Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Toward an understanding of the ambiguous electron paramagnetic resonance spectra of the iminoxy radical from *o*-fluorobenzaldehyde oxime: density functional theory and *ab initio* studies.

Autorzy

Maciej Witwicki

Julia Jezierska

Rok wydania

2015

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

119

Strony

9109-9120

DOI

10.1021/acs.jpca.5b06143

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Iminoxy radicals ($R_1R_2C{=}N{-}O^{\bullet}$) possess an inherent ability to exist as *E* and *Z* isomers. Although isotropic hyperfine couplings for the species with R_1 = H allow one to distinguish between *E* and *Z*, unequivocal assignment of the parameters observed in the EPR spectra of the radicals without the hydrogen atom at the azomethine carbon to the right isomer is not a simple task. The iminoxyl derived from *o*-fluoroacetophenone oxime (R_1 = CH_3 and R_2 = *o*-FC_6H_5) appears to be a case in point. Moreover, for its two isomers the rotation of the *o*-FC_6H_5 group brings into existence the *syn* and *anti* conformers, depending on the mutual orientation of the F atom and $C{=}N{-}O^{\bullet}$ group, making a description of hyperfine couplings to structure even more challenging. To accomplish this, a vast array of theoretical methods (DFT, OO-SCS-MP2, QCISD) was used to calculate the isotropic hyperfine couplings. The comparison between experimental and theoretical values revealed that the *E* isomer is the dominant radical form, for which a fast interconversion between *anti* and *syn* conformers is expected. In addition, the origin of the significant A_F increase with solvent polarity was analyzed.

Adres publiczny

http://dx.doi.org/10.1021/acs.jpca.5b06143

Strona internetowa wydawcy

https://www.acs.org/content/acs/en.html

Plik został wygenerowany dnia 2026-11-10 21:07:54

Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/0EhGaDJ.