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Supporting information for article:

Two topologically different 3D Cu^{II} metal–organic frameworks assembled from the same ligands: control of reaction conditions

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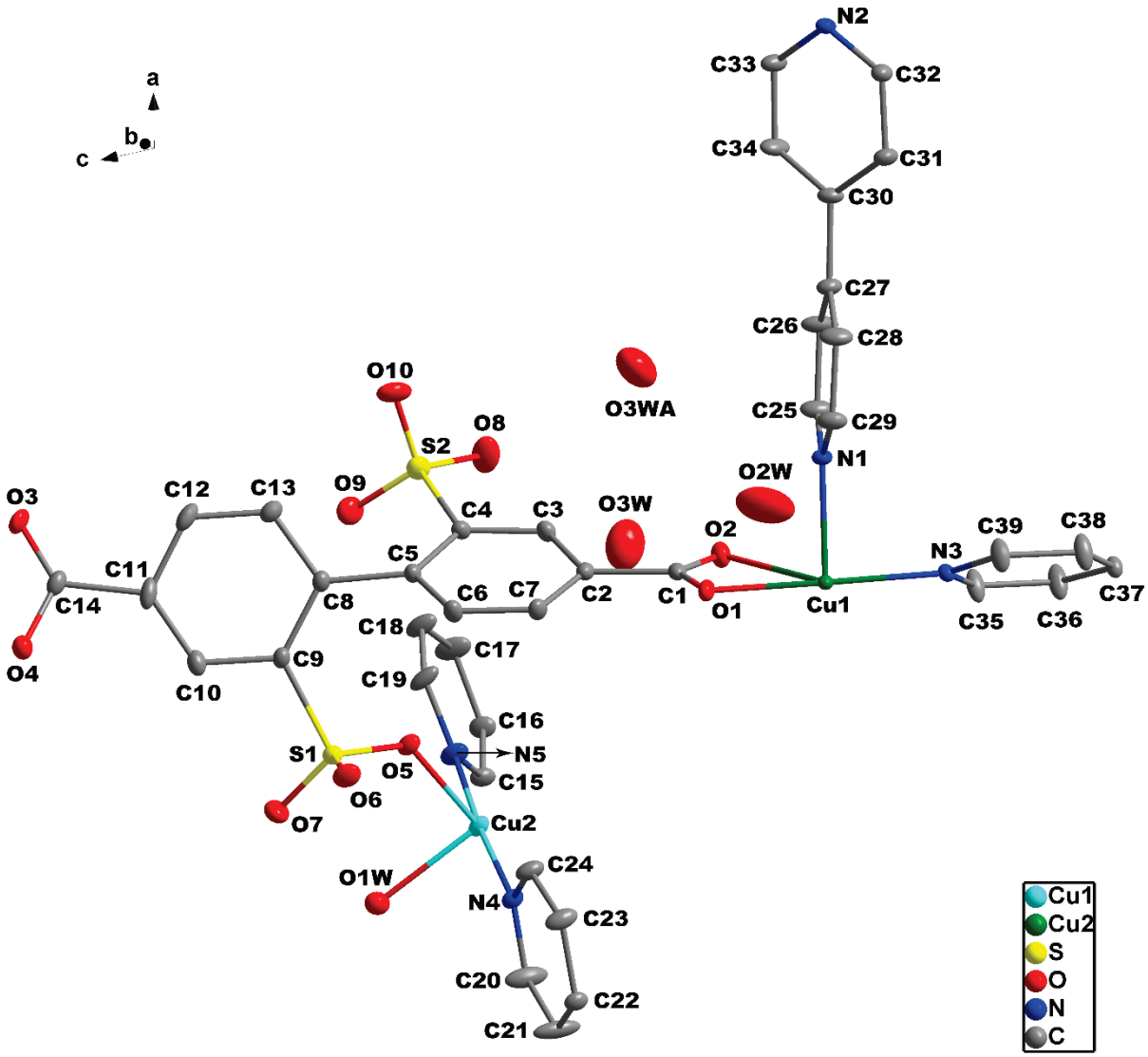

Figure S1 The asymmetric unit for (**1**). Displacement ellipsoids are drawn at the 30% probability level (Hydrogen and disordered atoms were omitted for clarity).

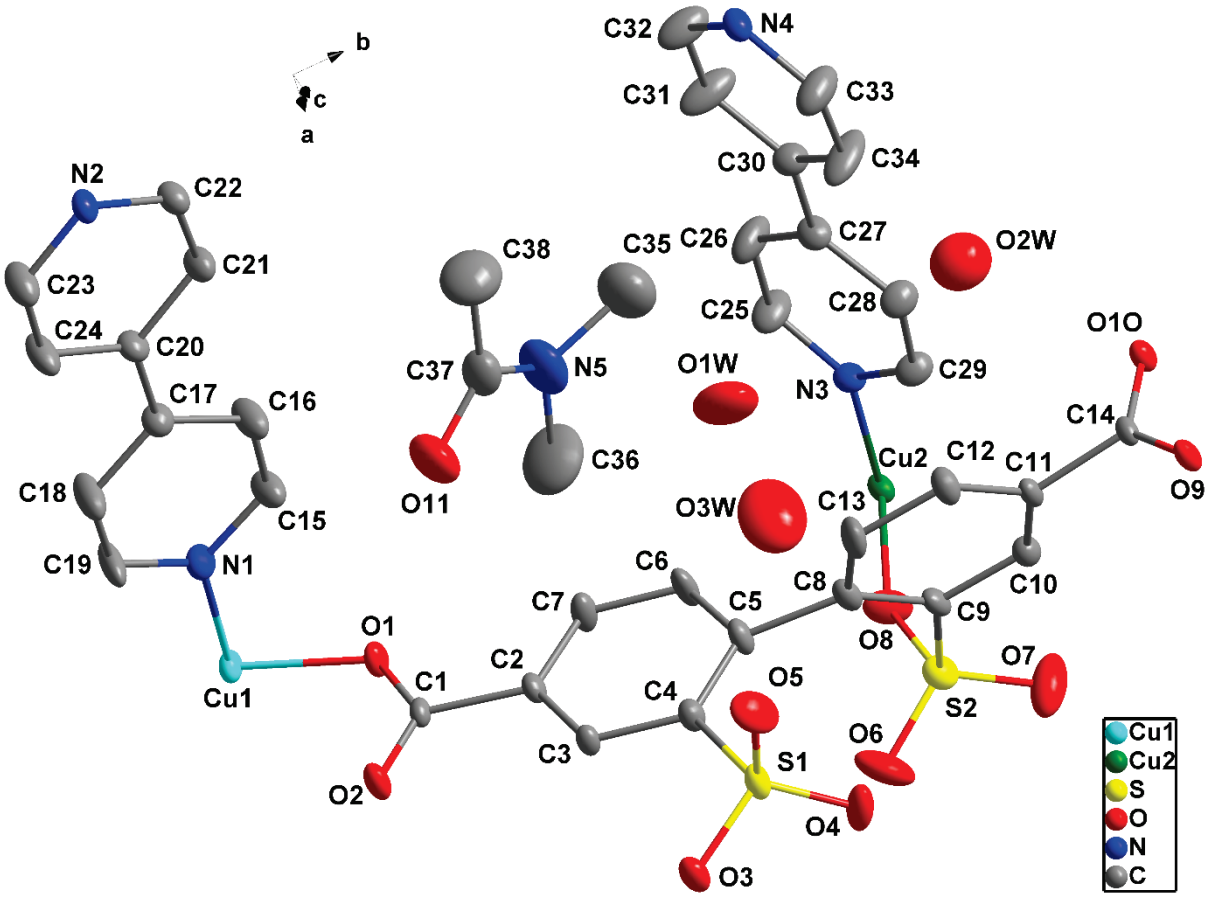

Figure S2 The asymmetric unit for (**2**). Displacement ellipsoids are drawn at the 30% probability level (Hydrogen and disordered atoms have been omitted for clarity).

