

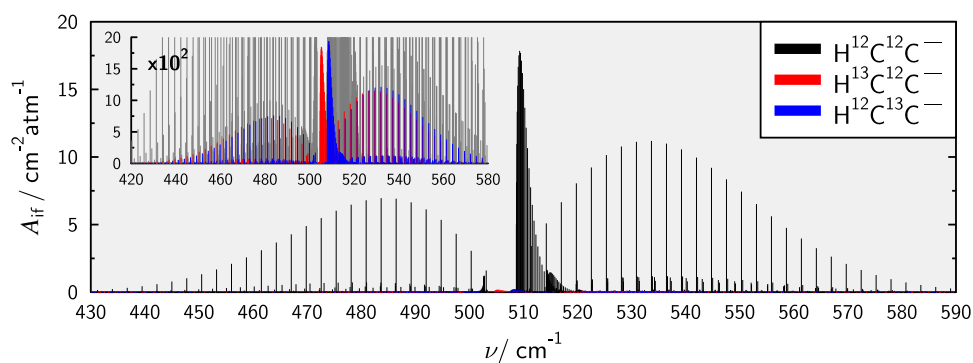
## AB INITIO ROVIBRATIONAL SPECTROSCOPY OF THE ACETYLIDE ANION

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The linear chains of type  $C_{2n}H^-$  are the most extensive group of interstellar anions with  $C_{10}H^-$  being detected quite recently.<sup>1</sup> In contrast, the smallest member of the series, the acetylide anion  $HCC^-$ , has not been observed so far in astronomical sources. Furthermore, experimental spectroscopic data on this fundamental ion are scarce with the ground state rotational spectrum being the only high-resolution result.<sup>2,3</sup>

This contribution tries to fill this gap and provide a thorough theoretical investigation of the rovibrational spectrum of the acetylide anion  $HCC^-$  based on high-level electronic structure methods and variational rovibrational calculations. The potential energy surface and dipole moment surface are constructed from a well established composite procedure that combines explicitly correlated coupled cluster calculations with corrections due to core-valence correlation, scalar relativistic effects, and higher-order excitation effects to converge the description of the potential energy and dipole moment.

Accurate spectroscopic parameters determined from variational calculations are presented. In comparison to the few available reference data the present results show excellent agreement with ground state rotational constants within 0.005 % of the experimental value. Intensities determined from the variational calculations suggest the bending fundamental transition  $\nu_2$  around  $510\text{ cm}^{-1}$  to be the best target for detection (see spectrum below). The rather weak CD stretching fundamental  $\nu_1$  in deuterated isotopologues shows a second-order resonance with the  $(0, 2^0, 1)$  state and the consequences are discussed in some detail.



<sup>1</sup>[doi:10.3847/2041-8213/acb648](https://doi.org/10.3847/2041-8213/acb648), A. Remijan *et al.*, *Astrophys. J. Lett.*, **994**, L45 (2023).

<sup>2</sup>[doi:10.1051/0004-6361/20066964](https://doi.org/10.1051/0004-6361/20066964), S. Brünken *et al.*, *Astron. Astrophys.*, **464**, L33 (2007).

<sup>3</sup>[doi:10.1063/1.3043739](https://doi.org/10.1063/1.3043739), T. Amano, *J. Chem. Phys.*, **129**, 244305 (2008).