Supporting information for the article

Anion – pyridine-n-oxime interplay to control metal - metal separations in a series of Cu(II) coordination polymers

Lilia Croitor - *Institute of Applied Physics, Academy str., 5 MD2028, Chisinau, Republic of Moldova;* ORCID: **0000-0003-0757-7358** E-mail: croitor.lilia@gmail.com;

Eduard B. Coropceanu - *Tiraspol State University, Iablocikin str. 5, MD2069, Chisinau, Republic of Moldova* ORCID: **0000-0003-1073-828X** E-mail: coropceanu.eduard@ust.md;

Marina S. Fonari *– I*nstitute of Applied Physics, Academy str., 5, MD2028, Chisinau, Republic of Moldova ;* ORCID **0000-0002-2508-5368** E-mail: marina.fonari@ifa.md; fonari.xray@gmail.com

Experimental

Material and methods

Metal salts, precursors and solvents were purchased from commercial suppliers and used without further purification. Elemental analyses were performed on an Elementar Analysensysteme GmbH Vario El III elemental analyzer.

Synthesis of coordination polymers

{[Cu(SiF_6)(4-pyaoH)$_4$] dmf 0.5H_2O}$_n$ (1). To the hot solution of CuF_2 (10 mg, 0.1 mmol) dissolved in 15 mL of water in a glass beaker was added the solution of H_2suc (12 mg, 0.1 mmol) and 4-pyaoH (24 mg, 0.2 mmol) dissolved in 10 mL of dmf. The resulting mixture was heated and stirred for 20 min, then filtered off and left to evaporate slowly at room temperature. Blue prismatic crystals were then collected from the solution. Yield (based on Cu): ~ 23% (18 mg). Anal. Calc. for $C_{27}H_{32}CuF_6N_9O_{5.5}Si$ (%): C, 41.77; H, 4.16; N, 16.25. Found: C, 41.39; H, 4.19; N, 16.12.

{[Cu(mal)(4-pyaoH)$_2$] dmf}$_n$ (**2**) and **{[Cu(mal)$_2$](4-pyaoH$_2$)$_2$}$_n$ (3)**. CuF_2 (10 mg, 0.1 mmol), H_2mal (10 mg, 0.1 mmol) and 4-pyaoH (24 mg, 0.2 mmol) were dissolved in a solution of 20 mL water:dmf (1:1). The mixture was heated and stirred for 25 min, then filtered and left to evaporate slowly at room temperature. Deep green needles of 2 were collected from the solution. Yield (based on Cu): ~ 29% (14 mg). Anal. Calc. for $C_{18}H_{21}CuN_5O_7$ (%): C, 44.76; H, 4.38; N, 14.51. Found: C, 44.54; H, 4.23; N, 14.37.
Light green plate-like crystals of **3** were collected from the same solution. Yield (based on Cu): ~ 23% (12 mg). Anal. Calc. for $C_{18}H_{18}CuN_4O_{10}$ (%): C, 42.06; H, 3.53; N, 11.29. Found: C, 41.83; H, 3.27; N, 11.04.

[Cu(adi)(3-pyaoH)$_2$(H$_2$O)]$_n$ (**4**). To CuF_2 (10 mg, 0.1 mmol) dissolved in 10 mL of water was added the solution of H_2adi (15 mg, 0.1 mmol) and 3-pyaoH (24 mg, 0.2 mmol) dissolved in 15 mL of methanol. The resulting mixture was heated and stirred for 20 min, then filtered off and left to evaporate slowly at room temperature. Blue prismatic crystals were then collected from the solution. Yield (based on Cu): ~ 37% (15 mg). Anal. Calc. for $C_{18}H_{22}CuN_4O_7$ (%): C, 45.99; H, 4.72; N, 11.93. Found: C, 45.76; H, 4.64; N, 11.58.

[Cu(adi)(3-pyaoH)$_2$]$_n$ (5). The mixture of CuF_2 (10 mg, 0.1 mmol), H_2adi (15 mg, 0.1 mmol) and 3-pyaoH (24 mg, 0.2 mmol) was dissolved in 30 mL of methanol:dmf (2:1) mixture, heated and stirred for 30 min, then filtered off and left to evaporate slowly at room temperature. Then blue plate-like crystals were collected from the solution. Yield (based on Cu): ~ 31% (14 mg). Anal. Calc. for $C_{18}H_{20}CuN_4O_6$ (%): C, 47.83; H, 4.46; N, 12.39. Found: C, 47.78; H, 4.41; N, 12.27.

