CONNECTING WATER CLUSTERS TO ICE

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What is the most stable form of bulk ice and how stable is it? Many believe that it is the ferroelectric, proton-ordered, $Cmc2_1$ form called Ice XI. The structure and energetics of families of water clusters carved from Ice XI are studied as a function of cluster size and compared to other families of cluster structures. Zero point energy is extremely important in these hydrogen bonding energetics and will be examined as a function of cluster size. The work has determined: the approximater cluster size at which the bulk structure becomes more stable than other cluster families, that the bulk structure is unstable at the surface, and a value for the stability of Ice XI. The stability of Ice XI will be considered relative to experimental determinations of the enthalpy of sublimation of ice.