Supplementary Materials: Synthesis, Crystal Structure, Luminescence and Magnetism of Three Novel Coordination Polymers Based on Flexible Multicarboxylate Zwitterionic Ligand

Yulu Ma, Lin Du, Kaimin Wang and Qihua Zhao

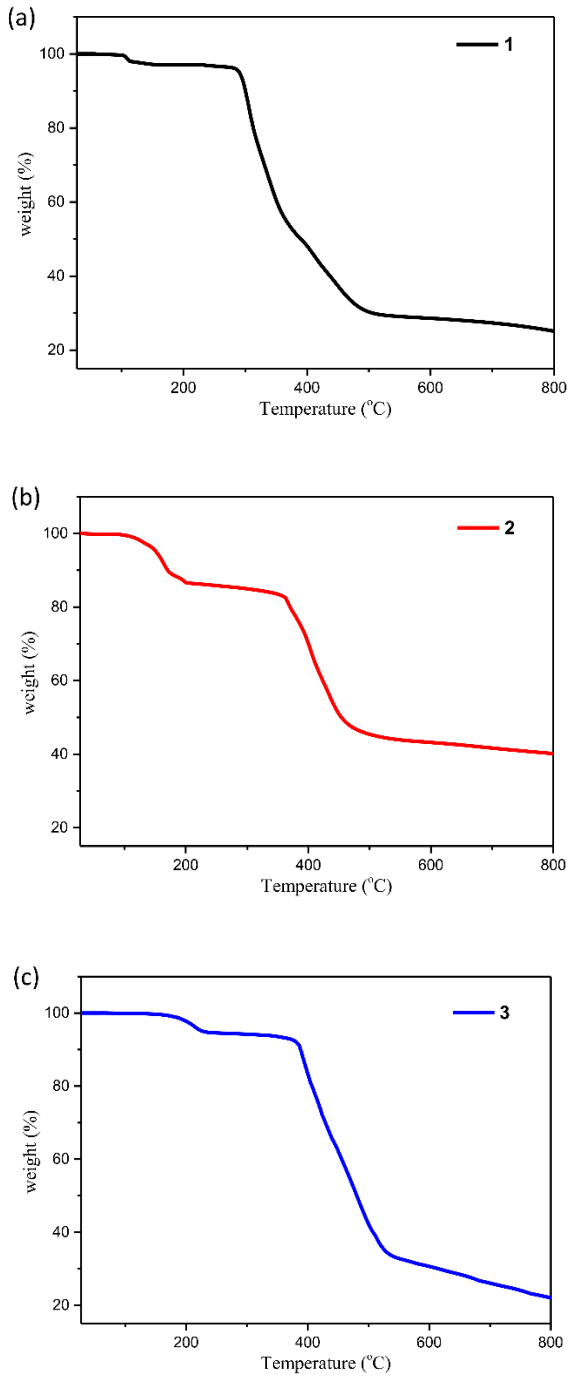


Figure S1. (**a**) The TGA curves of compound **1**; (**b**) The TGA curves of compound **2**; (**c**) The TGA curves of compound **3**.

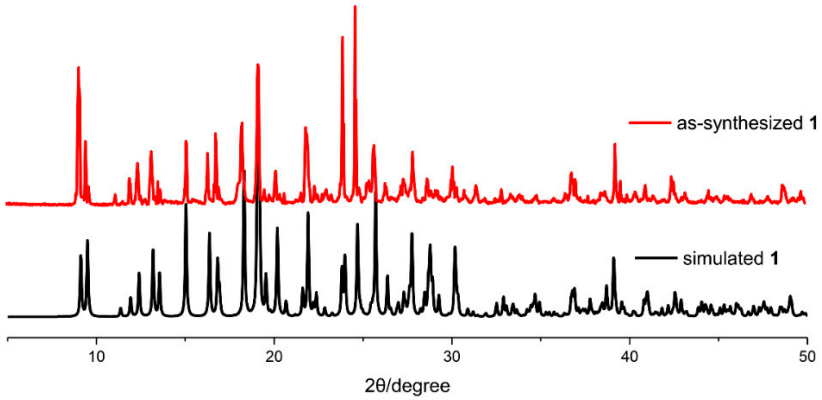


Figure S2. The PXRD experimental and as-simulated patterns of compound **1**.

