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Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Factor analysis of deuterium isotope effects on ^{13}C NMR chemical shifts in Schiff bases.

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Rok wydania

2005

Czasopismo

Chemistry-A European Journal

Numer woluminu

11

Strony

4758-4766

DOI

10.1002/chem.200401350

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

We have analyzed deuterium isotope effects on ^{13}C chemical shifts in a series of *o*-hydroxy Schiff bases by applying factor analysis. Two orthogonal factors were obtained that explain about 80 and 10 % of the variance of the data. The numerical values of these factors can be related to ^{1}H NMR chemical shifts of the proton involved in the intramolecular bonds δ(XH) (X=O or N). Such a relation allows one to identify clusters of compounds with different tautomeric forms of hydrogen bonding. Application of a similar approach to solution ^{13}C NMR chemical shifts produces three important factors, which have a different structure to factors describing isotope effects. This illustrates well the different nature of chemical shifts and isotope effects. The three factors explain about 54, 15, and 13 % of variance. They can be rationalized and are strongly related to the electronic properties and location of substituents.

Adres publiczny

https://doi.org/10.1002/chem.200401350

Strona internetowa wydawcy

onlinelibrary.wiley.com

Plik został wygenerowany dnia 2026-08-24 18:10:53

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/o1rtW7h.