

VIBRATIONAL AND ROTATIONAL ACTION SPECTROSCOPY OF $\text{H}_2\text{C}_3\text{H}^+$

WESLLEY G. D. P. SILVA, DIVITA GUPTA, *I. Physikalisches Institut, Universität zu Köln, Köln, Germany*; JOSÉ LUIS DOMÉNECH, *Instituto de Estructura de la Materia, (IEM-CSIC), Madrid, Spain*; ELINE PLAAR, STEPHAN SCHLEMMER, OSKAR ASVANY, *I. Physikalisches Institut, Universität zu Köln, Köln, Germany*.

The high-resolution rovibrational and pure rotational spectra of $\text{H}_2\text{C}_3\text{H}^+$ are reported here for the first time. The spectra were collected in a 4K 22-pole cryogenic ion trap (COLTRAP) instrument using the novel leak-out spectroscopy (LOS) method.^a Rovibrational signatures within the fundamental ν_1 (C-H stretch) and the combination $\nu_3+\nu_5$ (C-C stretches) bands were detected in the 3 μm spectral region using a continuous wave optical parametric oscillator and were successfully assigned, aided by previous theoretical calculations.^b These observations allowed accurate spectroscopic constants for the ground and vibrationally excited states to be determined. Significant differences were observed in the values of the rotational constant A , which decreases by about 2.7% and 5.0% in the ν_1 and $\nu_3+\nu_5$ bands, respectively, in comparison to ν_0 . By analyzing the changes in A , information about the molecular structure of $\text{H}_2\text{C}_3\text{H}^+$ upon excitation of the C-H and C-C stretches was obtained, which indicates that the HCH angle may have an increase of approximately 3° in ν_1 and 6° in $\nu_3+\nu_5$. Guided by the ground state constants obtained from the infrared (IR) measurements, 14 pure rotational lines were observed in the 90-200 GHz frequency range using a double resonance scheme, in which the ions are excited simultaneously by the IR and a mm-wave radiation. These rotational measurements allowed even more accurate ground state spectroscopic parameters to be determined and open up the possibility for the first (radio)astronomical search of $\text{H}_2\text{C}_3\text{H}^+$ in the interstellar medium. Finally, the capability of the novel LOS method in isolating isomers in the ion trap will be discussed with a focus on the abundances of $\text{H}_2\text{C}_3\text{H}^+$ and its cyclic sibling, $c\text{-C}_3\text{H}_3^+$.

^aSchmid, P. C., Asvany, O., Salomon, T., Thorwirth, S., and Schlemmer, S. 2022, *J. Phys. Chem. A*, 126, 8111.

^bHuang, X., Taylor, P. R., and Lee, T. J. 2011, *The Journal of Physical Chemistry A*, 115, 5005.