Supplementary Information

Design and Synthesis of Coordination Polymers with Cu(II) and Heterocyclic N-Oxides

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FT-IR spectra of synthesized compounds

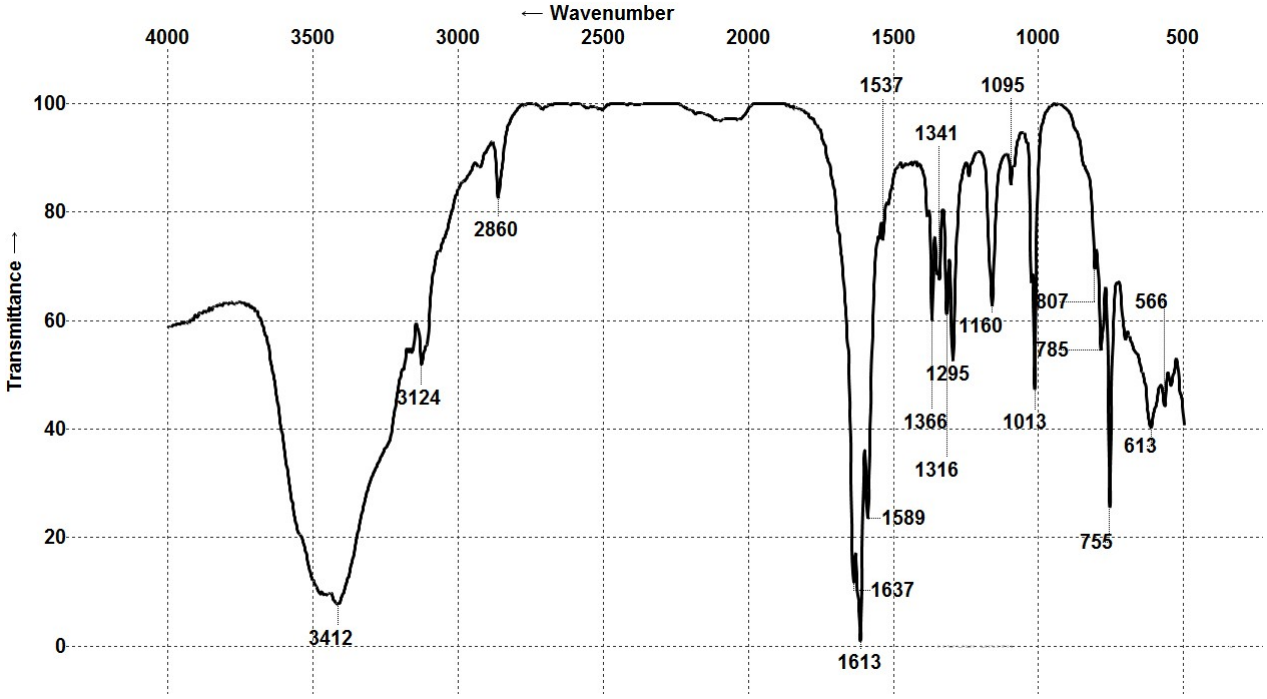

Figure S1. FT-IR spectra of compound **1**.

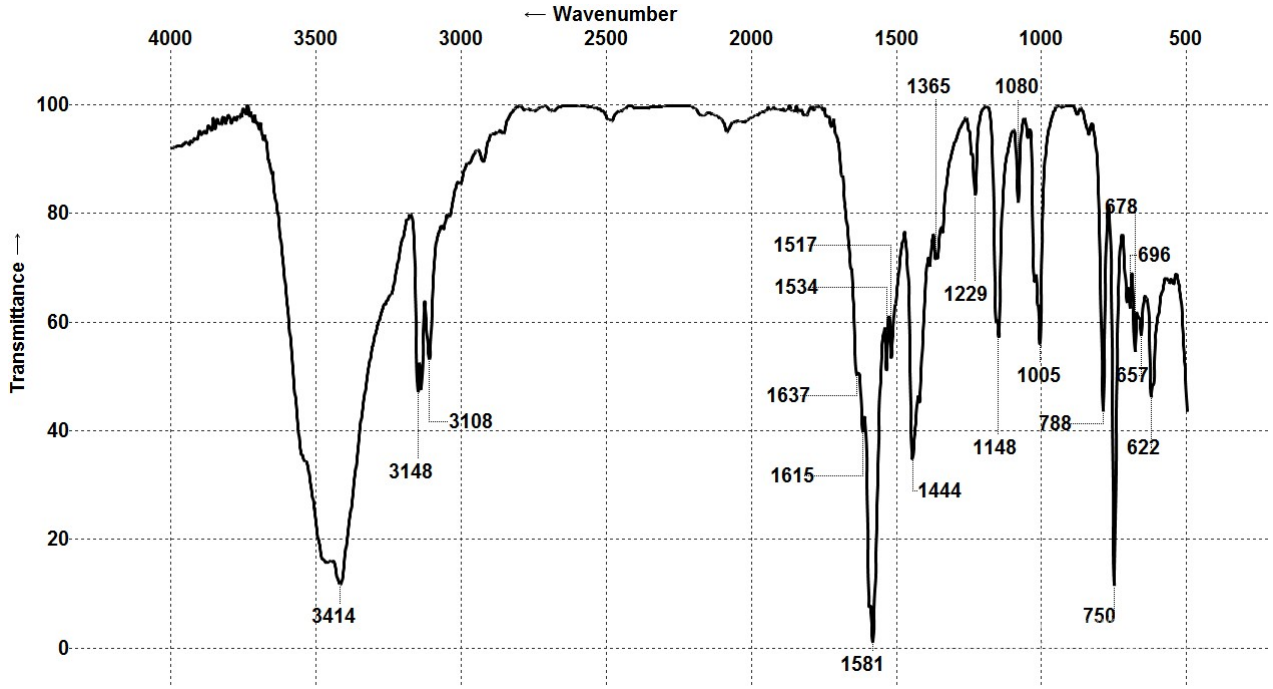

Figure S2. FT-IR spectra of compound **2**.