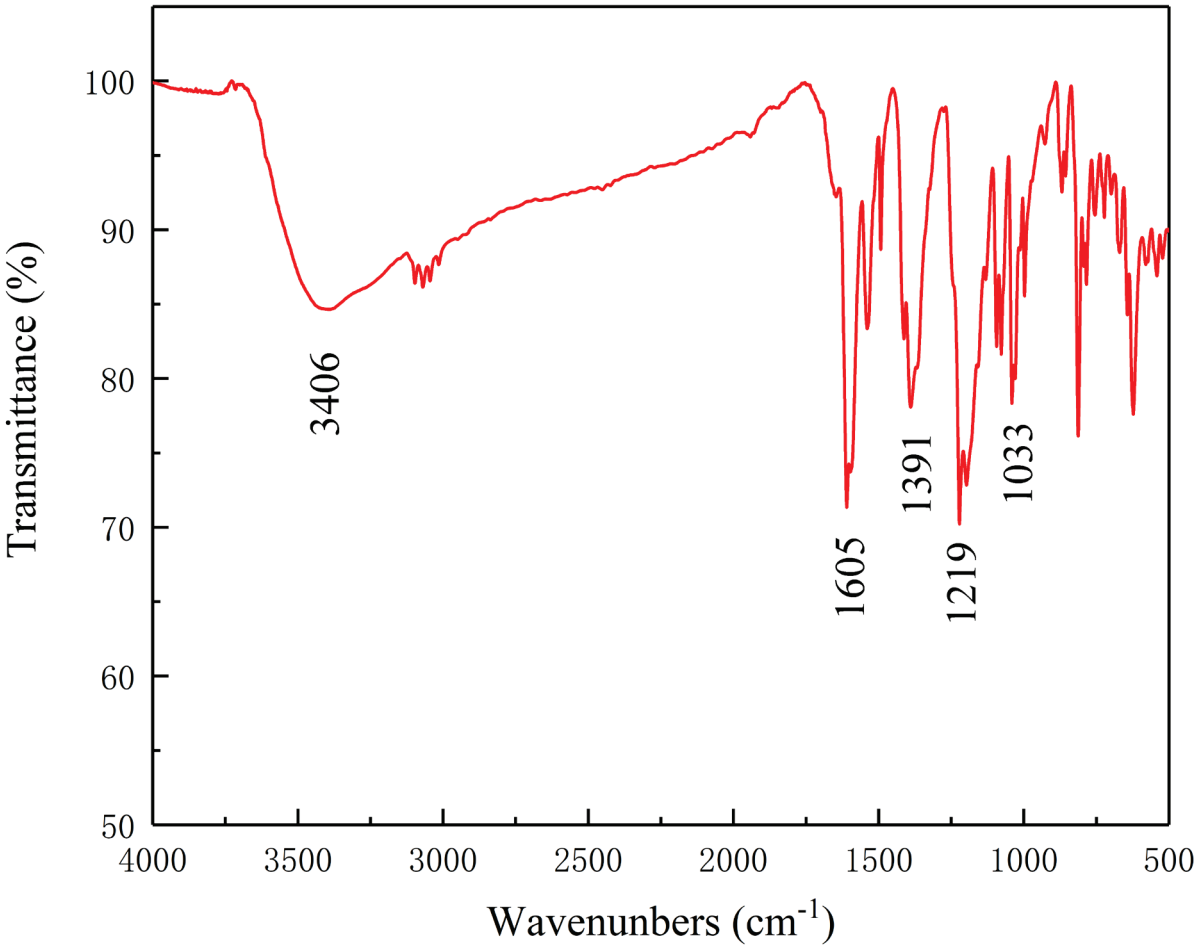

Figure S3 The IR spectrum of (**1**)