{[Cu(adi)(3-pyaoH)$_2$] 0.6MeOH 0.3H$_2$O}$_n$ (**6**). The mixture of CuF_2 (10 mg, 0.1 mmol), H_2adi (15 mg, 0.1 mmol) and 3-pyaoH (24 mg, 0.2 mmol) was dissolved in 40 mL of methanol:water (1:1), heated and stirred for 15 min, then filtered off and left to evaporate slowly at room temperature. Blue plate-like crystals were collected from the solution. Yield (based on Cu): ~ 24% (11 mg). Anal. Calc. for $C_{18.6}H_{23}CuN_4O_{6.9}$ (%): C, 48.87; H, 4.86; N, 11.76. Found: C, 48.71; H, 4.67; N, 11.62.

{[Cu(seb)(3-pyaoH)$_2$] H$_2$seb 2H$_2$O}$_n$ (7). CuF_2 (10 mg, 0.1 mmol) was dissolved in 20 mL of water by heating and stirring for 10 min. Then to the resulting solution was added solution of H_2seb (20 mg, 0.1 mmol) and 3-pyaoH (24 mg, 0.2 mmol) in 15 mL methanol. The mixture was heated and stirred for 10 min, then filtered off and left to evaporate slowly at room temperature, resulting in the formation of blue elongated plate-like crystals. Yield (based on Cu): ~ 21% (16 mg). Anal. Calc. for $C_{32}H_{50}CuN_4O_{12}$ (%): C, 51.50; H, 6.75; N, 7.51. Found: C, 51.27; H, 6.57; N, 7.38.

[Cu(ClO$_4$)(2-pyao)(2-pyaoH)]$_n$ (**8**). To the solution of $Cu(ClO_4)_2 \cdot 6H_2O$ (37 mg, 0.1 mmol) dissolved in 10 mL water was added methanolic solution (15 mL) of malonic acid (10 mg, 0.1 mmol) and 2-pyaoH (24 mg, 0.2 mmol). The resulting mixture was heated and stirred for 15 min, then filtered off and left to evaporate slowly at room temperature. Blue plate-like crystals were collected from the solution. Yield (based on Cu): ~ 26% (11 mg). Anal. Calc. for $C_{12}H_{11}CuN_4O_6$ (%): C, 35.47; H, 2.73; N, 13.80. Found: C, 35.32; H, 2.67; N, 13.59.

{[Cu(oxa)(2-pyaoH)] H$_2$O}$_n$ (**9**). To the solution of CuF_2 (10 mg, 0.1 mmol) dissolved in 10 mL water was added methanolic solution (15 mL) of H_2ox (9 mg, 0.1 mmol) and 2-pyaoH (24 mg, 0.1 mmol). The resulting mixture was heated and stirred for 20 min, then filtered off and left to evaporate slowly at room temperature. Green plate-like crystals were collected from the solution. Yield (based on Cu): ~ 41% (12 mg). Anal. Calc. for $C_8H_8CuN_2O_6$ (%): C, 32.94; H, 2.76; N, 9.61. Found: C, 32.78; H, 2.54; N, 9.43.

{[Cu_3(μ_3-OH)(2-pyao)$_3$(fum)]·6.5H_2O}$_n$ (10). To CuF_2 (10 mg, 0.1 mmol) dissolved in 10 mL water was added 2-pyaoH (24 mg, 0.2 mmol) dissolved in 10 mL methanol. The resulting solution was heated and stirred for 30 min, then added H_2fum (12 mg, 0.1 mmol) dissolved in 10 mL of methanol. The mixture was heated and stirred for 10 min more, then filtered off and left to evaporate slowly at room temperature. Dark blue plate crystals were collected from the solution. Yield (based on Cu): ~ 18% (14 mg). Anal. Calc. for $C_{22}H_{31}Cu_3N_6O_{14.5}$ (%): C, 32.94; H, 3.90; N, 10.48. Found: C, 32.61; H, 3.76; N, 10.37.
All compounds are soluble in water, methanol, DMF and DMSO.

