Supplementary Material (ESI) for Dalton Transactions

Electronic Supplementary Information

Diverse structures and adsorption properties of quasi-Werner-type copper(II) complexes with flexible and polar axial bonds

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Experimental Section

SEM. Scanning electron microscopy (SEM) observations were performed with a JEOL Model JSM-6510 SEM system operating at 1 kV. Dried samples were deposited on carbon tape.

Table S1. Selected Bond Distances (Å) for α-[$Cu(PF_6)_2$(4-mepy)$_4$] (α-**1**) and {[Ni(4-mepy)$_4$]·$2PF_6$}.

α-**1**			
P(1)–F(1)[a]	1.632(2)	P(1)–F(2)	1.598(2)
P(1)–F(3)	1.570(3)	P(1)–F(4)	1.581(3)
P(1)–F(5)	1.575(2)	P(1)–F(6)	1.571(2)
P(2)–F(7)[a]	1.622(2)	P(2)–F(8)	1.572(2)
P(2)–F(9)	1.588(3)	P(2)–F(10)	1.580(2)
P(2)–F(11)	1.509(2)	P(2)–F(12)	1.564(2)
P(3)–F(13)[a]	1.627(2)	P(3)–F(14)	1.581(2)
P(3)–F(15)	1.582(2)	P(3)–F(16)	1.591(2)
P(3)–F(17)	1.589(3)	P(3)–F(18)	1.583(2)
P(4)–F(19)[a]	1.630(2)	P(4)–F(20)	1.587(2)
P(4)–F(21)	1.579(2)	P(4)–F(22)	1.578(2)
P(4)–F(23)	1.579(3)	P(4)–F(24)	1.585(3)
{[Ni(4-mepy)$_4$]·$2PF_6$}			
P–F(1)[a]	1.588(8)	P–F(2)	1.556(9)
P–F(3)	1.567(11)	P–F(4)	1.466(12)
P–F(5)	1.593(13)	P–F(6)	1.543(9)

[a] These F atoms are located on the axial sites of each metal ion.

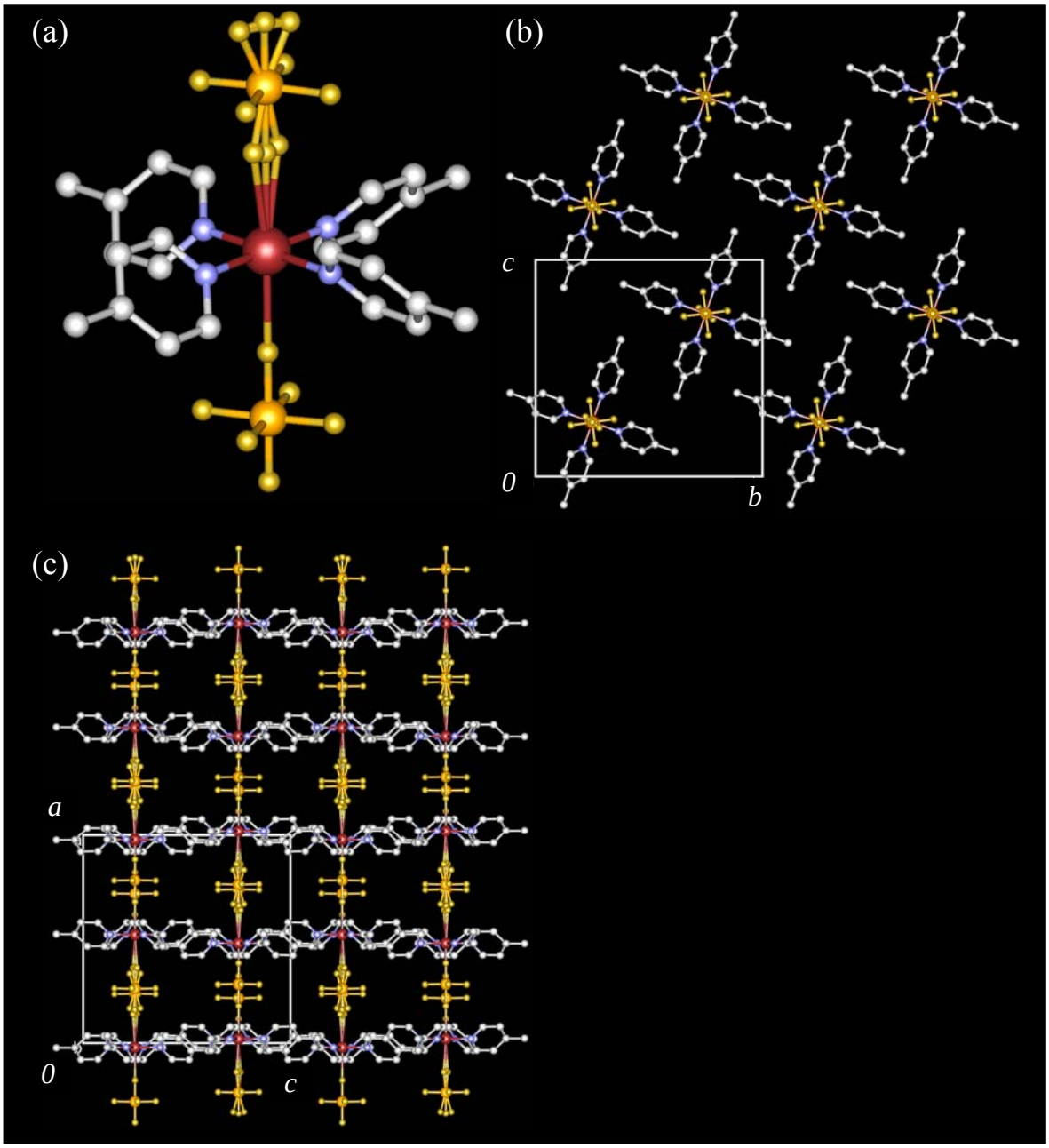
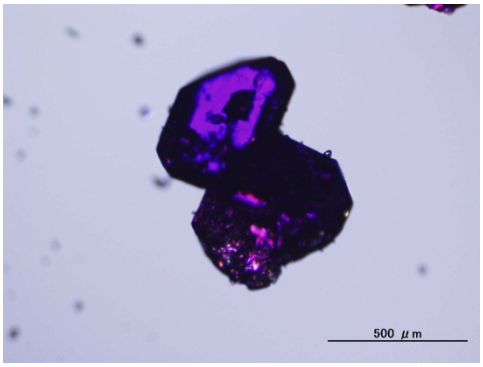
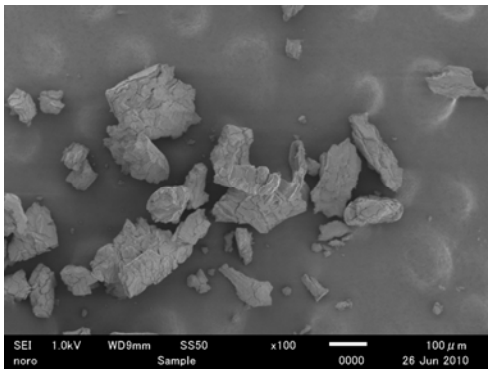


