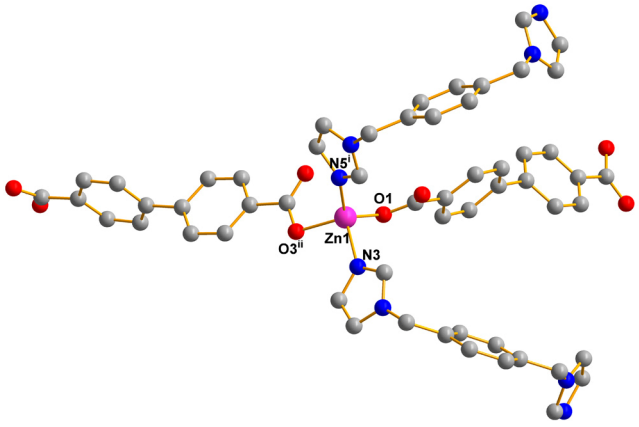

Figure S3. The coordination configuration of Zn(II) atom in crystal **2** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) x+1/2, y, -z+1/2; (ii) -x+1/2, -y, z-1/2.

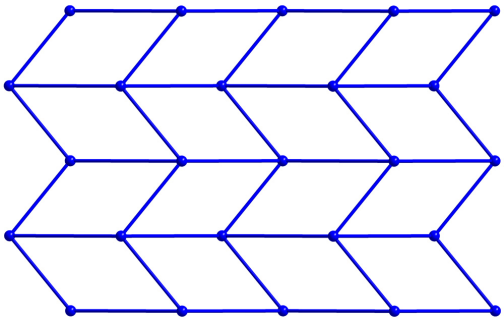

Figure S4. (4, 4) net of crystal 2.

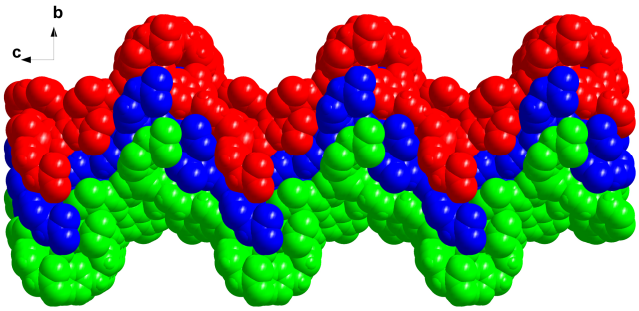

Figure S5. 3D supermolecular structure of crystal **2**.

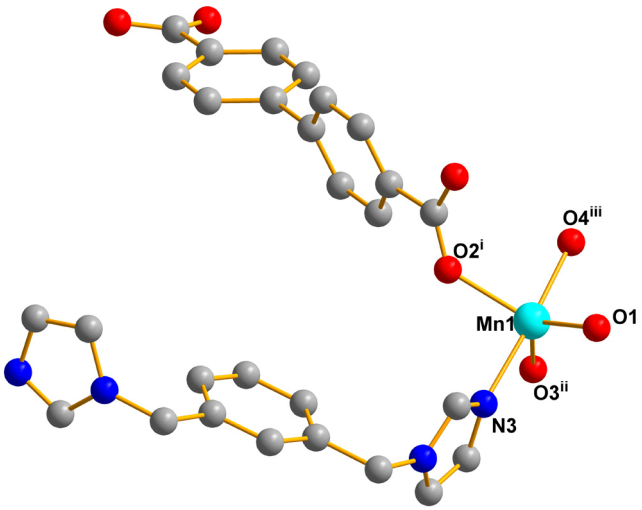

Figure S6. The coordination configuration of Mn(II) atom in crystal **4** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) -x+2, -y+1, -z; (ii) x-1/2, y-1/2, z; (iii) -x+5/2, y-1/2, -z+1/2.

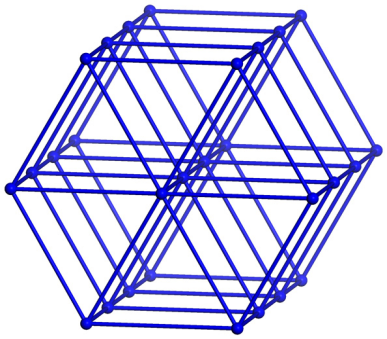

Figure S7. Hex topology of crystal **4**.