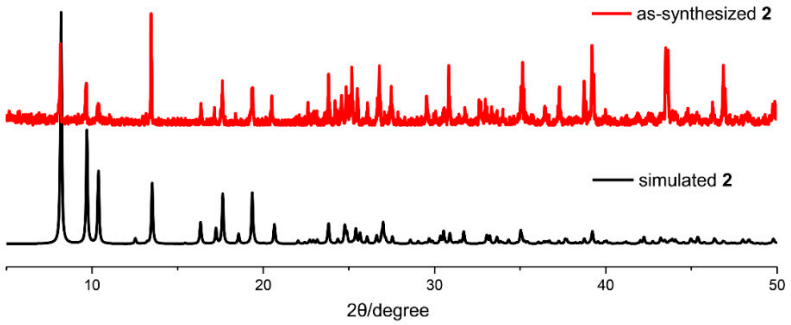


Figure S3. The PXRD experimental and as-simulated patterns of compound **2**.

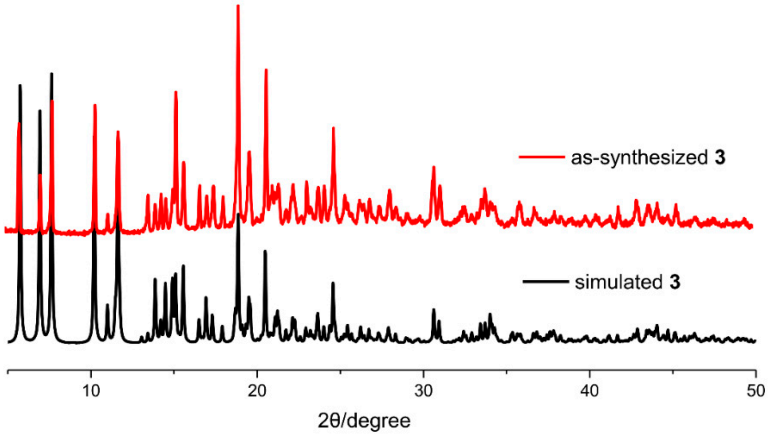


Figure S4. The PXRD experimental and as-simulated patterns of compound **3**.

