Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Density functional theory study of intramolecular hydrogen bonding and proton transfer ino-hydroxyaryl ketimines.

Autorzy

Aleksander Filarowski

Aleksander Koll

Poul Erik Hansen

Małgorzata Kluba

Rok wydania

2008

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

112

Strony

3478-3485

DOI

10.1021/jp076991l

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The potential energy surface and the reaction pathway for the intramolecular hydrogen transfer in o-hydroxyaryl ketimines are characterized using DFT methods. Structural changes in the proton-transfer process in quasi-aromatic hydrogen bonding are described. A transition state and a state with a low proton-transfer barrier were studied in sterically compressed o-hydroxyaryl ketimines (2(N-methyl-alpha-iminoethyl)phenols) possessing two potential minimums. The potentials for proton vibration in the OH and HN tautomers of o-hydroxyaryl ketimines were investigated and anharmonic frequencies were determined. Solvent and substituent effects were analyzed. The energies of the various conformers of the OH and HN tautomers were compared with the related forms of o-hydroxyaryl aldimine.

Słowa kluczowe

Hydrogen, Reaction mechanisms, Energy, Noncovalent interactions, Molecular structure

Adres publiczny

https://doi.org/ 10.1021/jp076991l

Strona internetowa wydawcy

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

Plik został wygenerowany dnia 2026-06-22 19:05:49

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