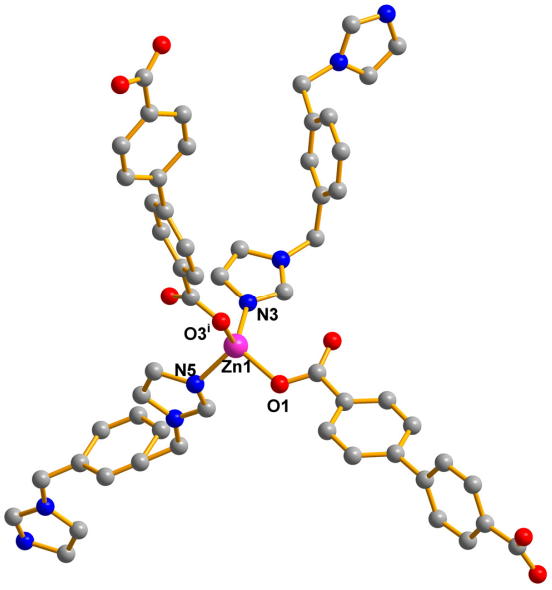

Figure S8. The coordination configuration of Zn(II) atom in crystal **5** (nitro groups of NBPDC, hydrogen atoms, and disordered atoms have been omitted for clarity). Symmetry codes: (i) x, -y-2, z+1/2.

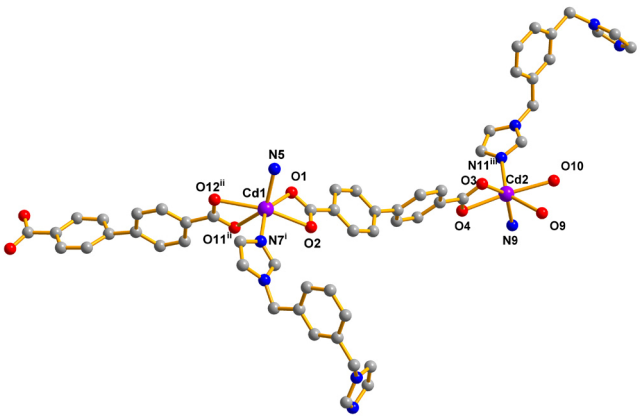

Figure S9. The coordination configuration of Cd(II) atom in crystal **6** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) x+1, y, z; (ii) x-1, y+2, z; (iii) -x, -y-1, -z+2.

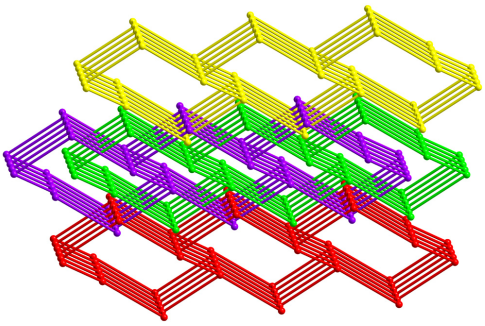

Figure S10. Four-fold interpenetrating $\{6^3\}\{6^5.8\}$ topology of crystal **6**.

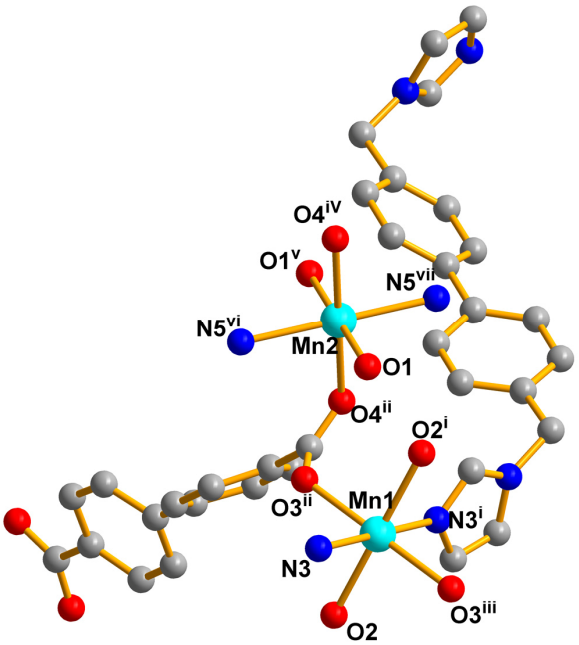

Figure S11. The coordination configuration of Mn(II) atom in crystal **7** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) -x, -y+2, -z+1; (ii) x, y-1, z; (iii) -x, -y+3, -z+1; (iv) -x-1, -y+3, -z+1; (v) -x-1, -y+2, -z+1; (vi) x+1, -y+3/2, z+1/2; (vii) -x-2, y+1/2, -z+1/2.

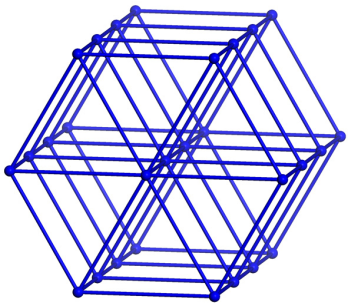

Figure S12. Hex topology of crystal **7**.