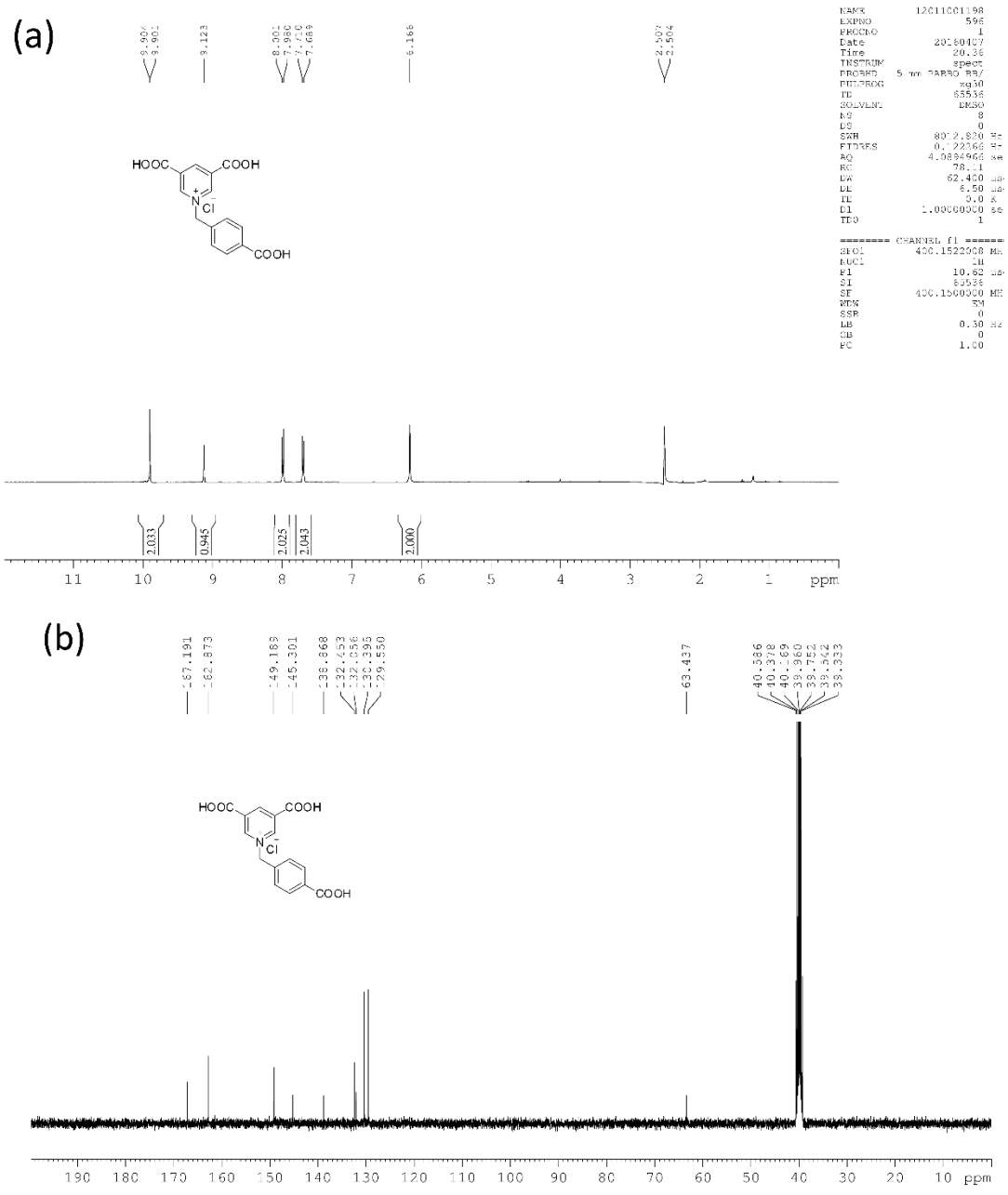
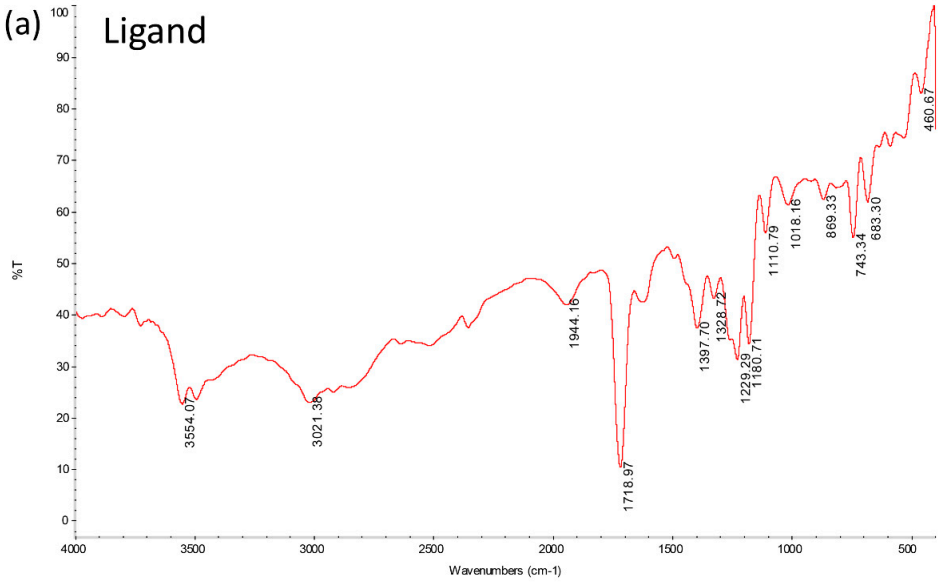
