

Deciphering the conformational preferences of selenocystine: The crucial role of noncovalent interactions

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Streszczenie

Conformational studies were conducted for (*R,R*)-selenocystine in the gas phase. The analysis was performed using various methods and software. From the obtained sets of conformers, 10 structures with the lowest energies were selected and reoptimized using Density Functional Theory (DFT) methods. Harmonic and anharmonic vibrational frequencies were also calculated for each conformer. Energies of the lowest-energy conformers were recalculated at the second-order Møller–Plesset perturbation theory (MP2) and Coupled-Cluster Singles, Doubles, and perturbative Triples (CCSD(T)) levels of theory and the global minimum was determined. The Boltzmann-averaged vibrational spectra were obtained from static calculations, as well as from ab initio molecular dynamics simulations. The NCI method was used to analyze noncovalent interactions in several conformers. The present study suggests that the results of conformational analysis depend on the method and software used. It was also shown that intramolecular interactions play an important role in stabilizing the (*R,R*)-selenocystine molecule in the gas phase.

Słowa kluczowe

Selenocystine, Conformational analysis, Born–Oppenheimer molecular dynamics, Vibrational analysis, Hydrogen bonding, Chalcogen bonding

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