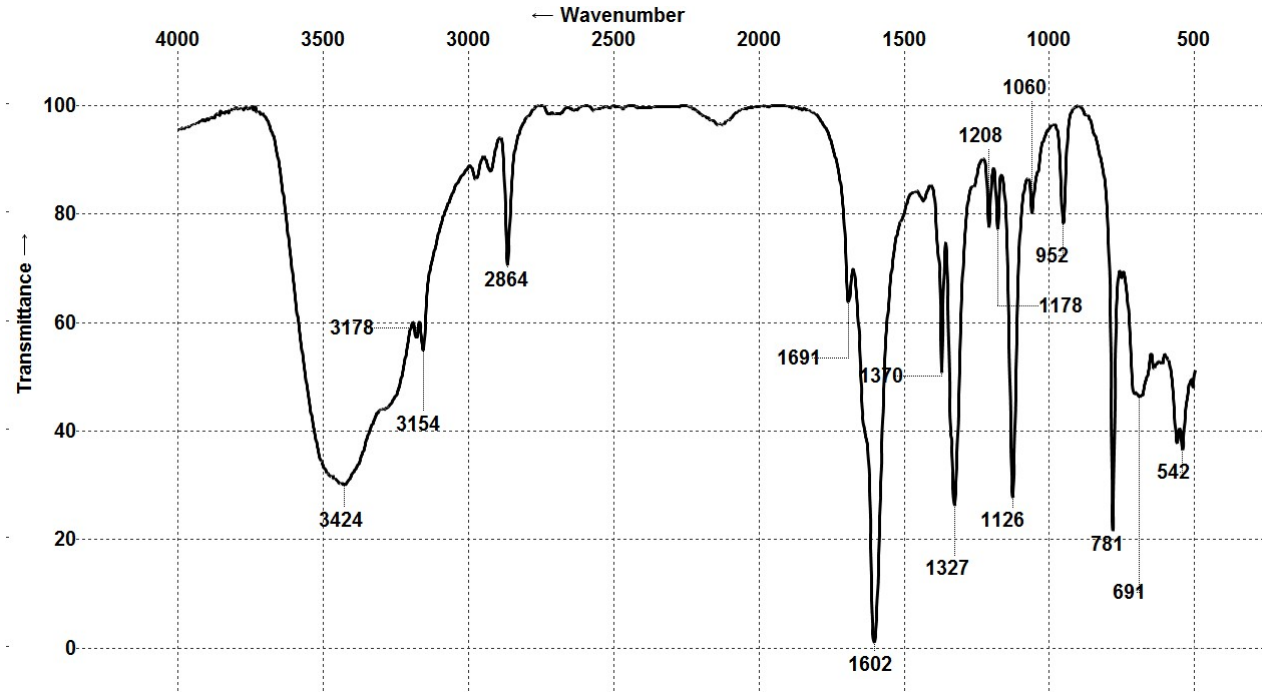

Figure S3. FT-IR spectra of compound **3**.

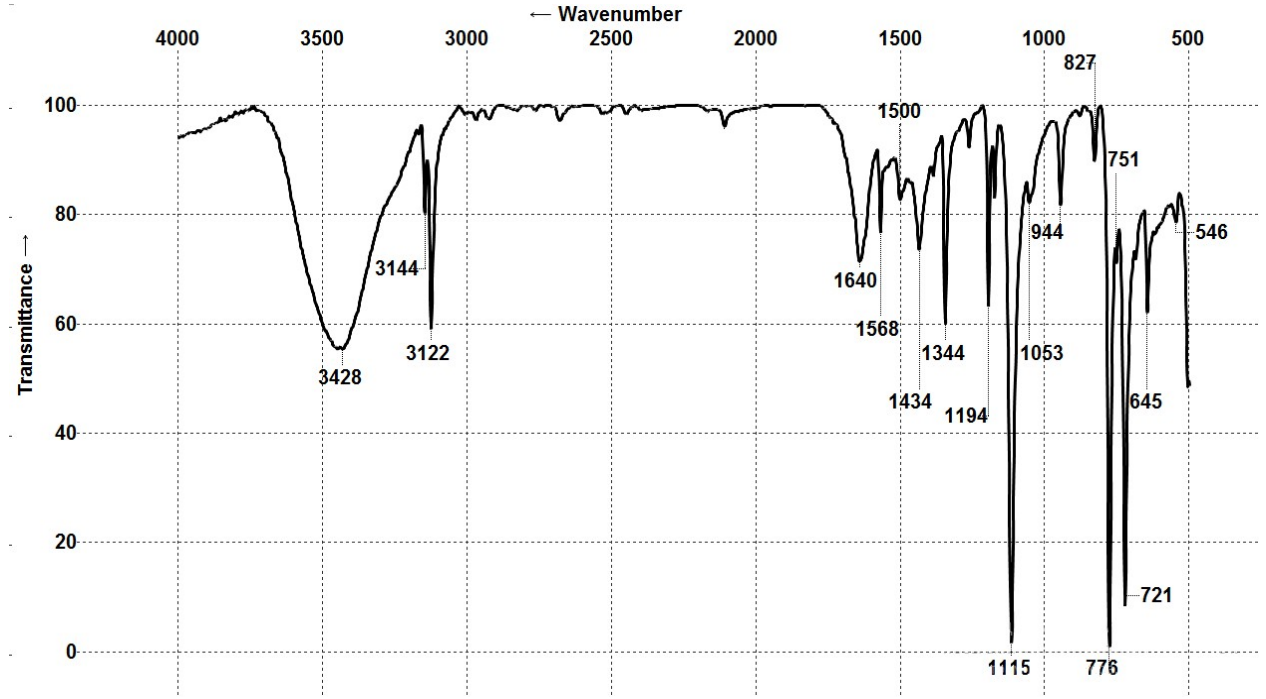

Figure S4. FT-IR spectra of compound **4**.

