

SUPPLEMENTARY MATERIAL

Unique Occurrence of Cationic and Anionic Bis-1,2-Diaminocyclohexane Copper(II) Units in a Double Complex Salt

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Table S1. Intramolecular hydrogen bonds /Å,° in the anionic moiety of[Cu(dach)₂(H₂O)₂][Cu(dach)₂(SO₄)₂] \cdot 6H₂O.

Symmetry operator (1-x,1-y,1-z) generates equivalent atoms that is marked with “#”.

D-H	A	D-H	H \cdots A	D \cdots A	DH \cdots A
N9-H9A	O4#	0.97	2.32	3.239(2)	158
N16-H16A	O3	0.97	2.18	3.119(2)	162

Table S2. Intermolecular hydrogen bonds /Å,° between the complex units of the complex[Cu(dach)₂(H₂O)₂][Cu(dach)₂(SO₄)₂] \cdot 6H₂O.

Symmetry operator (-2+x,-1+y,z) generates equivalent atoms that is marked with “#”, (-x,1-y,1-z) marked with “#2”, (1-x,1-y,1-z) marked with “#3”, (-1+x,y,z) marked with “#4”, (2-x,1-y,1-z) marked with “#5” and (-1+x,-1+y,z) marked with “#6”.

D-H	A	D-H	H \cdots A	D \cdots A	DH \cdots A
N1-H1A	O1#	0.97	2.03	2.922(2)	152
N1-H1B	O1#2	0.97	1.96	2.922(2)	171
N8-H8A	O1#3	0.97	2.14	3.0238(19)	151
N8-H8A	O4#3	0.97	2.68	3.546(2)	150
N9-H9B	O3#4	0.97	2.12	3.0575(19)	162
N16-N16B	O4#5	0.97	2.15	3.002(2)	146
O1W1-H1W1	O3#	0.83	2.20	3.028(2)	174
O1W1-H2W1	O2#6	0.84	1.87	2.7090(19)	172

Table S3. Intermolecular hydrogen bonds /Å, ° with the participation of non-coordinating water molecules in [Cu(dach)₂(H₂O)₂][Cu(dach)₂(SO₄)₂] \cdot 6H₂O.

Symmetry operator (x,y,-1+z) generates equivalent atoms that is marked with “#”, (-x,-y,-z) marked with “#2”, (x,y,1+z) marked with “#3”, (1-x,1-y,1-z) marked with “#4”, (1+x,y,z) marked with “#5” and (1-x,1-y,2-z) marked with “#6”.

D-H	A	D-H	H \cdots A	D \cdots A	DH \cdots A
C13-H13A	O1W4#	0.97	2.60	3.391(4)	139
N8-H8B	O1W2#2	0.97	2.37	3.260(3)	153
O1W2-H1W2	O1W4#	0.91	1.96	2.754(4)	145
O1W2-H2W2	O1W1#2	0.90	1.93	2.816(3)	169
O1W3-H1W3	O1W2#3	0.92	2.42	2.777(4)	103
O1W3-H2W3	O3#4	0.90	2.01	2.889(3)	164
O1W4-H1W4	O1W3#5	0.95	1.81	2.742(4)	165
O1W4-H2W4	O1W3#6	0.94	2.53	3.390(4)	154

