

Molecular models of high-pressure ices using MOL-TALOS

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In order to understand the structure of water, especially under high-pressure conditions, many researchers used structures of H₂O ices (for example, Kamb, 1968, in Structural Chemistry and Molecular Biology, p. 507-542 Freeman). H₂O ice has more than fourteen polymorphs and two amorphous phases. Except for ice X, these phases exist at a pressure range lower than a few GPa (see an updated comprehensive review by Dr. Martin Chaplin at www.lsbu.ac.uk/water). Therefore, the phase diagram of H₂O at relatively low-pressure region is complex.

Here, we made new molecular models of a cage-type hexamer unit of water, ice VI and ice VII using commercially available plastic ball-and-rod assemblies MOL-TALOU (Teaching And Learning Of Understanding, http://www.talous-world.com/english/talous_a.htm) in which blue large balls, green balls, blue tubes, and white tubes represent oxygen atoms, hydrogen atoms, single bonds, and hydrogen bonds, respectively. The oxygen atoms have four legs with 109 degree which is not identical to those of water and ices but similar to those. In our poster presentation, we will show those molecular models, and discuss about the features seen in the molecular models of water and high-pressure ices.