Crystallographic data collection and structure determination

Single crystals were mounted on a glass fiber using Paratone oil. Data collections were carried out on an Oxford Diffraction Xcalibur four-circle kappa geometry single-crystal diffractometer with Sapphire 3 CCD detector, using a graphite monochromated MoKα (λ = 0.71073 Å) radiation, and applying the CrysAlisPro Software system at 295(2) K. Data reduction, including absorption correction, was done by CrysAlisPro program. The structures were solved by SHELXS program [*G.M. Sheldrick, A short history of SHELX, Acta Crystallogr. Sect. A Found. Crystallogr. 64 (2008) 112–122. https://doi.org/10.1107/S0108767307043930*]. The coordinates and the anisotropic thermal parameters for all non-hydrogen atoms were refined by full-matrix least-squares methods based on F^2 using the SHELXL program. The C-bound H-atoms were generated geometrically using the riding model with the isotropic factor set 1.2Ueq of the parent atom, while O-bound H-atoms were found in mixed mode, either located in the difference Fourier map at the final stages of the refinement or generated geometrically using the riding model. The disordering problems were resolved in several structures. In **1** the solvent dmf and water molecules were refined with incomplete occupancies, and H-atoms in these molecules were not found. In **5-7** the oximic group of 3-pyaoH ligand is disordered over two positions, and for the minor components found with the probabilities of 0.062(4) in **5**, 0.115(4) in **6**, and 0.137(4) in **7** the oximic oxygen atom is excluded from Cu(II) coordination. In **8** two oxygen atoms of ClO_4^- anion that obeys a two-fold symmetry are disordered over two positions with probabilities 0.58(2) and 0.42(2). Crystals **10** displayed poor X-ray diffraction. The repeated trials for the different crystals displayed the identical unit-cell and the best structure solution was found for the twinned crystal. The solved crystal structure was unambiguous although the complete refinement was impossible because of poor crystal quality, so only the crystal model was discussed for **10**. CCDC 2174312 - 2174321 contain the supplementary crystallographic data for this paper. The Figures were produced using MERCURY program [*C.F. Macrae, I.J. Bruno, J.A. Chisholm, P.R. Edgington, P. McCabe, E. Pidcock, L. Rodriguez-Monge, R. Taylor, J. Van De Streek, P.A. Wood, Mercury CSD 2.0 - New features for the visualization and investigation of crystal structures, J. Appl. Crystallogr. 41 (2008) 466–470. https://doi.org/10.1107/S0021889807067908*].

Table S1. Crystal data and structure refinement parameters for compounds **1-10**.

Compound	**1**	**2**	**3**	**4**	**5**
CCDC numbers	2174318	2174316	2174312	2174314	2174319
Empirical formula	$C_{27}H_{32}CuF_6N_9O_{5.50}Si$	$C_{18}H_{21}CuN_5O_7$	$C_{18}H_{18}CuN_4O_{10}$	$C_{18}H_{22}CuN_4O_7$	$C_{18}H_{20}CuN_4O_6$
Formula weight	776.24	482.94	513.90	469.93	451.92
Crystal system	Tetragonal	Orthorhombic	Triclinic	Monoclinic	Monoclinic
Space group	*P*4/*ncc*	$Pna2_1$	*P*-1	*C*2/*c*	$P2_1/c$
a,*Å*	16.1144(6)	7.5251(3)	5.1679(7)	15.9487(9)	7.9490(4)
b,*Å*	16.1144(6)	14.0673(6)	10.3878(18)	6.1547(4)	14.2074(10)
c,*Å*	16.2242(10)	20.2503(7)	10.5431(14)	21.6085(10)	8.5744(4)
α, °	90	90	113.875(15)	90	90
β , °	90	90	90.888(11)	107.375(5)	97.604(4)
γ, °	90	90	99.321(12)	90	90
V, $Å^3$	4213.0(4)	2143.65(15)	508.66(14)	2024.3(2)	959.83(9)
Z	4	4	1	4	2
D(calcd) Mg/m^3	1.224	1.496	1.678	1.542	1.564
μ, mm^{-1}	0.616	1.068	1.141	1.128	1.182
F(000)	1592	996	263	972	466
Reflections collected	8773	4794	2673	3112	3142
Independent reflections	1850 [*R*(int)=0.0750]	3293 [*R*(int)=0.0291]	1780 [*R*(int)=0.0402]	1770 [*R*(int)=0.0284]	1679 [*R*(int)=0.0223]
Data / restraints / parameters	1850 / 42 / 152	3293 / 2 / 285	1780 / 0 / 151	1770 / 0 / 140	1679 / 0 / 139
GOF on F^2	1.037	0.994	1.005	1.047	1.057
R_1, wR_2 ($I > 2\sigma(I)$)	0.0636, 0.1195	0.0415, 0.0914	0.0492, 0.1048	0.0390, 0.0901	0.0384, 0.0929
R_1, wR_2 (all data)	0.1591, 0.1875	0.0556, 0.1000	0.0692, 0.1147	0.0481, 0.0963	0.0509, 0.1018
$\Delta\rho_{max}/\Delta\rho_{min}$ ($e\cdot Å^{-3}$)	0.408 / -0.247	0.305 /-0.249	0.334 /-0.426	0.444 /-0.266	0.309 /-0.249

Table S1 (continuation).

