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Intermolecular potential for phenol based on the test particle model

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Abstract

An intermolecular potential to describe the interaction between phenol molecules was constructed using the test particle model (T-model). The T-model potential was used in the calculation of the equilibrium structures and energies of phenol dimers and trimers. The absolute and local energy minima on the T-model potential energy surface were examined by ab initio calculations with the second-order Møller–Plesset perturbation (MP2) theories. The equilibrium structures of phenol dimers computed from the T-model potential agree well with the MP2 results, and are compatible with those deduced from rotational coherence spectroscopy. The hydrogen bonds (H-bonds) in phenol–water 1:1 complexes were also investigated using the T-model potentials and MP2 calculations. The results are in good agreement with the previous ab initio calculations with a larger basis set and experiment in the gas phase. Structures and energies of liquid phenol, as well as phenol in aqueous solution, were studied using Molecular Dynamics (MD) and Monte Carlo (MC) simulations, respectively. The results are discussed in comparison with available theoretical and experimental results on the same and similar systems.