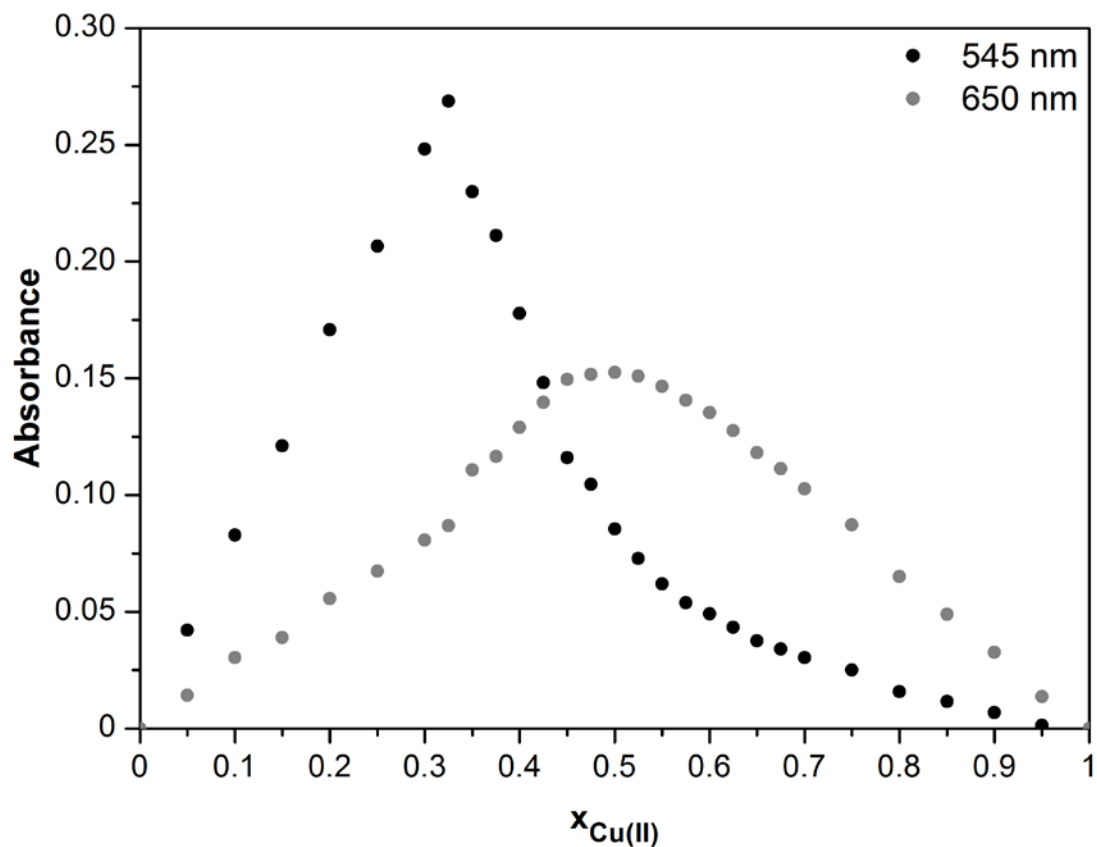
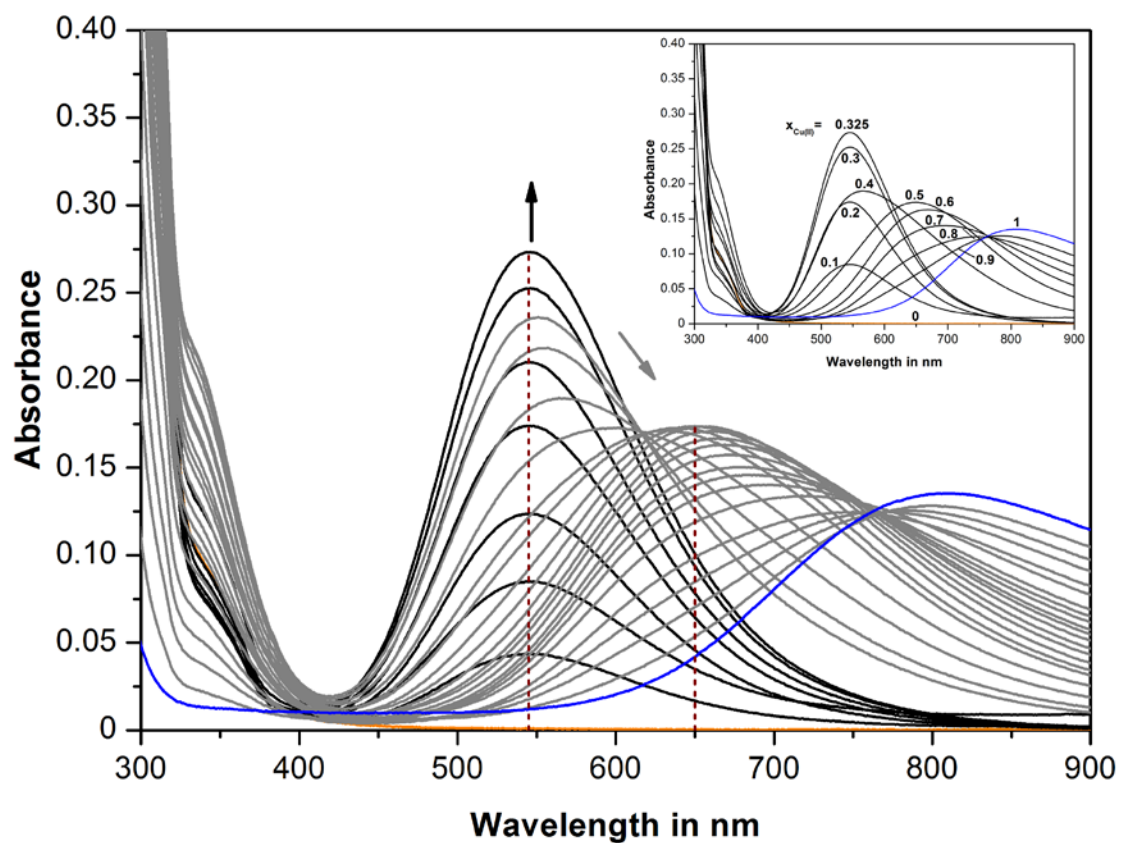


Figure S1. UV/Vis spectra (top) and Job plot (bottom) for complexation of copper sulfate (blue) with dach (orange) in water. $[\text{dach}] + [\text{Cu(II)}] = 1 \times 10^{-2} \text{ M}$ ($x_{\text{Cu(II)}} = 0 \dots 1$), $t = 30 \text{ min}$.

