Solvent-Driven Dimensionality Control in Molecular Systems Containing Cu^{II}, 2,2'-Bipyridine, and an Oxamato-Based Ligand

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Supporting Information

Analyses of 1

Calcd for $C_{40}H_{32}Cu_2N_8O_{14}$ (**1**): C, 49.23; H, 3.31; N, 11.48; Cu, 13.02. Found: C, 48.86; H, 3.39; N, 11.24 Cu, 14.10%.

IR (KBr): 3085, 3253s, 1682s,1633, 1602, 1445, 1353, 763, 726.

Analyses of 2

Calcd for $C_{22}H_{20}CuN_4O_7S$ (**2**): C, 48.22; H, 3.68; N, 10.22; Cu, 11.60. Found: C, 47.48; H, 3.83; N, 9.87; Cu, 11.17%.

IR (KBr): 3075s, 3351, 1685, 1659, 1636, 1605, 1447, 1361, 1031, 774, 728

Table S1: Crystallographic parameters of compounds **1-2**

	1	**2**
Empirical Formula	$C_{40}H_{28}Cu_2N_8O_{12}\cdot 2(H_2O)$	$C_{21}H_{17}CuN_4O_7S$
F.W.	975.82	532.99
Crystal size (mm)	0.13 × 0.10 × 0.03	0.72 × 0.15 × 0.09
Crystal System	Monoclinic	Orthorhombic,
Space group	$P2_1/n$	*Pcca*
T(K)	150(2)	293 K
a (Å)	11.030 (2)	13.5402 (8)
b (Å)	13.570 (3)	11.3945 (7)
c (Å)	13.623 (3)	16.0434 (9)
α (Å)	90°	90°
β (Å)	113.40 (3)°	90°
γ (Å)	90°	90°
V (Å^3)	1871.4 (6)	2475.2 (3)
Z	2	4
*D*calcd (g cm^{-3})	1.732	1.430
μ (mm^{-1})	2.158	1.013
F(000)	996	1088
Index ranges	-13≤ h≤ 13, -14≤ k≤ 15, -16≤ l≤ 16	-16≤ h≤ 16, -14≤ k≤ 14, -19≤ l≤ 20
Reflections collected	33041	13505
Independent reflections	3253 [R(int) = 0.062]	2536 [R(int) = 0.0484]
R (F_o^2) [I> 2σ(I)]	0.0379	0.0484
R_w (F_o^2) [I> 2σ(I)]	0.0903	0.1289

Table S2: Selected bond distances (Å) and angles (º) for **1**[#]

Cu1—O1	1.9538 (19)	Cu1—O3	1.9840 (19)
Cu1—N1	1.977 (2)	Cu1—O5^{i}	2.178 (2)
Cu1—N2	1.982 (2)		
O1—Cu1—N1	166.15 (9)	N2—Cu1—O3	169.55 (9)
O1—Cu1—N2	96.34 (9)	O1—Cu1—O5i	89.56 (8)
N1—Cu1—N2	82.04 (10)	N1—Cu1—O5i	104.28 (9)
O1—Cu1—O3	83.51 (8)	N2—Cu1—O5i	95.43 (9)
N1—Cu1—O3	95.59 (9)	O3—Cu1—O5i	95.01 (8)

Hydrogen bonds*,[&]

D—H···A	D—H / Å	H···A / Å	D···A / Å	D—H···A / º
O7—H7*A*···O6	0.88 (2)	1.91 (2)	2.744 (3)	159 (4)
O7—H7*B*···O5^{ii}	0.87 (2)	1.93 (2)	2.799 (3)	176 (4)
N3—H3···O7^{iii}	0.86	2.04	2.865 (3)	162
C14—H14···O7^{iii}	0.93	2.32	3.111 (4)	143
N4—H4···O2^{iv}	0.86	2.09	2.940 (3)	168
C16—H16···O1^{iv}	0.93	2.59	3.511 (4)	170

[#]Estimated standard deviations in the last significant digits are given in parentheses. *D and A stand for donor and aceptor, respectively. [&] Symmetry code: (i) -*x*, -*y*+1, -*z*+2; (ii) -*x*, -*y*+1, -*z*+3; (iii) -*x*+1/2, *y*-1/2, -*z*+5/2; (iv) *x*-1/2, -*y*+1/2, *z*+1/2.