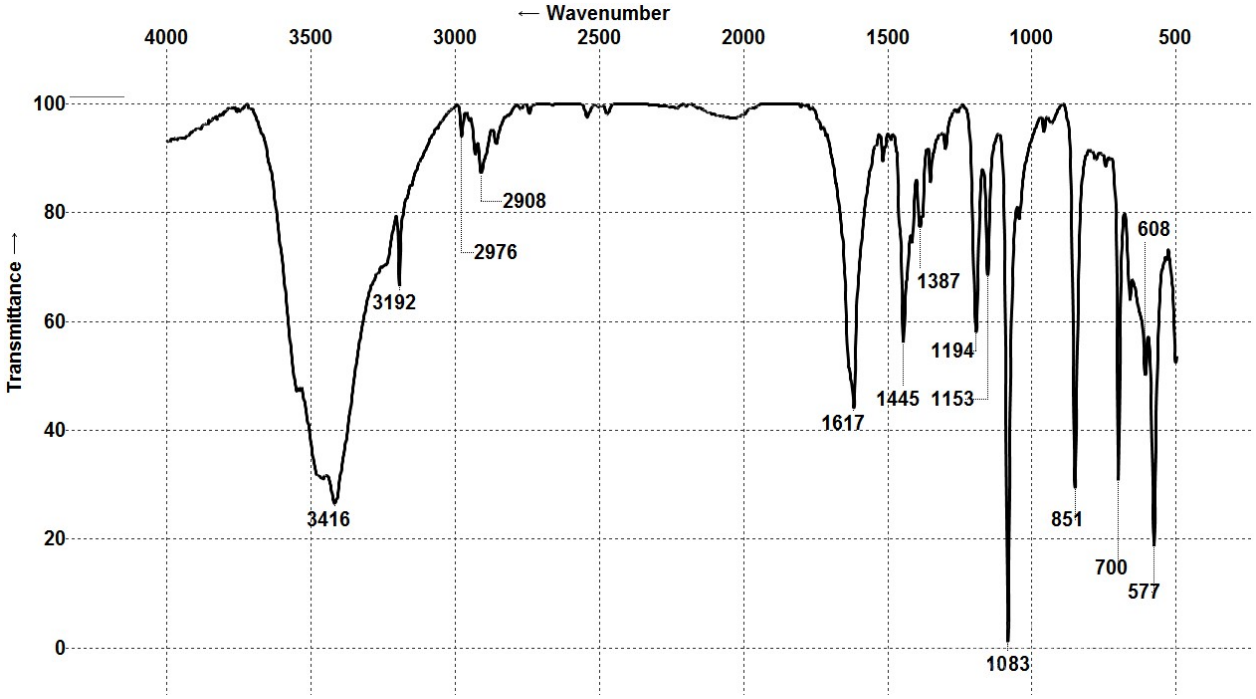

Figure S5. FT-IR spectra of compound **5**.

Powder X-ray diffraction of synthesized compounds

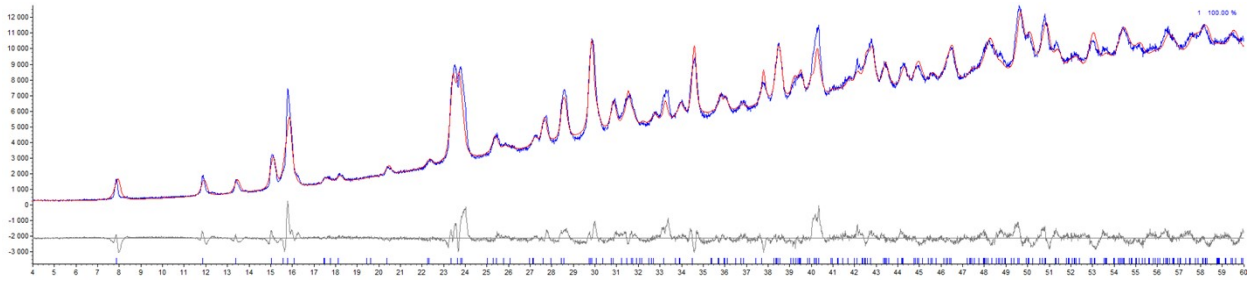

Figure S6. PXRD pattern of compound **1**. Rietveld analysis shows phase purity. R_{wp}/R_{bragg} = 5.269 / 3.859. The blue line in the experimental pattern, the fuchsia line is the calculated pattern, and the grey line is the difference curve.

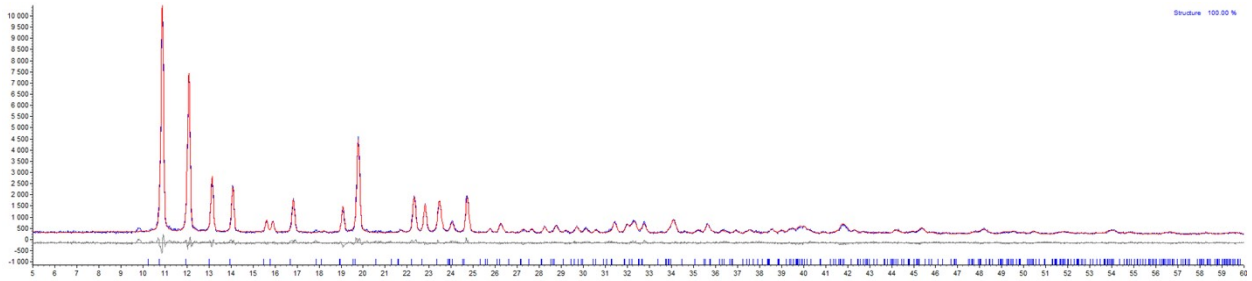

Figure S7. PXRD pattern of compound **2**. Rietveld analysis shows phase purity. R_{wp}/R_{bragg} = 7.083/1.624. The blue line in the experimental pattern, the fuchsia line is the calculated pattern, and the grey line is the difference curve.

