Uniwersytet Wrocławski

Repozytorium

Plik pochodzi z repozytorium Wydziału Chemii Uniwersytetu Wrocławskiego

Toward accurate prediction of amino acid derivatives structure and energetics from DFT: glycine conformers and their interconversions

Autorzy

Chong Shu

Zhongming Jiang

Małgorzata Biczysko

Rok wydania

2020

Czasopismo

Journal of Molecular Modeling

Numer woluminu

26

Strony

129/1-129/13

DOI

10.1007/s00894-020-4342-7

Kolekcja

Naukowa

Język

Angielski

Typ publikacji

Artykuł

Streszczenie

This work provides the accurate reference data for structural and energetic properties relevant for computational studies of amino acids and polypeptides. Glycine due to its small size allows for detailed theoretical explorations of its whole conformational space. The reference energies are computed at the CCSD(T)/CBS+CV level on the best estimated geometries of all local minima and the transition states. For the minima, we complete the set of reference structures reported in Phys. Chem. Chem. Phys., 2013, 15, 10094, by determining the CCSD(T)/(CBS+CV)^{MP2} quality geometries for the two highest energy conformers VIIp/tcc and VIIIn/gtc. These data stand as the reference to asses reliability and accuracy of less expensive computational models, with particular focus on dispersion-corrected hybrid and double-hybrid DFT approaches, considering several basis sets of double- and triple-ζ quality. Based on results for minima the B2LYP-D3(BJ)/aug-cc-pVTZ level is set as the reference for transition states geometries. Considering accuracy of both single point energies and structural parameters B2PLYP(-D3BJ) and DSDPBEP86 in conjunction with aug-cc-pVTZ basis set can be recommended for reference studies of amino-acids and small poly-peptides, while B3LYP(-D3(BJ)) shown to be the most robust from considered hybrid DFT approaches.

Słowa kluczowe

DFT, Double hybrid functionals, Dispersion, Structure, Amino acids, Benchmark, Coupled clusters, CBS limit, Glycine conformes, Transition states, Interconversion

Adres publiczny

http://dx.doi.org/10.1007/s00894-020-4342-7

Strona internetowa wydawcy

http://link.springer.com

Plik został wygenerowany dnia 2026-11-15 02:35:42
Adres w repozytorium https://old.chem.uni.wroc.pl/pl/repozytorium/0wTX8go.