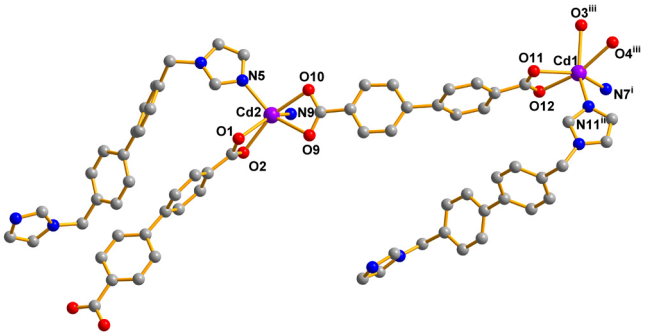

Figure S13. The coordination configuration of Cd(II) atom in crystal **8** (nitro groups of NBPDC, and hydrogen atoms have been omitted for clarity). Symmetry codes: (i) x-1, y+1, z-1; (ii) x-1, y, z; (iii) x, y+1, z-1.

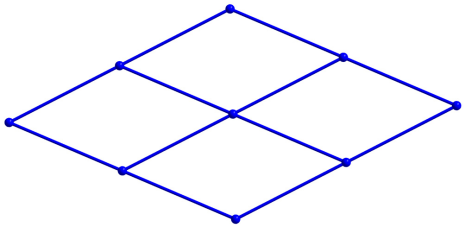

Figure S14. (4, 4) topology of crystal **8**.

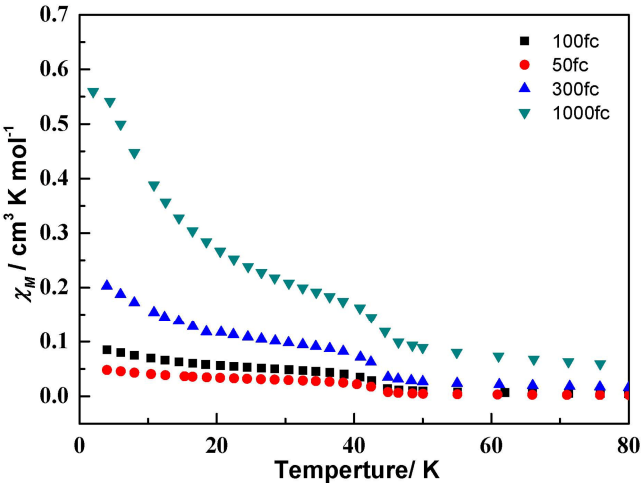

Figure S15. Plots of temperature dependence of χm at different fields at 2-80 K.of **1**.

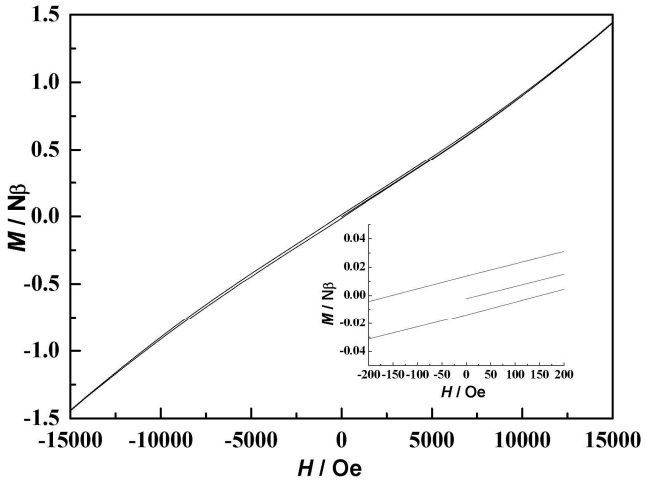

Figure S16. The hysteresis loop of **1** measured at 2 K in the ±1.5 T range.

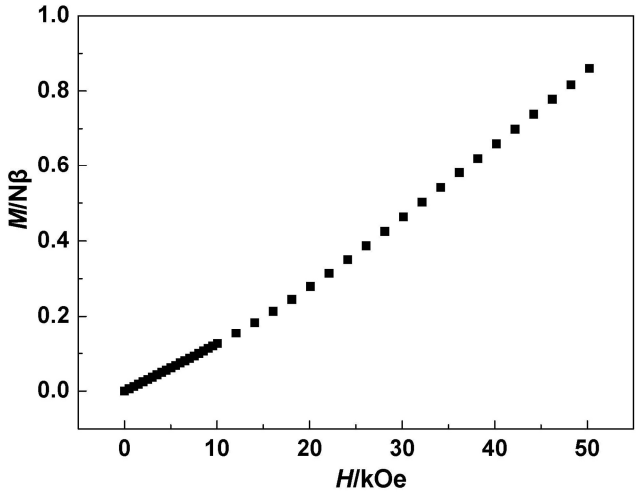

Figure S17. Plots of the magnetization (M) vs H of **4** at 2 K.

