E2-30 Solvation enthalpy of benzene in argon fluid: a computer simulation study

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A Molecular Dynamics simulation has been carried out for argon fluid containing 1 benzene molecule at the temperature of 180 K and pressure 1.7 atm. The solute molecule, benzene, was modelled by a rigid body of D_{6h} symmetry. Solvent-solvent and solvent-solute interactions were calculated using 4 parameter potential functions.

The radial distribution function of the solvent in the solution was compared with that of the pure solvent. Diffusion coefficients of solvent molecules in the solution and in the pure solvent were calculated. The solvation enthalpy of benzene in argon fluid at 180 K and 1.7 atm is 42.3 kJ/mol. Further, the results show that the solvation of benzene like solute in a non polar solvent is energetically driven and does not show a major structural and dynamical change of the properties of the solvent.