Compound	**6**	**7**	**8**	**9**	**10**
CCDC numbers	2174321	2174313	2174315	2174317	2174320
Empirical formula	$C_{18.60}H_{23}CuN_4O_{6.90}$	$C_{32}H_{50}CuN_4O_{12}$	$C_{12}H_{11}ClCu\ N_4O_6$	$C_8H_8CuN_2O_6$	$C_{22}H_{31}Cu_3N_6O_{14.50}$
Formula weight	476.55	746.30	406.24	291.70	802.15
Crystal system	Triclinic	Triclinic	Orthorhombic	Monoclinic	Monoclinic
Space group	*P*-1	*P*-1	*Pccn*	$P2_1/c$	$P2_1/c$
a,Å	8.0458(7)	8.2351(7)	7.0897(5)	8.9697(4)	10.4648(12)
b,Å	8.4741(6)	10.7703(10)	12.7224(7)	14.8584(5)	17.6569(18)
c,Å	8.6258(6)	11.2831(9)	17.1140(11)	7.6158(4) Å	16.962(2)
α, °	84.174(6)	71.752(8)	90	90	90
β , °	62.420(8)	77.454(7)	90	102.409(5)	96.147(11)
γ, °	82.413(7)	74.439(8)	90	90	90
V, Å^3	516.18(8)	905.83(15)	1543.65(17)	991.29(7)	3116.2(6)
Z	1	1	4	4	4
D(calcd) Mg/m^3	1.533	1.368	1.748	1.955	1.710
μ, mm^{-1}	1.106	0.668	1.626	2.224	2.105
F(000)	247	395	820	588	1632
Reflections collected	2887	5520	3216	3235	7024
Independent reflections	1810 [*R*(int)=0.0239]	3532 [*R*(int)=0.0286]	1364 [*R*(int)=0.0222]	1736 [*R*(int)=0.0285]	3226 [*R*(int)=0.0859]
Data / restraints / parameters	1810 / 1 / 154	3532 / 4 / 239	1364 / 12 / 132	1736 / 3 / 160	3226 / 277 / 369
GOF on F^2	1.076	1.026	1.020	1.017	1.087
R_1, wR_2 ($I > 2\sigma(I)$)	0.0398, 0.0995	0.0524, 0.0991	0.0350, 0.0747	0.0359, 0.0869	0.1645, 0.3106
R_1, wR_2 (all data)	0.0446, 0.1034	0.0742, 0.1104	0.0597, 0.0859	0.0466, 0.0925	0.2290, 0.3441
$\Delta\rho_{max}/\Delta\rho_{min}$ (e·Å^{-3})	0.562 /-0.271	0.314 /-0.233	0.251 /-0.200	0.485 /-0.378	1.961 /-1.126

Table S2. Bond lengths [Å] and angles [°] for **1-9**.

1			
Cu(1)-N(1)	2.015(4)	Cu(1)-F(1)	2.320(5)
Cu(1)-N(1)#1	2.015(4)	Si-F(1)	1.681(5)
Cu(1)-N(1)#3	2.015(4)	Si-F(2)	1.681(2)
Cu(1)-N(1)#2	2.015(4)	Si-F(3)	1.681(2)
N(1)-Cu(1)-F(1)	89.78(10)	F(1)-Si-F(3)	180.0
N(1)-Cu(1)-N(1)#2	89.999(1)	F(2)-Si-F(1)	89.60(11)
N(1)-Cu(1)-N(1)#1	179.6(2)	F(2)-Si-F(3)	90.40(11)
Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+1/2, z;			