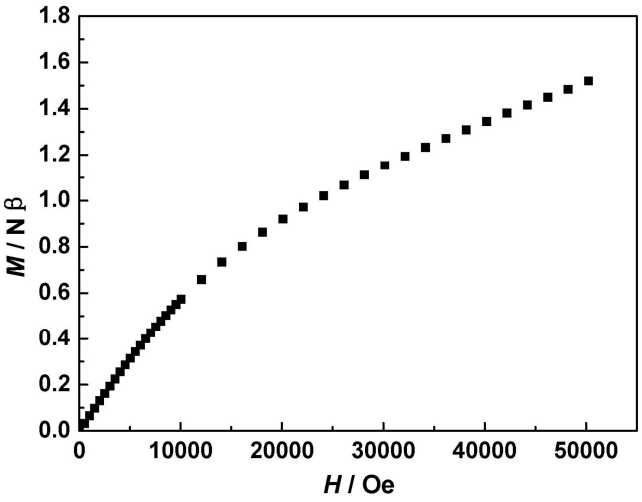

Figure S18. Plots of the magnetization (M) vs H of **7** at 2 K.

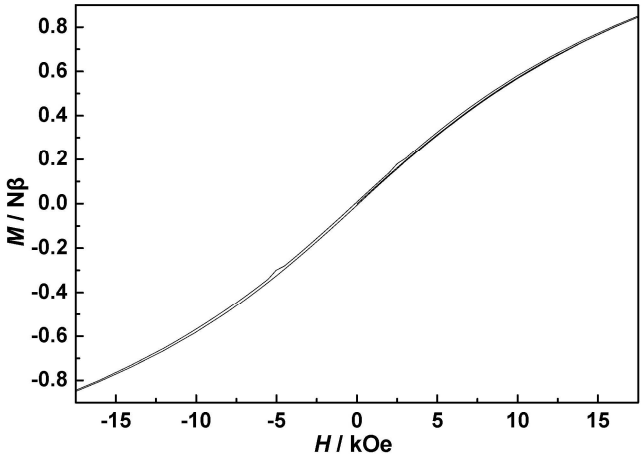

Figure S19. The hysteresis loop of **7** measured at 2 K in the ±1.5 T range.

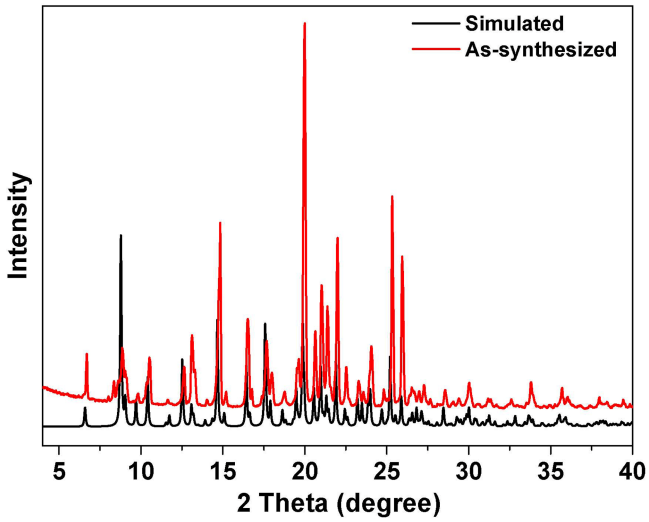

Figure S20. The XRD Figure of compound **1**.

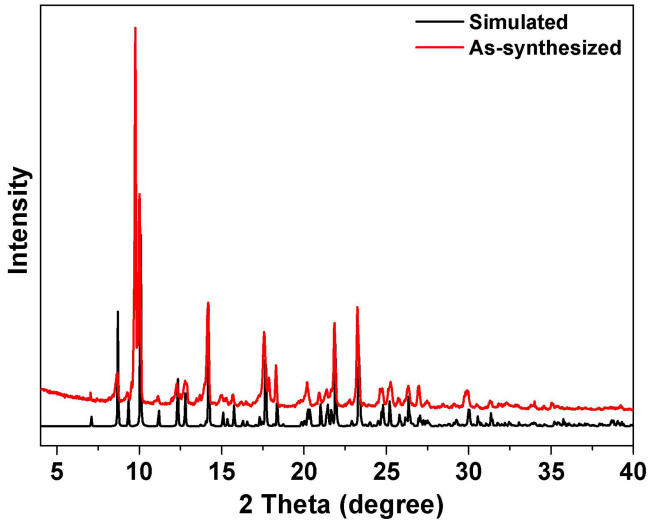

Figure S21. The XRD Figure of compound **2**.

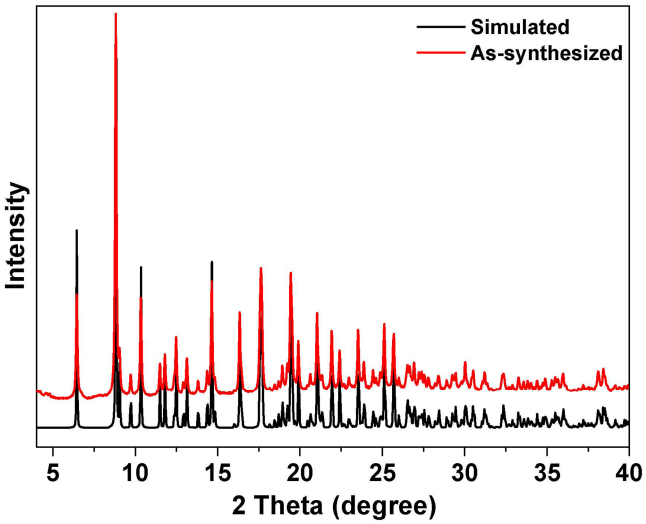

Figure S22. The XRD Figure of compound **3**.

