

Characterization of a well-resolved water layer containing (H₂O)₄₀ water morphology via dianion templating

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Abstract

A well-resolved 2D supramolecular water layer, which self-assembled by (H₂O)₄₀ water morphology templating via tartrate dianion, has been observed in the compound [Cu₂(tar)(2,2'-bipy)₄tar · 12H₂O(1) [tar = tartrate dianion]. Hydrogen bonding interactions between the 2D layers of water and binuclear moieties create a unique, infinite 3D supramolecular edifice.

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Being water plays an indispensable role for human life and in biological and chemical processes, investigations on the structure, properties and functions of water have received more scientific attention than any other substance [1–4]. In this context, “discrete” water clusters within the lattice of a crystal host have been extensively studied, both theoretically and experimentally, in attempts to providing insight into the structure and properties of liquid water or ice [5–7]. Many examples dealing with the structure of some interesting polymeric water morphologies, which were observed in crystal hydrates of organic compounds or coordination complexes, have been reported [8–12]. Recent studies are focused on unraveling structural morphologies of water cocrystallized with various chemical entities, that mainly because the lattice of a crystal host

offers an attractive environment for stabilizing various topologies of water clusters, and thereby provide quantitative characterization of the hydrogen bonded networks that exist in liquid water. Very recently, two-dimensional (2D) water/ice layers containing 6-, 10-, 12-, 18-, and 45-membered water rings have been observed in the solid state [13–20]. Without doubt, the above studies have significantly advanced our knowledge toward understanding the behavior of bulk water. However, water is still not a fully understood substance and studies toward understanding the growth of larger water clusters, and how these clusters link themselves to form a larger network of water molecules is still a challenging scientific endeavor [21–23].

In general, the incorporation of water clusters or networks into polymeric architectures is accomplished using synthons, which are rich in hydrogen bond donor/acceptor groups [24], with inter- and intra-molecular hydrogen bonding and other noncovalent interactions being the main driving forces for the assembly of such systems. The tar dianion contains two carboxylate and two hydroxyl groups that can be harnessed in hydrogen bonding networks, and it can also serve as a template in the formation of hydrogen

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bond-driven polymeric systems. Indeed, structural elucidations and understanding hydrogen bonding properties of supramolecular networks of water and water-anion at nanometer scales have been a topic of significant challenge [2]. Well characterized high water morphology via dianion templating clusters are rare [15,16,19], although structural elucidations of such clusters is imperative to gaining insight into the anomalous properties and, to understanding the hydrogen bonding and dynamics of water-anion binary mixtures. Herein, we describe the formation of well-resolved, infinite 2D-layered water of $(\text{H}_2\text{O})_{40}$ cluster by using tar as a template, where each $(\text{H}_2\text{O})_{40}$ cluster consists of two six-membered rings, two four-membered rings, two three-membered rings, and further associated to two trimers and two water tetramers. Hydrogen bonding interactions between the 2D layers of water and binuclear moieties create a unique, infinite 3D supramolecular framework.

The compound $[\text{Cu}_2(\text{tar})(2,2'\text{-bipy})_4]\text{tar} \cdot 12\text{H}_2\text{O}$ (**1**) was prepared [25] by reacting $\text{Na}(\text{H}_2\text{tar})$, 2,2'-bipyridine and $\text{Cu}(\text{AcO})_2 \cdot 2\text{H}_2\text{O}$ at room temperature, and characterized by X-ray crystallography [26], elemental analysis, vibrational spectroscopy, thermal analysis and magnetic measurement.

Single-crystal X-ray diffraction analysis reveals that compound **1** contains one $[\text{Cu}_2(\text{tar})(2,2'\text{-bipy})_4]^{2+}$ cation, one tartrate dianion, and twelve lattice water molecules in the asymmetric unit. Each Cu(II) is five-coordinate, having triangular bipyramid geometry with equatorial coordination from two nitrogen atoms from two different 2,2'-bipy ligands and one oxygen atom from the tartrate dianion, and the other two nitrogen atoms occupy the axial sites (Fig. 1).

The most startling feature for **1** is that an ordered 2D hydrogen bonded water layer is observed in the *ac*-plane (Fig. 2). Hydrogen bonding association generates a centrosymmetric $(\text{H}_2\text{O})_{40}$ water cluster (Fig. 3), which consists of

