

Strengthening of the intramolecular OHN hydrogen bonds in Schiff bases as a result of steric repulsion.

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Three ortho hydroxy Schiff bases 2-(*N*-methyl- α -iminoethyl)-phenol (**I**), 2-(*N*-benzyl- α -iminoethyl)-phenol (**II**) and 2-(*N*-benzyl- α -iminopropyl)-phenol (**III**) were synthesised in which the hydrogen atoms in C–C(H)N group were replaced by an alkyl substituent. The crystal structures were determined and ab initio calculations at the B3LYP/6-31G** basis set were performed. One of the shortest known O–H $\cdots$ N hydrogen bonds were found with O $\cdots$ N distance equal to 2.459(3), 2.497(3) and 2.494(3) Å, respectively in **I**, **II** and **III**. Steric repulsion of substituted alkyl results in this unusual strengthening of the hydrogen bonds. FT-IR spectra in solution and in the solid state in function of the temperature were determined. Strong influence of the temperature on the character of the hydrogen bond was observed.

Słowa kluczowe

Schiff bases, Crystal structure, Ab initio, Steric repulsion,
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Adres publiczny

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