MONTE CARLO STUDY OF HYDRATION EFFECTS OF POLAR MOLECULES IN INFINITELY DILUTED SOLUTIONS

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S u m m a r y

The radial distribution functions (RDF) for the aqueous solutions of methanol and dimethyloxygen are calculated by using the Monte Carlo method, and the local structures of the solutions are analyzed. The latter have a higher density than bulk water. The Coulomb part of the average interaction energy in the system decreases in the transition from the water-methanol system to the water-dimethyloxygen one.