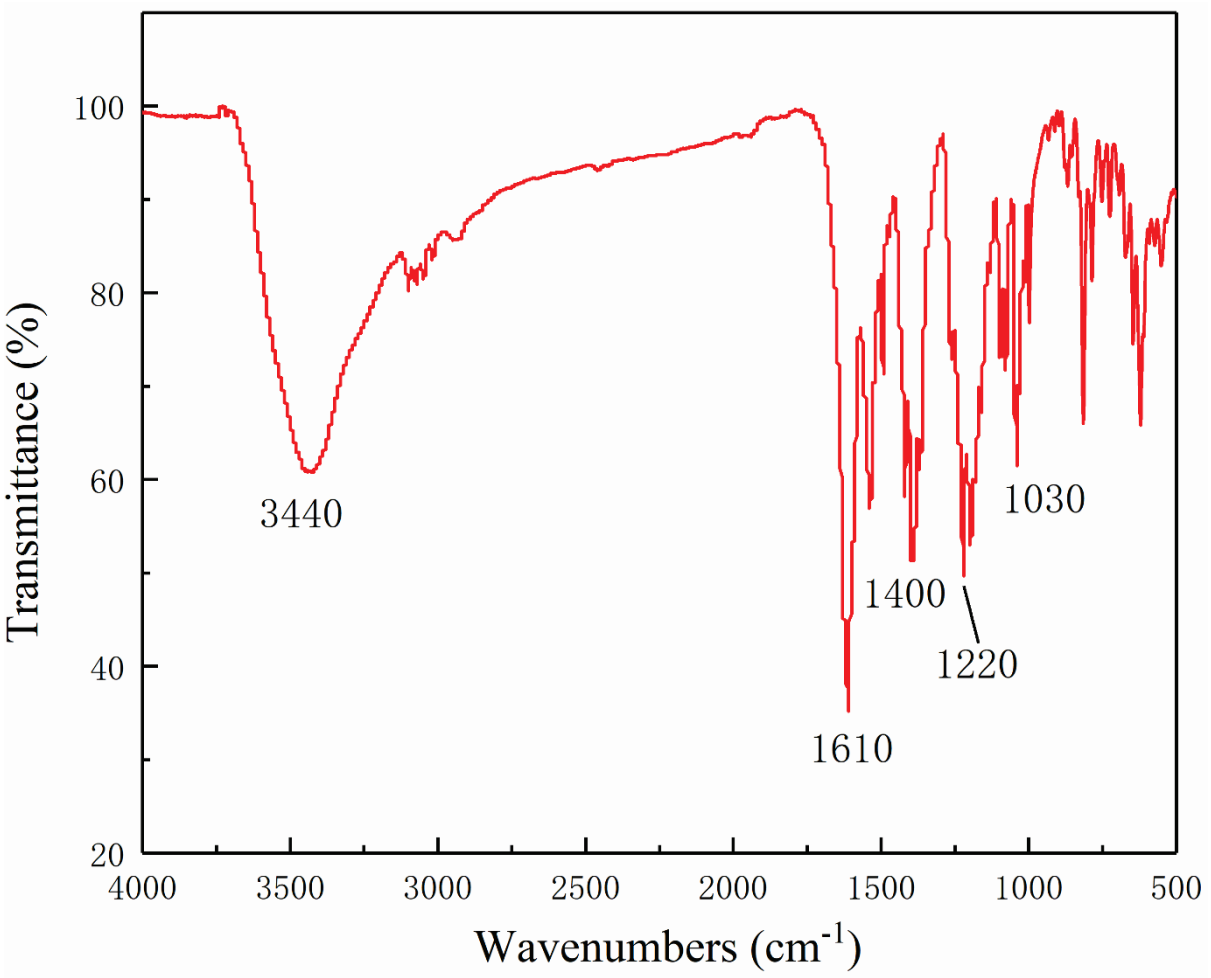

Figure S4 The IR spectrum of (**2**)

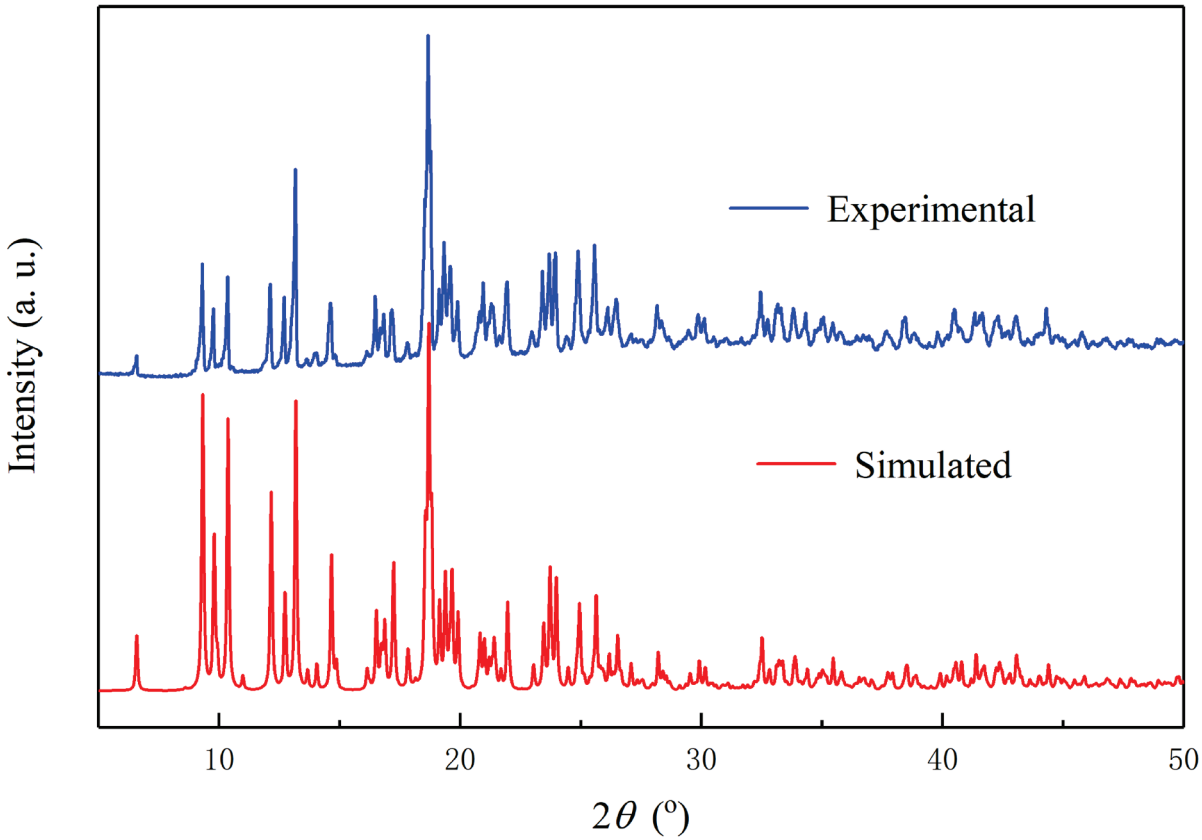

Figure S5 Simulated and experimental PXRD patterns for (**1**)

