Supporting Information

Two- and Three-Dimensional Nickel(II) and Copper(II) Metal–Organic Frameworks Based on 1*H*-Pyrazole-4-carboxylate

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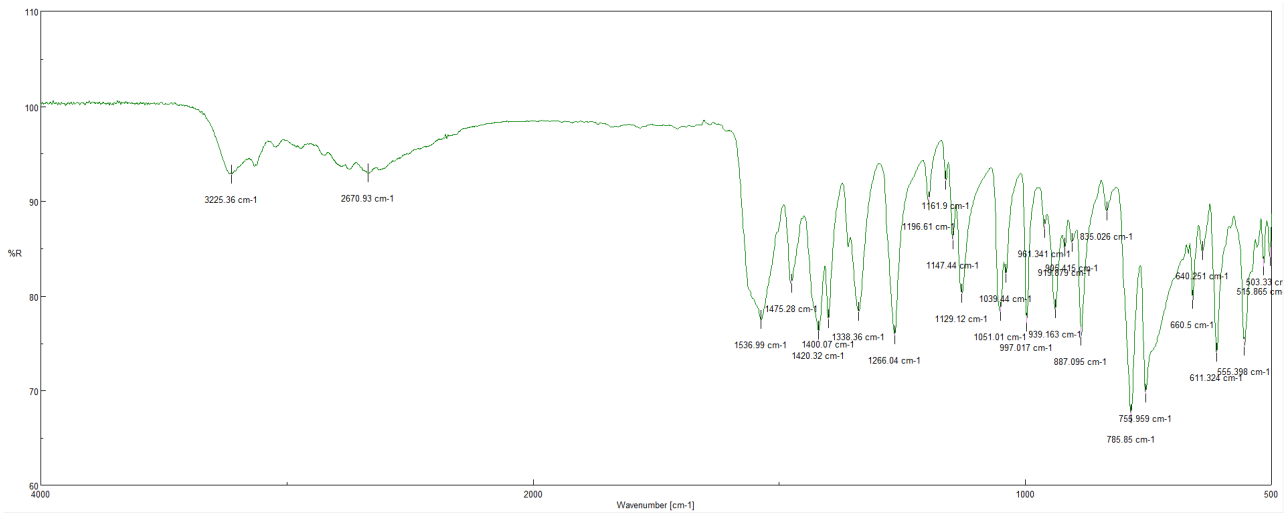
(a)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Wavenumber [cm-1]
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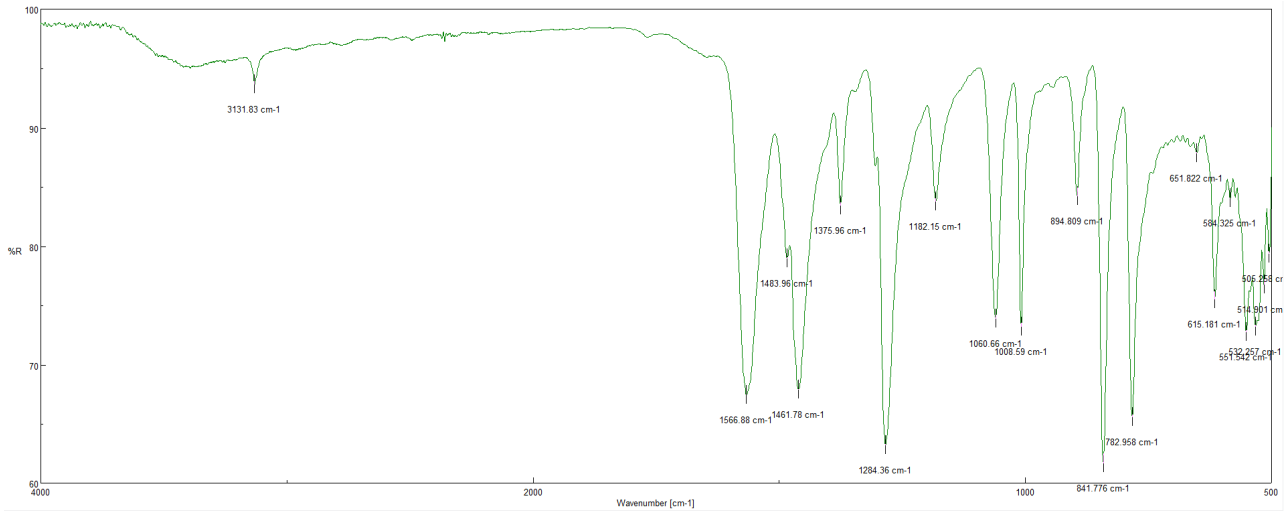
1400.07 cm-1
1338.36 cm-1
1266.04 cm-1
1196.61 cm-1
1161.9 cm-1
1147.44 cm-1
1129.12 cm-1
1051.01 cm-1
1039.44 cm-1
997.017 cm-1
939.163 cm-1
887.095 cm-1
835.026 cm-1
785.85 cm-1
759.959 cm-1
660.5 cm-1
640.251 cm-1
611.324 cm-1

