

Molecular dynamics study of the tautomeric equilibrium in the 4-nitro-and 2,4,6-trichloro derivatives of 2-(*N*, *N*-dialkyloaminomethyl)phenol.

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Streszczenie

Molecular dynamics thermodynamic integration (MDTI) method and quantum chemical calculations at the density functional theory B3LYP 6-31+(d,p) level, which included the Tomasi model of the solvent reaction field, were applied to study the tautomeric equilibrium of Mannich base in methanol solution. The values obtained for the free-energy difference are in good agreement with experimental data. However, the results from quantum mechanical calculations were not as good as the results of MDTI simulations owing to inappropriate treatment of intermolecular hydrogen bonds between the solute molecule and the first shell of solvent molecules in the Tomasi model of the solvent reaction field. The radial distribution functions between solute atoms and solvent atoms confirmed the formation of hydrogen bonds between the solute molecule and surrounding methanol molecules and indicated that the zwitterionic form is associated more with an organized solvent structure at the level of the first solvation shell than is the molecular form.

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<http://link.springer.com>