Table S3: Selected bond distances (Å) and angles (º) for **2**[#]

Cu1—O1	1.983 (2)	Cu1—N1^{i}	2.005 (3)
Cu1—O1^{i}	1.983 (2)	Cu1—O3	2.333 (2)
Cu1—N1	2.005 (3)	Cu1—O3^{i}	2.333 (2)
O1—Cu1—O1^{i}	93.23 (15)	N1—Cu1—O3	95.72 (11)
O1—Cu1—N1	93.12 (11)	N1—Cu1—N1^{i}	81.29 (16)
O1—Cu1—N1^{i}	171.09 (11)	N1—Cu1—O3^{i}	96.41 (10)
O1—Cu1—O3^{i}	91.77 (10)	N1^{i}—Cu1—O3^{i}	95.73 (11)
O1—Cu1—O3	77.16 (9)	O3—Cu1—O3^{i}	163.98 (13)

Hydrogen bonds*,[&]

D—H···*A*	*D*—H / Å	H···*A* / Å	*D*···*A* / Å	*D*—H···*A* / º
N2—H2···O4	0.86	2.18	2.979 (4)	155
C5—H5···O4	0.93	2.60	3.255 (5)	128

[#]Estimated standard deviations in the last significant digits are given in parentheses. *D and A stand for donor and aceptor, respectively. [&] Symmetry code: (i) -*x*+3/2, -*y*+1, *z*