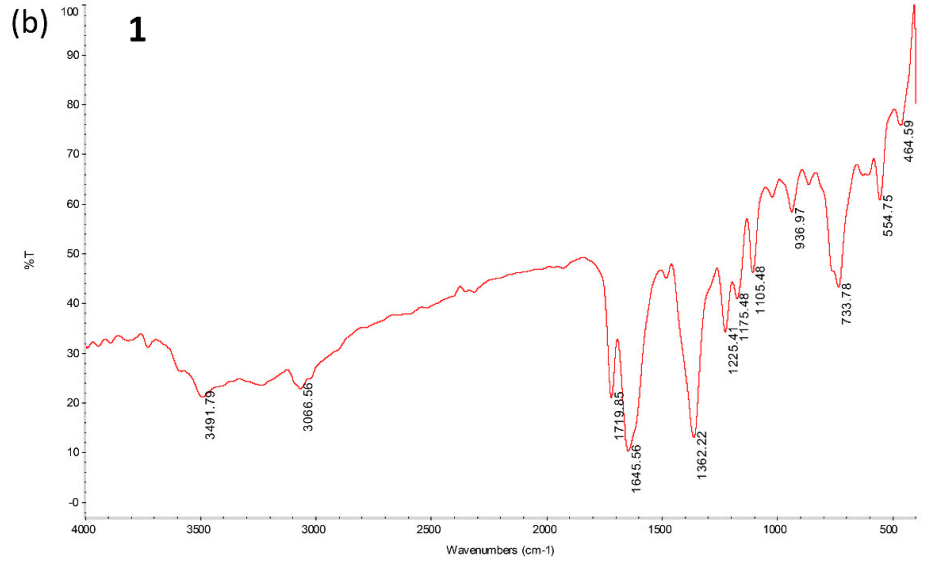
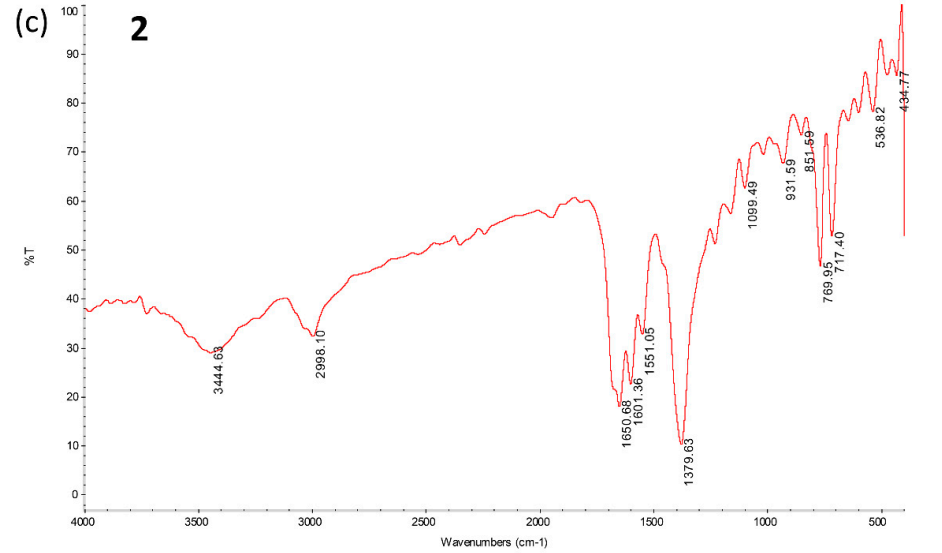


