

STUDY OF STRUCTURAL PECULIARITIES OF  
HYDROPHOBIC HYDRATION OF NONPOLAR  
MOLECULES IN WATER

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S u m m a r y

The radial distribution functions (RDF) of a water-propane solution are calculated by using Monte Carlo simulations. The RDF give the information about intramolecular interactions and hydrogen bonds in the two-component water-propane solution. The sizes of the first and second hydration spheres are determined. The influence of nonpolar solvent molecule on the water's local structure and the net of hydrogen bonds is analyzed.