

Structural and Vibrational Properties of Amino Acids from Composite Schemes and Double-Hybrid DFT: Hydrogen Bonding in Serine as a Test Case

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Streszczenie

The structures, relative stabilities, and vibrational wavenumbers of the two most stable conformers of serine, stabilized by the O-H...N, O-H...O=C and N-H...O-H intramolecular hydrogen bonds, have been evaluated by means of state-of-the-art composite schemes based on coupled-cluster (CC) theory. The so-called "cheap" composite approach (CCSD(T)/(CBS+CV)MP2) allowed determination of accurate equilibrium structures and harmonic vibrational wavenumbers, also pointing out significant corrections beyond the CCSD(T)/cc-pVTZ level. These accurate results stand as a reference for benchmarking selected hybrid and double-hybrid, dispersion-corrected DFT functionals. B2PLYP-D3 and DSDPBEP86 in conjunction with a triple- ζ basis set have been confirmed as effective methodologies for structural and spectroscopic studies of medium-sized flexible biomolecules, also showing intramolecular hydrogen bonding. These best performing double-hybrid functionals have been employed to simulate IR spectra by means of vibrational perturbation theory, also considering hybrid CC/DFT schemes. The best overall agreement with experiment, with mean absolute error of 8 cm⁻¹, has been obtained by combining CCSD(T)/(CBS+CV)MP2 harmonic wavenumbers with B2PLYP-D3/maug-cc-pVTZ anharmonic corrections. Finally, a composite scheme entirely based on CCSD(T) calculations (CCSD(T)/CBS+CV) has been employed for energetics, further confirming that serine II is the most stable conformer, also when zero-point vibrational energy corrections are included.

Słowa kluczowe

Basis sets, Composites, Molecular structure, Peptides and proteins, Quantum mechanics

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