formalism for describing rigid-body vibrational motions of arbitrary objects. Multi-group TLS models are broadly applicable to describe inter-domain and other internal vibrational modes of proteins. The web-based analysis tool TLSMD (http://skuld/bmsc/washington.edu/~tlsmd) generates experimentally based multi-group TLS models from a refined protein structural model and associated atomic displacement parameters. These may be used to analyze the presence and physical significance of TLS motion in existing structures, to guide additional crystallographic refinement, or to generate target models of protein flexibility for use in computational protein-protein or protein-ligand docking. The utility of TLSMD in refinement, particularly at low resolution, is now solidly established. I will present examples of applying TLSMD in other contexts to extract information on protein dynamics, domain structure, hinge locations, and binding site flexibility.

Keywords: crystallographic refinement, docking computation, dynamic properties

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Supramolecular stabilization of well-ordered water clusters

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Water may play an important role in the stabilization of molecular crystals and coordination polymers. Our view has been that information of biological significance may be obtained by a thorough study of water in such environments. We have previously published a number of articles in which trimers, octamers, and decamers have been discussed. Also of importance in supramolecular assemblies are water dimers and even monomers. The essential question is which stabilizes which? Do the water clusters stabilize the supramolecular architecture or does the supramolecular architecture stabilize the water clusters? These questions are not really philosophical, as the discussion will demonstrate. The discussion will also point out the use of metal coordination and hydrogen bonding forces to effect stabilization. However, exciting new results on the importance of weaker interactions will be revealed.

Keywords: supramolecular, water clusters, weak intertions

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Hydration structure changes around proteins at work

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Proteins fold and function in water known as a complex liquid displaying unusual physicochemical properties caused by hydrogen bonds between water molecules. To understand why water is necessary for structures and functions of proteins and biological macromolecules, interfacial structures between water and biomolecules, so-called hydration structures must be investigated. X-ray crystallography has been contributing to visualize the hydration structures of proteins (Nakasako (1999) J. Mol. Biol. 289, 547.; Nakasako (2004) Phil. Trans. B. Roy. Soc. Lond. 359, 1191.), it is, however, still difficult to observe directly the reorganization accompanying protein motion to understand the physical mechanism underlying the reorganization. In the present study, I would like to discuss how the reorganization of hydration structures occur to accommodate to the domain motions of a multi-domain enzyme, glutamate dehydrogenase composed of six identical subunits with two separate domains. X-ray crystal structure analyses suggest the possibility that a set of hydration water molecules adsorbing on the depth of the active site cleft regulate the domain movements. A large-scale molecular dynamics simulation for the enzyme demonstrates that the domain movements are rear events and occur very short period within 50 psec. In addition to the simulation, the frequencies of the domain movements are measured by atomic force microscopy for the surface of the enzyme crystals. The results provide probabilities of the domain movement of the enzyme. To understand totally the results from the three different types of experiments, it is plausible that hydration water molecules inhibit the molecular motions of the enzyme in solution.

Keywords: hydration structure, cryogenic X-ray crystallograhy, molecular dynamics simulation

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Water embedded in metal-polycarboxylate crystal host

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Because water plays an indispensable role in life-sustaining processes, investigations on its structure, properties and functions have received more scientific attention than any other substance. The study of the possible structures of water clusters in different surroundings is important to understand the nature of water-water interactions in the bulk water or ice,[1] as well as in many biological, chemical, and physical processes. This realization has led to theoretical and experimental explorations of several small water clusters in the solid state. In the course of our research interest on the preparation of policarboxylate coordination polymers and their magnetic properties, several water motifs have been obtained and characterized showing the contribution of water to the stability of the host, and the cooperative association of the water clusters and crystal host in the formation of the water clusters. Because it is impossible for water clusters in solution and in the solid state to be discrete, the precise structural data and the cooperative association of the water clusters and crystal host may be helpful in improving our understanding of the contribution of water clusters to the stability and function of the biological assemblies, as well as anomalous properties of water.

[1]S. W. Benson, E. D. Siebert, J. Am. Chem. Soc., 1992, 114, 4269.