

ANALYSIS OF THE LOWEST IN-PLANE BEND AND FIRST EXCITED TORSIONAL STATE OF CH₃CH₂CN^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 (CH₃CH₂CN) 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.

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