

ANALYSIS OF THE CORIOLIS- AND FERMI-COUPLED TRIAD NEAR 315 cm^{-1} OF BENZONITRILE ($\text{C}_6\text{H}_5\text{CN}$)

MARIA ZDANOVSKAIA, BRIAN J. ESSELMAN, R. CLAUDE WOODS, ROBERT J. McMAHON, *Department of Chemistry, University of Wisconsin-Madison, Madison, WI, USA*; ZBIGNIEW KISIEL, *ON2, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland*.

We previously presented the least-squares fit of the benzonitrile ($\text{C}_6\text{H}_5\text{CN}$, C_{2v} , $\mu_a = 4.5\text{ D}$) ground vibrational state, which was fit to a partial octic Hamiltonian, as well as the first analysis of its two Coriolis-coupled, lowest-energy fundamental states, ν_{22} and ν_{33} .¹ Herein, we present the continuation of this work: the analysis and fitting of the Coriolis- and Fermi-coupled triad of the overtone and combination states ($\nu_{22} = 2$, $\nu_{33} = 2$, and $\nu_{22} + \nu_{33}$) near 315 cm^{-1} . Approximately 3000 transitions are assigned for each state, including multiple resonances, and their least-squares fitting results in precise energy separations that are in agreement with those expected based on the energy separation determined for ν_{22} and ν_{33} .

1. Zdanovskaia, M. A.; Esselman, B. J.; Lau, H. S.; Bates, D. M.; Woods, R. C.; McMahon, R. J.; Kisiel, Z. The 103 - 360 GHz Rotational Spectrum of Benzonitrile, the First Interstellar Benzene Derivative Detected by Radioastronomy. *J.Mol.Spectrosc.* **2018**, 351, 39-48.