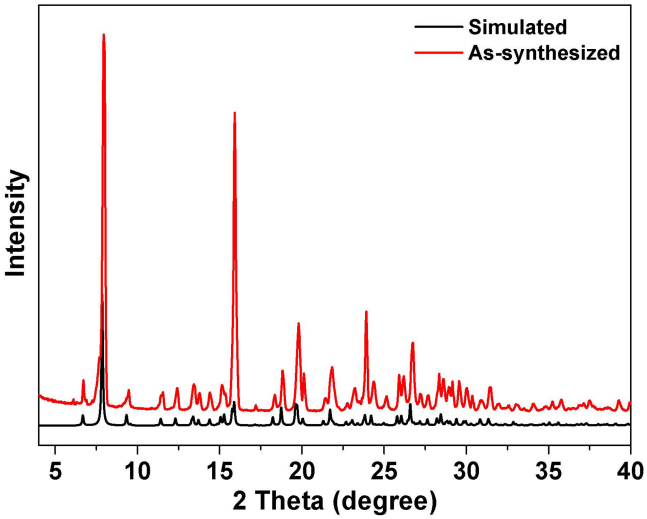

Figure S23. The XRD Figure of compound **4**.

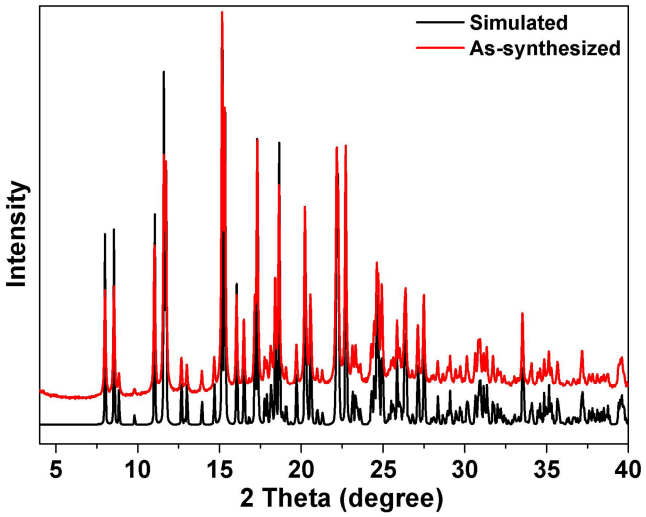

Figure S24. The XRD Figure of compound **5**.

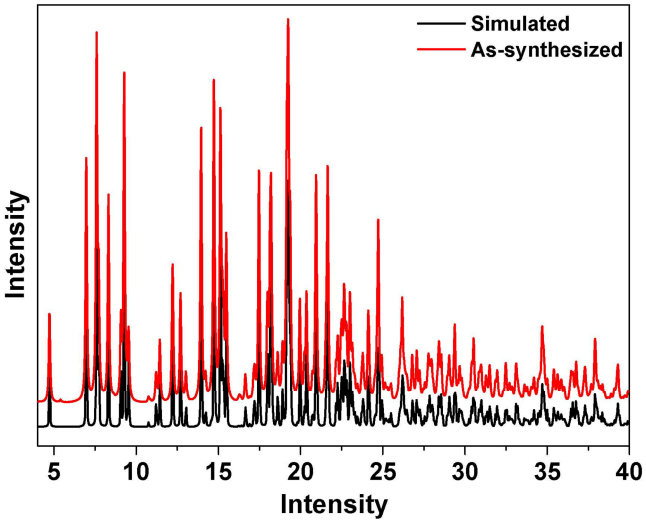

Figure S25. The XRD Figure of compound **6**.

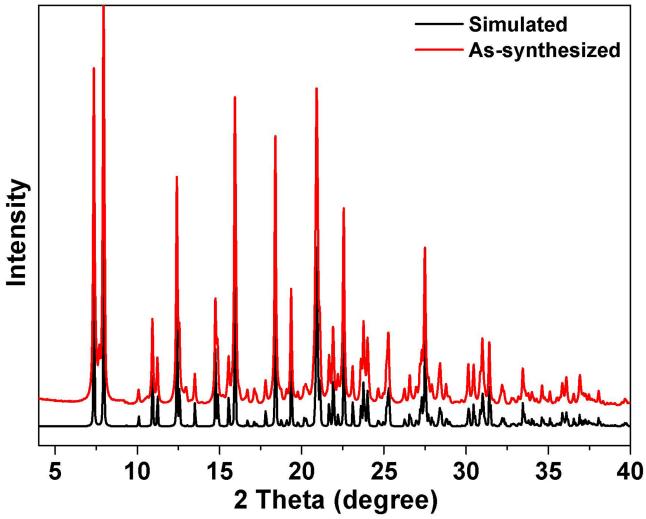

Figure S26. The XRD Figure of compound **7**.

