THE SUBMILLIMETER SPECTRUM OF CH_3CH_2CN IN ITS GROUND VIBRATIONAL STATE[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 routinely observed with large column densities and at surprisingly high temperatures in hot core sources. The development of new, more sensitive observatories such as Herschel, ALMA and SOFIA have made it important to extend the laboratory data for propionitrile to coincide with the capabilities of the new instruments. In the present work, the laboratory measurements of the rotational spectrum of propionitrile have been extended to 1.6 THz. A global analysis of 4606 ground state transitions, which includes 2159 newly assigned transitions, has been fit to within experimental error to $J = 138$, $K = 45$, using both Watson $A-$reduced and Watson $S-$reduced Hamiltonians. The newly assigned transitions are primarily $b-$type, high K and very high J asymmetry split ^aR-branch transitions. The derived constants show a decided advantage of the Watson $S-$reduction in the analysis of this near-prolate ($\kappa = 0.96$) asymmetric top. The spectrum and molecular constants will be presented.

[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.