magnetochemistry

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Supplementary Materials

One-dimensional chain-type Dicopper Coordination Polymer Linked by 1,4-Di(4-pyridyl)benzene; Synthesis, Crystal Structure, Magnetic Property, and Gas-adsorption Property

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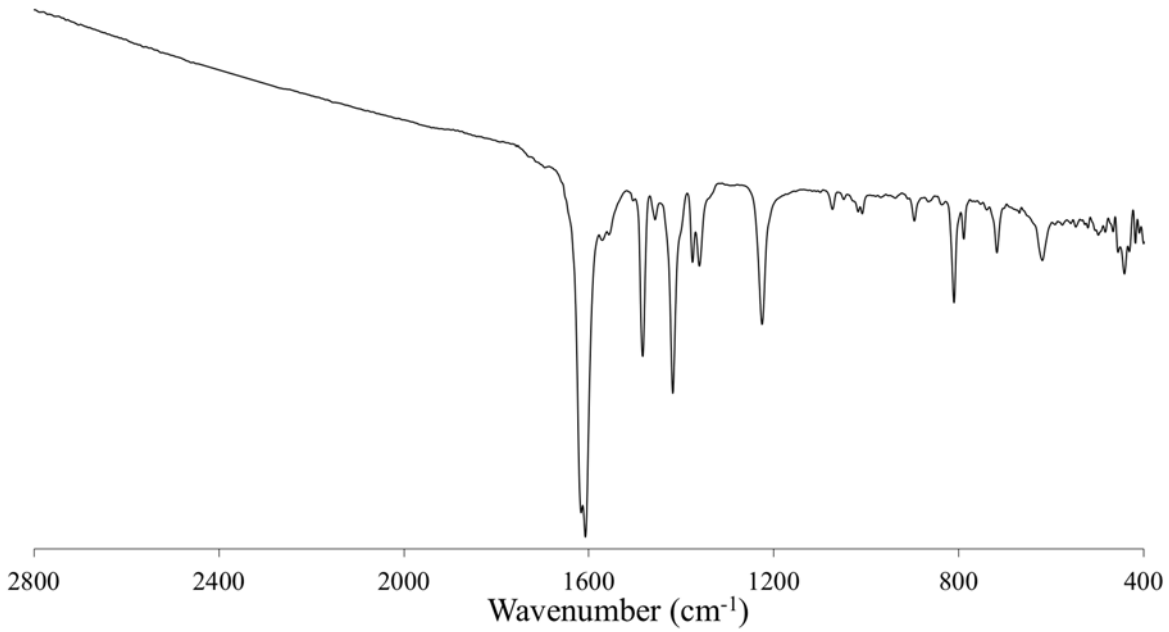

Figure S1. IR spectrum of **1** (in KBr) at 300 K.