(b)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1284.36 cm-1
1182.15 cm-1
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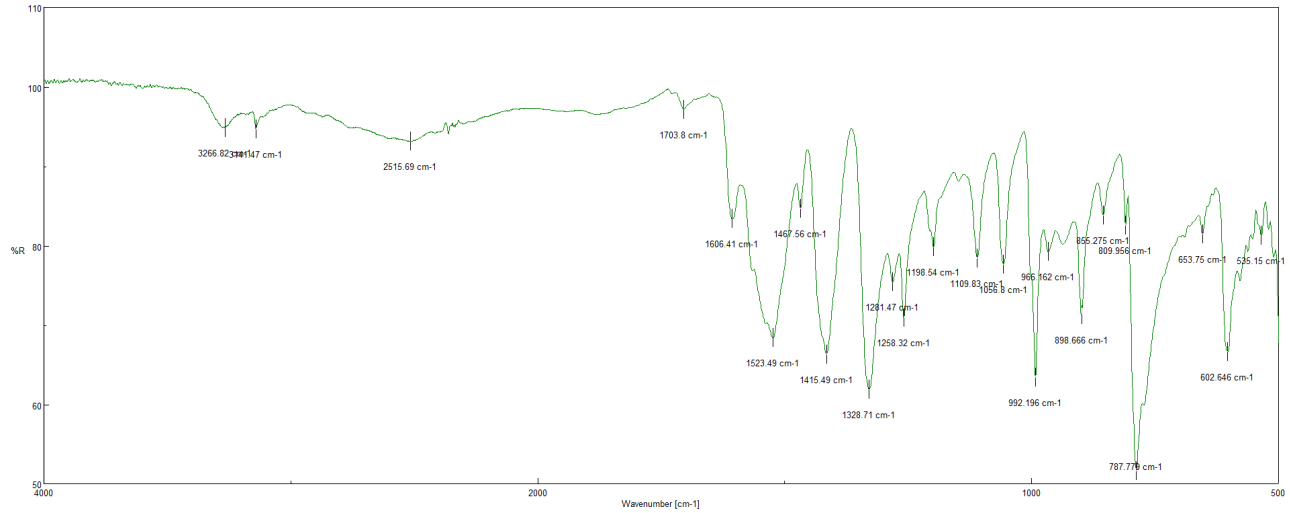
894.809 cm-1
841.776 cm-1
782.958 cm-1
651.822 cm-1
615.181 cm-1