#2 y,-x+1/2, z ; #3 -y+1/2, x, z			
2			
Cu(1)-O(5)	1.926(4)	Cu(1)-N(1)	2.023(5)
Cu(1)-O(3)	1.946(4)	Cu(1)-O(4)#1	2.227(5)
Cu(1)-N(3)	2.016(4)		
O(5)-Cu(1)-O(3)	91.59(19)	O(5)-Cu(1)-N(1)	151.2(2)
O(5)-Cu(1)-N(3)	90.5(2)	O(3)-Cu(1)-N(1)	86.7(2)
O(3)-Cu(1)-N(3)	177.53(19)	N(3)-Cu(1)-N(1)	92.2(2)
Symmetry transformations used to generate equivalent atoms: #1 x+1/2, -y+1/2, z			
3			
Cu(1)-O(1)	1.904(2)	Cu(1)-O(3)	1.927(2)
O(1)-Cu(1)-O(3)	94.21(10)	O(1)#1-Cu(1)-O(3)	85.79(10)
O(3)-Cu(1)-O(3)	180.0		
Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y, -z+1			
4			
Cu(1)-O(2)	1.9353(17)	Cu(1)-N(1)	2.057(2)
Cu(1)-O(1W)	2.291(4)		
O(2)#1-Cu(1)-O(2)	174.43(12)	N(1)#1-Cu(1)-N(1)	164.54(14)
O(2)-Cu(1)-N(1)#1	89.28(8)	O(2)-Cu(1)-O(1W)	87.22(6)
O(2)-Cu(1)-N(1)	91.47(8)	N(1)-Cu(1)-O(1W)	97.73(7)
Symmetry transformations used to generate equivalent atoms: #1 -x+1, y, -z+1/2			
5			
Cu(1)-O(2)	1.9297(19)	Cu(1)-N(1)	2.041(2)
O(2)-Cu(1)-N(1)	91.22(8)	O(2)#1-Cu(1)-N(1)	88.78(8)
Symmetry transformations used to generate equivalent atoms: #1 -x+1, -y+2, -z			
6			
Cu(1)-O(2)	1.942(2)	Cu(1)-N(1)	2.029(2)
O(2)-Cu(1)-N(1)	89.08(9)	O(2)-Cu(1)-N(1)#1	90.92(9)
Symmetry transformations used to generate equivalent atoms: #1 -x+2, -y, -z+1			
7			
Cu(1)-O(2)	1.9387(17)	Cu(1)-N(1)	2.019(2)
O(2)-Cu(1)-N(1)	89.04(8)	O(2)-Cu(1)-N(1)#1	90.96(8)
Symmetry transformations used to generate equivalent atoms: #1 -x, -y, -z+1			
8			
Cu(1)-N(2)	1.980(3)	Cu(1)-O(2)	2.471(15)
Cu(1)-N(1)	2.024(3)		
N(2)-Cu(1)-N(2)#1	91.58(18)	N(2)-Cu(1)-O(2)	96.3(6)
N(2)-Cu(1)-N(1)	80.75(12)	N(2)#1-Cu(1)-O(2)	95.9(4)
N(2)#1-Cu(1)-N(1)	168.60(10)	N(1)-Cu(1)-O(2)	93.3(3)
Symmetry transformations used to generate equivalent atoms: #1 -x+1/2, -y+3/2, z			
9			
Cu(1)-O(5)	1.925(2)	Cu(1)-N(2)	2.025(2)

Cu(1)-O(2)	1.948(2)	Cu(1)-O(3)#1	2.359(2)
Cu(1)-N(1)	1.970(3)		
O(5)-Cu(1)-O(2)	85.00(9)	O(5)-Cu(1)-O(3)#1	95.08(9)
O(5)-Cu(1)-N(1)	170.99(11)	O(2)-Cu(1)-O(3)#1	90.50(9)
O(2)-Cu(1)-N(1)	95.72(10)	N(1)-Cu(1)-O(3)#1	93.89(10)
O(5)-Cu(1)-N(2)	97.98(10)	N(2)-Cu(1)-O(3)#1	96.30(10)
O(2)-Cu(1)-N(2)	172.28(10)	N(1)-Cu(1)-N(2)	80.22(10)
Symmetry transformations used to generate equivalent atoms: #1 x,-y+3/2,z+1/2			

Table S3. Hydrogen bonds for **1-7** and **9** [Å and °].

