

Matrix-isolation FT-IR and theoretical investigation of the vibrational properties of the sterically hindered *ortho*-hydroxy acylaromatic *Schiff* bases.

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Streszczenie

FT-IR and FT-Raman spectra of the *ortho*-hydroxy acylaromatic *Schiff* bases (2-(α -(*N*-methylimino)ethyl)-4-chloro-6-nitrophenol – I, 2-(α -(*N*-methylimino)ethyl)-4,6-dichlorophenol – II), and their isotoposubstitutions have been recorded in the range of 4000–50 cm⁻¹. The spectra were interpreted by a normal coordinate analysis based on B3LYP/6-31++G(d,p) density functional calculations and experimental deuterio substitution. Proton transfer equilibrium between the enolic and keto tautomers of two sterically hindered *Schiff* bases has been studied combined experimental (FT-IR matrix-isolation and FT-Raman) and theoretical (DFT/B3LYP/6-31++G(d,p)) methods.

Słowa kluczowe

Intramolecular hydrogen bond, *ortho*-Hydroxy ketimine, Acylaromatic, *Schiff* base, Matrix-isolation

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