# ACCURATE SPECTROSCOPIC CHARACTERIZATION OF UNSATURATED CARBON-CHAINS OF ASTROCHEMICAL IMPORTANCE

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The molecular universe of Astrochemistry is expanding at a surprisingly rapid pace. However, to univocally identify the transitions of the studied molecule within an astronomcial survey –which are, typically, densely packed with lines– an extremely accurate knowledge of the rotational frequencies is required. Therefore, an accurate spectroscopic characterization of *E*- and *Z*-cyanovinylacetylene (CVA), allenylacetylene (AA) and propadienone (PD) has been carried out to guide their detection in the interstellar medium. An eventual first detection, as it would be for PD and *Z*-CVA, as well as new findings (on *E*-CVA and AA, which have been recently identified in TMC-1) in different astronomical regions, can be of great help in the refining of the models of the interstellar objects. Indeed, PD is the only isomer of the $[H_2C_3O]$ family which has not been observed in the ISM, while unsaturated carbon chains like CVA and AA can play important roles in reactivity, e.g., the pathways leading to the formation of aromatic molecules.

In this work, we relied on a solid computational study to complete the experimental data available in literature. The accurate equilibrium geometries of the four species have been determined, exploiting composite schemes rooted in the coupled-cluster theory. Harmonic and anharmonic force field calculations gave access to the set of centrifugal distortion parameters; the importance of an accurate estimate of the sextic ones is presented. Exploiting a pyrolysis system to generate the four species in the gas-phase and using a frequency-modulation spectrometer working in the millimeter/sub-millimeter wave range, we were able to record and analyze the rotational spectrum up to 400 GHz, providing accurate rotational frequencies and a thorough characterization of the spectroscopic parameters.