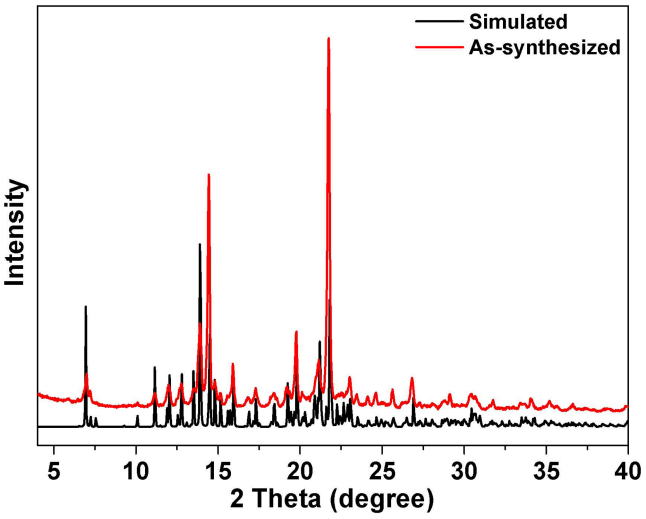

Figure S27. The XRD Figure of compound **8**.

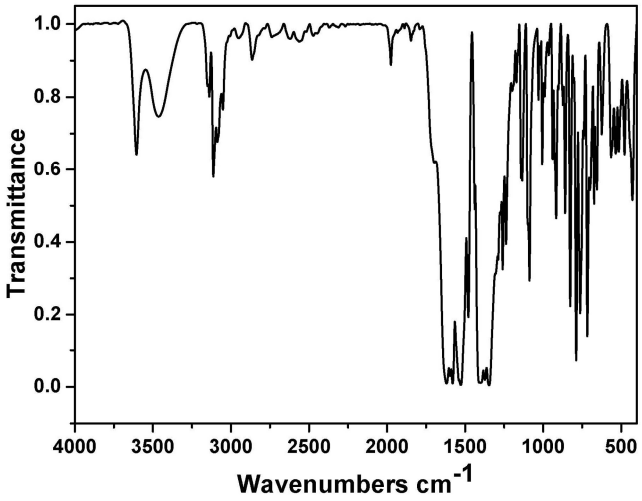

Figure S28. IR figure of compound **1**.

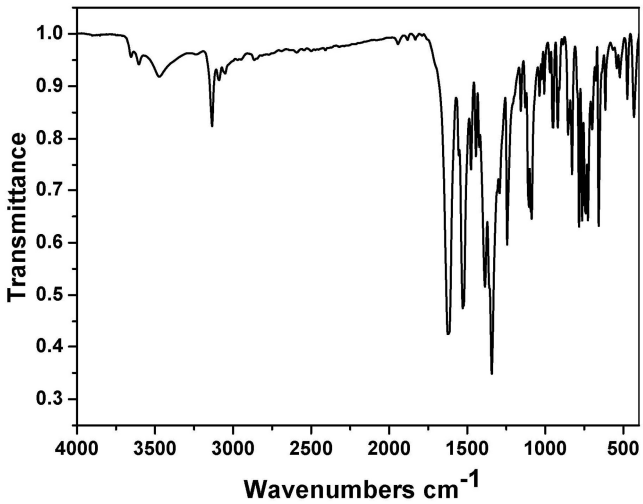

Figure S29. IR figure of compound **2**.

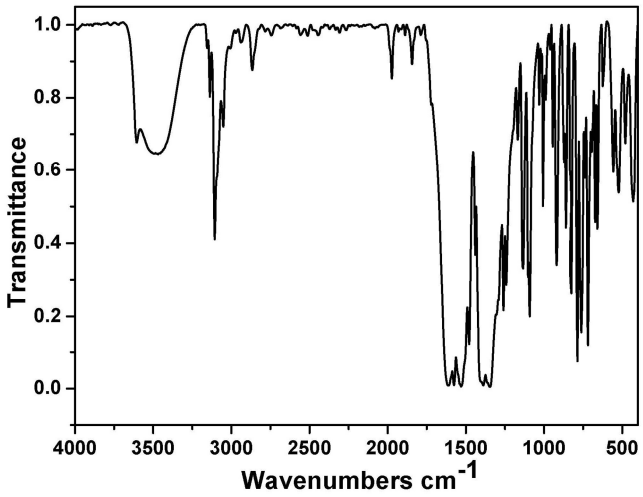

Figure S30. IR figure of compound **3**.