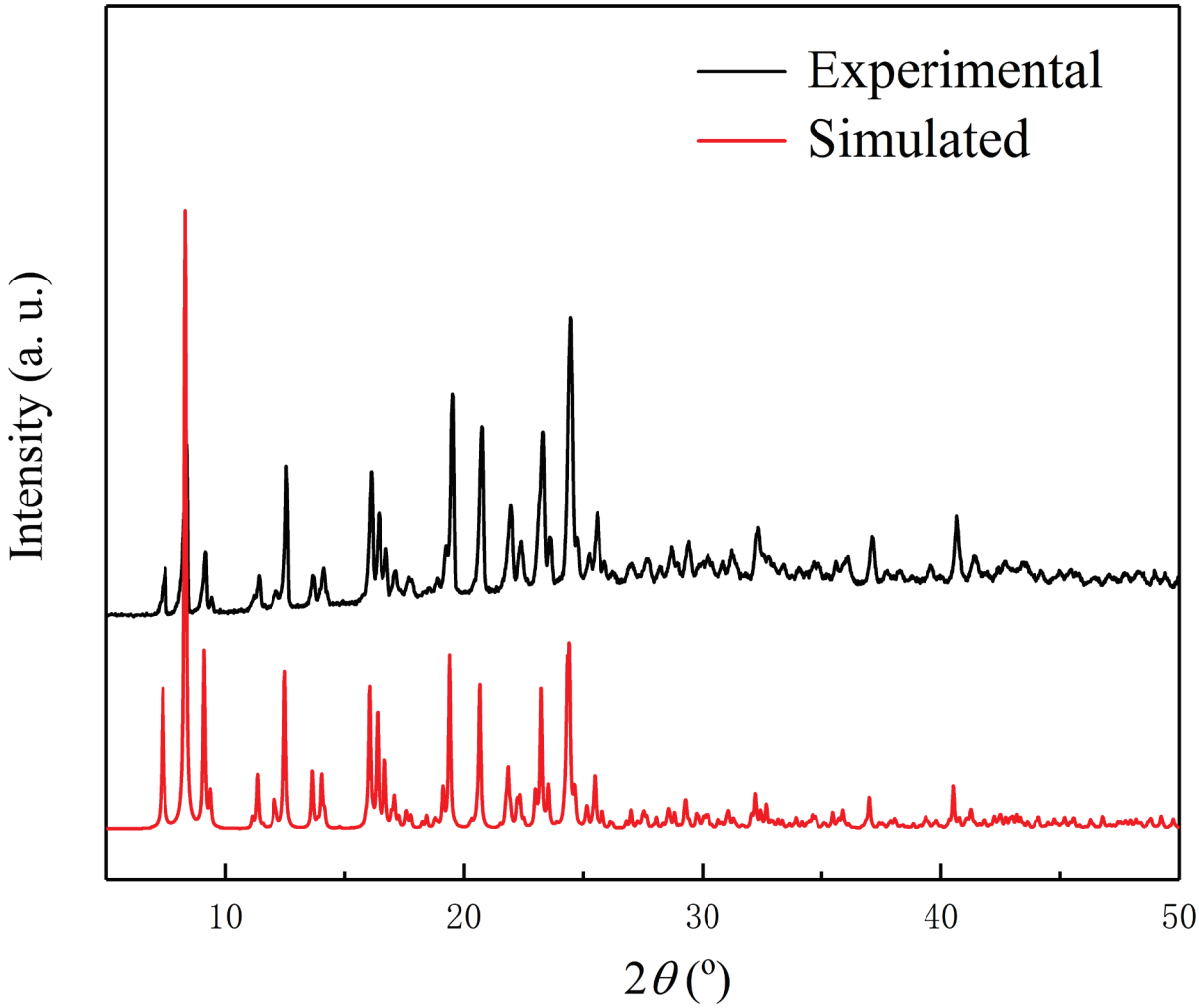

Figure S6 Simulated and experimental PXRD patterns for (**2**)

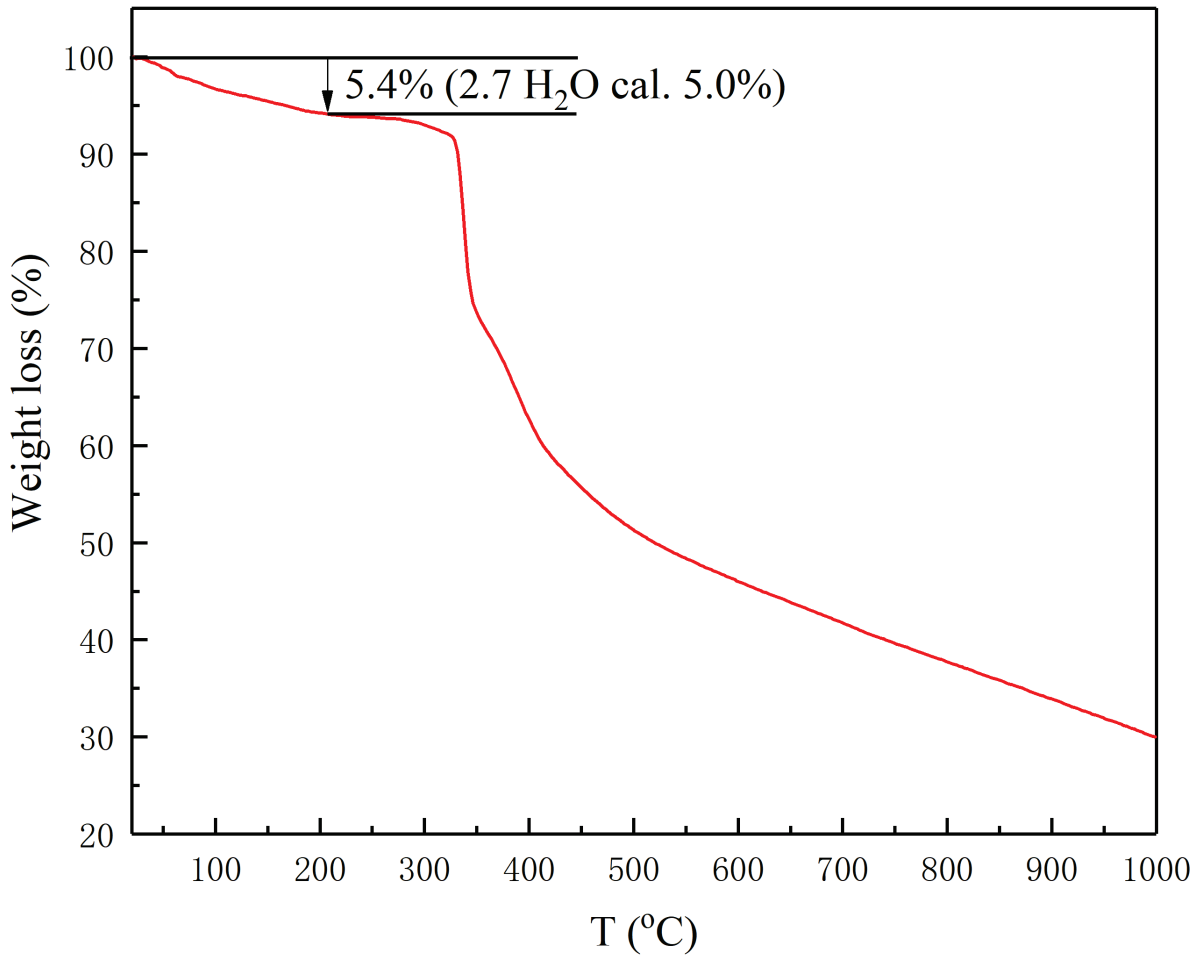

Figure S7 TGA curve for (**1**)