Fig. S1. Crystal structure of γ-**1**⊃2benzene: (a) the molecular structures, (b) the sheet arrangement in the projection along the *a*-axis, and (c) the packing view in the projection along the *b*-axis. The hydrogen atoms and benzene guests are omitted for clarity.

(a)



(b)



(c)

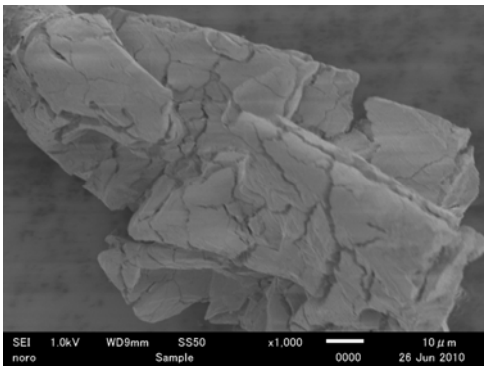


Fig. S2. Morphology of crystals in (a, optical microscope image) α-**1** and (b and c, SEM images) α-**1'**.

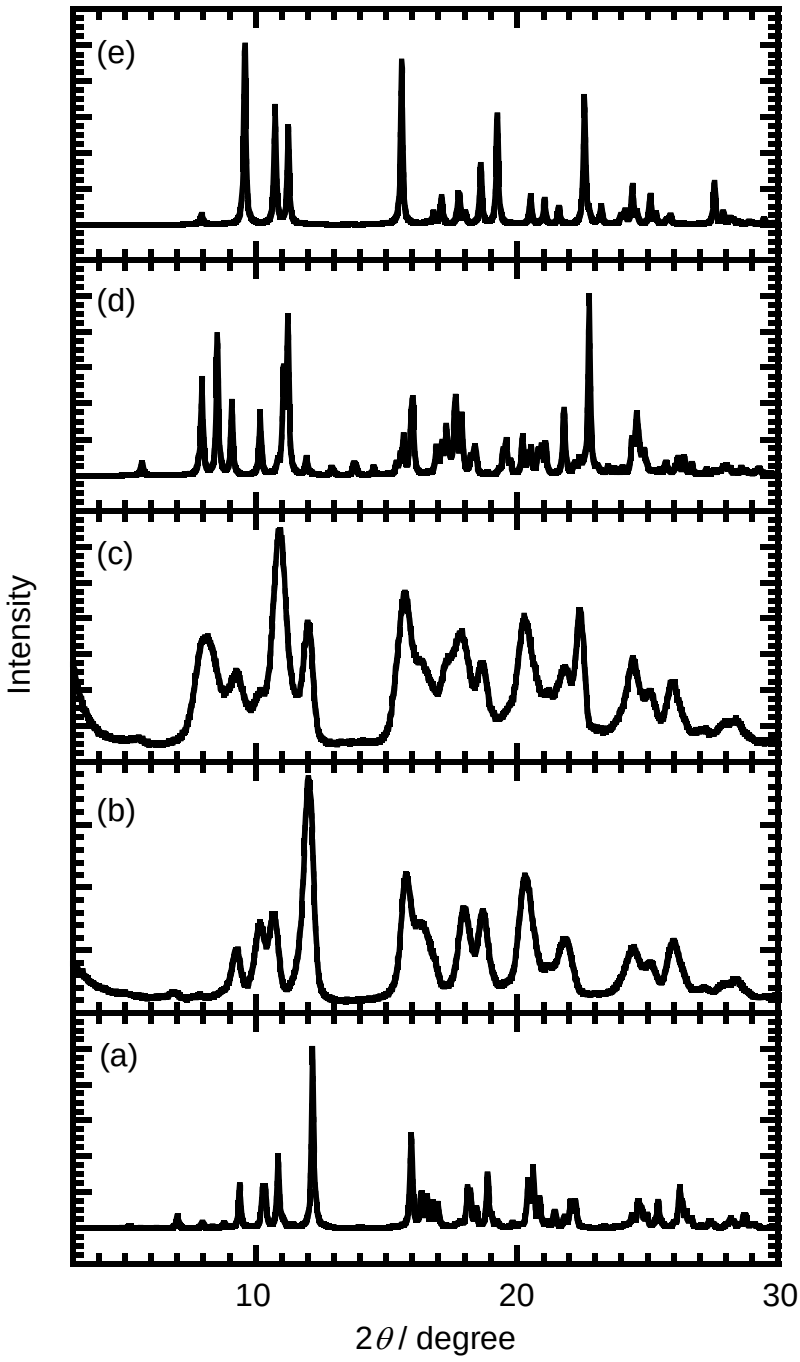


Fig. S3. XRD patterns of (a) simulated α-**1** from single-crystal analysis, (b) α-**1'**, (c) γ-**1**⊃2benzene, which was obtained by an exposure of α-**1** to a benzene vapor for 4 hours, and (d and e) simulated γ-**1**⊃0.5H_2O·2benzene (d) and γ-**1**⊃2benzene (e) from single-crystal analysis. During the XRD measurement of γ-**1**⊃2benzene, some guest benzene molecules may be removed from the sample, which is the reason why the XRD pattern of γ-**1**⊃2benzene is not consistent with that of simulated γ-**1**⊃2benzene from single-crystal analysis.

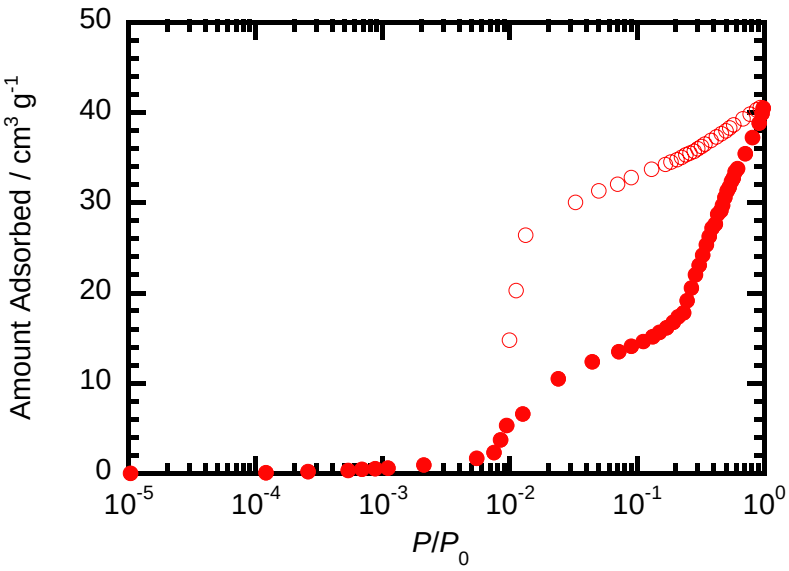


Fig. S4. Adsorption (filled symbols) and desorption (open symbols) isotherms for CO_2 gas in α-**1'** at 195 K plotted against a logarithmic relative pressure.