

Strengthening of the intramolecular hydrogen bond in 7-ethylsalicylidene aniline due to steric repulsion.

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Rok wydania

2002

Czasopismo

Journal of Molecular
Structure-Theochem

Numer woluminu

577

Strony

153-159

DOI

10.1016/S0166-
1280(01)00658-3

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

In a newly synthesized orthohydroxy Schiff base, 7-ethylsalicylidene aniline (ESA), the hydrogen atom in C–C(H)N group is replaced by an ethyl group. The crystal structures of ESA determined by X-ray crystallography and ab initio calculations at the level of B3LYP/6-31G** are performed. The results obtained indicate that the steric effects lead to the strengthening of intramolecular hydrogen bond (O–H···N) of ESA. We have compared the results of ESA with the results of another two previously studied Schiff bases, 2-(*N*-methyl- α -iminoethyl)-phenol (I) and 2-(*N*-benzyl- α -iminoethyl)-phenol (II). We have also constructed the potential energy surfaces on which the proton is supposed to move and analyzed the reaction path.

Słowa kluczowe

Schiff base, Ab initio, Steric repulsion

Adres publiczny

[https://doi.org/10.1016/S0166-1280\(01\)00658-3](https://doi.org/10.1016/S0166-1280(01)00658-3)

Strona internetowa wydawcy

<http://www.elsevier.com>