Figure S5. (**a**) ^{1}H NMR (400 Hz, DMSO-*d*6) spectra of H_3CbdcpCl, (**b**) ^{13}C NMR (100 Hz, DMSO-*d*6) spectra of H_3CbdcpCl.


(a)
Ligand
%T
Wavenumbers (cm-1)
3554.07
3021.38
1944.16
1718.97
1397.70
1328.72
1229.29
1180.71
1110.79
1018.16
869.33
743.34
683.30
460.67


(b)
1
%T
Wavenumbers (cm-1)
3491.79
3066.56
1719.85
1645.56
1362.22
1225.41
1175.48
1105.48
936.97
733.78
554.75
464.59


(c)
2
%T
Wavenumbers (cm-1)
3444.63
2998.10
1650.68
1601.36
1551.05
1379.63
1099.49
931.59
851.59
769.95
717.40
536.82
434.77

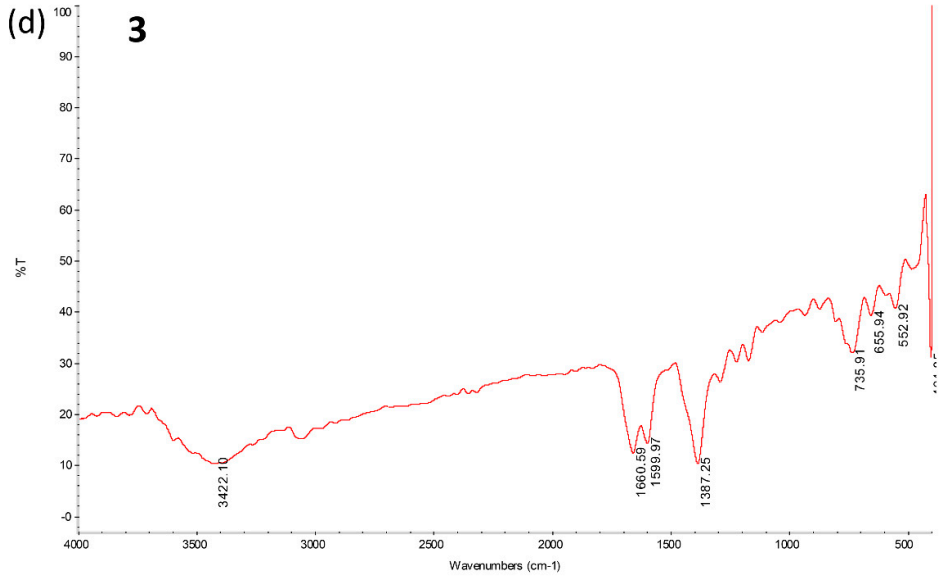


Figure S6. (**a**) The IR spectra of ligand H_3CbdcpCl; (**b**) The IR spectra of complex **1**; (**c**) The IR spectra of complex **2**; (**d**) The IR spectra of complex **3**.

Table S1. Bond lengths (Å) and angles (°) for **1**–**3**.