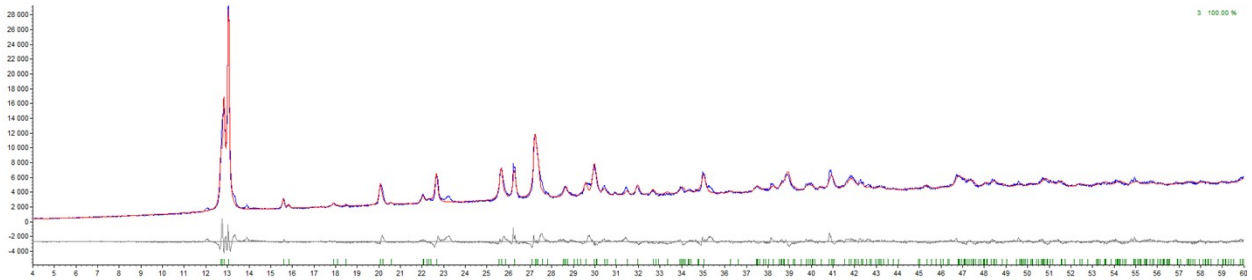

Figure S8. PXRD pattern of compound **3**. Rietveld analysis shows phase purity. R_{wp}/R_{bragg} = 5.008/1.420. The blue line in the experimental pattern, the fuchsia line is the calculated pattern, and the grey line is the difference curve.

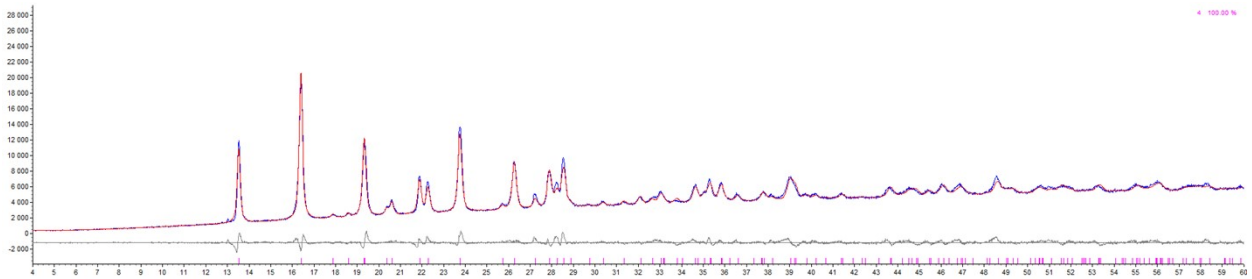

Figure S9. PXRD pattern of compound **4**. Rietveld analysis shows phase purity. R_{wp}/R_{bragg} = 4.163/1.985. The blue line in the experimental pattern, the fuchsia line is the calculated pattern, and the grey line is the difference curve.

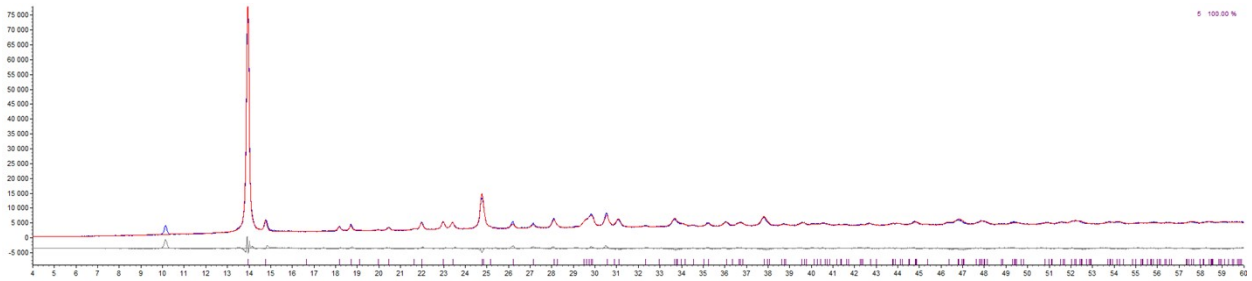

Figure S10. PXRD pattern of compound **5**. Rietveld analysis shows phase purity. R_{wp}/R_{bragg} = 4.952 / 1.771. The blue line in the experimental pattern, the fuchsia line is the calculated pattern, and the grey line is the difference curve.