D-H…A	H…A, **Å**	D…A, **Å**	∠D-H…A, °	Symmetry transformation for acceptor
1				
O(1)-H(1)···F(2)	1.99	2.723(5)	148.5	*-y*, *-x*, *-z*+1/2
O(1)-H(1)···F(2)	2.37	2.942(4)	127.2	*x*-1/2, *-y*, *-z*+1/2
2				
O(1)-H(1)···O(6)	1.94(4)	2.801(8)	165(11)	*-x*+1/2, *y*-1/2, *z*+1/2
O(2)-H(2)···O(1K)	1.86	2.660(10)	166.1	*-x*+5/2, *y*+1/2, *z*+1/2
3				
O(5)-H(5)···O(2)	1.82	2.611(4)	162.3	*x*+1, *y*, *z*
N(1)-H(1)···O(1)	2.57	3.139(4)	124.1	*-x*, *-y*, *-z*
N(1)-H(1)···O(3)	1.95	2.790(4)	165.9	*x*-1, *y*, *z*-1
4				
O(1W)-H(1W)···O(3)	2.158	2.891	170.67	*-x*+1, *y*+1, *-z*+1/2
O(1)-H(1O1)···O(3)	1.916	2.720(3)	166.64	*-x*+1/2, *-y*+1/2, *-z*
5				
O(1)-H(1)···O(3)	1.76	2.554(3)	163.6	*-x*, 2*-y*, *-z*
6				
O(1)-H(1)···O(3)	1.75	2.547(3)	163.6	*x*-1, *y*, *z*
7				
O(1)-H(1)···O(3)	1.83	2.638(3)	167.7	*x*+1, *y*, *z*
O(5)-H(5)···O(3)	1.77	2.577(3)	166.5	*-x*, *-y*+1, *-z*+1
O(1W)-H(1X)···O(5)	2.25(3)	2.989(3)	143(5)	*-x*+1, *-y*+1, *-z*
O(1W)-H(2X)···O(4)	2.03(3)	2.826(4)	153(5)	
9				
O(1)-H(1)···O(1W)	1.78	2.556(4)	157.8	*-x*+1, *-y*+2, *-z*+1
O(1W)-H(1W)···O(4)	2.16(5)	2.746(4)	138(6)	*x*, *y*, *z*+1
O(1W)-H(2W)···O(5)	2.13(5)	2.737(4)	137(5)	*-x*+1, *-y*+2, *-z*+1

