

Solvent influence on the transformation of intramolecular hydrogen bonds in 2-hydroxy-5-methyl-3-nitroacetophenone.

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Streszczenie

DFT (B3LYP/6-31+G(d,p)) calculations performed on 2-hydroxy-5-methyl-3-nitroacetophenone (**I**) indicate that the isomer with the intramolecular hydrogen bond (IMHB) to the nitro group (**Ia**) is more stable by $7.3 \text{ kJ}\cdot\text{mol}^{-1}$ than that with the H-bond to the acetyl group (**Ib**). The calculated polarities of both isomers are quite different with the dipole moment of **Ib** being five times higher. Dipole moment and infrared studies of the **Ia** $\rightleftharpoons$ **Ib** conformational equilibrium in different solvents show that the IMHB transformation is controlled by the solvent polarity. In polar dichloromethane and acetonitrile the **Ia** $\rightleftharpoons$ **Ib** equilibrium is strongly shifted towards the polar **Ib** isomer. The simple continuum dielectric model for a heterogeneous medium and polarizable solute allows a quantitative explanation of the influence of the solvent on the **Ia** $\rightleftharpoons$ **Ib** equilibrium.

Słowa kluczowe

2-Hydroxy-5-methyl-3-nitroacetophenone, intramolecular hydrogen– bonds, conformational equilibrium, dipole moments, infrared spectra, solvent effect

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