

Quantum semiempirical parametrization of the molecular dynamics thermodynamics integration method in a case of the proton transfer reaction in the 2-[N,N-dimethylaminomethyl]-phenol.

Autorzy

Adam Fedorowicz

Aleksander Koll

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In this paper, the results of application of quantum semiempirical parametrization in molecular dynamics simulations of the intramolecular proton transfer reaction in the 2-[N,N-dimethylamino]-phenol in methanol solution are presented. Free energy difference of the proton transfer reaction in the studied systems was calculated and compared with the experimental data. The local changes in the solvent structure connected with intramolecular proton transfer reaction in the solute molecule were found. However, it appears that these changes have only local extent, as they do not influence the bulky solvent structure.

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