Electronic Supplementary Material (ESI) for CrystEngComm

Co-crystal of $[CuCl_4]^{2-}$ and L1 and its inclusion compounds with three different guests (L1 = N, N, N′, N′ - tetra-p-methoxybenzyl – ethylenediamine)

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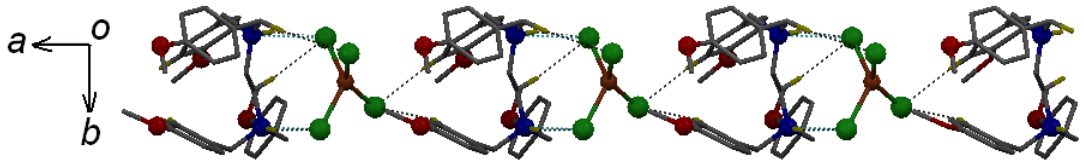
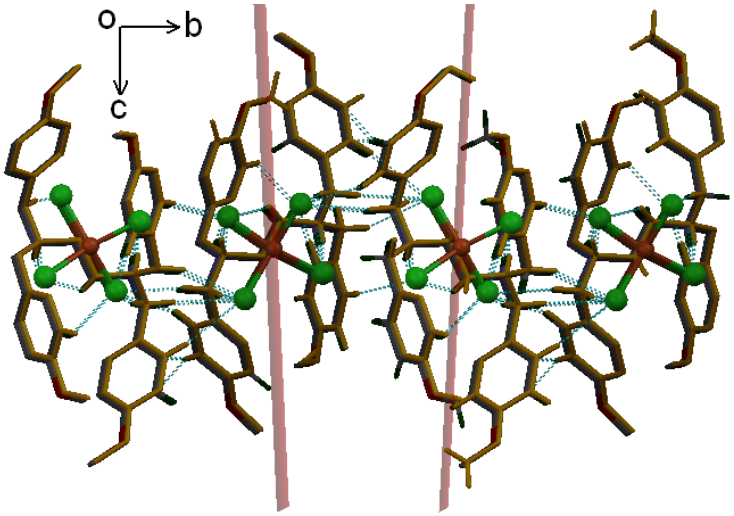


(a)



(b)

Fig.S1 Crystal 3: (a) Linear $\{[H_2L1]^{2+}\cdot[CuCl_4]^{2-}\}_n$ polymer chains. (b) The 2D layers, (c) The adjacent chains (running into the page) in **3** are arranged with a dihedral angle of 21 º.