Bond Lengths (Å) for 1					
Zn(1)-O(7)	1.953(3)	O(3)-C(7)	1.244(4)	N(1)-C(4)	1.344(4)
Zn(1)-O(1)	1.958(3)	O(4)-C(7)	1.265(4)	N(1)-C(3)	1.358(4)
Zn(1)-O(10)	1.965(3)	O(5)-C(15)	1.229(5)	N(1)-C(8)	1.503(4)
Zn(1)-O(4)A	1.992(3)	O(6)-C(15)	1.343(5)	N(2)-C(18)	1.339(4)
O(4)-Zn(1)C	1.992(3)	O(7)-C(21)	1.276(4)	N(2)-C(19)	1.353(4)
O(1)-C(6)	1.280(4)	O(8)-C(21)	1.232(4)	N(2)-C(23)	1.502(4)
O(2)-C(6)	1.227(5)	O(9)-C(22)	1.237(4)	C(1)-C(5)	1.380(5)
Bond Angles (°) for 1					
O(7)-Zn(1)-O(1)	101.65(11)	C(7)-O(4)-Zn(1)C	116.6(2)	C(4)-N(1)-C(3)	121.6(3)
O(7)-Zn(1)-O(10)	115.91(11)	N(2)-C(18)-C(17)	119.9(3)	C(4)-N(1)-C(8)	118.8(3)
O(1)-Zn(1)-O(10)	111.87(12)	N(2)-C(19)-C(20)	119.9(3)	C(3)-N(1)-C(8)	119.5(3)
O(7)-Zn(1)-O(4)A	103.11(11)	C(21)-O(7)-Zn(1)	114.8(2)	O(5)-C(15)-O(6)	123.0(4)
O(1)-Zn(1)-O(4)A	120.21(11)	C(22)-O(10)-Zn(1)	112.8(2)	O(2)-C(6)-O(1)	126.7(4)
O(10)-Zn(1)-O(4)A	104.34(11)	O(3)-C(7)-O(4)	127.4(3)	C(18)-N(2)-C(19)	122.3(3)
C(6)-O(1)-Zn(1)	119.1(2)	O(11)-C(30)-O(12)	124.5(4)	O(11)-C(30)-C(27)	123.5(4)
N(2)–Zn(1)–O(5)	85.46(10)	C(14)–O(4)–Zn(1)A	82.3(2)		
O(2)–Zn(1)–O(5)	171.00(10)	C(19)–N(2)–Zn(1)	123.2(2)		
N(3)–Zn(1)–O(5)	88.58(10)	C(15)–N(2)–Zn(1)	120.1(2)		
Bond Lengths (Å) for 2					
Mn(1)-O(1)	2.145(2)	O(3)-Mn(1)G	2.214(2)	O(4)-C(14)	1.247(4)
Mn(1)-O(5)B	2.159(2)	O(4)-Mn(1)H	2.222(2)	O(5)-C(15)	1.257(4)
Mn(1)-O(6)E	2.172(2)	O(5)-Mn(1)B	2.159(2)	O(6)-C(15)	1.247(3)
Mn(1)-O(2)A	2.186(2)	O(6)-Mn(1)I	2.172(2)	N(1)-C(13)	1.352(4)
Mn(1)-O(3)C	2.214(2)	O(1)-C(1)	1.269(4)	N(1)-C(9)	1.355(4)
Mn(1)-O(4)D	2.222(2)	O(2)-C(1)	1.256(4)	N(1)-C(8)	1.496(3)
O(2)-Mn(1)F	2.186(2)	O(3)-C(14)	1.259(4)	C(1)-C(2)	1.504(4)
Bond Angles (°) for 2					
O(1)-Mn(1)-O(5)B	94.98(8)	O(1)-Mn(1)-O(4)D	80.25(8)	C(15)-O(6)-Mn(1)I	156.9(2)
O(1)-Mn(1)-O(6)E	94.68(8)	O(5)B-Mn(1)-O(4)D	85.04(8)	N(1)-C(8)-C(5)	111.0(2)
O(5)B-Mn(1)-O(6)E	164.62(8)	O(6)E-Mn(1)-O(4)D	108.41(8)	N(1)-C(9)-C(10)	120.0(3)
O(1)-Mn(1)-O(2)A	87.85(8)	O(2)A-Mn(1)-O(4)D	165.33(8)	N(1)-C(13)-C(12)	119.8(3)
O(5)B-Mn(1)-O(2)A	87.49(8)	O(3)C-Mn(1)-O(4)D	77.61(8)	O(4)-C(14)-O(3)	127.3(3)
O(6)E-Mn(1)-O(2)A	80.93(8)	C(1)-O(1)-Mn(1)	124.56(19)	O(4)-C(14)-C(10)	115.6(3)
O(1)-Mn(1)-O(3)C	157.02(8)	C(1)-O(2)-Mn(1)F	121.41(19)	O(2)-C(1)-O(1)	124.6(3)
O(5)B-Mn(1)-O(3)C	89.23(8)	C(14)-O(3)-Mn(1)G	129.29(19)	C(13)-N(1)-C(9)	122.1(2)
O(6)E-Mn(1)-O(3)C	86.53(8)	C(14)-O(4)-Mn(1)H	121.37(19)	C(13)-N(1)-C(8)	119.0(2)
O(2)A-Mn(1)-O(3)C	114.94(8)	C(15)-O(5)-Mn(1)B	126.12(19)	C(9)-N(1)-C(8)	118.9(2)

