

## Supporting Information

### Convenient Crystal Growth, Structural Determination, and Magnetic Properties of Layered Copper Hydroxides Containing Aromatic Sulfonates

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1. Crystal Structures

S2

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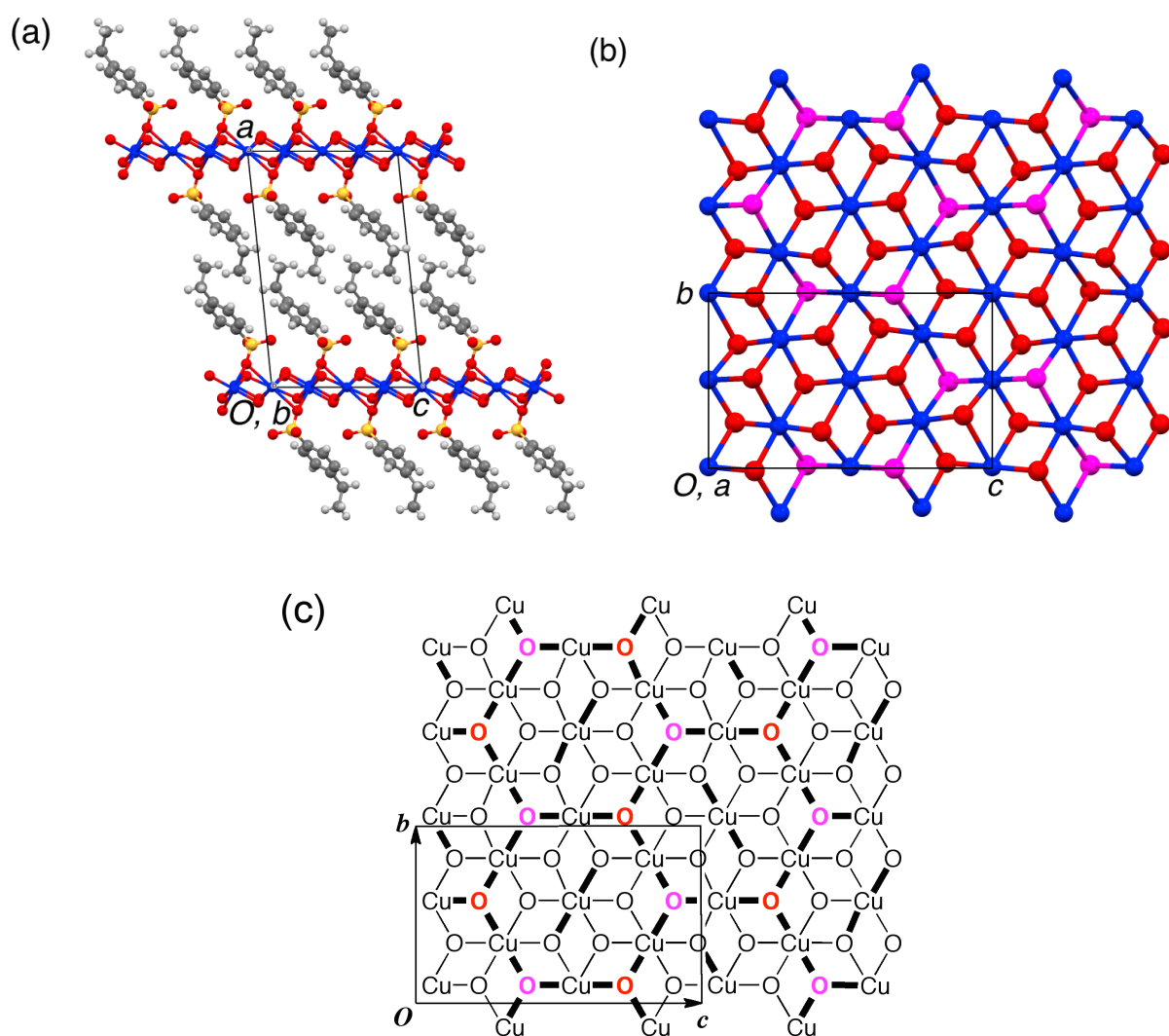


