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Hydrophobic Hydration – Information from Solvation of Small Molecules as a Source of Structural Models for Macromolecular Crystallography. Janusz Lipkowski^a, Konstantin Udachin^b, Dariusz Świerczyński^a, Jerzy Ostyk-Narbutt^c, ^aInst. Phys. Chem., Polish Acad. Sci., Warszawa, Poland, klatrat@ichf.edu.pl, ^bStecie Inst. Mol. Sci., NRC Ottawa, Canada, ^cInst. Radiation Chem. and Techn., Warszawa, Poland.

In the present paper an up-to-date review of hydrophobic hydrates will be given, some new, yet unpublished, experimental data will be presented as well.

As known from literature, complex cavities may be formed *via* different deformations of arrangement of water molecules: either by combination of dodecahedra to form Jeffrey-type complex cavities or by incorporating foreign species. Strong ionic environment exerts significant deforming influence as well. Thus, the resulting structural pattern is a combination of hydrophobic hydration, ionic strength and foreign species incorporated into the framework.

The illustrations will be based on recent, partly unpublished X-ray structures of hydrates of macrocyclic compounds (crowns, calixarenes) and their intermolecular complexes, coordination complexes and fatty acids. Statistics on water coordination number in these compounds will be presented as well.

The importance of the structural patterns to stabilize selected structures has been experimentally demonstrated, e.g. in extraction studies in the water/organic systems, proton or ionic conductivities in the systems and redox equilibria, with water aggregates serving as proton or electron sponges.