(c)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Wavenumber [cm-1]
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1328.71 cm-1
1281.47 cm-1
1258.32 cm-1
1198.54 cm-1
1109.83 cm-1
1056.8 cm-1
992.196 cm-1
966.162 cm-1
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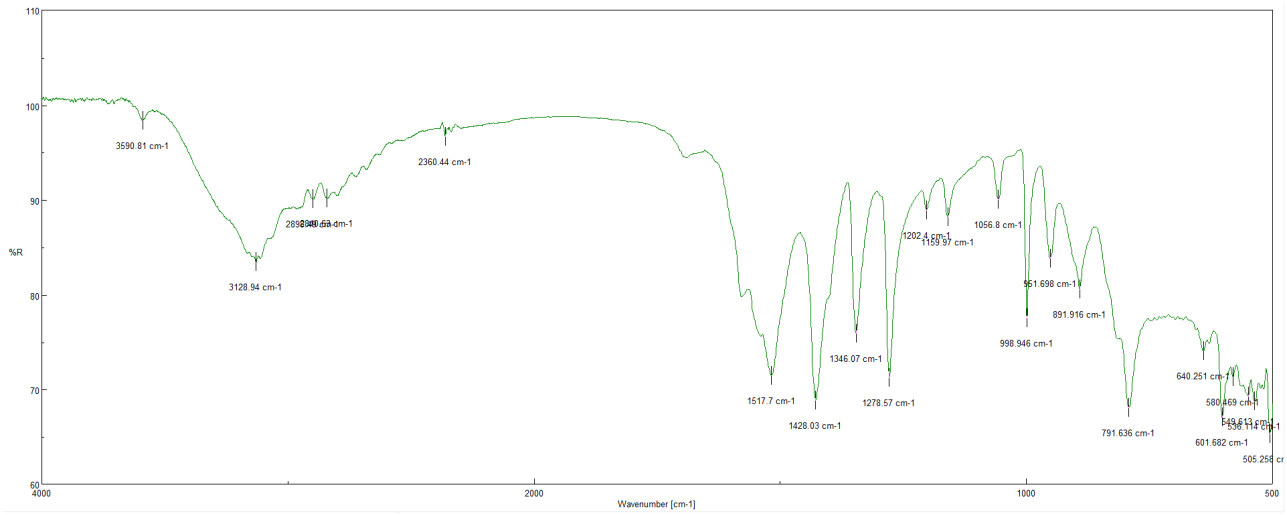
856.275 cm-1
809.956 cm-1
787.776 cm-1
653.75 cm-1
602.646 cm-1

(d)



(e)

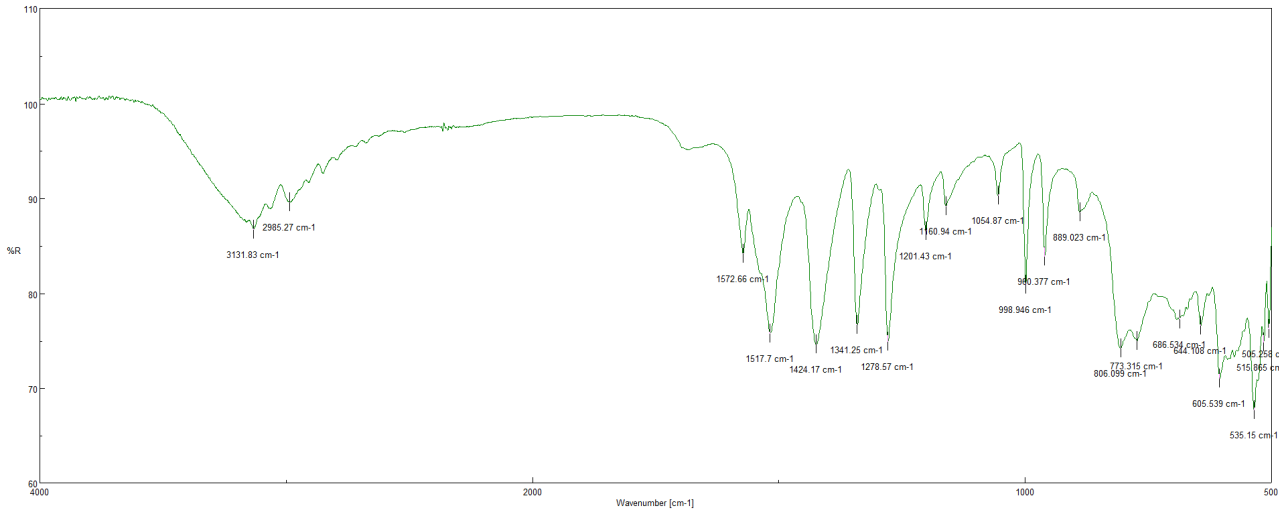


Figure S1. FT-IR spectra of (a) **1**, (b) **2**, (c) **3**, (d) *trans*-**4**, and (e) *cis*-**4**.