Figure S1. Crystal Structure of **2**. The hydrogen atoms of hydroxide ions are omitted. Spheres correspond to Cu (blue), O (red), C (dark grey), S (yellow), and H (light grey). (a) Stacking of the copper hydroxide layers and the organic anion layers. (b) Projection of the atomic arrangement of the copper hydroxide layer along the *a* axis. (c) Schematic representation of the copper hydroxide layer and the Cu–O–Cu bridges of **2** showing the Cu–O bonds and the direction of the  $d_{z^2}$  orbitals of Cu(II) ions in the copper hydroxide layer. Coloured O's correspond to the oxygen atom of *p*-ethylbenzenesulfonate anion. The bold lines are the axial bonds. The red and magenta symbols correspond to the oxygen atoms of the aromatic ions that are located to the front and back of the inorganic layer, respectively.

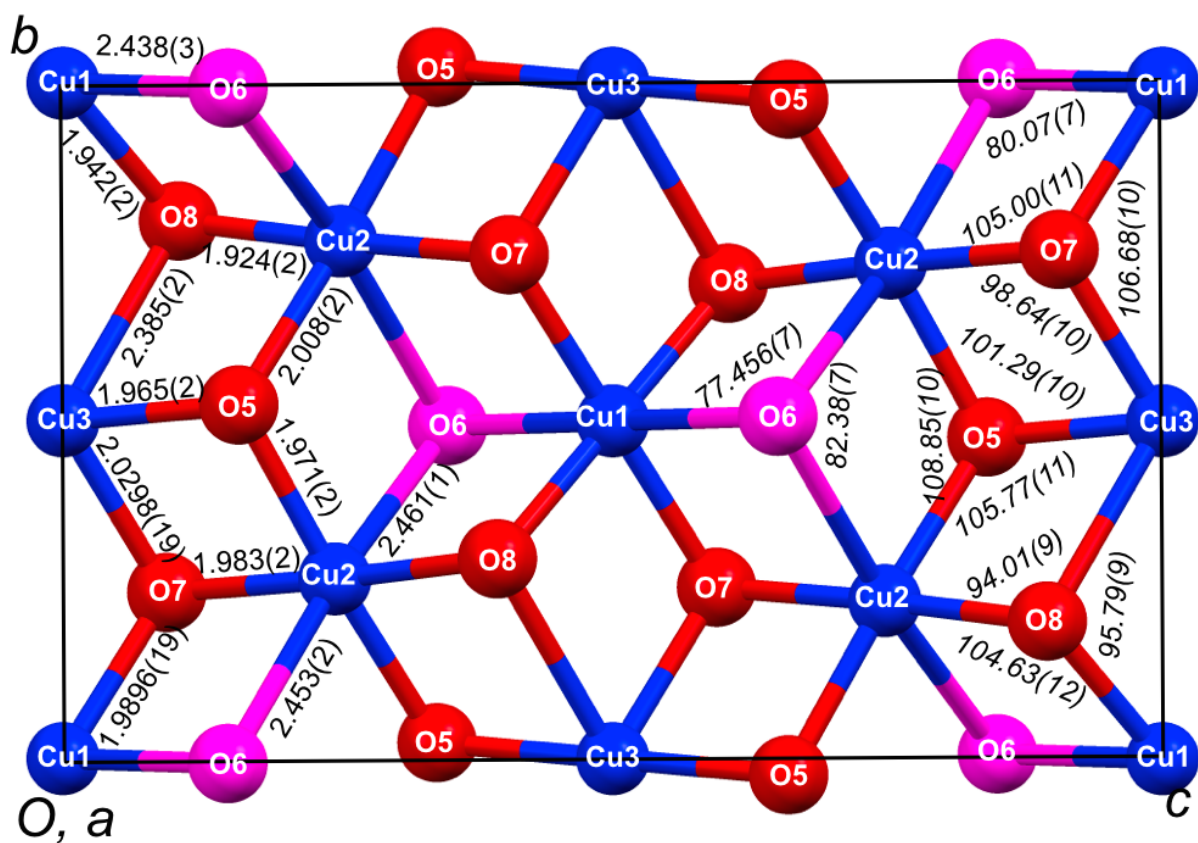


Figure S2. Selected Cu-O bond lengths (Å) and Cu-O-Cu bridging angles (°) in **1**. The bond lengths and bridging angles are described in plain and italic characters, respectively.

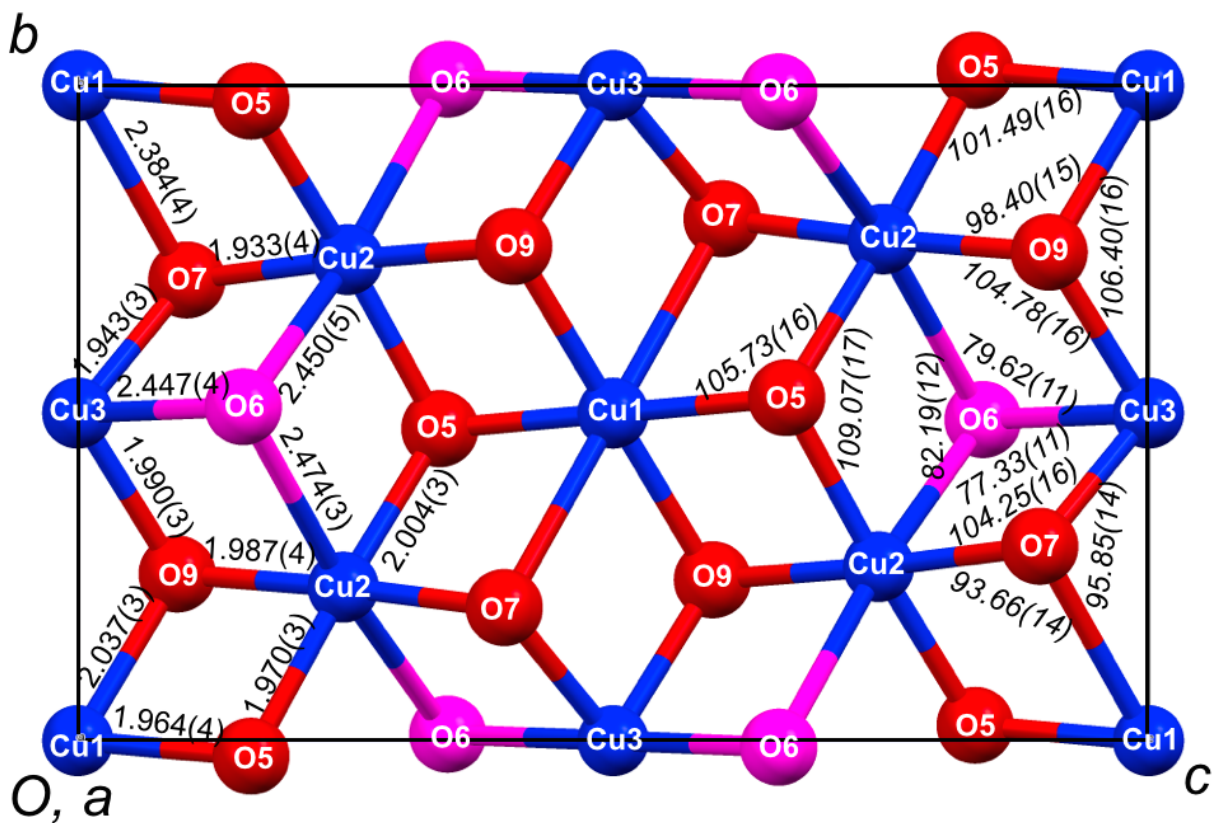


Figure S3. Selected Cu–O bond lengths (Å) and Cu–O–Cu bridging angles (°) in **2**. The bond lengths and bridging angles are described in plain and italic characters, respectively.



