Theoretical study on the polarizability and hyperpolarizability of hydrogen bonded complexes of nitropyridines with hydrogen fluoride.

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Rok wydania

2009

Czasopismo

Journal of Molecular Structure-Theochem

Numer woluminu

916

Strony

72-75

DOI

10.1016/j.theochem.2009.09.008

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The static polarizability, and the static and dynamic hyperpolarizability of molecular hydrogen bonded complexes of nitropyridines with the hydrogen fluoride molecule and their ion pairs are investigated by *ab initio* time-dependent Hartree–Fock and Finite Field methods. The nonlinear electro-optical properties are calculated for a series of basis sets: 4−31G, 6−31G, 6−31G(*d*), 6−31G(*d*,*p*) and 6−311G(*d*,*p*). The calculated results show that the average value of the polarizability is almost independent of the form of the hydrogen bond, whereas a very large enhancement of the first and second hyperpolarizability due to proton transfer is found in the studied complexes.

Słowa kluczowe

Nonlinear optics, Time-dependent Hartree–Fock (TDHF) method, Finite Field (FF) method, Polarizabilities, Hyperpolarizabilities, Hydrogen bond

Adres publiczny

https://doi.org/10.1016/j.theochem.2009.09.008

Strona internetowa wydawcy

http://www.elsevier.com