Liquid phase dispersing of synthesized compounds

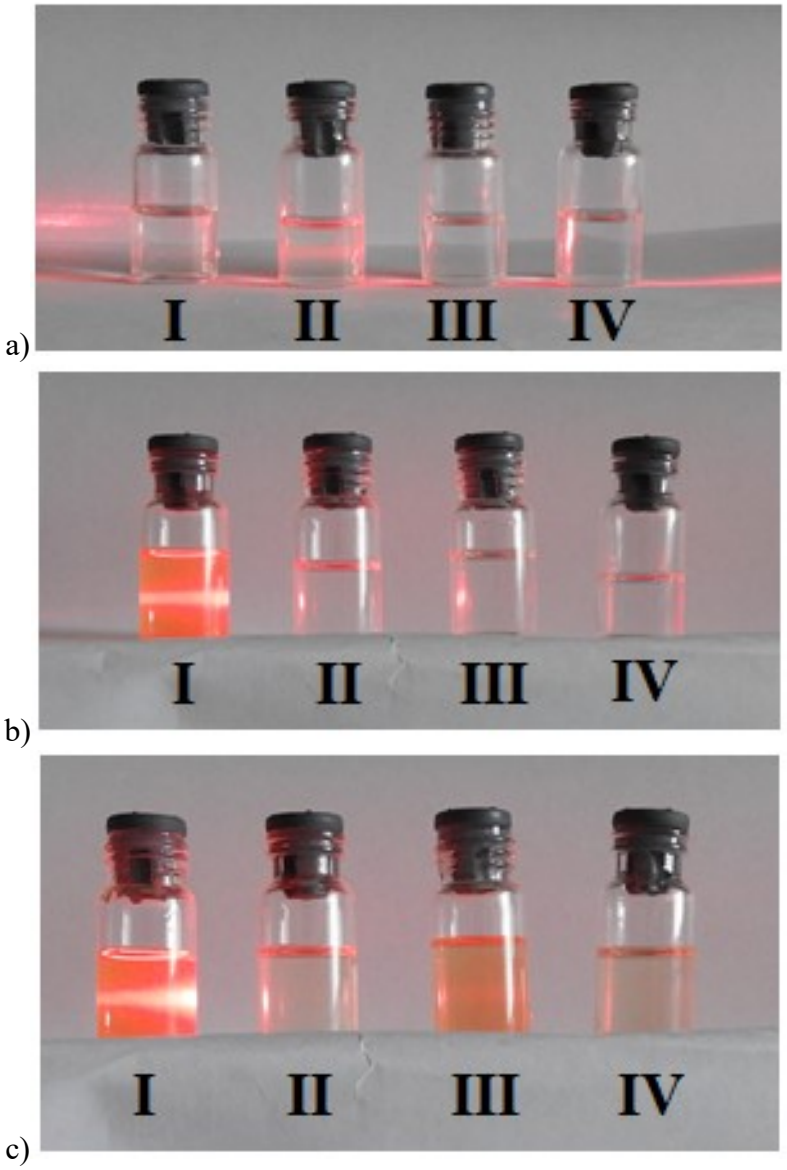

Figure S11. The Tyndal effect test (red laser) for sonicated $Cu(H_2O)(HCO_2)(L1)]\cdot 0{,}5H2O$ (**1**) [I], $[Cu(L3)_2]$ (**5**) [II], $[Cu(H_2O)(HCO_2)(L2)]\cdot H_2O$ (**3**) [III], and $[Cu(L2)_2]$ (**4**) [IV] in acetone (a), ethanol (b), and DMF (c)

Parameters of valence bonds, H-bonds, and interlayer van der Waals interactions

Table S1 "Compositions and topological parameters of 623 structures of complexes with Cu-O←NC_2 group" is presented as a separate file "Table S1.xlsx"

Table S2. Crystal data and structure refinement for **1–5**.

Parameter	**1**	**2**	3	**4**	**5**
Empirical formula	$C_4H_7CuN_2O_{5.5}$	$C_{16}H_{18}Cu_3N_8O_{12}$	$C_5H_{10}CuN_2O_6$	$C_8H_{10}CuN_4O_4$	$C_{10}H_{14}CuN_4O_4$
Formula weight	234.66	705.00	257.69	289.74	317.79
a (Å)	22.5046(18)	7.396(3)	9.6088(19)	5.868(5)	9.832(9)
b (Å)	10.0382(9)	17.171(7)	9.929(2)	8.771(7)	9.541(9)
c (Å)	6.9385(6)	9.335(4)	9.850(2)	10.174(9)	12.769(10)
β (°)	90	94.808(10)	91.297(7)	101.18(3)	90
V (Å^3)	1567.4(2)	1181.5(8)	939.5(3)	513.7(7)	1197.8(19)
Crystal system	Orthorhombic	Monoclinic	Monoclinic	Monoclinic	Orthorhombic
Space group, Z	*P n m a, 8*	*P 2$_1$/c, 2*	*P 2$_1$/n, 4*	*P 2$_1$/n, 2*	*P b c a, 4*
D_{cal}(g cm^{-3})	1.989	1.982	1.822	1.873	1.762
μ (mm^{-1})	2.781	2.756	2.332	2.136	1.841
Reflections collected	11277	17003	18004	5125	14505
Independent reflections (R_{int})	2394 (0.034)	5160 (0.174)	2867 (0.042)	1529 (0.035)	1566 (0.048)
Obs.refl./restraints/ parameters	2037 / 0 / 130	2213 / 0 / 179	2577 / 0 / 119	1287 / 0 / 80	1129 / 0 / 90
R,[a] % [$F^2 > 2\sigma(F^2)$]	0.044	0.072	0.041	0.029	0.042
wR_2,[b] % (F^2)	0.116	0.148	0.103	0.090	0.093
GOF	1.09	0.99	1.08	1.00	1.09
F(000)	944	706	524	294	652

[a] $R = \Sigma \left| \left| F_o \right| - \left| F_c \right| \right| / \Sigma \left| F_o \right|$. [b] $wR2 = [\Sigma(w(F_o^2 - F_c^2)^2)/\Sigma(w(F_o^2))]^{1/2}$. [c] $GOF = [\Sigma w(F_o^2 - F_c^2)^2/(N_{obs} - N_{param})]^{1/2}$

