

Interference of H-bonding and substituent effects in nitro- and hydroxy-substituted salicylaldehydes.

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Streszczenie

Two intramolecular interactions, i.e., (1) hydrogen bond and (2) substituent effect, were analyzed and compared. For this purpose, the geometry of 4- and 5-X-substituted salicylaldehyde derivatives (X = NO(2), H or OH) was optimized by means of B3LYP/6-311 + G(d,p) and MP2/aug-cc-pVDZ methods. The results obtained allowed us to show that substituents (NO(2) or OH) in the para or meta position with respect to either OH or CHO in H-bonded systems interact more strongly than in the case of di-substituted species: 4- and 3-nitrophenol or 4- and 3-hydroxybenzaldehyde by ~31%. The substituent effect due to the intramolecular charge transfer from the para-counter substituent (NO(2)) to the proton-donating group (OH) is ~35% greater than for the interaction of para-OH with the proton-accepting group (CHO). The total energy of H-bonding for salicylaldehyde, and its derivatives, is composed of two contributions: ~80% from the energy of H-bond formation and ~20% from the energy associated with reorganization of the electron structure of the systems in question.

Słowa kluczowe

intramolecular hydrogen bond, DFT, MP2

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<http://link.springer.com>