

Keywords: water structure, metal coordination complexes, weak interactions

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Diffused scattering and dynamic disorder observed nucleotide hydrates

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Nucleotides are the basic components of nucleic acids. Nucleotides crystallize as hydrates. Layered structures made of molecular layers of nucleotides and inorganic layers of counter ions and crystal water molecules are constructed. In some cases, diffused scatterings attribute to dynamic disorder of inorganic layers were observed, and phase transitions occurred around 200 K. Freezing of hydration water around biomolecules causes attention in connection to the glass transition of proteins. Disodium uridine 5'-monophosphate heptahydrate ($\text{Na}_2\text{UMP}\cdot 7\text{H}_2\text{O}$) was one of the representative cases. Fundamental diffractions streak along the c^* axis and weak diffused diffractions due to a super-lattice were observed at 300 K (Fig. 1). Phase transition occurred around 220 K, and diffused diffractions changed to spots. There were 42 water molecules and 12 sodium ions in an asymmetric unit of the averaged structure at 300 K. In the low temperature phase, the numbers became four-fold, *i.e.*, 168 water molecules and 48 sodium ions in an asymmetric unit. The hydrogen bonding and sodium coordination networks in nucleotide hydrates were analyzed, and the origin of the dynamic disorder will be discussed.

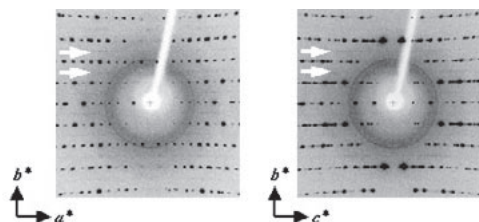


Figure 1 Oscillation photographs of $\text{Na}_2\text{UMP}\cdot 7\text{H}_2\text{O}$ at 300K

Keywords: nucleotide, disorder of hydrogen-bonding network, hydrates

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Incompatible host-guest strategy to enclathrate water clusters into polyoxometalate crystals

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Many compounds crystallize as hydrated forms when precipitated from aqueous or water-containing solutions. Water plays an important role in constructing such crystals. One extreme example of them is the clathrates of hydrophobic gaseous molecules. Another extreme example may be water molecules enclathrated in hydrophobic environments. Recently, we have discovered

discrete water clusters enclathrated in fairly hydrophobic voids constructed by the tetraphenylphosphonium cations, which may be regarded as examples of water clusters in hydrophobic environments. The tetraphenylphosphonium cations self-assemble by the C-H $\cdots\pi$ interactions to form three-dimensional host framework with periodical voids of about 1 nm in diameter, to which guest polyoxometalate anions (e.g. $\text{V}_{10}\text{O}_{28}^{6-}$ and $\text{PV}_{14}\text{O}_{42}^{11-}$) are incorporated. However, the sizes and charges of the voids and the anions are incompatible and thus some of the voids remain unoccupied. These voids lead to the formation of discrete water clusters. Temperature dependent single crystal X-ray diffraction illustrated the melting behavior of the water cluster. In one of these examples, the distribution of the clusters become ordered or disordered depending on the crystallization conditions, resulting in the disappearance/appearance of the diffuse scattering recorded on its single crystal diffraction images.

Keywords: water structure, hydrogen bonds, polyoxometalates

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Stop-action movie of UvrD helicase unwinding DNA

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Molecular mechano-chemical coupling is a fundamental process in biology. To capture molecular locomotion by X-ray crystallography, we determined a dozen crystal structures of UvrD-DNA complexes in the absence or presence of ATP hydrolysis analogs. After combining multiple structures representing each functional state and accounting for crystal lattice effects, we obtained a stop-action movie of UvrD helicase unwinding DNA one base pair per ATP hydrolyzed. For the first time, we show that each ATP-hydrolysis cycle delivers a power stroke in two parts. Binding of ATP is coupled with unwinding of one base pair, and release of ADP and Pi is coupled with translocation of the newly unpaired single base. Combining our new mutagenesis, structural and kinetic studies with published data, we have put forward the model of dual active states of UvrD for its dual functions (dsDNA unwinding and RecA removal from ssDNA) in DNA replication and repair.

Keywords: mechano-chemical coupling, motor protein, helicase

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Stop codon recoding mechanism revealed by the suppressor tRNA^{Pyl}/PylS complex structure

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The genetic code strictly assigns 64 codon triplets to the 20 canonical amino acids, except for three stop codons, UAG (amber), UGA (opal)