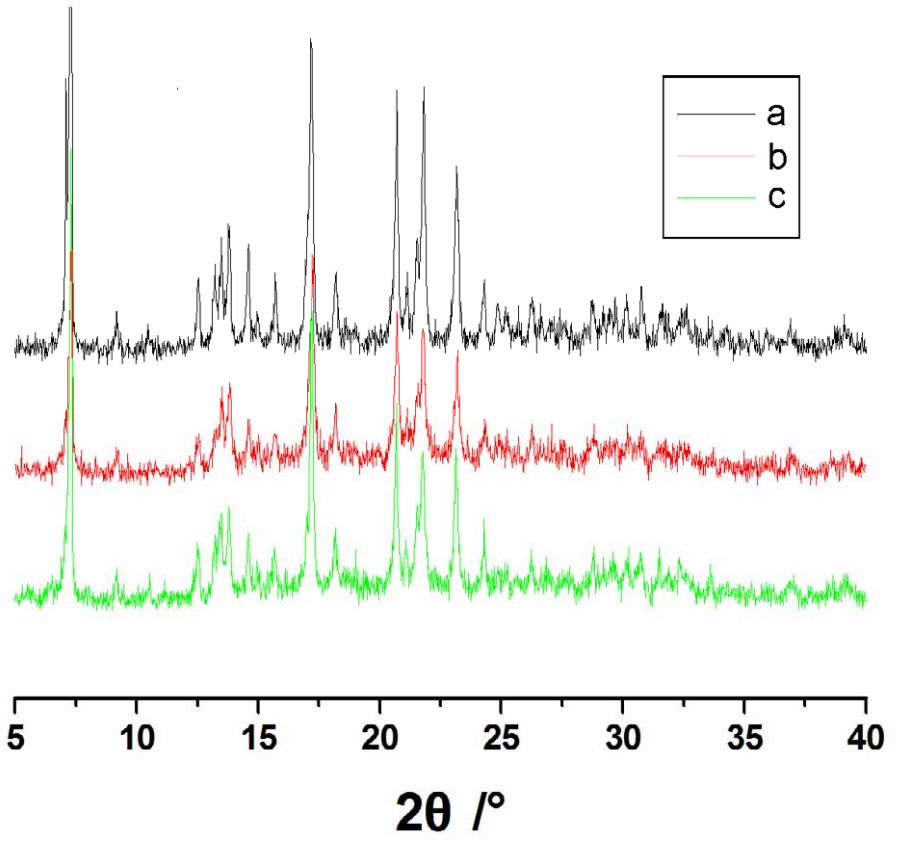


Fig. S2 Comparison of the powder X-ray diffraction patterns of the solid products by adding benzene (a) or toluene (b) and (c) PXRD patters for crystal 1, indicating that the inclusion property is size-selective, benzene or toluene cannot be included.

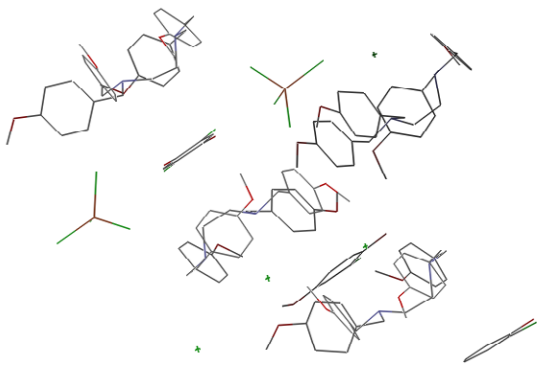
The inclusion compound with guest of hydroquinone

Experiment:

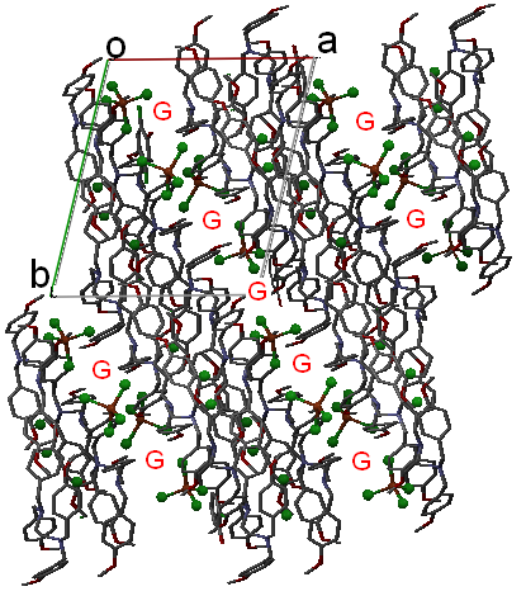
0.0662g L1, 10 mL methanol, 0.0436 g CuCl2·2H2O, and 1 mL concentrated hydrochloric acid were added into a 50mL Erlenmeyer flask, then 0.0241 g hydroquinone were added and shaken until the contents were dissolved. The flask was allowed to stand for about 2-3 days at room temperature, producing yellow and block crystals. Powder X-ray diffraction and melting point indicate the crystallization of crystal **1**. Another 2.5 mL hydrochloric acid was added, and the crystals were dissolved and recrystallized for twice or three times. The flask was allowed to stand for nearly one month, giving dark brown and flake crystals. m.p. 117-122 ºC.

IR (KBr), $\bar{\upsilon}_{max}$ /cm^{-1}: 3458(s,OH), 2096 (w, ArH), 2837, 2551(m,N^{+}H), 2933 (w, CH_2), 2957(w, CH_3), 1612, 1515, 1458 (s, Ar),1255,1032 (s, O-C). ^{1}H NMR (DMSO, 300 MHz) δ: 3.366 (4H, s, CH_2), 3.776 (12H, s, -OCH_3), 4.165 (8H, s, CH_2), 6.88~7.42 (24H, overlapped, 16H from ArH of L1 and 8H from ArH of hydroquinon**)** , 11.271(2H, s, N^{+}H).

The product complex tends to be amorphous. The poor crystal quality made the structure determination difficult, in which the obscure structure can be roughly seen from one solution. X-ray crystallography revealed that the structure crystallizes as a triclinic crystal system, and the space group is Pī. One asymmetric unit contains two dianion $[CuCl_4]^{2-}$, four doubly protonated **L1**, four anions of Cl^{-}, two molecules of 2,5-dichloride - hydroquinon, and one molecules of hydroquinon.



(a)



(b)

Fig. S3 The inclusion compound with guest of hydroquinone. (a) Structure of one asymmetric unit. (b) structural packing of the inclusion complex viewed along c axis.