Table S3. The geometrical parameters of valence bonds and angles in the structure of compound **1**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.9755(18)	O4	C1	1.277(5)
Cu1	O2[1]	2.0173(18)	O5	C1	1.226(6)
Cu1	O3	1.921(3)	N1	C2	1.327(6)
Cu1	O4	1.937(2)	N1	C4	1.364(7)
Cu1	O6	2.271(3)	N2	C2	1.331(5)
O1	Cu1[2]	1.9755(18)	N2	C3	1.356(6)
O1	N1	1.353(4)	N3	C5	1.334(4)
O2	Cu1[3]	2.0173(18)	N3	C6	1.362(5)
O2	Cu1[4]	2.0173(18)	C3	C4	1.362(7)
O2	N2	1.363(4)	C5	N3[5]	1.334(4)
O3	N3	1.353(3)	C6	C6[5]	1.359(8)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cu1	O2[1]	73.68(10)	C1	O4	Cu1	110.8(3)
O1	Cu1	O6	92.65(15)	O1	N1	C4	125.1(4)
O2[1]	Cu1	O6	99.02(13)	C2	N1	O1	123.9(4)
O3	Cu1	O1	160.25(11)	C2	N1	C4	111.0(4)
O3	Cu1	O2[1]	87.38(9)	C2	N2	O2	123.4(4)
O3	Cu1	O4	100.44(11)	C2	N2	C3	111.0(4)
O3	Cu1	O6	95.87(13)	C3	N2	O2	125.6(3)
O4	Cu1	O1	97.01(12)	O3	N3	C6	125.9(3)
O4	Cu1	O2[1]	165.74(12)	C5	N3	O3	123.7(3)
O4	Cu1	O6	92.08(12)	C5	N3	C6	110.1(3)
Cu1[2]	O1	Cu1	107.68(14)	O5	C1	O4	124.8(4)
N1	O1	Cu1	126.16(7)	N1	C2	N2	105.7(4)
N1	O1	Cu1[2]	126.16(7)	N2	C3	C4	106.4(4)
Cu1[3]	O2	Cu1[4]	104.49(13)	C3	C4	N1	105.9(4)
N2	O2	Cu1[3]	114.41(14)	N3[5]	C5	N3	106.6(4)
N2	O2	Cu1[4]	114.41(14)	C6[5]	C6	N3	106.6(2)
N3	O3	Cu1	120.7(2)				

[1]+X,+Y,1+Z; [2]+X,1/2-Y,+Z; [3]+X,1/2-Y,-1+Z; [4]+X,+Y,-1+Z; [5]+X,3/2-Y,+Z

Table S4. The parameters of interlayer H-bonds in the structure of compound **1**.

Contacting atoms	*Distance H···A, Å*	*Angle D-H···A, °*
Interface 1I-1I, $O7_{ws}H7\cdots O4_f$(C1)	1,909	168,79
Interface 1I-1I, $O6_wH6B\cdots O7_{ws}$	2,115	158,90
Interface 1I-1I, $O6_wH6A\cdots O3$(N3)	1,865	163,26
Interface 1I-1I, $C2H2\cdots O7_{ws}$	2,336	165,93
Interface 1II-1II, $C6H4\cdots O5_f$ (C1)	2,340	164,41

w – coordinated water
ws – solvate water
f – formiate anion

Table S5. The parameters of interlayer van der Waals (vdw) interactions in the structure of compound **1**.

Contacting atoms	*Distance, Å*
(C1)H1···H1(C1)	3,173
(C1)H1···H2(C2)	2,887
(C1)H1···H5(C5)	2,864
($O6_w$)H6B···$O6_w$	3,029
($O6_w$)H6B···H7($O7_{ws}$)	2,205
($O6_w$)H6B···H5(C5)	2,907
($O6_w$)H6B···C5	2,929
(C1)H1···H4(C4)	3,554
(C1)H1···$O5_f$(C1)	2,758
(C1)H1···H3(C3)	2,713
(C2)H2···H5(C5)	2,705
(C4)H4···O5(C1)	3,600
(C4)H4···H6(C6)	2,840
(C5)H5···O2(N2)	2,542
($O7_{ws}$)H7···C5	3,308
($O7_{ws}$)H7···C6	3,525
($O7_{ws}$)H7···N3	3,520
($O7_{ws}$)H7···O6	3,099
$O6_w$···$O6_w$	2,947

w – coordinated water
ws – solvate water
f – formiate anion

Table S6. The geometrical parameters of valence bonds and angles in the structure of compound **2**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1[1]	1.944(3)	O4	N4	1.366(5)
Cu1	O1	1.944(3)	O5	C7	1.256(6)
Cu1	O5	1.955(4)	O6	C7	1.249(6)
Cu1	O5[1]	1.955(4)	N1	C1	1.342(6)
Cu2	O1[1]	2.392(4)	N1	C2	1.368(6)
Cu2	O2[2]	1.961(3)	N2	C1	1.330(6)
Cu2	O3	1.929(4)	N2	C3	1.364(6)
Cu2	O4[3]	1.945(3)	N3	C4	1.344(6)
Cu2	O6	1.945(3)	N3	C5	1.350(7)
O1	Cu2[1]	2.392(4)	N4	C4	1.338(7)
O1	N1	1.358(5)	N4	C6	1.360(7)
O2	Cu2[4]	1.961(3)	C2	C3	1.358(7)
O2	N2	1.357(5)	C5	C6	1.367(8)
O3	N3	1.355(5)	C7	C8	1.509(7)
O4	Cu2[5]	1.945(3)			

