Supplementary Materials

for

Bis(3-aminobenzenesulfonato-N)-diaqua-bis(*N,N′*-dimethylformamide-O)-copper(II)

Susanta Hazra * and Anirban Karmakar

Centro de Química Estrutural, Institute of Molecular Science, Técnico Lisboa, Universidade de Lisboa, Av. Rovisco Pais, 1049–001 Lisbon, Portugal; anirbanchem@gmail.com
* Correspondence: susanta.hazra@tecnico.ulisboa.pt

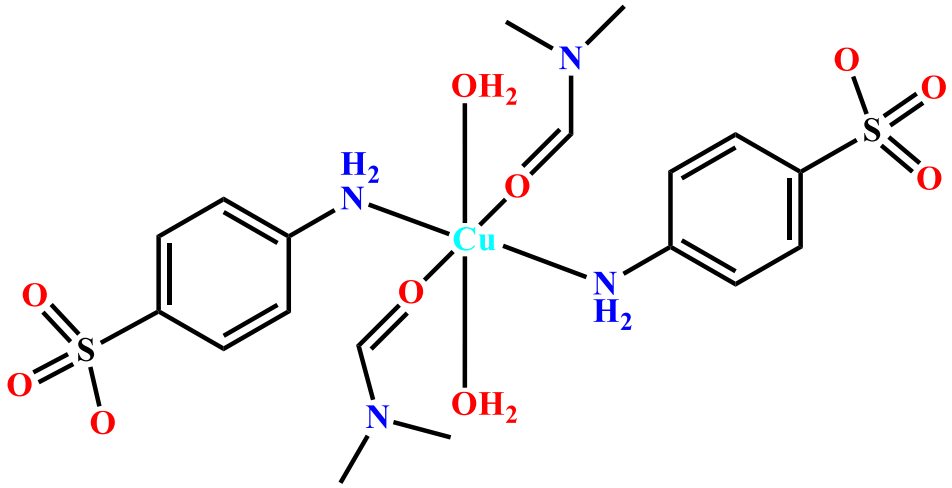

Chart S1: Chemical diagram of $[Cu(L2)_2(DMF)_2(H_2O)_2]$ (**2**).

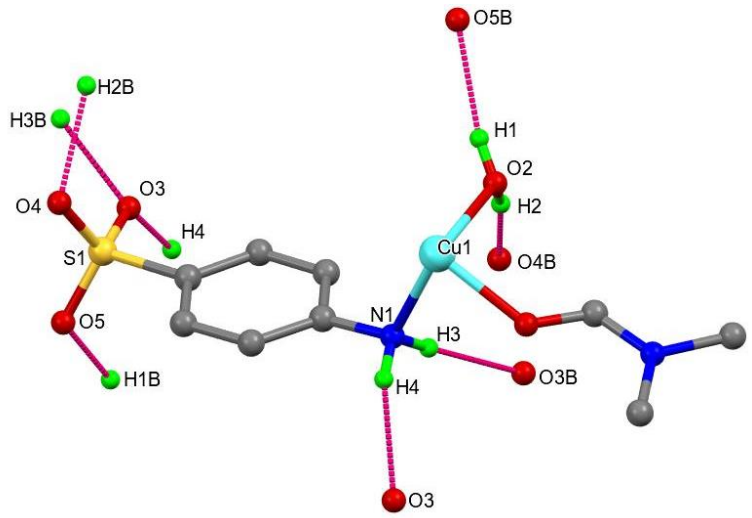

Figure S1. H-bonding interactions in the asymmetric unit of **2**.