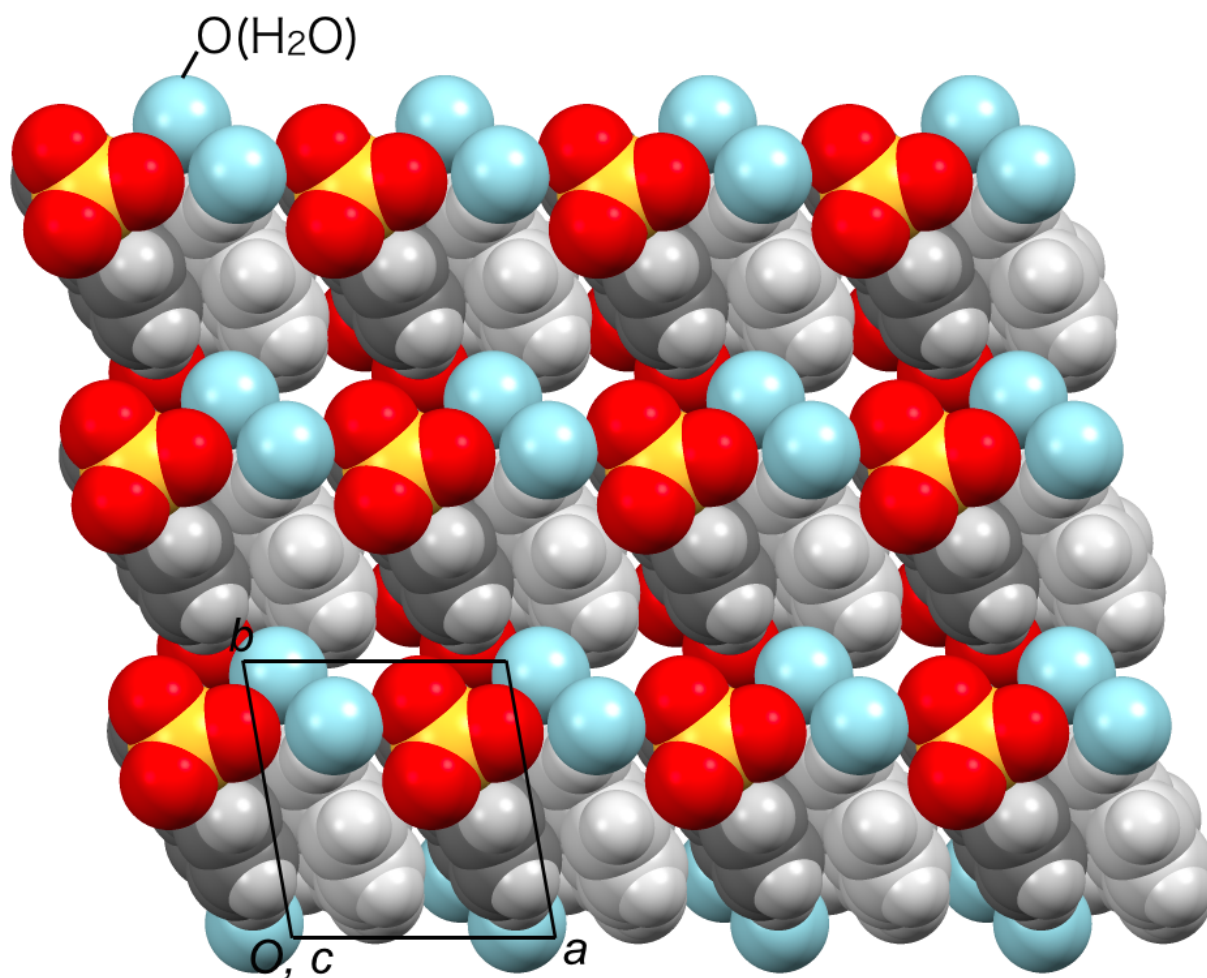


Figure S5. The molecular orientation of 1-naphthalenesulfonate anions and water molecules between the inorganic layers in **3**. The organic anion with the sulfonate group located to the back are colored by light gray. There are short interatomic O•••O contacts of the water molecules, and of the water molecule and the sulfonate group due to formation of hydrogen bonds.