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	Cu1	O1	180.00(14)	C7	O6	Cu2	130.5(3)
O1[1]	Cu1	O5[1]	91.56(14)	O1	N1	C2	126.4(4)
O1	Cu1	O5[1]	88.44(14)	C1	N1	O1	124.1(4)
O1	Cu1	O5	91.57(14)	C1	N1	C2	109.6(4)
O1[1]	Cu1	O5	88.43(14)	O2	N2	C3	125.2(4)
O5	Cu1	O5[1]	180.0	C1	N2	O2	124.3(4)
O2[2]	Cu2	O1[1]	101.53(13)	C1	N2	C3	110.4(4)
O3	Cu2	O1[1]	99.89(14)	C4	N3	O3	123.7(4)
O3	Cu2	O2[2]	87.47(15)	C4	N3	C5	110.0(4)
O3	Cu2	O4[3]	170.92(16)	C5	N3	O3	126.3(4)
O3	Cu2	O6	91.91(15)	C4	N4	O4	124.8(4)
O4[3]	Cu2	O1[1]	88.99(14)	C4	N4	C6	110.5(4)
O4[3]	Cu2	O2[2]	92.66(15)	C6	N4	O4	124.7(5)
O4[3]	Cu2	O6	86.39(15)	N2	C1	N1	106.6(4)
O6	Cu2	O1[1]	88.42(14)	C3	C2	N1	106.9(4)
O6	Cu2	O2[2]	170.00(15)	C2	C3	N2	106.4(5)
Cu1	O1	Cu2[1]	93.25(14)	N4	C4	N3	106.2(4)
N1	O1	Cu1	116.4(3)	N3	C5	C6	107.3(5)
N1	O1	Cu2[1]	121.0(3)	N4	C6	C5	106.0(5)
N2	O2	Cu2[4]	112.7(3)	O5	C7	C8	115.6(4)
N3	O3	Cu2	118.2(3)	O6	C7	O5	127.0(5)
N4	O4	Cu2[5]	119.3(3)	O6	C7	C8	117.5(5)
C7	O5	Cu1	129.4(3)				

[1]2-X,1-Y,1-Z; [2]2-X,1/2+Y,3/2-Z; [3]1+X,+Y,+Z; [4]2-X,-1/2+Y,3/2-Z; [5]-1+X,+Y,+Z

Table S7. The geometrical parameters of valence bonds and angles in the structure of compound **3**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.943(2)	N1	C2	1.334(6)
Cu1	O3	1.9031(19)	N1	C4	1.371(7)
Cu1	O4[1]	1.9851(17)	N2	C2	1.344(6)
Cu1	O4[2]	1.9752(17)	N2	C3	1.353(7)
Cu1	O5	2.328(3)	C2	C5	1.462(9)
O1	C1	1.267(4)	C3	C4	1.393(8)
O2	C1	1.223(4)	N1A	C2A	1.316(7)
O3	N1	1.353(4)	N1A	C4A	1.385(8)
O3	N1A	1.330(4)	N2A	C2A	1.309(7)
O4	Cu1[3]	1.9752(17)	N2A	C3A	1.392(8)
O4	Cu1[4]	1.9851(17)	C2A	C5A	1.477(9)
O4	N2	1.367(4)	C3A	C4A	1.309(10)
O4	N2A	1.385(4)			

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cu1	O4[1]	165.50(8)	C2	N1	C4	110.7(4)
O1	Cu1	O4[2]	95.21(8)	C2	N2	O4	120.5(4)
O1	Cu1	O5	94.76(10)	C2	N2	C3	112.5(4)
O3	Cu1	O1	99.97(8)	C3	N2	O4	127.0(4)
O3	Cu1	O4[1]	90.85(7)	N1	C2	N2	105.4(4)
O3	Cu1	O4[2]	161.53(8)	N1	C2	C5	126.5(5)
O3	Cu1	O5	94.98(11)	N2	C2	C5	128.1(5)
O4[1]	Cu1	O4[2]	72.54(8)	N2	C3	C4	104.8(5)
O4[1]	Cu1	O5	93.87(9)	N1	C4	C3	106.6(5)
O4[2]	Cu1	O5	94.18(10)	O3	N1A	C4A	123.3(5)
C1	O1	Cu1	114.87(19)	C2A	N1A	O3	127.7(4)
N1	O3	Cu1	115.6(2)	C2A	N1A	C4A	108.9(5)
N1A	O3	Cu1	121.0(2)	O4	N2A	C3A	129.2(5)
Cu1[3]	O4	Cu1[4]	107.46(8)	C2A	N2A	O4	122.1(4)
N2	O4	Cu1[4]	122.3(2)	C2A	N2A	C3A	108.7(5)
N2	O4	Cu1[3]	124.9(2)	N1A	C2A	C5A	126.4(6)
N2A	O4	Cu1[4]	127.2(2)	N2A	C2A	N1A	108.2(5)
N2A	O4	Cu1[3]	120.3(2)	N2A	C2A	C5A	125.4(6)
O2	C1	O1	126.3(3)	C4A	C3A	N2A	107.1(6)
O3	N1	C4	124.2(4)	C3A	C4A	N1A	107.1(6)
C2	N1	O3	125.1(4)				

[1]1/2-X,1/2+Y,3/2-Z; [2]1/2+X,1/2-Y,-1/2+Z; [3]1/2-X,-1/2+Y,3/2-Z; [4]-1/2+X,1/2-Y,1/2+Z

Table S8. The parameters of interlayer H-bonds in the structure of compound **3**.

Contacting atoms	*Distance H···A, Å*	*Angle D-H···A, °*
$O5_wH5A\cdots O2_f(C1)$	1.991	164,07
$O5_wH5B\cdots O6_{ws}$	1.923	160,86
$O6_{ws}H6B\cdots O2_f(C1)$	1,988	168,87
$O6_{ws}H6A\cdots O1_f(C1)$	2,089	169,49
$O5_wH5B\cdots O6_{ws}$	1,923	160,86

w – coordinated water
ws – solvate water
f – formiate anion

Table S9. The parameters of interlayer van der Waals (vdw) interactions in the structure of compound **3**.