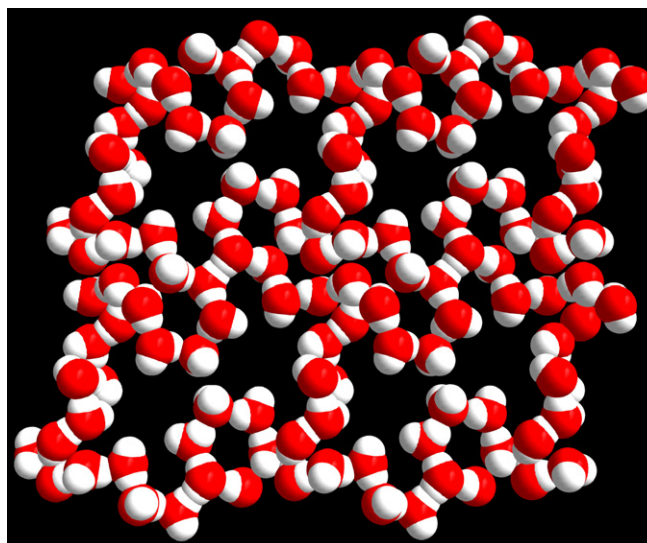


Fig. 2. Perspective view of supramolecular $(\text{H}_2\text{O})_{40}$ water layer in **1**.

two O13, two O14, two O17, two O18, two O20 and four O15, four O16, four O19, four O21, four O22, four O24 and six O23 centers. The $(\text{H}_2\text{O})_{40}$ morphology are fused two six-membered rings, two four-membered rings, two three-membered rings, and further associated to two water trimers and two water tetramers, which result in a 2D supramolecular $(\text{H}_2\text{O})_{40}$ morphology with a corrugated sheet. A closer view of the $(\text{H}_2\text{O})_{40}$ cluster illustrates that each water monomer acts as both hydrogen bond donor and hydrogen bond acceptor. In the supramolecular $(\text{H}_2\text{O})_{40}$ morphology, the $\text{O} \cdots \text{O}$ distance ranges from 2.318 to 3.040 Å, resulting in an average $\text{O} \cdots \text{O}$ distance of 2.769 Å, which is very close to the corresponding value of 2.759 Å in ice I_h [27]. The $\text{O} \cdots \text{O} \cdots \text{O}$ angles range from 111.9 to 139.83°, considerably deviating from the preferred

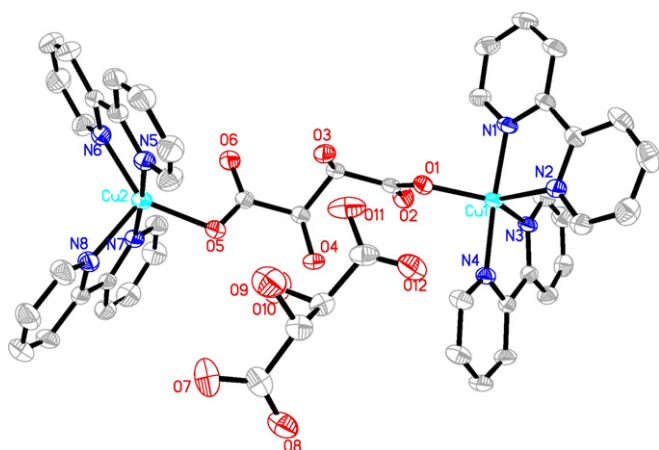


Fig. 1. The local coordinate environment of copper center in **1**. Selected distances (Å): Cu(1)–O(1) 2.007(3), Cu(2)–O(5) 2.047(3), Cu(1)–N(1) 1.995(3), Cu(1)–N(2) 2.145(4), Cu(1)–N(3) 2.057(4), Cu(1)–N(4) 1.973(3), Cu(2)–N(5) 1.977(4), Cu(2)–N(6) 2.058(4), Cu(2)–N(7) 1.993(4), Cu(2)–N(8) 2.148(4).

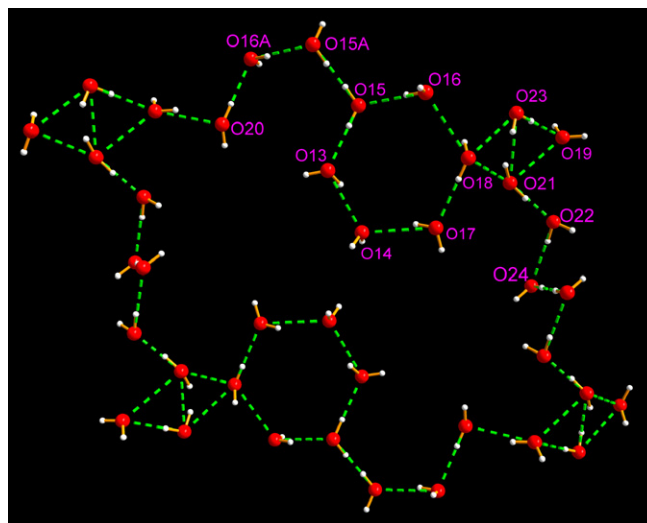


Fig. 3. Perspective view of supramolecular $(\text{H}_2\text{O})_{40}$ morphology in compound **1**. Colors are as follows: red, oxygen; white, hydrogen, green (H-bonding interactions). (For interpretation of the references to colour in this figure legend, the reader is referred to the web version of this article.)

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