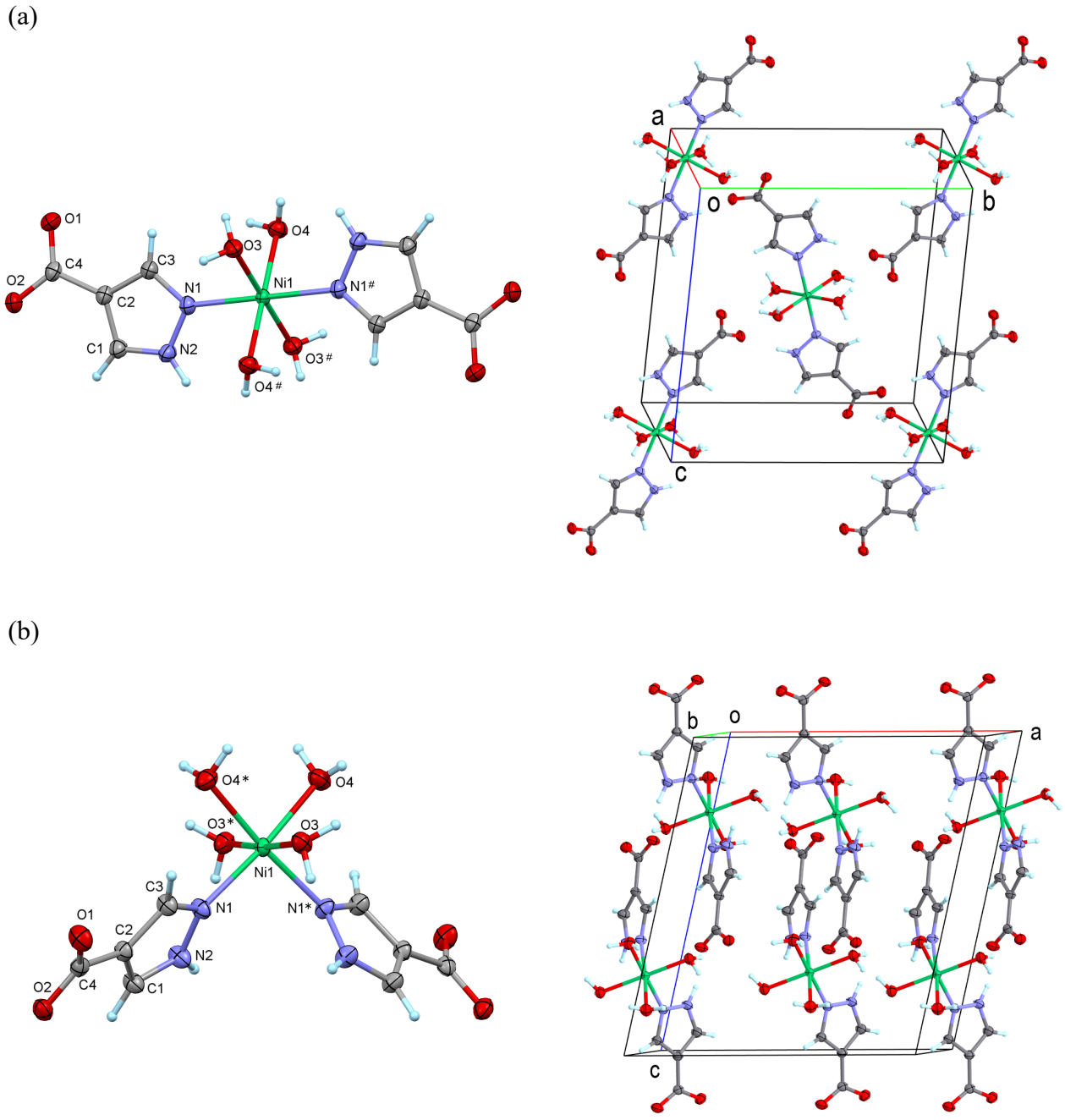


Figure S2. Molecular and crystal structures of (a) *trans*-**4** and (b) *cis*-**4**. Thermal ellipsoids are drawn at the 50% probability. Symmetry codes of # and * are (1 – *x*, 1 – *y*, 1 – *z*) and (1 – *x*, *y*, 1/2 – *z*), respectively.

