Solvent and substitution influence on the character of tautomers resulting from proton transer reaction in some phenol derivatives.

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Rok wydania

2004

Czasopismo

Structural Chemistry

Numer woluminu

15

Strony

353-361

DOI

10.1023/B:STUC.0000037890.17802.9a

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The work verifies the application of a “resonance model” in description of the structure of tautomers in the so-called resonance-assisted hydrogen bonds. The results of B3LYP/6-31G + G(d,p) calculations are presented for *N*-methyl-2-hydroxy benzylidene amine and its 2,- and 2,4-chloroderivatives (Schiff bases) as well as for related Mannich bases. The influence of surrounding permittivity and the phenol acidity on the structure is discussed. It is demonstrated that enhancement of both the factors leads to the increase of the content of keto resonance forms in Mannich bases. In the case of Schiff bases, a decrease of the content of such forms with surrounding permittivity increase has been found. The differences in dipole moments of particular forms explain such tendencies.

Adres publiczny

https://doi.org/10.1023/B:STUC.0000037890.17802.9a

Strona internetowa wydawcy

http://link.springer.com