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Abstracts

A quantum chemical investigation of electro-optical properties and spectroscopic features of propargylimine

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Propargylimine (HC≡CH–CH=NH), detected toward the Galactic Center molecular cloud G+0.693–0.027, is a potential a nitrogen-bearing 3C-atom species in prebiotic chemistry. In this study, we present a comprehensive computational investigation of its thermodynamics, reaction mechanism, electro-optical properties, global reactivity descriptors, and vibrational spectroscopic signatures. The formation of Z and E conformers of propargylimine was explored through radical–radical association pathway in the gas phase using density functional theory (DFT) (M06-2X/aug-cc-pVTZ), and benchmarked with CCSD(T)/aug-cc-pVTZ single-point calculations. Thermodynamic parameters, electro-optical properties, global reactivity descriptors, and molecular electrostatic potential surfaces were evaluated to assess its chemical stability and detectability. The simulated infrared spectrum provides characteristic vibrational markers, particularly the C=N stretch at 1691.9 cm−1 and N–H stretching bands (∼3430–3447 cm−1), which may facilitate astronomical identification. UV absorption features and the electronic absorption properties of propargylimine were investigated using time-dependent (TD)-DFT. This work offers a theoretical framework for understanding its formation and spectroscopic features, reinforcing its role as a chemically robust molecule in the nitrogen-bearing chemistry and molecular complexity in Galactic Center molecular clouds.

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Hyperfine-Resolved Rovibrational and Rotational Spectroscopy of OH + (3Sigma+)

Weslley G. D. P. Silva, Lea Schneider, Urs U. Graf, Holger S. P. Müller, Pavol Jusko, Arshia M. Jacob, Dominik Riechers, Stephan Schlemmer, Oskar Asvany

The OH+ (3Sigma+) radical cation has been investigated by combining a 4 K 22-pole ion trap apparatus with high-resolution IR and THz radiation sources. Applying different types of action spectroscopic methods, the fundamental vibrational band in the 3 mum range and the spin manifold of the 1 - 0 rotational transition around 1 THz have been extended and refined. Additionally, the spin manifold of the 2 - 1 rotational transition, scattered around 2 THz, has been measured for the first time with microwave accuracy. Although all hyperfine components of the pure rotational transitions are affected by considerable Zeeman splittings, a simulation of their contours allowed us to extract the field-free center frequencies with high accuracy. A global fit combining rovibrational and pure rotational transitions from the literature with those newly obtained in this work was performed, leading to improvements in the spectroscopic constants of OH+, particularly those in the ground vibrational state.

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TMC-1: probing the onset of chemical complexity in space

Marcelino Agundez, Jose Cernicharo

In recent years, the obsessive interest in the observation of TMC-1 has brought a boost in our knowledge of the chemistry of cold dark clouds. The number of molecules detected in this particular cloud has been more than doubled. Two observational programmes, GOTHAM and QUIJOTE, are responsible for this spectacular achievement. Here we provide an overall view of QUIJOTE, which is a line survey carried out in the Q band (31-50 GHz) with the Yebes 40m radiotelescope, summarize the actual observational status of TMC-1, and discuss the chemistry of this remarkable source. We highlight the successes and failures of state-of-the-art chemical models to describe its chemical composition, with a particular emphasis on the origin of PAHs, which is yet far from being understood.

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