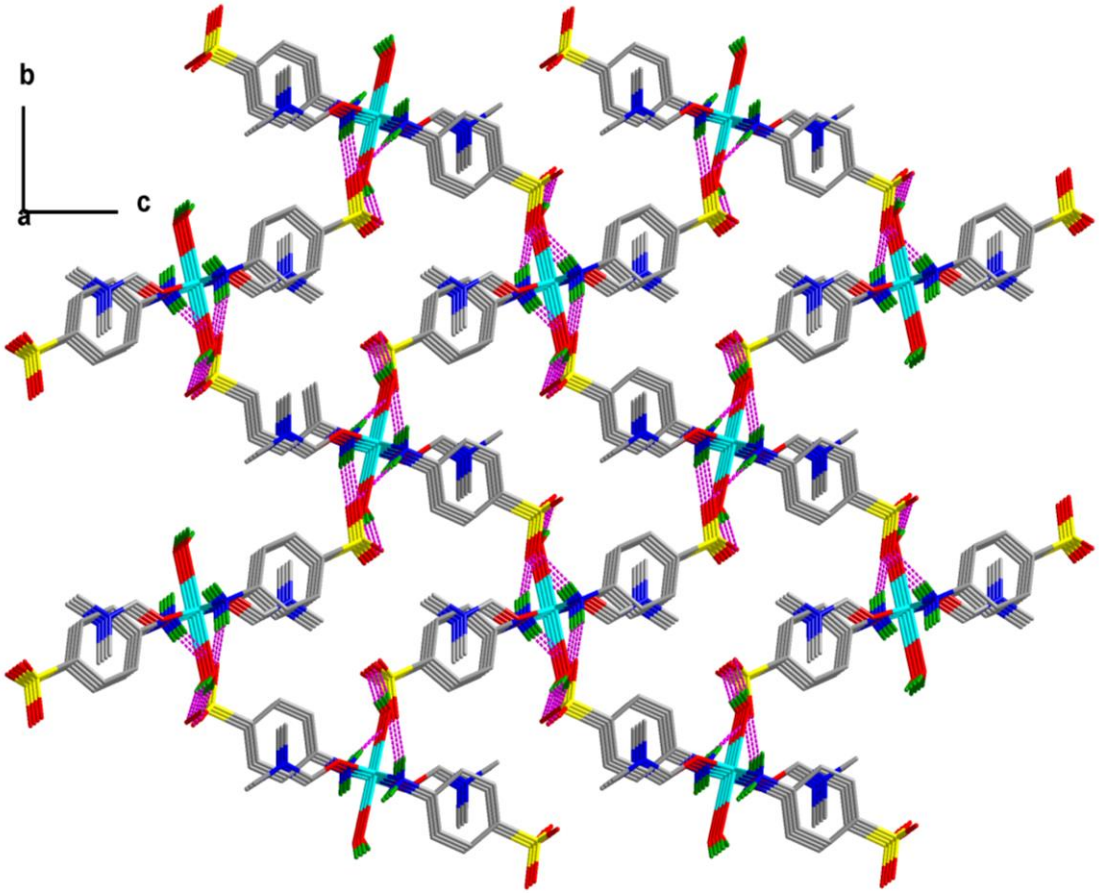

Figure S2. The H-bonded 3D network in **2** down the *a*-axis (idealized).

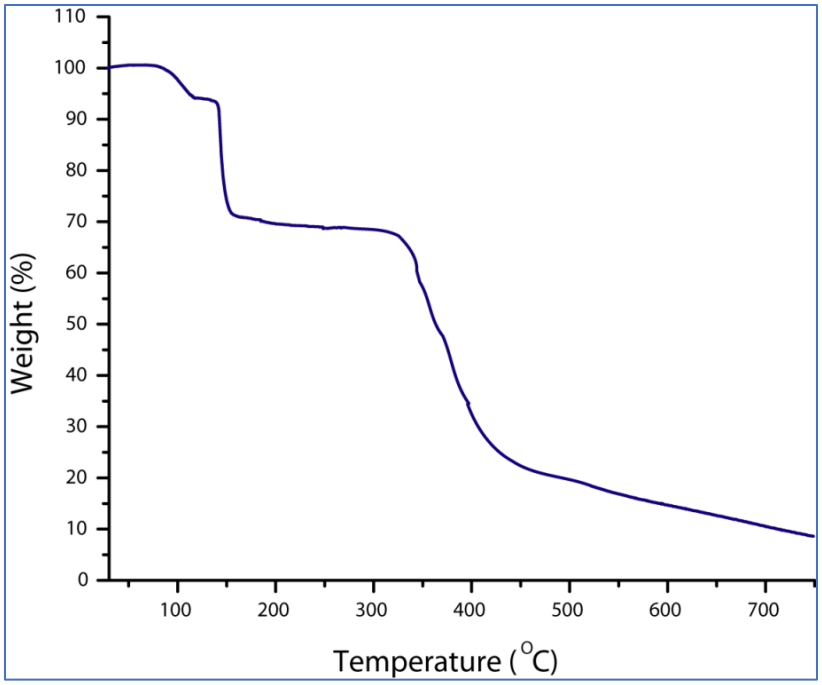

Figure S3. Thermogravimetric curve for **1**.

