

Strengthening of the intramolecular O...H...N hydrogen bond in 2-(N-benzyl- α -iminoethyl)-naphthol as a result of steric repulsion.

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Streszczenie

One new ortho-hydroxy Schiff base, 2-(N-benzyl- α -iminoethyl)-naphthol (BEIN) in which the hydrogen atom in the C-C(H)=N group is replaced by a methyl substituent, is synthesized. The crystal structure is determined and ab initio calculations with B3LYP/6-31G** basis sets are performed. The O...N distance found in the O-H...N hydrogen bond turns out to be quite short and is equal to 2.499 Å. This shortening is due to the steric repulsion of methyl substituent group and results in strengthening of the hydrogen bond.

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