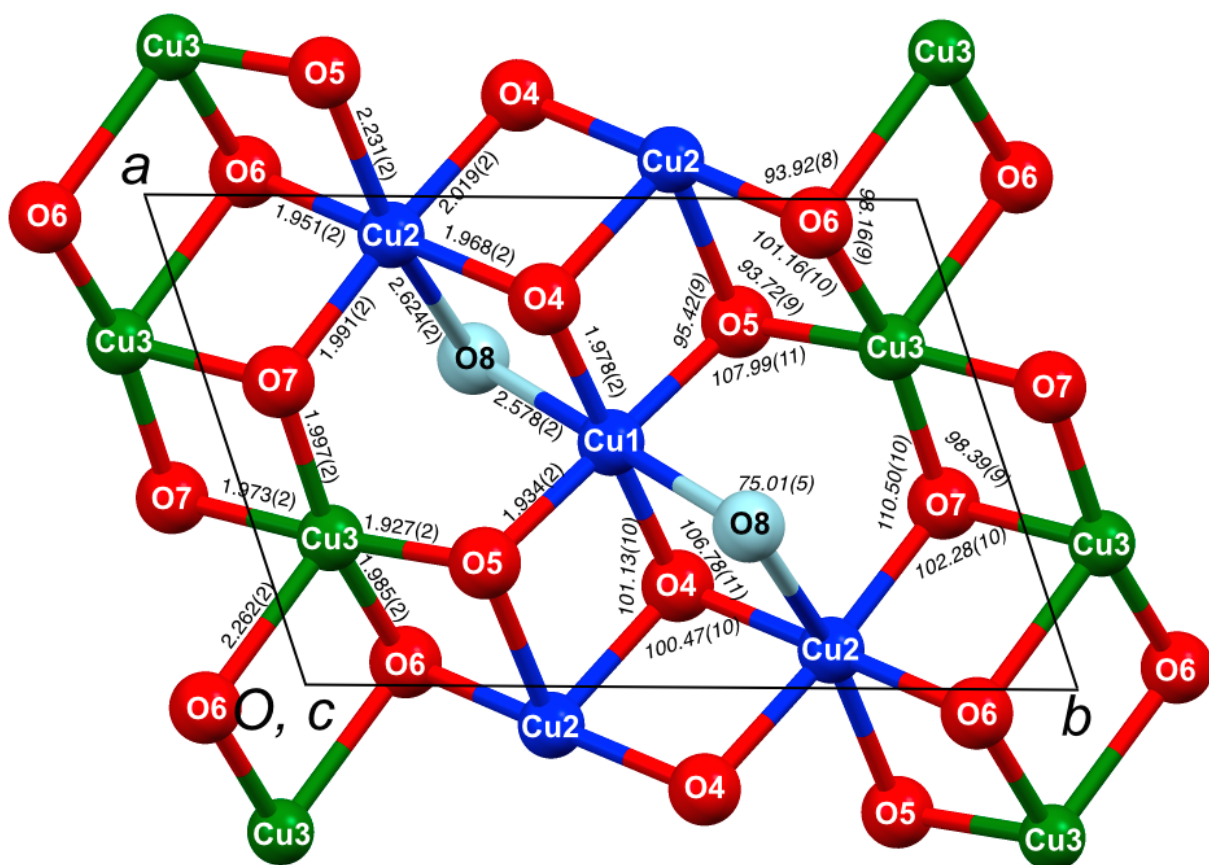


Figure S6. Selected Cu–O bond lengths (Å) and Cu–O–Cu bridging angles (°) in **4**. The bond lengths and bridging angles are described in plain and italic characters, respectively.