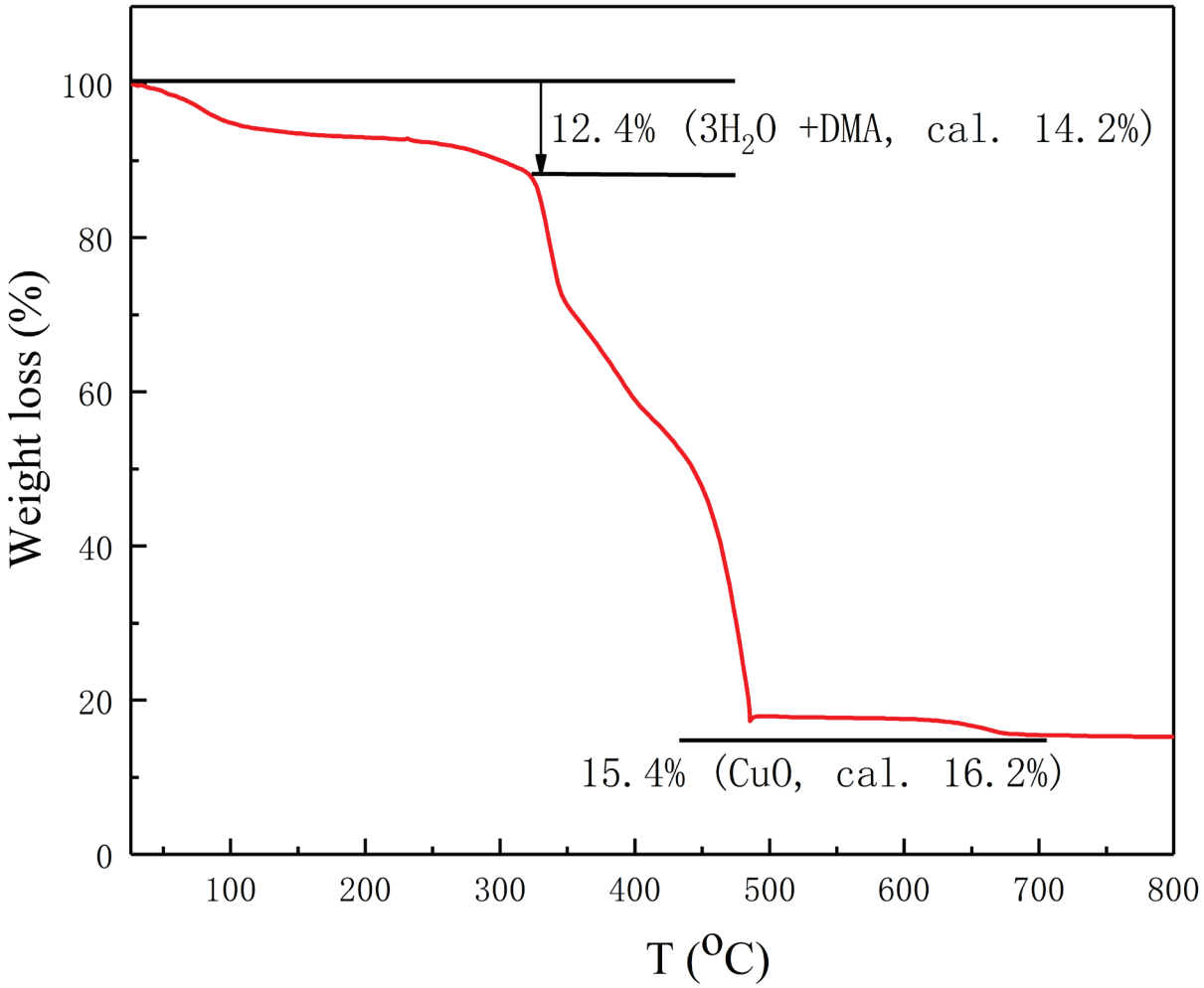

Figure S8 TGA curve for (**2**)

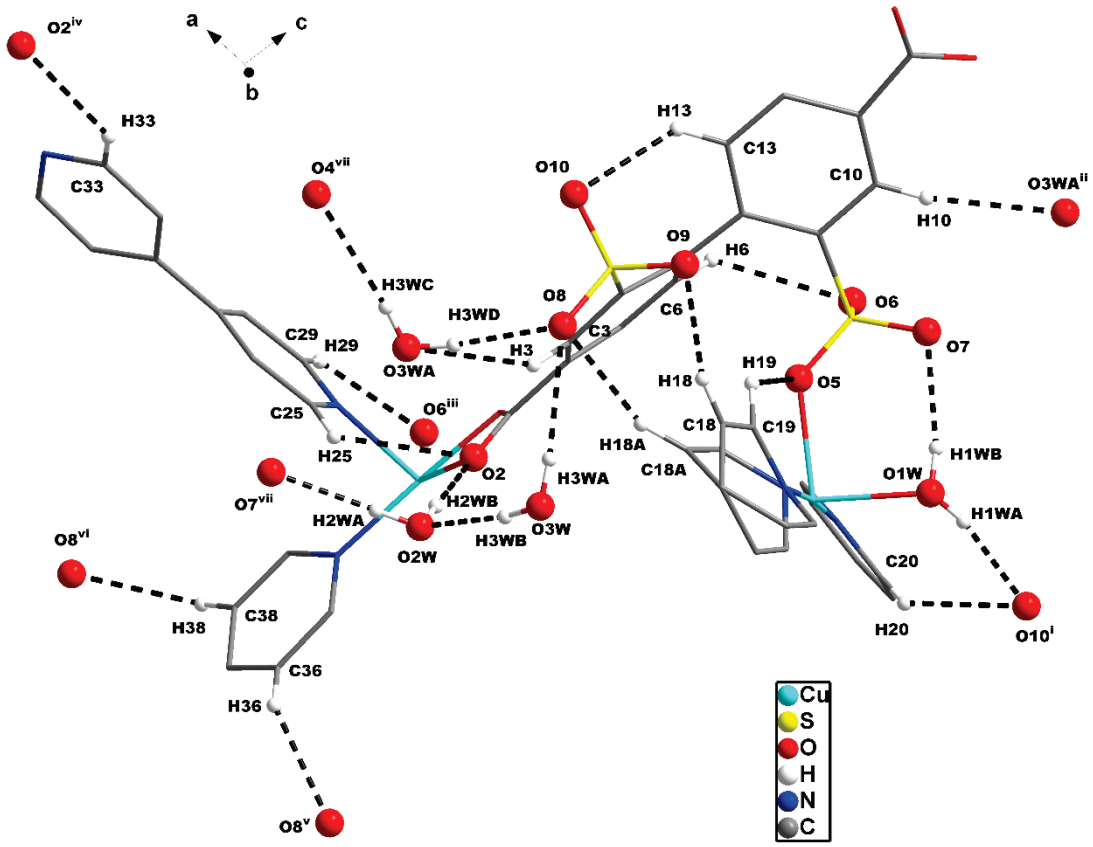

Figure S9 The hydrogen bonds of (**1**)

