Structural and electronic structure differences due to the O–H···O and O–H···S bond formation in selected benzamide derivatives: a first-principles molecular dynamics study.

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2009

Czasopismo

Theoretical Chemistry Accounts

Numer woluminu

124

Strony

319-330

DOI

10.1007/s00214-009-0612-2

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Density functional theory-based methods were employed to obtain static and dynamical descriptions of the molecular properties of 2-hydroxy-*N*-methylbenzamide and 2-hydroxy-*N*-methylthiobenzamide; compounds containing O–H···O and O–H···S strong, intramolecular hydrogen bonds. These compounds are important as analogues of commercial analgesic and antipyretic medicines. In the current study the classical Kohn–Sham method was applied to develop static models describing the geometric parameters and proton potentials. The topological analysis of the electron density was performed via atoms in molecules theory. Subsequently, Car–Parrinello molecular dynamics investigations were performed in vacuo and in the solid state. The geometric and spectroscopic properties were investigated and compared with available experimental data. The influence of quantum effects on the intramolecular hydrogen bond properties were studied via path integral molecular dynamics in the solid state for 2-hydroxy-*N*-methylbenzamide. We found that the proton behavior depends strongly on the type of acceptor: the sulfur-containing bridge has significantly smaller proton flexibility than the oxygen-bearing analogue, which is reflected in the electronic structure and bridge dynamics.

Słowa kluczowe

Intramolecular hydrogen bond, Atoms in molecules, Car–Parrinello molecular dynamics (CPMD), Path integrals molecular dynamics (PIMD

Adres publiczny

https://doi.org./10.1007/s00214-009-0612-2

Strona internetowa wydawcy

http://link.springer.com