

Microsolvation of 2-Thiouracil: Molecular Structure and Spectroscopic Parameters of the Thiouracil–Water Complex

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Streszczenie

State-of-the-art quantum-chemical computations have been employed to accurately determine the equilibrium structure and interaction energy of the 2-thiouracil–water complex, thus extending available reference data for biomolecule solvation patterns. The coupled-cluster level of theory in conjunction with a triple- ζ basis set has been considered together with extrapolation to the basis set limit, performed by employing second-order Møller–Plesset perturbation theory, and inclusion of core-correlation and diffuse-function corrections. On the basis of the comparison of experiment and theory for 2-thiouracil [Puzzarini et al. Phys. Chem. Chem. Phys. 2013, 15, 16965–16975], structural changes due to water complexation have been pointed out. Molecular and spectroscopic properties of the 2-thiouracil–water complex have then been studied by means of the composite computational approach introduced for the molecular structure evaluation. Among the results achieved, we mention the accurate determination of the molecular dipole moment and of the spectroscopic parameters required for predicting the rotational spectrum.

Słowa kluczowe

Energy levels, Equilibrium, Molecular structure, Spectroscopy

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