Study of Water and Dimethylformamide Interaction by Computer Simulation

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Monte Carlo simulations of water-dimethylformamide (DMF) mixtures were performed in the isothermal and isobaric ensemble at 298.15 K and 1 atm. The intermolecular interaction energy was calculated using the classical 6-12 Lennard-Jones pairwise potential plus a Coulomb term. The TIP4P model was used for simulating water molecules, and a six-site model previously optimised by us was used to represent DMF. The potential energy for the water-DMF interaction was obtained via standard geometric combining rules using the original potential parameters for the pure liquids. The radial distribution functions calculated for water-DMF mixtures show well characterised hydrogen bonds between the oxygen site of DMF and hydrogen of water. A structureless correlation curve was observed for the interaction between the hydrogen site of the carbonyl group and the oxygen site of water. Hydration effects on the stabilisation of the DMF molecule in aqueous solution have been investigated using statistical perturbation theory. The results show that energetic changes involved in the hydration process are not strong enough to stabilise another configuration of DMF than the planar one.

Key words: Monte Carlo Simulation; Solvent Effects; Statistical Perturbation Theory; Hydration of Peptides.

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