Table S1. Comparison of selected bond lengths (Å) and angles (°) in $[Cu(L1)_2(DMF)_2(H_2O)_2]$ (**1**) and $[Cu(L2)_2(DMF)_2(H_2O)_2]$ (**2**). Symmetry: *i*) 2–x, 2–y, 2–z (in **1**); B) –x, –y, 2–z (in **2**).

1		**2**	
Cu1–N1	2.0720(12)	Cu1–N1	2.061
Cu1–O5	1.9705(11)	Cu1–O1	1.978
Cu1–O4	2.3333(14)	Cu1–O2	2.430
N1–Cu1–N1^i	180.0	N1–Cu1–N1B	180.0
O4–Cu1–O4^i	180.0	O1–Cu1–O1B	180.0
O5–Cu1–O5^i	180.0	O2–Cu1–O2B	180.0
O4–Cu1–O5	88.15(6)	O1–Cu1–O2B	87.12
O4–Cu1–O5^i	91.85(6)	O1–Cu1–O2	92.88
O4–Cu1–N1	86.24(6)	O1–Cu1–N1	85.28
O4–Cu1–N1^i	93.76(6)	O1–Cu1–N1B	94.72
O5–Cu1–N1	86.57(5)	O2–Cu1–N1	92.13
O5–Cu1–N1^i	93.43(5)	O2–Cu1–N1B	87.87
N1–Cu1–N1^i	180.0	N1–Cu1–N1B	180.0
O4–Cu1–O4^i	180.0	O1–Cu1–O1B	180.0
O5–Cu1–O5^i	180.0	O2–Cu1–O2B	180.0
O4–Cu1–O5	88.15(6)	O1–Cu1–O2B	87.12

Table S2. Geometries [distances in (Å) and angles in (°)] of the H-bonds in $[Cu(L1)_2(DMF)_2(H_2O)_2]$ (**1**) and $[Cu(L2)_2(DMF)_2(H_2O)_2]$ (**2**). Symmetry: *ii*) 1.5–x, 0.5+y, 1.5–z; *iii*) x, 1+y, z; *iv*) 0.5+x, 1.5–y, 0.5+z (in **1**) and B).

D–H···A	D···A	H···A	D–H···A
	1		
N1–H5···O3^{ii}	2.904	1.983	162.40
N1–H6···O2^{iii}	3.149	2.307	167.10
O4–H4A···O2^{iii}	2.820	2.040	155.53
O4–H4B···O1^{iv}	2.794	2.003	162.93
	2		
N1–H3···O3B	2.999	2.104	172.97
N1–H4···O3	3.042	2.189	158.02
O2–H1···O5B	2.927	2.108	170.70
O2–H2···O4B	2.921	2.087	172.31

Table S3. Crystallographic data for $[Cu(L1)_2(DMF)_2(H_2O)_2]$ (**1**).

Formula	$C_9H_{15}Cu_{0.5}N_2O_5S$
Formula Weight	295.06
Crystal color	Green
Crystal system	Monoclinic
Space group	*P*21/n
a/Å	11.4788(10)
b/Å	8.5348(8)
c/Å	12.9741(11)
β/°	108.009(3)
V/Å^3	1208.79(19)
Z	4
T/K	296(2)
2θ/°	6.06–61.10
μ (Mo Kα)/mm^{-1}	1.137
ρ_{calcd}/g cm^{-3}	1.621
F(000)	614
Absorption-correction	Multi-scan
Index ranges	$-16<h<16$
	$-12<k<12$
	$-18<l<17$
Reflections collected	34902
Independent reflections	3654
R_{int}	0.0199
R_1[a]/ wR_2[b] [I > 2σ(I)]	0.0410/0.1076
R_1[a]/ wR_2[b] [for all F_o^2]	0.0430/0.1103
GOF on F^2	1.083