

INSIGHTS INTO THE INFRARED SPECTRUM OF A PREBIOTIC SPECIES: THE CASE OF AMINOACETONITRILE

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Aminoacetonitrile is an interstellar molecule with a prominent prebiotic role, already detected in the chemically-rich molecular cloud Sagittarius B2(N) and postulated to be present in the atmosphere of the largest Saturn's moon, Titan. To further support its observation in such remote environments and laboratory experiments aimed at improving our understanding of interstellar chemistry, we report a thorough spectroscopic characterization of aminoacetonitrile. Fundamental bands as well as spectroscopic and molecular parameters have been accurately computed by exploiting a composite scheme rooted in the coupled-cluster theory that accounts for the extrapolation to the complete basis set limit and core-correlation effects. From the experimental side, we report the analysis of the three strongest fundamental bands of aminoacetonitrile observed between 500 and 1000 cm^{-1} in high-resolution infrared spectra. More generally, all computed band positions are in excellent agreement with the present and previous experiments. The only exception is the ν_{15} band, for which we provide a revision of the experimental assignment, now in good agreement with theory.