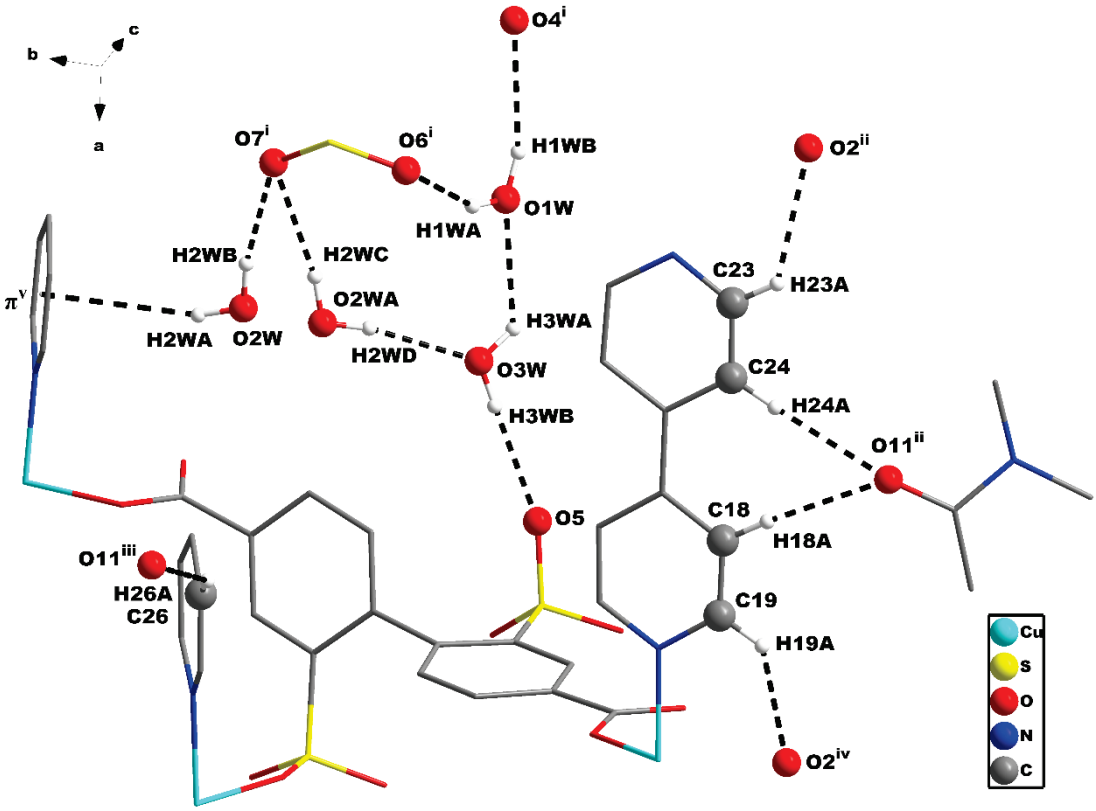

Figure S10 The hydrogen bonds of (**2**)

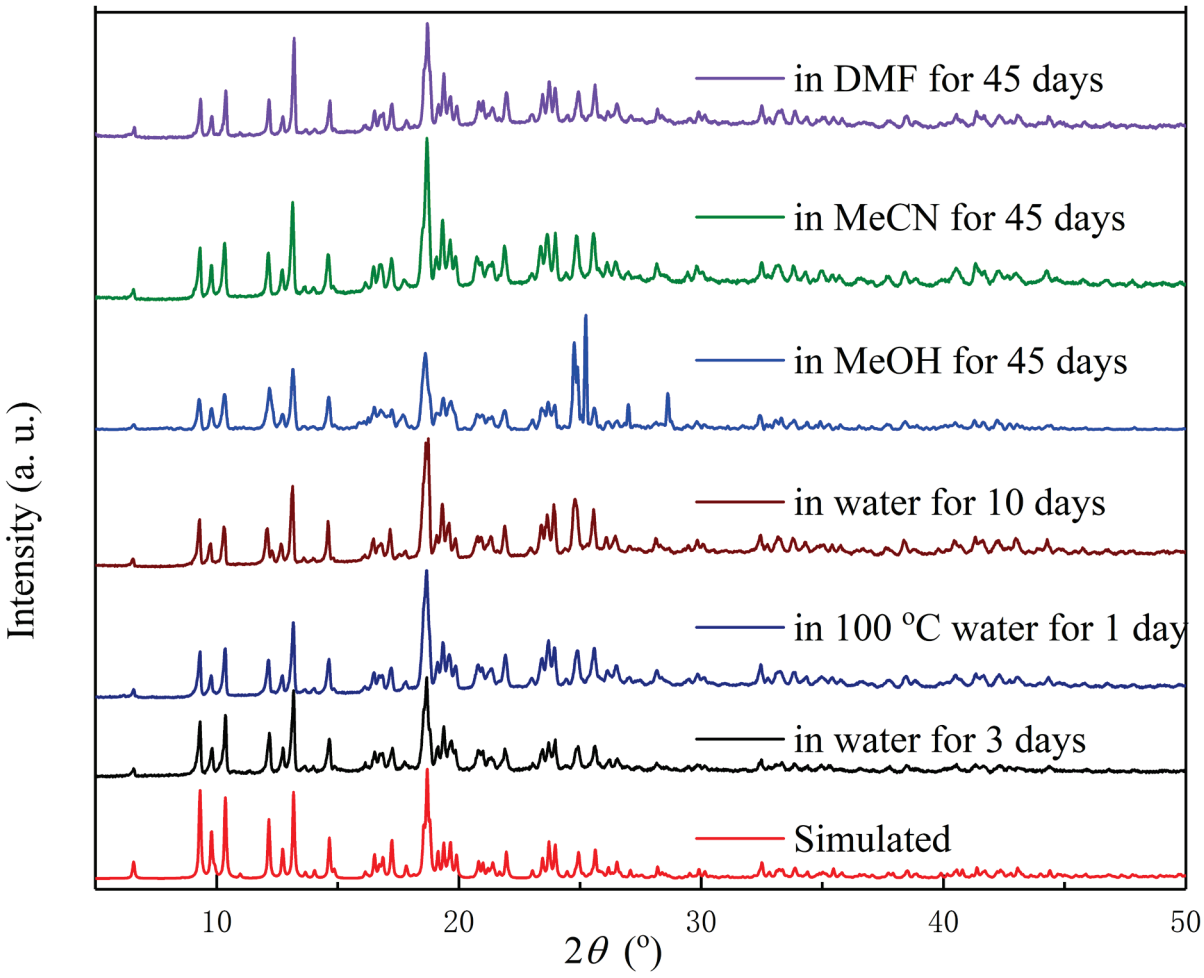

Figure S11 PXRD patterns of (**1**): treated in water for 3-10 days at r.t.; treated in water for 1 day at 100 °C and in methanol (MeOH), acetonitrile (MeCN), N,N′-dimethylformamide (DMF) for 45 days at r.t.

