Steric enhancement of the strength of intramolecular hydrogen bond in 3-Cl substituted 2-(*N*-dimethylaminomethyl) phenols.

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Streszczenie

The structure modification and energetic consequences of the formation of intramolecular hydrogen bonds in the series of chloro substituted 2-(*N*-dimethylaminomethyl) phenol are discussed on the basis of result of ab initio and DFT calculations. A specific behaviour of derivatives containing the 3-Cl substituent was detected, suggesting formation of the stronger hydrogen bond than in analogous derivatives without such a substituent. It was found that steric repulsion of 3-Cl atom moves the methylamino group towards the OH group, leading to shortening of the OH···N hydrogen bridge. The geometric and electronic consequences of such shortening of the hydrogen bond are similar to the effects of the increase of acid–base interactions. The estimation of the corrections on steric interaction in the procedure of the energy of intramolecular hydrogen bond calculation appears to be much more complicated than in the series of the compounds not containing the 3-Cl substituent.

Adres publiczny

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