

Models of Interfacial Metalloprotein Hydrate Structures Containing Water Chains and Clusters.

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One-dimensional chains of hydrogen-bonded water molecules, or proton wires, are of interest because of their role in proton permeation involving transmembrane proteins such as cytochrome oxidase, bacteriorhodopsin, as well as carbonic anhydrase. Rapid translocation of H⁺ along water chains appears to be important in controlling proton flux in these and related systems, however, we still know very little about the mechanism and structure of protonated species involved in these proton relay systems. The objective of this study is to examine the structure and properties of several metal hydrates containing biologically relevant imidazole ligands as models of metal complex-hydrate interfaces known or proposed to be present in biological systems. The study will demonstrate that imidazole compounds can form biologically relevant hydrate structures containing both one-dimensional chains and clusters of water molecules stabilized by hydrogen bonding in supramolecular solid state channels, which model the chain and pool structures of water observed in proteins such as bacteriorhodopsin, and carbonic anhydrase. This work was supported by the NSF (CHE-0328406), and the Kentucky Science and Engineering Foundation (KSEF-275-RDE-003).