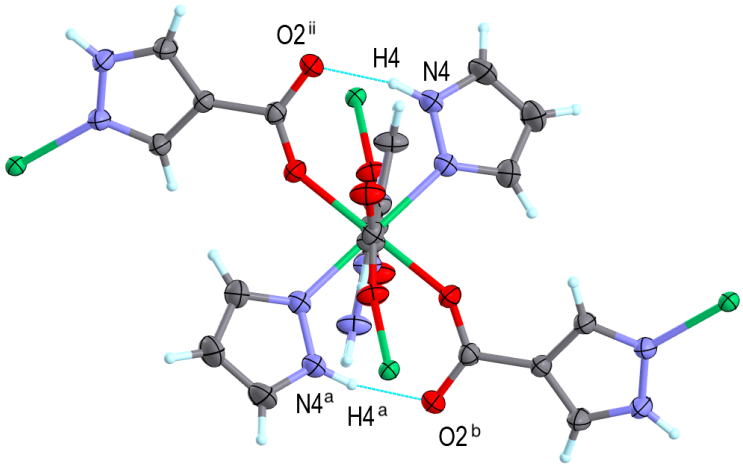
Table S1. Selected Crystallographic data of *trans*- and *cis*-**4**.

Complex	*trans*-**4**	*cis*-**4**
Formula	$C_8H_{14}N_4NiO_8$	$C_8H_{14}N_4NiO_8$
Formula weight	352.94	352.94
Dimension /mm^3	0.210×0.151×0.117	0.102×0.083×0.067
T / K	299	300
Crystal system	orthorhombic	monoclinic
Space group	*Pbca*	*C*2/*c*
a /Å	6.7762(3)	12.6240(6)
b /Å	13.2851(6)	7.3667(3)
c /Å	14.2804(6)	13.8231(6)
β /°	90	103.215(4)
V /Å^3	1285.56(10)	1251.47(10)
Z	4	4
D_{calc} /g cm^{-3}	1.824	1.873
Unique data	1819	1706
μ(MoKα) /mm^{-1}	1.559	1.601
R (F)[a] ($I > 2\sigma(I)$)	0.0289	0.0332
$R_w(F^2)$[b] (all data)	0.0828	0.0944
Goodness-of-fit	1.063	1.094
CCDC reference	2435384	2435385

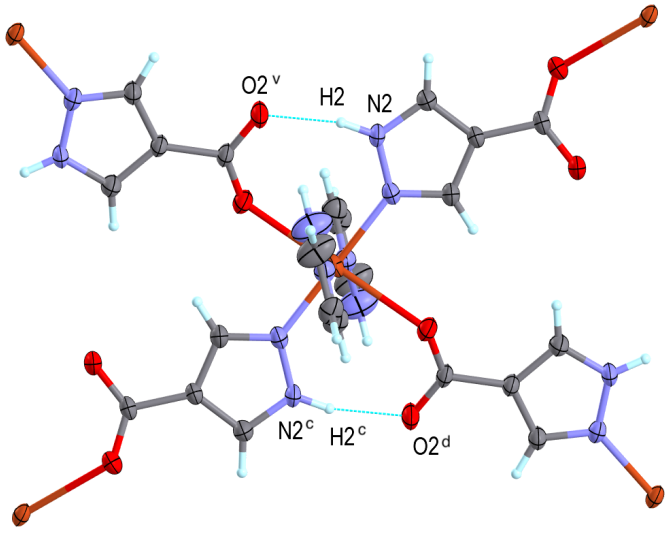
a) $R = \Sigma||F_o| - |F_c||/\Sigma|F_o|$.

b) $R_w = [\Sigma w|F_o^2 - F_c^2|^2/\Sigma w(F_o^2)^2]^{1/2}$.

