

Rotational isomerism of butanols: infrared, near-infrared and DFT study.

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Streszczenie

Infrared and near-infrared spectra of all butanols were recorded in dilute CCl_4 solutions as a function of temperature. The stability of the *trans* and *gauche* conformers was evaluated from the temperature dependence of the relative band intensities. The spectra reflect various conformations of the free OH group, whereas the influence of C–C rotations on ν_{OH} and $2\nu_{\text{OH}}$ bands was not observed. The position of these bands determines the type of conformer resulting from immediate environment of OH group, whereas the relative population of particular conformers strongly depends on steric effects of the groups in α - and β -position.

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