Gas phase FT-IR spectra and structure of aminoalcohols with intramolecular hydrogen bonds. I. The shape of the ν(OH) vibrational bands in $R_2NC_3H_6OH$ (R=H, CH_3).

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Streszczenie

Gas phase FT-IR spectra of 3-dimethylamino-1-propanol (**1**) and 3-amino-1-propanol (**2**) are recorded. It is found that the forms with intramolecular hydrogen bonds strongly predominate up to 100°C in both compounds. The origin of multicomponent structure of *ν*(OH) bands is discussed on the assumption of conformational equilibria as well as the coupling between the *ν*(OH) vibration mode with the low frequency chelate ring deformation modes affecting the N⋯O distance. DFT ab initio calculations are performed at 6-31G(d,p) and 6-311++G(2d,2p) levels. It is concluded that the *ν*(OH) band structure in **1** results from high/low frequency modes coupling.

Słowa kluczowe

Ab initio, Aminopropanol, Conformation, Gas phase IR spectra, Hydrogen bond, Multicomponent bands structure

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