# Exploring the Dynamical Nature of Intermolecular Hydrogen Bonds in Benzamide, Quinoline and Benzoic Acid Derivatives

Autorzy

Kamil Wojtkowiak

Aneta Jezierska

Rok wydania

2022

Czasopismo

Molecules

Numer woluminu

27

Strony

8847/1-8847/16

DOI

10.3390/molecules27248847

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

The hydrogen bonds properties of 2,6-difluorobenzamide, 5-hydroxyquinoline and 4-
hydroxybenzoic acid were investigated by Car–Parrinello and path integral molecular dynamics
(CPMD and PIMD), respectively. The computations were carried out in vacuo and in the crystalline
phase. The studied complexes possess diverse networks of intermolecular hydrogen bonds (N-H. . . O,
O-H. . .N and O-H. . . O). The time evolution of hydrogen bridges gave a deeper insight into bonds
dynamics, showing that bridged protons are mostly localized on the donor side; however, the proton
transfer phenomenon was registered as well. The vibrational features associated with O-H and N-H
stretching were analyzed on the basis of the Fourier transform of the atomic velocity autocorrelation
function. The spectroscopic effects of hydrogen bond formation were studied. The PIMD revealed
quantum effects influencing the hydrogen bridges providing more accurate free energy sampling.
It was found that the N. . .O or O. . .O interatomic distances decreased (reducing the length of the
hydrogen bridge), while the O-H or N-H covalent bond was elongated, which led to the increase in
the proton sharing. Furthermore, Quantum Theory of Atoms in Molecules (QTAIM) was used to give
insight into electronic structure parameters. Finally, Symmetry-Adapted Perturbation Theory (SAPT)
was employed to estimate the energy contributions to the interaction energy of the selected dimers.

Słowa kluczowe

hydrogen bond, non-covalent interactions, spectroscopic signatures, CPMD, PIMD, QTAIM, SAPT



Adres publiczny

http://dx.doi.org/10.3390/molecules27248847

Strona internetowa wydawcy

http://www.mdpi.com/journal/metals