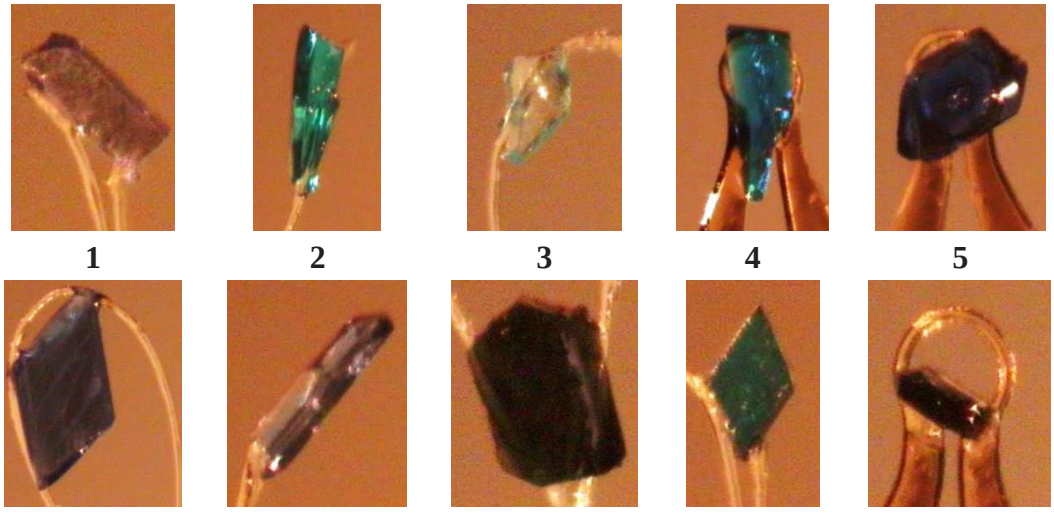


Figure S1. Images of crystals **1-10**

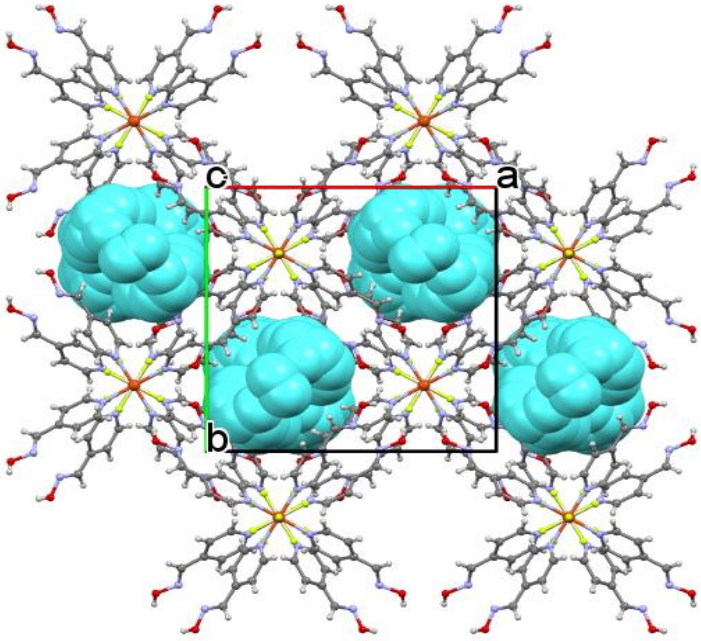


Figure S2. Crystal packing in $\{[Cu(SiF_6)(4\text{-pyaoH})_4]\cdot dmf\cdot 0.5H_2O\}_n$ (**1**) showing the association of coordination chains in the 3D H-bonded network *via* OH(3-pyaoH)···F hydrogen bonds with entrapping dmf and water solvents depicted as cyan space-filling models.

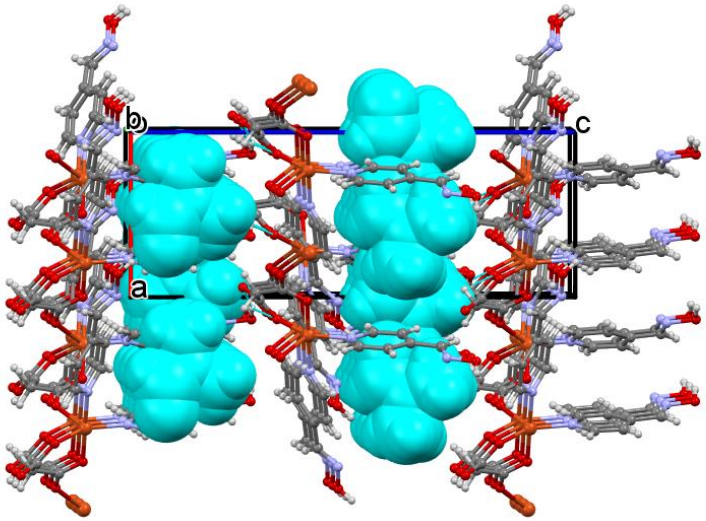


Figure S3. Crystal packing in {[Cu(mal)(4-pyaoH)$_2$]·dmf}$_n$ (**2**) with entrapped dmf solvent molecules depicted as cyan space-filling models.