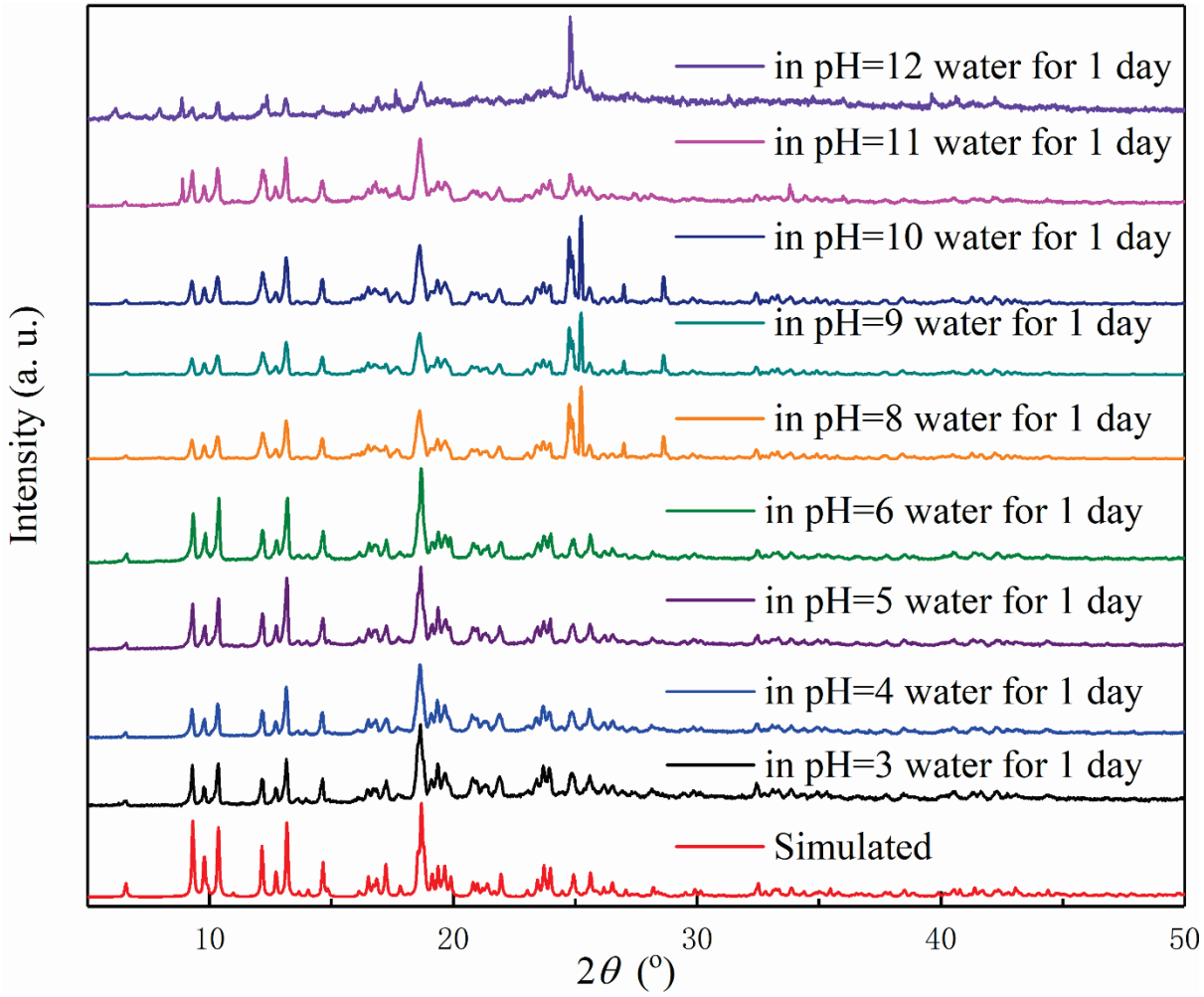

Figure S12 PXRD patterns of (**1**): treated in HCl (pH = 3-6) and NaOH (pH = 8-12) aqueous solutions for 1 day at r. t.

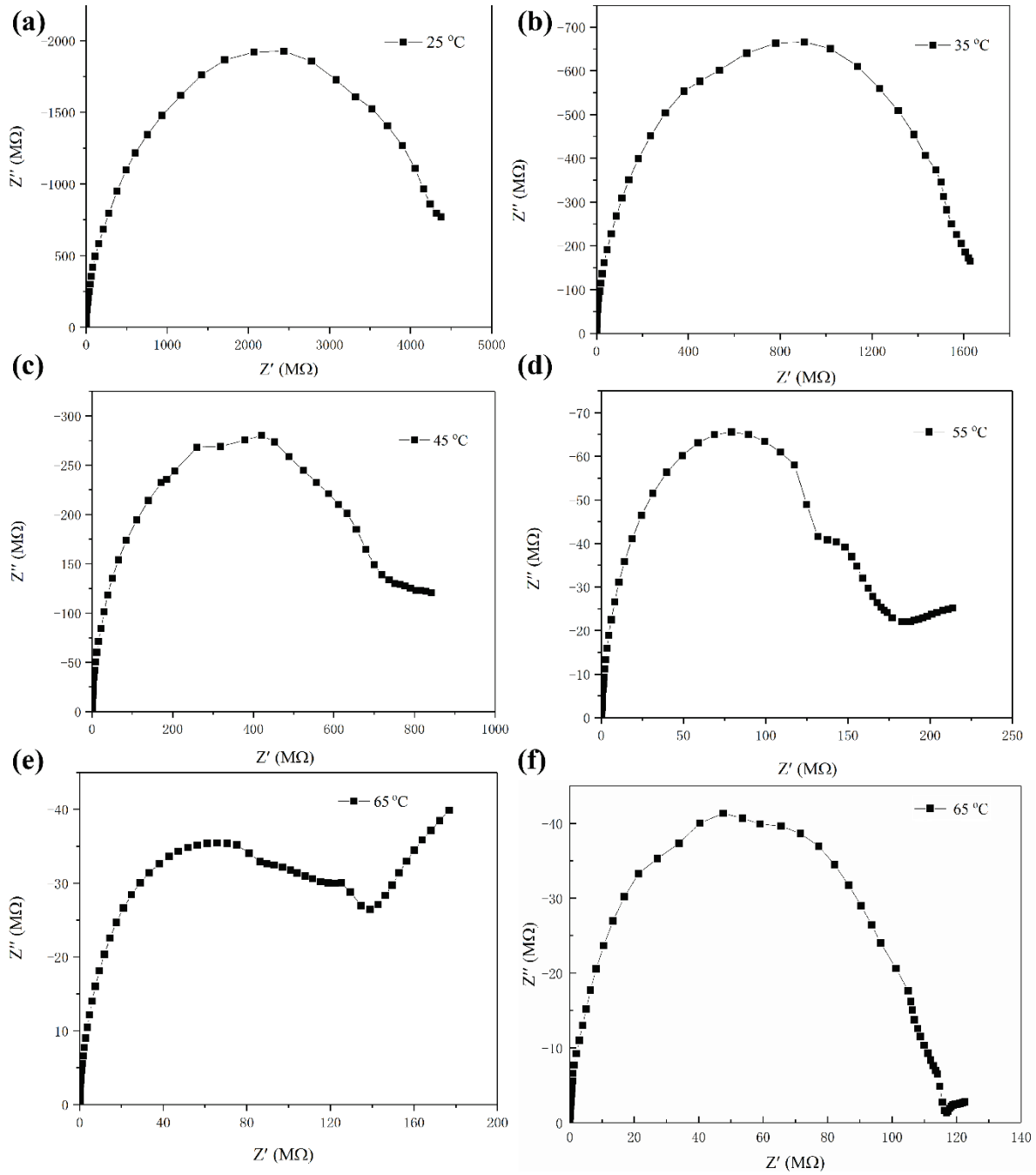

Figure S13. Nyquist plots for (**1**) at 95 % RH and under temperature from 25 to 65 °C (a)-(e), and (**1**) treated in HCl aqueous solutions (pH = 3) for 1 day at 95 % RH and 65 °C (f).

Table S1 Selected geometric parameters of MOF (**1**) (Å, °).

