

Hydrogen bridges of polycyclic aromatic systems with O–H...O bonds—a gas-phase vs. solid-state Car-Parrinello study.

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Rok wydania

2015

Czasopismo

Journal of Molecular
Modeling

Numer woluminu

21

Strony

15/1-15/7

DOI

10.1007/s00894-014-2550-8

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The current study belongs to a series of investigations of polycyclic aromatic compounds containing intramolecular hydrogen bonds. Close proximity of the coupled aromatic system and hydrogen bridges gives rise to resonance-assisted hydrogen bonding phenomena. Substituted naphthols are ideally suited for this kind of investigation. The parent compound, 1-hydroxy-8-methoxy-3-methylnaphthalene, and its derivative, 1-bromo-5-hydroxy-4-isopropoxy-7-methylnaphthalene, both with known crystal structure, are investigated. Car-Parrinello molecular dynamics (CPMD) is chosen as a theoretical background for this study. Gas phase and solid state simulations are carried out. The effect of Grimme's dispersion corrections is also included. The report presents time evolution of structural parameters, spectroscopic signatures based on the CPMD simulations, and comparison with available experimental data. We show that the proton transfer phenomena do not occur within the simulations, which is consistent with evaluation based on the acidity of the donor and acceptor sites. The effects of the substitution in the aromatic system and change of the environment (gas vs. condensed phase) are of similar magnitude.

Słowa kluczowe

Car-Parrinello molecular dynamics, Intramolecular O–H...O hydrogen bond, Naphthol derivatives, Vibrational features

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Adres publiczny

<http://dx.doi.org/10.1007/s00894-014-2550-8>

Strona internetowa wydawcy

<http://link.springer.com>