

DFT studies of the structure and vibrational spectra of NH tautomers of *trans* -*N,N'*-bis-salicylidene-1',2'-cyclohexanediamines.

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Streszczenie

The structure and vibrational spectra of the tautomeric NH form of *trans*-*N,N'*-bis-(*R*-salicylidene)-cyclohexanediamines (*R*^{1/4}H, 5-NO₂, 4,6-OCH₃, 3,5-Cl) and their analogues deuterated in the NH and CH imine groups were calculated using the DFT method at the 6-31G level. The complicated nature of the normal modes was shown. The influence of the substituents on the hydrogen bond strength and nonequivalence of the two hydrogen bonds present in Schiff base molecules are discussed.

Słowa kluczowe

Schiff bases, Tautomerism, theoretical vibrational spectra

Adres publiczny

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