Development of an OPLS-like Force Field for Monte Carlo Simulations of Alicyclic Compounds

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Molecular simulation methods are gradually becoming powerful tools for quantitative description of thermodynamic properties for various systems. Modern computational resources allow Monte Carlo (MC) simulations for complex organic molecules of different classes. The primary goal of the present work is to develop a force field (FF) for MC simulations capable of predicting enthalpies of vaporization and densities of alicyclic compounds. MC simulations were carried out in the *NPT*-ensemble for liquid and gas boxes at T = 298.15 K. Liquid densities and enthalpies of vaporization for the cyclopentane–cyclohexane, cyclopentanone−cyclohexanone, and γ-butyrolactone−δ-valerolactone pairs were used for optimization of the Lennard-Jones FF parameters. Atomic charges were obtained from quantum-chemical calculations. All other parameters were forwarded from the OPLS-AA-like force field [1]. The parameter optimization was performed with the use of the fractional factorial design. The number of factors and their levels were individually chosen for each numerical experiment and depended on the complexity of a particular functional group appearing in the studied molecule. A bootstrap procedure [1] was used to reduce the number of required simulations. The obtained force field was used for prediction of enthalpy of vaporization and liquid density for homologous series of cycloalkanes, cyclic ketones and lactones. The obtained results were in good agreement with the experimental values.

References

[1] E. Paulechka, K. Kroenlein, A. Kazakov, and M. Frenkel, A J. Phys. Chem. B. Vol. 116, P. 14389-14397 (2012).