Empirical Intermolecular Potential in N-Methylacetamide-Water Disolution: Molecular Dynamics Simulations

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The formulation of an intermolecular potential, suitable to perform extensive molecular dynamics (MD) simulations, has been applied to N-methylacetamide (NMA) interacting either with water or with another NMA molecule (disolution to with dofferent concentrations). The intermolecular potential energy is obtained by considering electrostatic and non electrostatic contributions. The first contribution, derived from sets of punctual charges distributed on the molecules, is calculated as a sum of Coulombic terms, each one representing the electrostatic interaction between two punctual charges placed on different molecules. The second contribution, associated to the van der Waals interaction, is calculated as a sum of effective potential functions (mainly including size repulsion and dispersion attraction), which are formulated by means of an Improved Lennard Jones function (the ILJ function [1-4]), representing the non electrostatic interaction between two dispersion centers (or sites) placed on different molecules. This formulation, appears to be appropiate to describe the energetic of both stable and less stable configurations of weakly interacting aggregates, including those binding with hydrogen bond.

The results show that the model potential is appropriate for describing the energetic of the various concentrations of NMA-H_2O disolution weakly interacting aggregates, including the formation of hydrogen bonds.

References

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