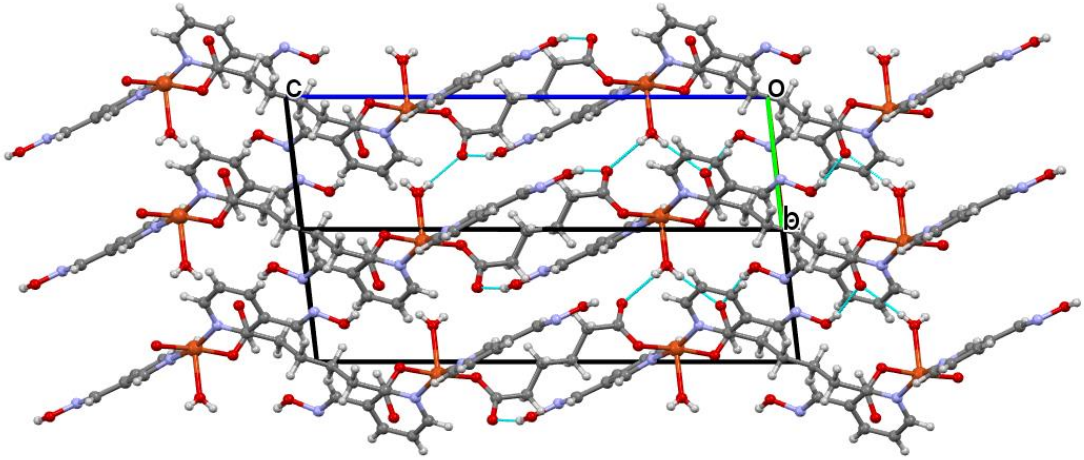
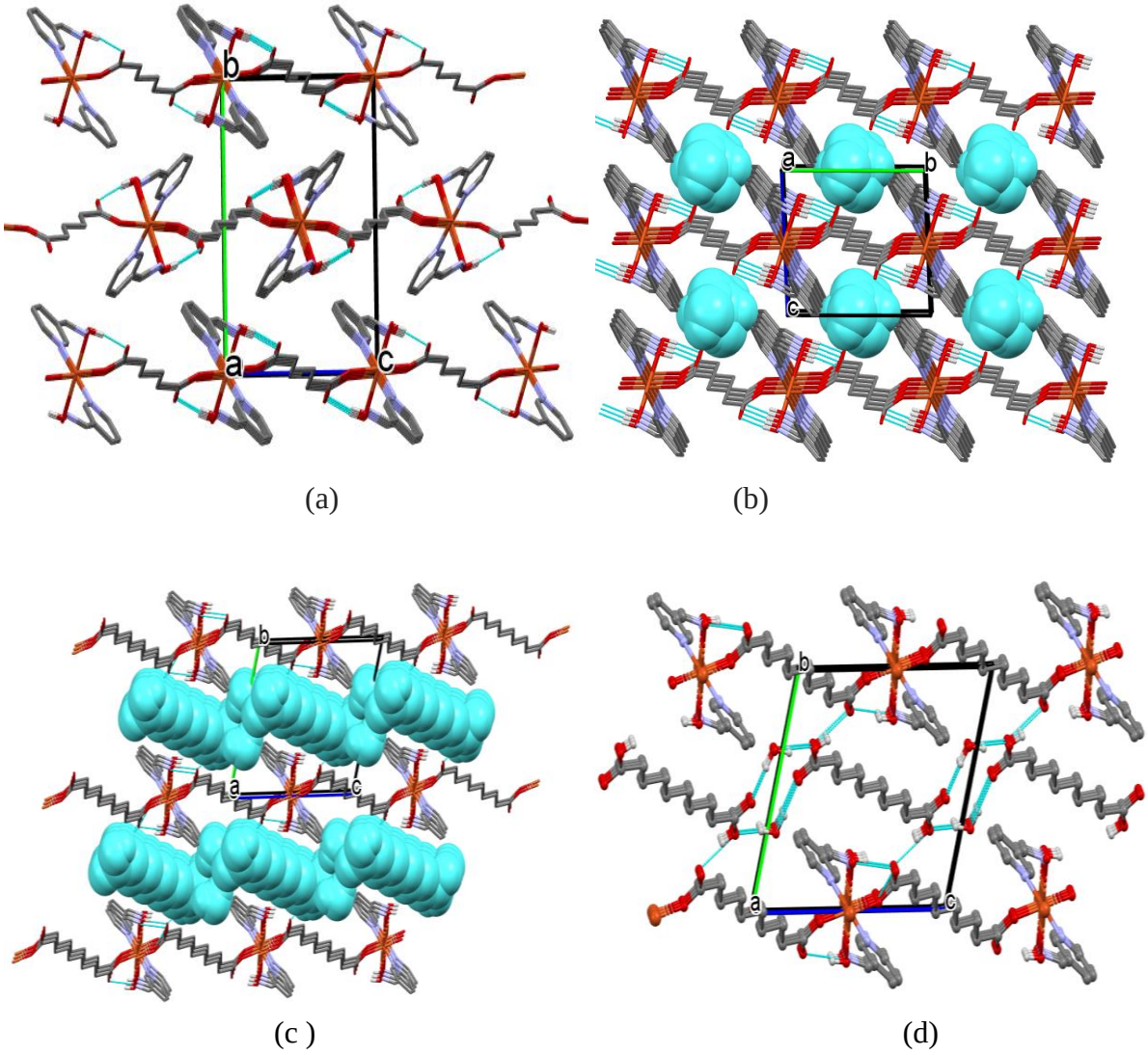


Figure S4. Crystal packing in [Cu(adi)(3-pyaoH)$_2$(H$_2$O)]$_n$ (**4**) showing the interconnection of coordination chains in the 3D H-bonded network *via* OH(3-pyaoH)···O(adi) and OH(H$_2$O)···O(adi) hydrogen bonds.



(a) (b)

(c) (d)

Figure S5. (a) Packing of coordination layers in **5**. (b) Packing of coordination layers in **6**. The accommodated MeOH and H_2O solvents are depicted as cyan space-filling models. (c) Packing of coordination layers in **7**. The accommodated H_2seb and H_2O guest molecules are depicted as cyan space-filling models. (d) View of H_2seb$\cdots H_2O$ infinite H-bonded chains situated in the interlayer space in **7**.