

THE ROTATIONAL SPECTRUM OF PROTONATED ETHYL CYANIDE

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Ethyl cyanide ($\text{CH}_3\text{CH}_2\text{CN}$) is a well-known constituent of interstellar clouds and has recently been detected in the atmosphere of Titan.^a It is so abundant in some interstellar clouds that its doubly substituted carbon-13 isotopologues, as well as highly excited vibrational satellites have been detected there.^b Because of the high abundance and high proton affinity of $\text{CH}_3\text{CH}_2\text{CN}$, protonated ethyl cyanide ($\text{CH}_3\text{CH}_2\text{CNH}^+$) is a plausible intermediate in the chemistry of interstellar clouds and planetary atmospheres. Here we report the detection of $\text{CH}_3\text{CH}_2\text{CNH}^+$ by Fourier transform microwave spectroscopy of a supersonic molecular beam. Thirteen *a*-type rotational transitions have been observed between 8 and 44 GHz, some with partially resolved nitrogen hyperfine structure. This data set allows determination of all three rotational constants, as well as several of the leading centrifugal distortion constants to high accuracy. The derived rotational constants and those calculated at the CCSD(T) level of theory agree to better than 0.2%. Nitrogen hyperfine structure in the lower rotational transitions is so compact that only the quadrupole coupling tensor element along the *a*-inertial axis (χ_{aa}) could be determined. With accurate laboratory data in hand, a radio astronomical search for $\text{CH}_3\text{CH}_2\text{CNH}^+$ in publicly available spectral line surveys as well as through dedicated observations can now be undertaken with high confidence.

^aCordiner, M. A., Palmer, M. Y., Nixon, C. A. et al. 2015, ApJL, 800, L14.

^bMargulès, L., Belloche, A., Müller, H. S. P. et al. 2016, A&A, 590, A93 and references therein.