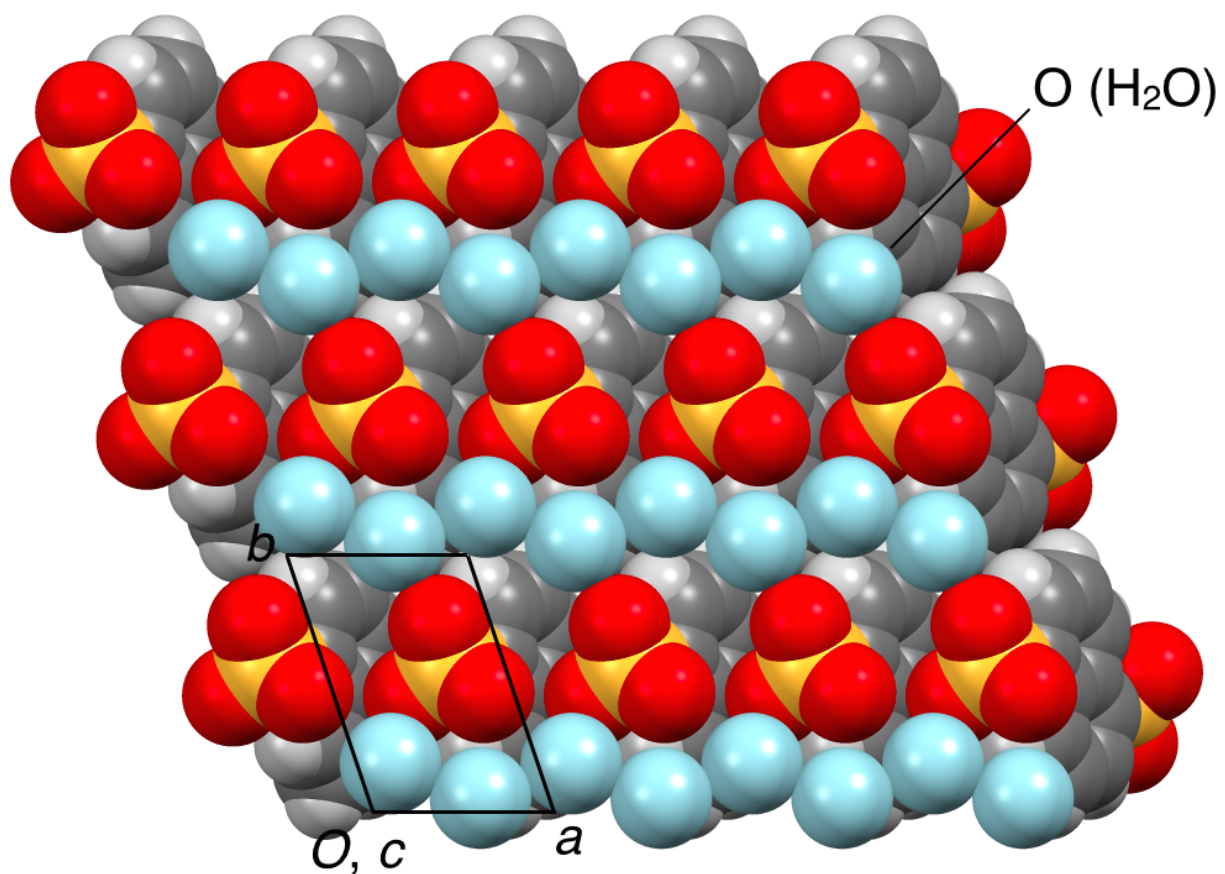


Figure S7. The molecular orientation of 1,5-naphthalenedisulfonate anions and water molecules between the inorganic layers in **4**. There are one-dimensional hydrogen bonding networks toward the *a* axis via short contacts between the oxygen atoms of the water molecules.