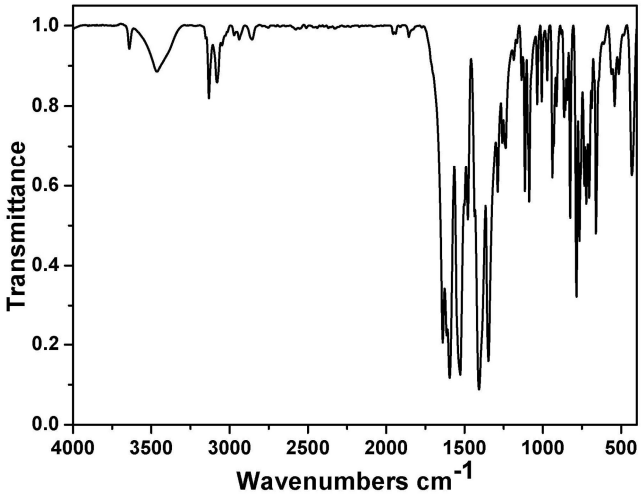

Figure S31. IR figure of compound **4**.

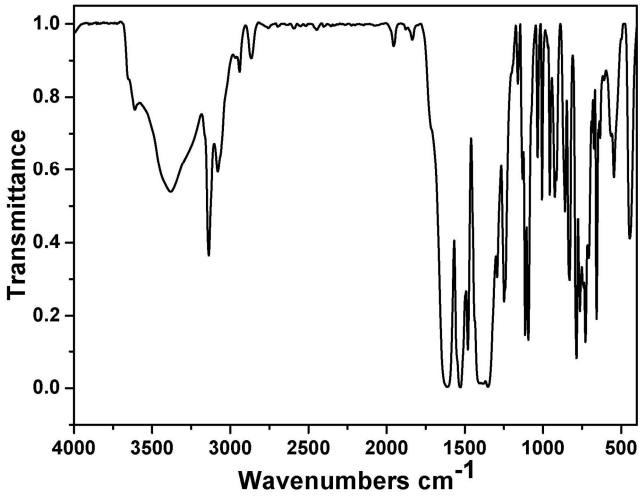

Figure S32. IR figure of compound **5**.

