Molecular dynamics study of the tautomeric equilibrium in the Mannich base.

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Streszczenie

The density functional theory ab initio quantum mechanical and molecular dynamics thermodynamic integration methods have been used to study the intramolecular proton transfer equilibrium in 2-[N,N-dimethylaminomethyl]-3,4,6-trichlorophenol. The model of slow proton transfer reaction was applied, where the geometry and charge data were linearly interpolated between two states calculated at the Becke3LYP 6-31G(d,p) level. This avoids the difficulties connected with the different time scales of proton transfer reaction and solvent relaxation processes. The calculated free energy differences obtained from ab initio calculations including the Tomasi model of the solvent reaction field (1.16 kcal mol^{-1}) and from ab initio plus molecular dynamic thermodynamic integration calculations (1.7 ± 1.8 kcal mol^{-1}) are in agreement with the experimental value 0.12 ± 0.02 kcal mol^{-1}.

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