Structural Properties of Water and that Solution from Crystalline to Subcritical States Based on Computer Simulation Data

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Liquid water and aqueous solutions play a significant role in technological and biological processes. In spite of comprehensive studies of water properties on the macroscopic level, we don't know the structure of water and all the peculiarities of intermolecular interactions on the microscopic level. The problem of constructing reliable and accurate interaction potentials for computer simulations of water remains unsolved. The configuration space for two molecules has six dimensions. This is one of the main factors that do not allow us to use quantum chemistry methods for scanning the potential energy surface (PES). But, even if we can solve the task for two molecules we know nothing about PES changes in the presence of extra molecules. It has been shown [1] that there are at least two additional (to linear dimmer) stationary points on PES. We named the first configuration as an inverted dimmer, the second one as a bifurcated dimmer. We built up a new effective pair additive potential (BMW) that has three minima on PES. We used Gauss functions for describing the shape of PES in the neighborhoods of the extra minima. Non tetrahedral twofold bonds correspond to transition states. Calculations of thermodynamic and structural properties of water at P = 0.1 MPa and temperature range from 268 to 368 K, and also at T=293-573 K and pressure up to 49.1 MPa were performed using the MC method in the NpT ensemble. The calculated radial distribution functions, partial and full structural factors were compared with the experimental data obtained by A. Soper (NDIS-97, NDIS-2000) and with the data calculated using other pair additive and polarizable potentials. It has been shown [2] the BMW potential gives closest to experimental data results. In the BMW model the H-bond networks have a large amount of non-tetrahedral fragments. A tetrahedral network pushes out non-tetrahedral fragments which form clusters. This phenomenon is one of the causes of water structure heterogeneity on the microscopic level. A method of computer simulation of water crystallization was proposed. The results of water (water solutions: hydrazine, methyllhydrazene, dime- thilhydrazine, aerozine, etc.) crystal phase calculations are presented. For investigative solutions we resaved lots of experimental data (density, thermal conductivity, specific heat capacity, viscosity, thermal temperature, enthalpy, entropy energy of Helmholtz, energy of Gibbs etc.)

[1] www.ensta.fr/~muguet.
[2] Yu.G. Bushuev, A.V. Davletbaeva and F.Muguet, *Molecules*, **8**, 226-242 (2003).