ANALYSIS OF THE LOWEST IN-PLANE BEND AND FIRST EXCITED TORSIONAL STATE OF CH_3CH_2CN[a]

CAROLYN S. BRAUER, JOHN C. PEARSON, BRIAN J. DROUIN, SHANSHAN YU, *JET PROPULSION LABORATORY, CALIFORNIA INSTITUTE OF TECHNOLOGY, 4800 OAK GROVE DR., PASADENA, CA 91109*.

Propionitrile (CH_3CH_2CN) is observed with large column densities in a number of high-mass star-forming cores, where core temperatures exceed 200 K. It is a near-prolate ($\kappa = 0.96$) asymmetric top with appreciable dipole moment components on both the $a-$ and $b-$axes ($\mu_a = 3.84$ D, $\mu_b = 1.23$ D).[a] This, combined with the presence of four fundamental modes as well as four overtones and combination bands all occurring below 600 cm^{-1}, results in a very rich spectrum. It is known to be a major contributor to spectral line confusion in ground-based observations and is expected to complicate observations by Herschel, SOFIA and ALMA, making it imperative to fully characterize the entire spectrum. The lowest in-plane bend, ν_{13}, is 206.9(0.5) cm^{-1},[b] and the first excited torsional state, ν_{21}, which is just 186 GHz above, have been detected in hot cores with antenna temperatures of a few Kelvin.[c] The close proximity of ν_{13} and ν_{21}, as well as their low-lying nature, offers a unique opportunity to study the vibration-torsion-rotation coupling problem in the case of two nearly degenerate vibrational states. As expected from C_s symmetry and their A' and A'' nature, these states exhibit strong $a-$ and $b-$symmetry Coriolis interactions, as well as interactions resulting from different sets of Eckhart-Sayvetz conditions being required in ν_{13} and ν_{21}. In the present work, the ν_{13} and ν_{21} states of propionitrile have been analyzed to high frequency and angular momentum quantum number. The spectrum, molecular constants,and insights into the vibration-torsion-rotation problem will be discussed.

[a]Research described in this paper was performed at the Jet Propulsion Laboratory, California Institute of Technology, under contracts and cooperative agreements with the National Aeronautics and Space Administration.

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