Bond Lengths (Å) for 3					
Cu(1)-O(1)	1.921(5)	Cu(2)-O(12)D	1.970(4)	C(1)-O(1)	1.251(8)
Cu(1)-O(7)	1.967(4)	Cu(2)-O(3)C	1.980(4)	C(1)-O(2)	1.258(8)
Cu(1)-O(6)A	1.986(4)	Cu(2)-O(4)B	1.983(4)	N(1)-C(13)	1.335(8)
Cu(1)-O(13)	2.017(5)	O(3)-Cu(2)E	1.980(4)	N(1)-C(9)	1.351(8)
Cu(1)-C(16)	2.544(7)	O(4)-Cu(2)B	1.983(4)	N(1)-C(8)	1.513(7)
Cl(1)-Cu(2)	2.376(3)	O(6)-Cu(1)A	1.986(4)	O(3)-C(15)	1.242(8)
Cu(2)-O(11)	1.962(4)	O(12)-Cu(2)D	1.970(4)	N(2)-C(20)	1.341(8)
Bond Angles (°) for 3					
O(1)-Cu(1)-O(7)	170.7(2)	O(12)D-Cu(2)-O(4)B	87.13(19)	C(5)-C(8)-N(1)	111.9(5)
O(1)-Cu(1)-O(6)A	86.97(19)	O(12)D-Cu(2)-O(3)C	90.39(19)	N(2)-C(20)-C(19)	120.3(6)
O(7)-Cu(1)-O(6)A	93.07(19)	O(11)-Cu(2)-Cl(1)	97.75(15)	N(2)-C(21)-C(17)	119.9(6)
O(1)-Cu(1)-O(13)	92.23(19)	O(12)D-Cu(2)-Cl(1)	96.57(15)	C(24)-C(23)-N(2)	109.6(5)
O(7)-Cu(1)-O(13)	89.55(19)	O(3)C-Cu(2)-Cl(1)	97.67(15)	O(9)-C(30)-O(10)	123.7(7)
O(6)A-Cu(1)-O(13)	168.6(2)	O(4)B-Cu(2)-Cl(1)	96.06(15)	O(9)-C(30)-C(27)	121.3(7)
C(1)-O(1)-Cu(1)	131.2(5)	C(15)-O(3)-Cu(2)E	124.7(4)	O(11)-C(22)-O(12)	126.1(6)
O(11)-Cu(2)-O(12)D	165.68(18)	C(15)-O(4)-Cu(2)B	119.5(4)	O(12)-C(22)-C(19)	117.3(5)
O(11)-Cu(2)-O(3)C	88.23(19)	C(14)-O(6)-Cu(1)A	101.1(4)	O(4)-C(15)-C(12)	115.9(6)
O(11)-Cu(2)-O(4)B	90.83(19)	C(22)-O(12)-Cu(2)D	121.6(4)	O(5)-C(14)-O(6)	125.7(6)

Symmetry transformations used to generate equivalent atoms for compound **1**: (A) x, y − 1, z; (B) x + 1, −y + 1, z + 1/2; (C) x, y + 1, z; (D) x − 1, −y + 1, z − 1/2. Compound **2**: (A) x, −y + 1/2, z + 1/2; (B) –x + 1, −y + 1, −z + 1; (C) x − 1, −y + 1/2, z − 1/2; (D) x − 1, y, z − 1; (E) –x + 1, y − 1/2, −z + 1/2; (F) x, −y + 1/2, z − 1/2; (G) x + 1, −y + 1/2, z + 1/2; (H) x + 1, y, z + 1; (I) –x + 1, y + 1/2, −z + 1/2. Compound **3**: (A) −x, −y, −z + 1; (B) −x, −y + 1, −z + 1; (C) x + 1, y + 1, z − 1; (D) –x + 1, −y + 2, −z; (E) x − 1, y − 1, z + 1.

Table S2. Hydrogen bonds for **1** (Å and °).

D-H...A	D (D-H)	D (H...A)	D (D...A)	<(DHA)
O(6)-H(6)...O(3)E	0.82	2.02	2.814(4)	161.7
O(12)-H(12)...O(9)F	0.82	2.46	3.085(4)	134.2
O(12)-H(12)...O(13)G	0.82	1.96	2.682(5)	146.8
O(13)-H(13A)...O(8)H	0.855(14)	2.03(2)	2.837(4)	156(6)
O(13)-H(13B)...O(2)B	0.853(14)	2.33(5)	2.835(5)	118(4)
O(13)-H(13B)...O(9)B	0.853(14)	2.30(3)	2.809(4)	119(3)

Symmetry transformations used to generate equivalent atoms: (A) x, y − 1, z; (B) x + 1, −y + 1, z + 1/2; (C) x, y + 1, z; (D) x − 1, −y + 1, z − 1/2; (E) x − 1, y, z − 1; (F) x + 1, y + 1, z + 1; (G) x, −y + 2, z + 1/2; (H) x + 1, y, z.