AIM analysis of intramolecular hydrogen bonding in*O*hydroxy aryl Schiff bases.

Autorzy

Aleksander Filarowski

Irena Majerz

Rok wydania

2008

Czasopismo

Journal of Physical Chemistry A

Numer woluminu

112

Strony

3119-3126

DOI

10.1021/jp076253x

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

AIM analysis was applied to study the changes in such topological parameters as the electron density at critical points of all the bonds of the molecule during the so-called nonadiabatic proton transfer in intramolecular hydrogen bonding in o-hydroxy aryl Schiff bases. Proton transfer is presented by a stepwise elongation and fixing of the hydroxyl bond with complete optimization of the rest of the parameters of the molecule by the B3LYP/6-311++G(d,p) method. A more detailed study of electron density changes at the critical points of the chelate and phenol rings in the stepwise proton-transfer process is presented. It was shown that the dependency of the electron density at the critical point of the chelate ring on tautomeric equilibrium is of a complicated character, whereas it is linear for the phenol ring. A complex study of the changes in the total electron density at the hydrogen bond, the quasi-aromatic ring, and in the whole molecule has been accomlished. The calculations of the intramolecular hydrogen bond by means of conformational and topological methods are discussed.

Słowa kluczowe

Coordination compounds, Energy, Noncovalent interactions, Molecular structure, Electron density

Adres publiczny

https://doi.org/10.1021/jp076253x

Strona internetowa wydawcy

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