

Toward the identification of cyano-astroCOMs via vibrational features: benzonitrile as a test case

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The James Webb Space Telescope (JWST) opened a new era for the identification of molecular systems in the interstellar medium (ISM) by vibrational features. One group of molecules of increasing interest is cyano-derivatives of aromatic organic molecules, which have already been identified in the ISM on the basis of the analysis of rotational signatures, and so, are plausible candidates for the detection by the JWST. Benzonitrile considered in this work represents a suitable example for the validation of a computational strategy, which can be further applied for different, larger, and not-yet observed molecules. For this purpose, anharmonic simulations of infrared (IR) spectra have been compared with recent FTIR experimental studies. The anharmonic computations using the generalized second-order vibrational perturbation theory (GVPT2) in conjunction with a hybrid force field combining the harmonic part of revDSD-PBEP86-D3/jun-cc-pVTZ with anharmonic corrections from B3LYP-D3/SNSD show very good agreement with those in the experiment, with a mean error of 11cm^{-1} for all fundamental transitions overall and only 2cm^{-1} for the $\text{C} \equiv \text{N}$ stretching fundamental at $4.49\ \mu\text{m}$. The inclusion of overtones up to three-quanta transitions also allowed the prediction of spectra in the near-infrared region, which shows distinct features due to $\text{C} \equiv \text{N}$ overtones at the $2.26\ \mu\text{m}$ and $1.52\ \mu\text{m}$. The remarkable accuracy of the GVPT2 results opens a pathway for the reliable prediction of spectra for a broader range of cyano-astroCOMs.

Słowa kluczowe

vibrational spectra, density functional theory, second-order vibrational perturbation theory, near-infrared, James Webb Space Telescope

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