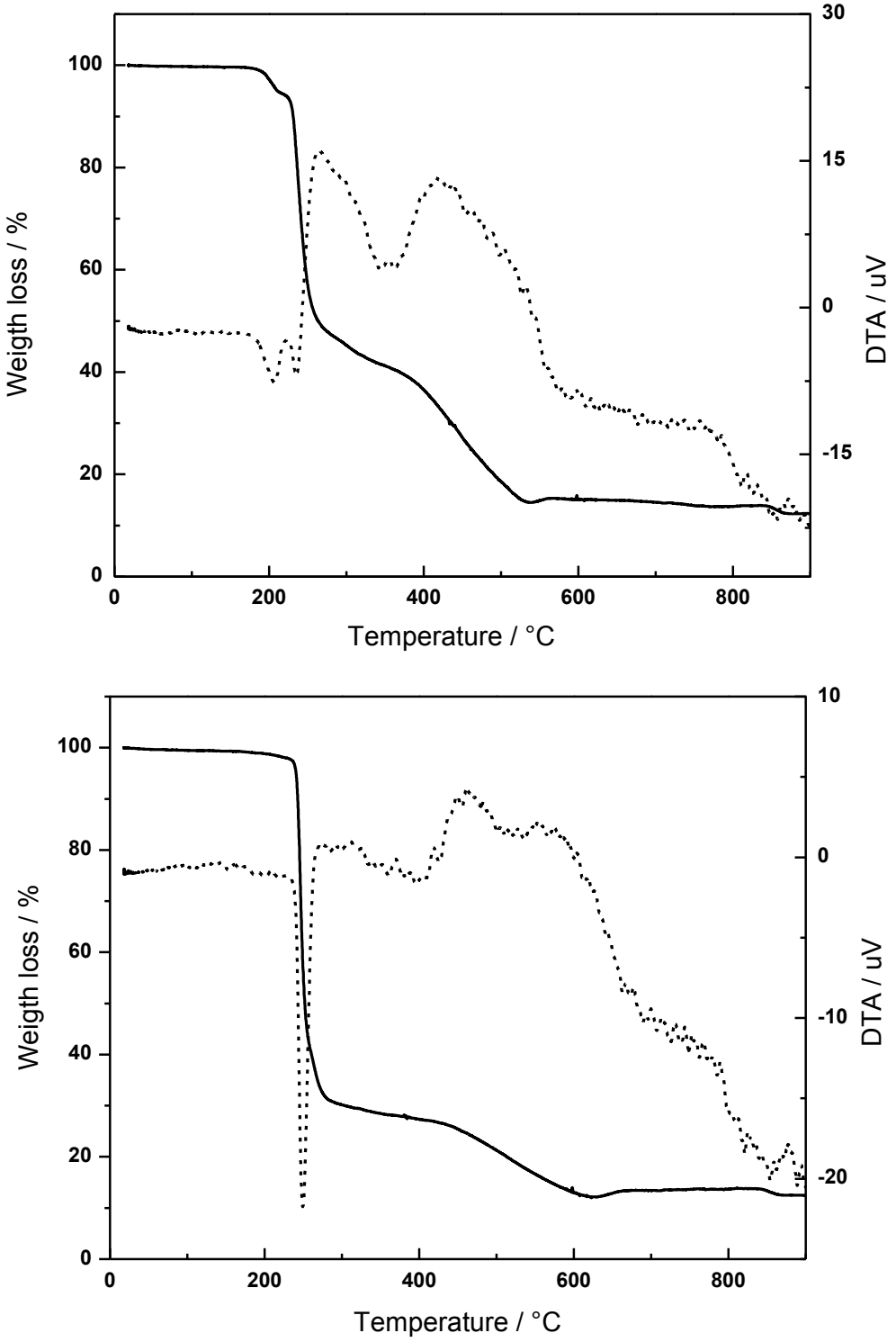

Figure S1: Thermogravimmetric (full line) and differential thermal analyses (dash lines) for **1**(top) and **2**(bottom).

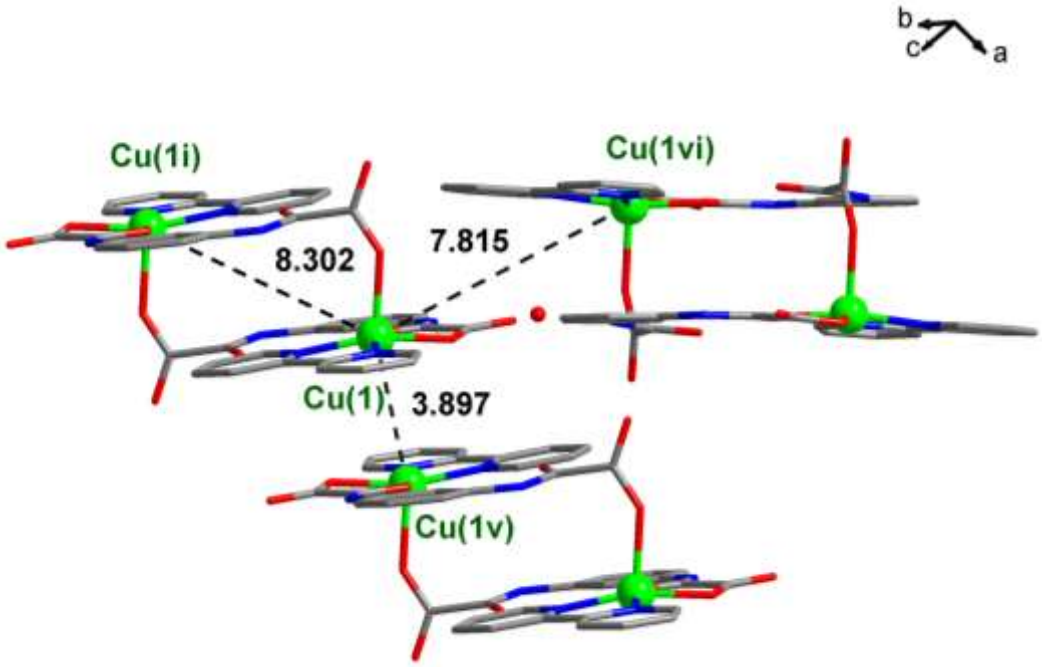

Figure S2: Intra and Intermolecular copper distances in **1**; symmetry codes (i) = -*x*, -*y*+1, -*z*+2; (v) = 1-*x*, 1-*y*, 2-*x* and (vi) =1/2-x, -1/2+y, 3/2-z**.**