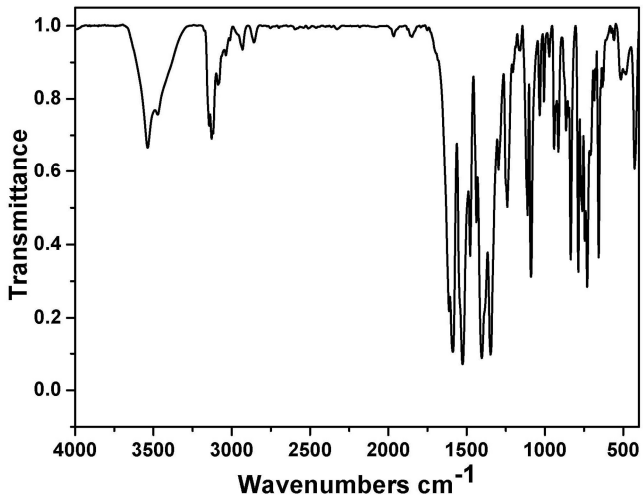

Figure S33. IR figure of compound **6**

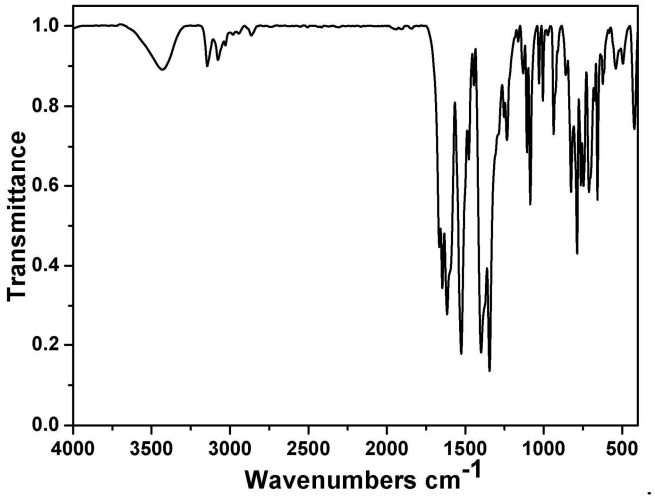

Figure S34. IR figure of compound **7**

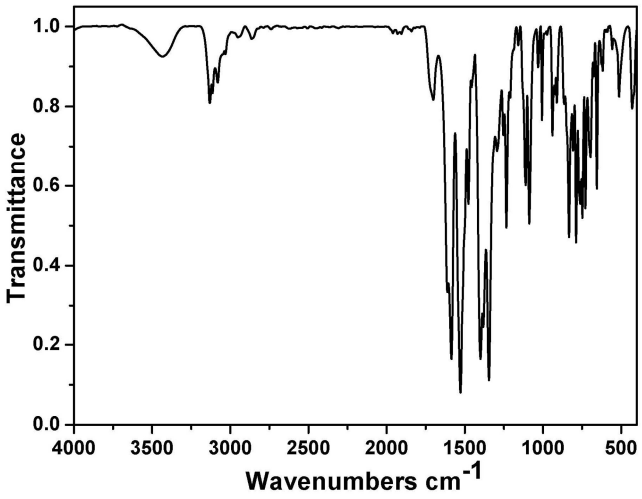

Figure S35. IR figure of compound **8**

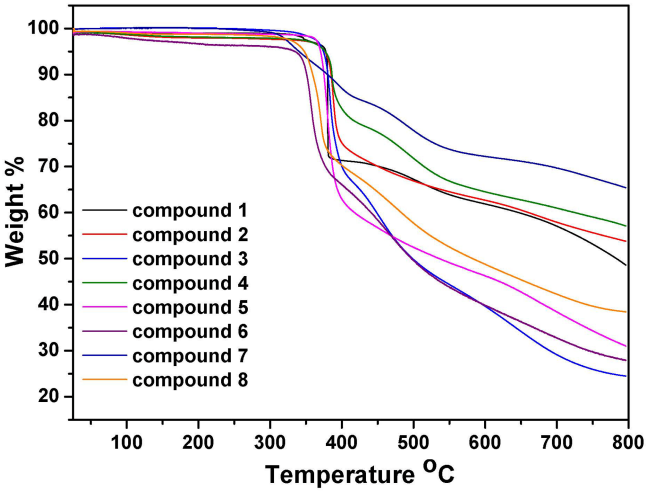

Figure S36. TG figure of compound **1-8**.

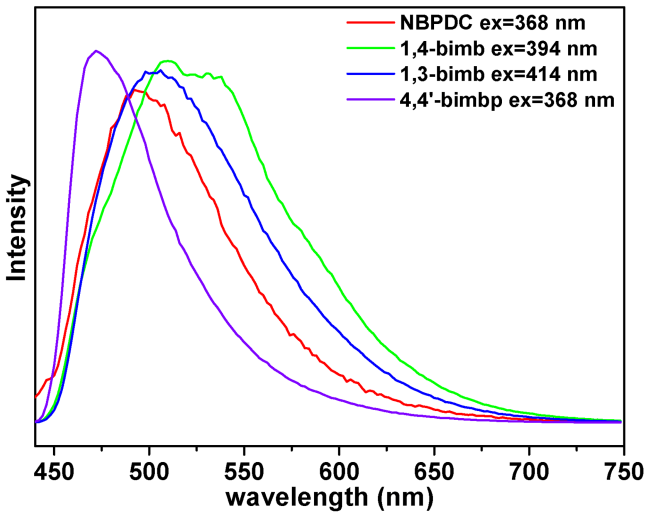

Figure S37. Emission spectra of the free ligands.

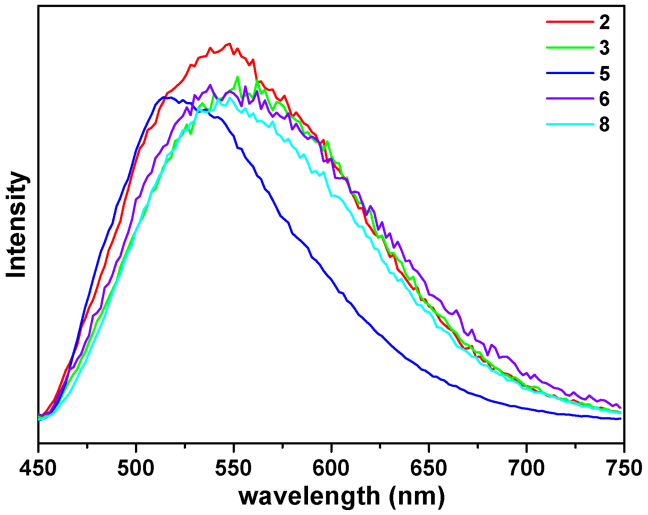

Figure S38. Emission spectra of **2**, **3**, **5**, **6**, **8**.

The photoluminescent properties of compounds **2, 3, 5, 6, 8** and the free ligands have been studied in the solid state at room temperature (Figure S37 and S38). The photoluminescent spectrum of coordination polymers are measured upon excitation at 430 nm. The emissions of coordination polymers may be due to the intraligand charge transfer (ILCT) of organic ligands.[1]

Reference

1 (a) H. Y. Bai, J. F. Ma, J. Yang, L. P. Zhang, J. C. Ma and Y. Y. Liu, *Cryst. Growth Des.* 2010, **10**, 1946; (b) J. G. Lin, S. Q. Zang, Z. F. Tian, Y. Z. Li, Y. Y. Xu, H. Z. Zhu and Q. J. Meng, *CrystEngComm* 2007, **9**, 915.