Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Microsolvation of histidine : a theoretical study of intermolecular interactions based on AIM and SAPT approaches.

Autorzy

Beata Kizior

Jarosław J. Panek

Aneta Jezierska

Rok wydania

2020

Czasopismo

Symmetry

Numer woluminu

12

Strony

1153/1-1153/19

DOI

10.3390/sym12071153

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

Histidine is unique among amino acids because of its rich tautomeric properties. It participates in essential enzymatic centers, such as catalytic triads. The main aim of the study is the modeling of the change of molecular properties between the gas phase and solution using microsolvation models. We investigate histidine in its three protonation states, microsolvated with 1:6 water molecules. These clusters are studied computationally, in the gas phase and with water as a solvent (Polarizable Continuum Model, PCM) within the Density Functional Theory (DFT) framework. The structural analysis reveals the presence of intra- and intermolecular hydrogen bonds. The Atoms-in-Molecules (AIM) theory is employed to determine the impact of solvation on the charge flow within the histidine, with emphasis on the similarity of the two imidazole nitrogen atoms—topologically not equivalent, they are revealed as electronically similar due to the heterocyclic ring aromaticity. Finally, the Symmetry-Adapted Perturbation Theory (SAPT) is used to examine the stability of the microsolvation clusters. While electrostatic and exchange terms dominate in magnitude over polarization and dispersion, the sum of electrostatic and exchange term is close to zero. This makes polarization the factor governing the actual interaction energy. The most important finding of this study is that even with microsolvation, the polarization induced by the presence of implicit solvent is still significant. Therefore, we recommend combined approaches, mixing explicit water molecules with implicit models.

Słowa kluczowe

histidine, microsolvation model, Hydrogen bonding, DFT, PCM, AIM, SAPT

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Adres publiczny

http://dx.doi.org/10.3390/sym12071153

Strona internetowa wydawcy

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

Plik został wygenerowany dnia 2026-11-12 02:30:15
Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/WVfTfy8.