Contacting atoms	*Distance, Å*
(O5w)H5A···H4(C4)	2.625
(O5w)H5A···H5C(C5)	3.022
(O5w)H5A···H4(C4)	3.731
(C3)H3···H5C(C5)	2.343
(C3)H3···H5E(C5)	2.608
(C3)H3···H5D(C5)	2.755
(C3)H3···$O6_{ws}$	2,522
(C4)H4···H5D(C5)	2.434
(C4)H4···H5E(C5)	2.634
(C4)H4···$O2_f$	3.171
(C4)H4···H4(C4)	3.631
(C5)H5C···$O6_{ws}$	2,959
(O6ws)H6A···H5A(O5)	2.581
(O6ws)H6A···H4(C4)	3.068
(O6ws)H6A···H3(C3)	3.678
(O6ws)H6A···C3	3.72
(O6ws)H6A···H1(C1)	3.798
(O6ws)H6B···H5A(O5)	2.338
(O6ws)H6B···H5E(C5)	2.937
(O6ws)H6B···H4(C4)	3.158
(O6ws)H6B···Cu1	3.355
(O6ws)H6B···H5C(C5)	3.374
(O6ws)H6B···H5D(C5)	3.437

w – coordinated water
ws – solvate water
f – formiate anion

Table S10. The geometrical parameters of valence bonds and angles in the structure of compound **4**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1	1.9279(19)	N1	C2	1.339(3)
Cu1	O1[1]	1.9279(19)	N1	C4	1.389(3)
Cu1	O2[2]	1.9362(19)	N2	C2	1.345(3)
Cu1	O2[3]	1.9362(19)	N2	C3	1.387(3)
O1	N1	1.361(2)	C1	C2	1.480(3)
O2	Cu1[4]	1.9362(19)	C3	C4	1.355(3)
O2	N2	1.357(2)			

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1	Cu1	O1[1]	180.0	C2	N1	C4	110.53(17)
O1[1]	Cu1	O2[2]	89.19(7)	O2	N2	C3	125.79(17)
O1	Cu1	O2[3]	89.19(7)	C2	N2	O2	123.42(16)
O1	Cu1	O2[2]	90.81(7)	C2	N2	C3	110.57(17)
O1[1]	Cu1	O2[3]	90.81(7)	N1	C2	N2	105.93(17)
O2[2]	Cu1	O2[3]	180.0	N1	C2	C1	127.8(2)
N1	O1	Cu1	118.64(12)	N2	C2	C1	126.22(19)
N2	O2	Cu1[4]	120.54(12)	C4	C3	N2	106.38(19)
O1	N1	C4	124.72(18)	C3	C4	N1	106.59(18)
C2	N1	O1	124.62(19)				

[1]1-X,-Y,1-Z; [2]1/2+X,1/2-Y,1/2+Z; [3]1/2-X,-1/2+Y,1/2-Z; [4]1/2-X,1/2+Y,1/2-Z

Table S11. The parameters of interlayer van der Waals (vdw) interactions in the structure of compound **4**.

Contacting atoms	*Distance, Å*
(C1)H1A···C4	2,714
(C1)H1A···H1C(C1)	3,085
(C1)H1A···H1B(C1)	3,083
(C1)H1A···H3(C3)	3,040
(C1)H1A···H4(C4)	2,586
(C1)H1B···H1C(C1)	2,233
(C1)H1C···H3(C3)	2,634
(C1)H1C···H4(C4)	2,710
(C3)H3···O1	3,237
(C3)H3···H3(C3)	3,057
(C3)H3···O2	2,530
(C3)H3···Cu1	2,794
(C4)H4···C3	3,155
(C3)H4···N2	2,896
(C3)H4···O2	2,869
(C4)H4···O1	3,731

Table S12. The geometrical parameters of valence bonds and angles in the structure of compound **5**.

Atom	Atom	Length/Å	Atom	Atom	Length/Å
Cu1	O1[1]	1.939(2)	N1	C1	1.338(3)
Cu1	O1	1.939(2)	N1	C3	1.382(3)
Cu1	O2[2]	1.946(2)	N2	C1	1.339(3)
Cu1	O2[3]	1.946(2)	N2	C2	1.376(3)
O1	N1	1.360(3)	C2	C3	1.375(4)
O2	Cu1[4]	1.946(2)	C2	C4	1.488(4)
O2	N2	1.363(3)	C3	C5	1.489(4)

Atom	Atom	Atom	Angle/°	Atom	Atom	Atom	Angle/°
O1[1]	Cu1	O1	180.0	O2	N2	C2	124.8(2)
O1	Cu1	O2[2]	88.37(8)	C1	N2	O2	124.9(2)
O1[1]	Cu1	O2[3]	88.37(8)	C1	N2	C2	110.3(2)
O1[1]	Cu1	O2[2]	91.63(8)	N1	C1	N2	106.9(2)
O1	Cu1	O2[3]	91.63(8)	N2	C2	C4	122.1(2)
O2[2]	Cu1	O2[3]	180.0	C3	C2	N2	106.5(2)
N1	O1	Cu1	116.23(15)	C3	C2	C4	131.4(3)
N2	O2	Cu1[4]	117.49(14)	N1	C3	C5	122.0(2)
O1	N1	C3	124.5(2)	C2	C3	N1	106.2(2)
C1	N1	O1	125.3(2)	C2	C3	C5	131.7(3)
C1	N1	C3	110.1(2)				

[1]1-X,-Y,1-Z; [2]1/2-X,-1/2+Y,+Z; [3]1/2+X,1/2-Y,1-Z; [4]-1/2+X,1/2-Y,1-Z

Table S13. The parameters of interlayer van der Waals (vdw) interactions in the structure of compound **5**.

Contacting atoms	*Distance, Å*
(C4)H4B···O2	2,796
(C4)H4B···H5C(C5)	2,601
(C1)H1···H4A(C4)	2,383
(C1)H1···H4B(C4)	2,675
(C1)H1···H5B(C5)	2,790
(C4)H4C···H5B (C5)	3,281
(C5)H5B ···O2	3,368
(C4)H4A···H5B(C5)	2,813
(C5)H5B ···O1	2,928
(C1)H1···H5C(C5)	3,016
(C4)H4A···H5A(C5)	3,020
(C4)H4B···H5A(C5)	3,021
(C4)H4C···H5C(C5)	2,962