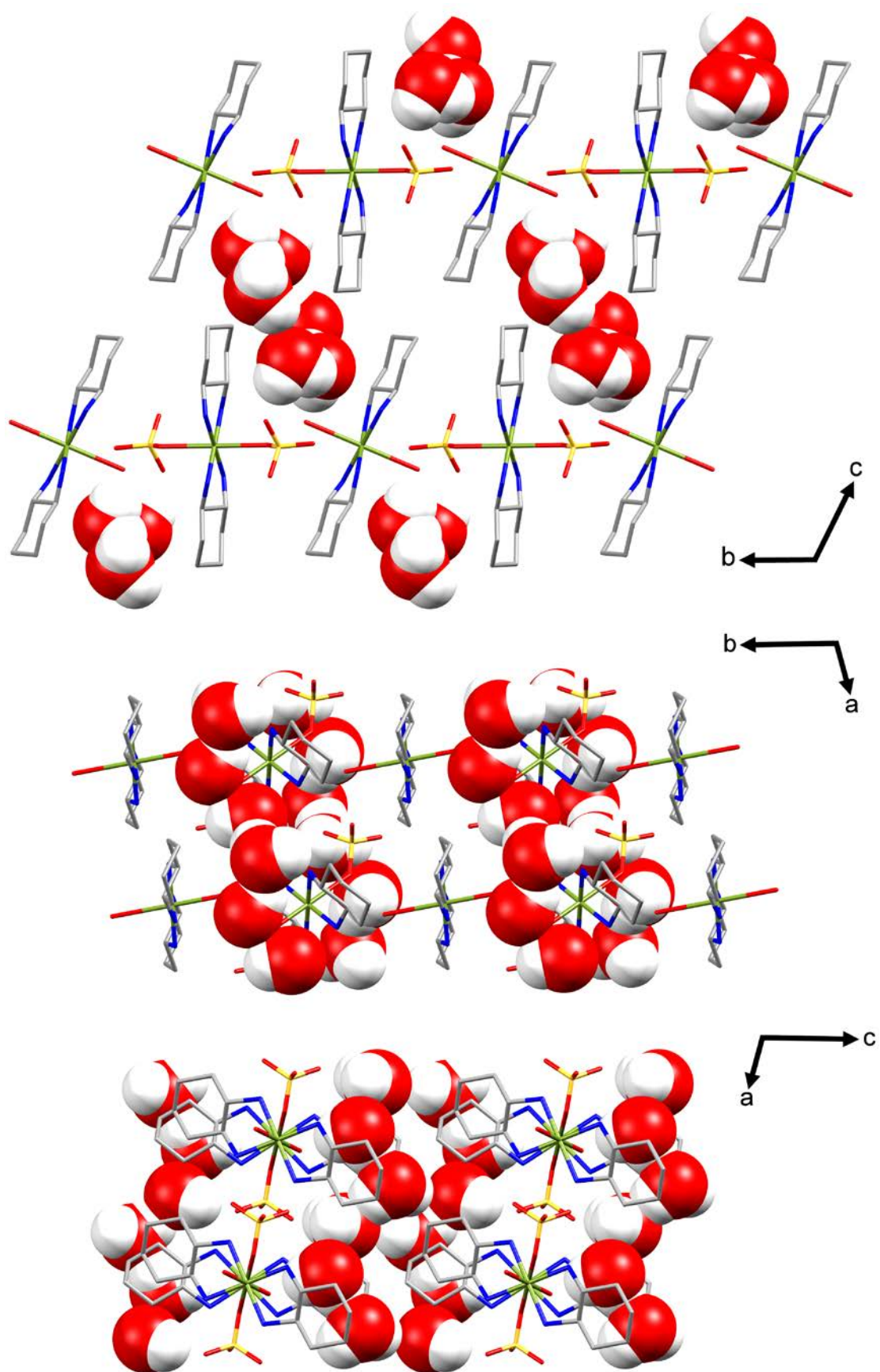


Figure S2. Crystal packing for $[\text{Cu}(\text{dach})_2(\text{H}_2\text{O})_2][\text{Cu}(\text{dach})_2(\text{SO}_4)_2] \cdot 6\text{H}_2\text{O}$.