Identification of DNA Bases and Their Cations in Astrochemical Environments: Computational Spectroscopy of Thymine as a Test Case

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Increased importance of vibrational fingerprints in the identification of molecular systems, can be highlighted by the upcoming interstellar medium (ISM) observations by the James Webb Space Telescope, or in a context of other astrochemical environments as meteorites or exoplanets, Mars robotic missions, such as instruments on board of Perseverance rover. These observations can be supported by combination of laboratory experiments and theoretical calculations, essential to verify and predict the spectral assignments. Astrochemical laboratory simulations have shown that complex organic molecules (COMs) can be formed from simple species by vacuum ultraviolet or X-ray irradiation expanding interest in searching for organic biological and prebiotic compounds. In this work an example of nucleobase, thymine, is selected as a test case for highlighting the utility of computational spectroscopic methods in astrochemical studies. We consider mid-infrared (MIR) and near-infrared (NIR) vibrational spectra of neutral (T) and cationic (T^+) thymine ground states, and vibrationally-resolved photoelectron (PE) spectra in the far UV range from 8.7 to 9.4 eV. The theoretical framework is based on anharmonic calculations including overtones and combination bands. The same anharmonic wavenumbers are applied into the simulations of vibrationally-resolved photoelectron spectra based on Franck-Condon computations. The infrared and vibrationally-resolved photoelectron spectra are compared with the available experimental counterparts to verify their accuracy and provide assignment of the observed transitions. Finally, reliable predictions of spectra, going beyond currently available experimental data, either dealing with energy ranges, resolution or temperature, which can support astrochemistry studies are provided.

Słowa kluczowe

vibrational spectra, vibrationally resolved electronic spectra, density functional theory, anharmonic, VPT2, Franck-Condon computations, NIR, photoionization

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