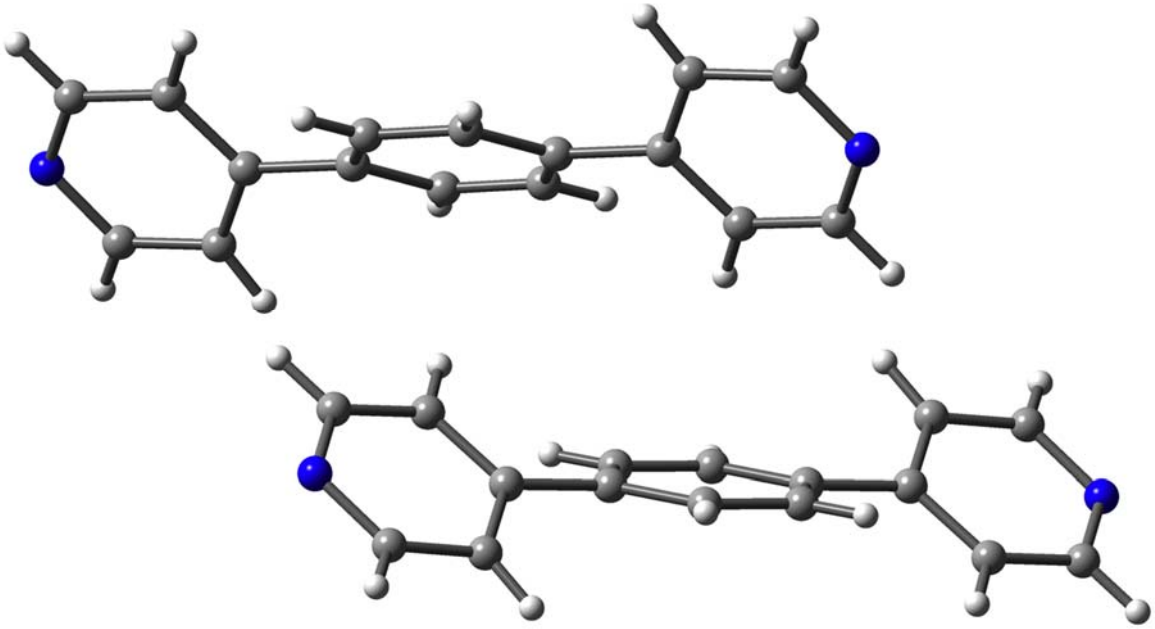

Figure S2. Calculated model structure of two dpybz ligands. (Here, blue, gray, and white colors are nitrogen, carbon, and hydrogen atoms, respectively.)

Table S1. Crystallographic data of **1**.

Complex	**1**
Formula	$C_{18}H_{24}CuNO_4$
M_r (g mol^{-1})	381.92
Crystal system	Monoclinic
Space group	*C* 2/*c*
a (Å)	24.149(3)
b (Å)	17.969(2)
c (Å)	10.4091(12)
α (°)	90
β (°)	90.560(3)
γ (°)	90
V (Å^3)	4516.6(9)
Z	8
D_{calc} (g cm^{-3})	1.123
μ (mm^{-1})	0.983
F(000)	1600.0
R_1, wR_2 ($I > 2\sigma(I)$)	0.0525, 0.1376
R_1, wR_2 (all data)	0.0652, 0.1478
GOF on F^2	1.088
CCDC No.	1841609

Table S2. Selected bond lengths (Å) and angles (°) of crystal structure of **1**.

Bond lengths (Å)			
Cu1-Cu1	2.5938(6)	C1-C2	1.537(4)
Cu1-O3	1.959(2)	C6-O4	1.254(3)
Cu1-O1	1.963(2)	C6-C7	1.531(4)
Cu1-O4	1.966(2)	C11-C12	1.389(4)
Cu1-O2	1.968(2)	C12-C13	1.383(4)
Cu1-N1	2.156(2)	C13-C14	1.392(4)
O1-C1	1.257(3)	C13-C16	1.487(3)
O2-C1	1.254(3)	C14-C15	1.381(4)
O3-C6	1.252(4)	C16-C17	1.395(4)
O4-C6	1.254(3)	C16-C18	1.403(4)
N1-C11	1.327(4)	C17-C18	1.386(3)
N1-C15	1.335(3)		
Bond angles (°)			
O3–Cu1–O1	91.18(11)	C11–N1–Cu1	119.96(17)
O3–Cu1–O4	169.10(8)	C15–N1–Cu1	121.95(18)
O1–Cu1–O4	87.70(11)	O2–C1–O1	124.6(3)
O3–Cu1–O2	88.08(11)	O2–C1–C2	117.5(2)
O1–Cu1–O2	169.17(8)	O1–C1–C2	117.7(2)
O4–Cu1–O2	90.98(11)	O3–C6–O4	124.8(3)
O3–Cu1–N1	95.67(9)	O3–C6–O7	117.6(3)
O1–Cu1–N1	96.12(8)	O4–C6–O7	117.6(3)
O4–Cu1–N1	95.23(9)	N1–C11–C12	122.9(2)
O2–Cu1–N1	94.70(8)	C13–C12–C11	119.6(3)
O3–Cu1–Cu1	84.08(6)	C12–C13–C14	117.3(2)
O1–Cu1–Cu1	84.96(6)	C12–C13–C16	120.9(2)
O4–Cu1–Cu1	85.02(6)	C14–C13–C16	121.8(2)
O2–Cu1–Cu1	84.22(6)	C15–C14–C13	119.4(2)
N1–Cu1–Cu1	178.89(6)	N1–C15–C14	123.0(3)
C1–O1–Cu1	122.65(19)	C17–C16–C18	118.7(2)
C1–O2–Cu1	123.31(18)	C17–C16–C13	120.8(2)
C6–O3–Cu1	123.74(19)	C18–C16–C13	120.5(2)
C6–O4–Cu1	122.2(2)	C18–C17–C16	120.9(2)
C11–N1–C15	117.8(2)	C17–C18–C16	120.4(2)