Cu1–O1	1.935(18)	Cu1–O2	2.747(2)
Cu1–O6^{ii}	2.357(2)	Cu2–O3^{i}	2.202(5)
Cu2–O4^{i}	2.035(8)	Cu2–O5	2.191(2)
Cu2–O1W	2.132(2)	Cu1–N1	2.045(2)

Cu1–N2^{iii}	2.051(2)	Cu1–N3	1.990(2)
Cu2–N4	2.007(2)	Cu2–N5	2.002(2)
O1–C1	1.279(4)	O2–C1	1.242(3)
O3–C14	1.241(10)	O4–C14	1.241(8)

O1–Cu1–N3	173.79(9)	N1–Cu1–N2^{iii}	171.69(9)
O6^{ii}–Cu1–O2	143.09(7)	N3–Cu1–O2	120.69(8)
N3–Cu1–O6^{ii}	95.78(8)	N2^{iii}–Cu1–O6^{ii}	95.12(8)
N1–Cu1–O6^{ii}	92.51(8)	O1–Cu1–N1	92.38(9)
N2–Cu1–O2^{i}	91.74(8)	O1–Cu1–N2^{iii}	90.91(9)
O1–Cu1–O6^{ii}	90.42(8)	N3–Cu1–N2^{iii}	88.24(9)
N3–Cu1–N1	87.67(9)	N1–Cu1–O2	84.12(8)
O1–Cu1–O2	53.18(7)	N5–Cu2–N4	175.28(9)
O1W–Cu2–O3^{i}	164.27(14)	O5–Cu2–O4^{i}	159.16(15)
O1W–Cu2–O4^{i}	105.50(15)	O5–Cu2–O3^{i}	100.58(14)
O1W–Cu2–O5	95.15(8)	N4–Cu2–O5	92.26(8)
N4–Cu2–O1W	92.03(9)	N5–Cu2–O5	91.29(8)
N5–Cu2–O1W	90.75(9)	N4–Cu2–O3^{i}	87.17(14)
N5–Cu2–O4^{i}	88.10(2)	N5–Cu2–O3^{i}	88.57(12)
N4–Cu2–O4^{i}	87.20(2)	O3^{i}–Cu2–O4^{i}	59.16(16)

Symmetry codes: i) *x*-1/2, 3/2-*y*, *z*-1/2; ii) 1-*x*, 1-*y*, 2-*z*; iii) *x*-1, y, z.

Table S2 Selected geometric parameters of MOF (**2**) (Å, °).

Cu1–O1	1.941(3)	Cu1–O2^{iii}	2.250(4)
Cu1–O9^{i}	2.052(3)	Cu2–O3^{i}	1.986(4)
Cu2–O8	2.177(4)	Cu2–O10^{iv}	1.966(3)
Cu1–N1	2.015(5)	Cu1–N2^{ii}	1.995(4)
Cu2–N3	2.020(4)	Cu2–N4^{ii}	2.002(4)

N2^{ii}–Cu1–N1	176.66(18)	O1–Cu1–O9^{i}	149.23(14)
O1–Cu1–O2^{iii}	126.25(14)	N2^{ii}–Cu1–O2^{iii}	91.98(15)
N1–Cu1–O2^{iii}	91.34(16)	N2^{ii}–Cu1–O9^{i}	90.82(16)
N1–Cu1–O9^{i}	89.87(16)	O1–Cu1–N1	89.09(16)
O1–Cu1–N2^{ii}	88.65(16)	O9^{i}–Cu1–O2^{iii}	84.52(13)
N4^{ii}–Cu2–N3	172.64(18)	O10^{iv}–Cu2–O3^{i}	163.75(14)
O10^{iv}–Cu2–O8	102.60(15)	N4^{ii}–Cu2–O8	95.17(17)
O3^{i}–Cu2–N3	94.46(17)	O3^{i}–Cu2–O8	93.64(16)
N3–Cu2–O8	91.54(17)	O10^{iv}–Cu2–N4^{ii}	89.79(15)
O3^{i}–Cu2–N4^{ii}	88.13(16)	O10^{iv}–Cu2–N3	85.80(16)

Symmetry codes: i) *x*, 1/2-*y*, *z*-1/2; ii) *x*+1, *y*, *z*; iii) 2-*x*, -*y*, 1-*z*; iv) 2-*x*, 1-*y*, 1-*z*.

Table S3 Hydrogen-bonding geometry (Å, °) for MOF (**1**).

D–H···A	d(D–H)	d(H···A)	d(D···A)	∠D–H···A
O1W–H1WA···O10^{i}	0.850	1.941	2.770	165
O1W–H1WB···O7	0.850	2.095	2.925	165
O2W–H2WA···O7^{vii}	0.850	2.004	2.854	180
O2W–H2WB···O2	0.850	1.995	2.845	180
O3W–H3WA···O8	0.850	2.387	3.232	173
O3W–H3WB···O2W	0.850	2.034	2.880	173
O3WA–H3WC···O4^{vii}	0.850	2.417	3.263	173
O3WA–H3WD···O8	0.850	2.124	2.955	165
C3–H3···O3WA	0.930	2.567	3.379	146
C10–H10···O3WA^{ii}	0.930	2.466	3.384	169
C18–H18···O9	0.930	2.324	3.000	129
C18A–H18A···O8	0.930	2.333	3.142	145
C19–H19···O5	0.930	2.478	3.078	122
C20–H20···O10^{i}	0.930	2.450	3.218	140
C25–H25···O2	0.930	2.490	3.094	123
C29–H29···O6^{iii}	0.930	2.443	3.114	129
C33–H33···O2^{iv}	0.930	2.578	3.306	135
C36–H36···O8^{v}	0.930	2.388	3.173	142
C38–H38···O8^{vi}	0.930	2.530	3.365	150

Symmetry codes: i) *x*-1, *y*, *z*; ii) *x*-1/2, 3/2-*y*, *z*+1/2; iii) 1-*x*, 1-*y*, 2-*z*; iv) *x*+1, *y*, *z*; iv) *x*-1/2, 3/2-*y*, *z*-1/2; v) 3/2-*x*, *y*-1/2, 3/2-*z*; vi) *x*+1/2, 3/2-*y*, *z*-1/2; vii) *x*+1/2, 3/2-*y*, *z*-1/2.

Table S4 Hydrogen-bonding geometry (Å, °) for MOF (**2**).

D−H···A	d(D−H)	d(H···A)	d(D···A)	∠D−H···A
O1W−H1WA···O6^{i}	0.85	1.921	2.703	152
O1W−H1WB···O4^{i}	0.85	2.411	3.200	157
O2W−H2WA···π^{v}	0.85	2.922	3.747	165
O2W−H2WB··· O7^{i}	0.85	2.009	2.850	170
O2WA−H2WC··· O7^{i}	0.85	2.192	3.031	169
O2WA−H2WD···O3W	0.85	2.081	2.921	170
O3W−H3WA ···O1W	0.85	2.326	2.870	122
O3W−H3WB···O5	0.85	2.221	3.070	178
C18−H18··· O11^{ii}	0.93	2.352	3.282	172
C19−H19··· O2^{iv}	0.93	2.447	3.039	122
C24−H24··· O11^{ii}	0.93	2.372	3.302	178
C26−H26··· O11^{iii}	0.93	2.533	3.369	150
C23−H23··· O2^{ii}	0.93	2.436	3.041	123

Symmetry codes: i) *x*-1, *y*, *z*; ii) 1-*x*, -*y*, 1-*z*; iii) *x*, 1/2-*y*, *z*-1/2; iv) 2-*x*, -*y*, 1-*z*; v) 1-*x*, 1-*y*, 1-*z*.

Table S5 Dihedral angles (°) for MOFs (**1**)-(**2**).

MOFs	Py/Py	Ph/Ph	CO_2^-/Ph
(**1**)	0, 43.84(1)	60.80(3)	17.70(6), 25.61(1)
(**2**)	3.37(2), 6.44(1)	71.85(5)	3.00(8), 70.71(5)