(a)



(b)



(c)

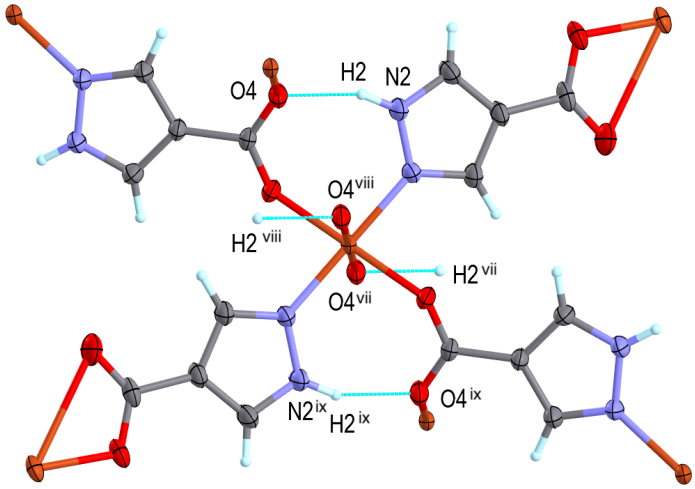


Figure S3. Hydrogen bonding structures of (a) **1**, (b) **2**, and (c) **3**. Hydrogen bonds are shown with dotted lines. Symmetry related hydrogen bonds are also shown. Symmetry operation codes for a, b, c, and d are (1–*x*, 1–*y*, 1–*z*), (1–*x*, –1/2+*y*, 1/2–*z*), (3/2–*x*, 3/2–*y*, 3/2–*z*), and (1–*x*, 1/2+*y*, 3/2–*z*), respectively. For other symmetry codes, see the main text.

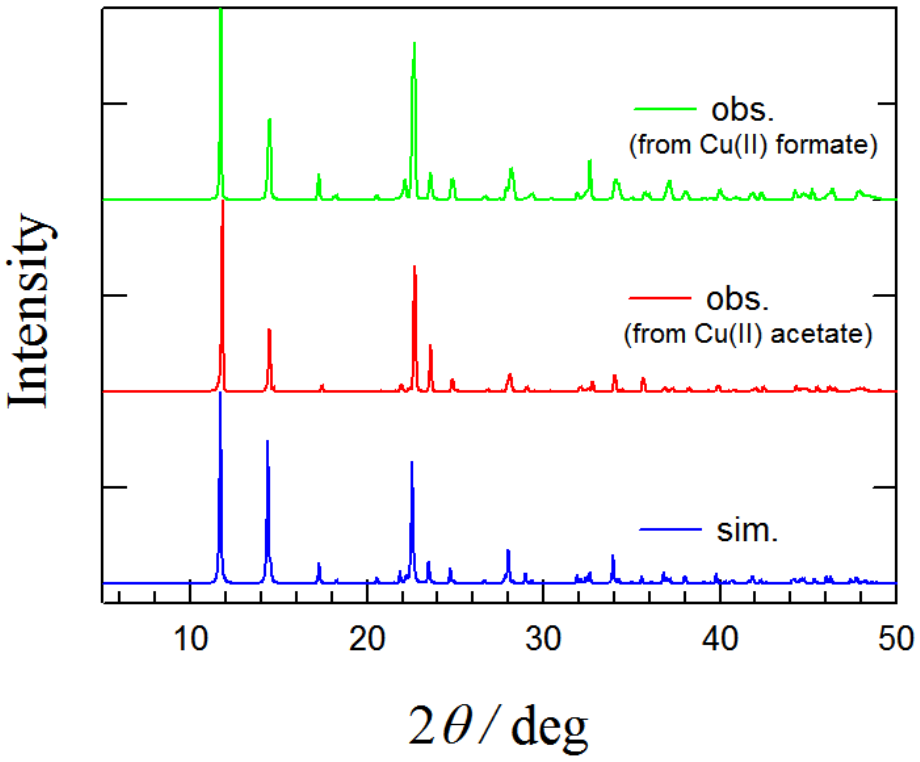


Figure S4. Powder XRD profiles for **3**. Color codes: observed for the sample prepared from copper(II) formate, green; observed for the sample prepared from copper(II) acetate, red; simulation from the single crystal crystallographic analysis at 100 K for the sample prepared from copper(II) acetate, blue.