

Bifunctional influence of 3-chloro substitution on structural and energetic characteristics of *N*-methyl-salicylidene imines.

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Energetic and structural effects of formation of intramolecular hydrogen bonds in the group of eight differently chloro-substituted ortho-hydroxy aromatic Schiff bases (*N*-methyl-salicylidene imines) containing the 3-chloro substituent in all compounds were studied. The aim was to explain the specific function of this substituent, giving rise to an especially large increase of the strength of intramolecular hydrogen bonds. DFT B3LYP/6–31 + G(d,p) calculations of the structures of particular conformers as well as the potential energy surfaces were carried out. The method of thermodynamic cycle-like scheme was adapted, where the three open conformers are used to estimate the steric corrections connected with formation of chelate rings in the fourth conformer. Problems arising for the estimation of the energy of intramolecular hydrogen bonds connected with the selection of reference states and various structural aspects are discussed in detail. 3-Chloro-substituted Schiff bases can be accounted as sterically enhanced intramolecular hydrogen bonds. Participation of steric and electronic functions in increasing of the energy of intramolecular hydrogen bonds was analyzed. Low energetic proton transfer reaction was found in these molecules, which can be potentially interesting from the point of view of possible thermochromic applications.

Słowa kluczowe

intramolecular hydrogen bonds, Energy of hydrogen bond, Steric effects, Structure of hydrogen bond, DFT calculations

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