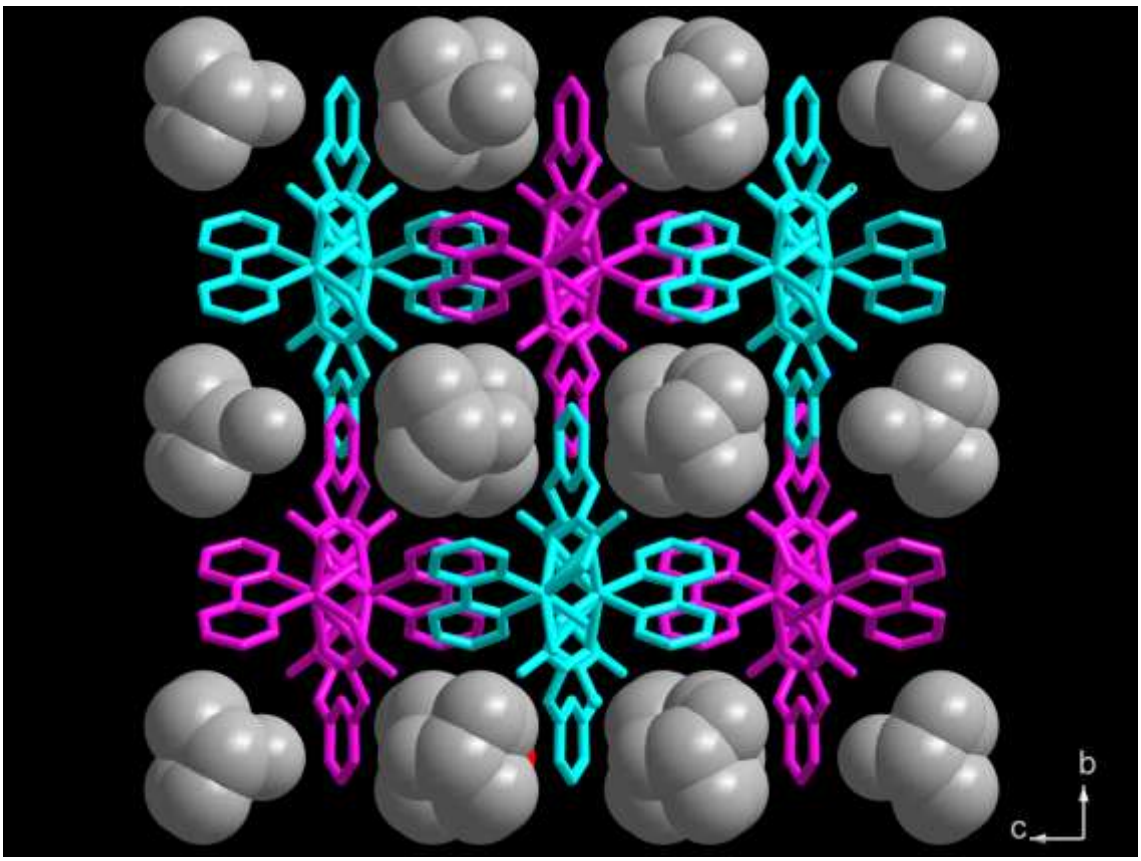

Figure S3: View of the packing in **2** down the crystallographic *a* axis showing the dmso (represented in space-filling) occupancy.