

MILLIMETER-WAVE SPECTRUM OF THE LOWEST ENERGY, VIBRATIONALLY EXCITED COUPLED DYAD OF *S-TRANS-Z-1-CYANO-1,3-BUTADIENE*

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Recently, the ground state spectroscopic constants of three cyanobutadiene isomers (C_5H_5N) were reported as plausible targets for detection in the interstellar medium.¹ Many hundreds of transitions were collected in the 130 – 375 GHz range for each isomer, but *s-trans-Z-1-cyano-1,3-butadiene* is the only isomer with an isolated ground state. *s-trans-Z-1-Cyano-1,3-butadiene* ($\mu_a = 3.6$ D, $\mu_b = 2.3$ D, MP2/6-311+G(2d,p) is a prolate ($\kappa = -0.91$), asymmetric top with C_s symmetry, and its ground state was fit to a partial octic, distorted rotor Hamiltonian model with over 5500 distinct transitions. The lowest-energy vibrationally excited state (ν_{19} , B_1) is predicted to be 129 cm^{-1} higher in energy than the ground state and is close in energy to the second-lowest energy vibrationally excited state (ν_{27} , B_2 , 135 cm^{-1} , MP2/6-311+G(2d,p)). These states form a Coriolis coupled dyad with intense coupling along the *a*- and *b*- principal axes causing the formation of sharp local resonances hundreds of MHz away from their unperturbed predicted frequencies. This presentation will detail the effects of strong Coriolis coupling in a dyad of vibrational states $< 6\text{ cm}^{-1}$ apart and the strategies used to assign and least-squares fit these transitions.

1. Zdanovskaia, M. A.; Dorman, P. M.; Orr, V. L.; Owen, A. N.; Kougiyas, S. M.; Esselman, B. J.; Woods, R. C.; McMahon, R. J. Rotational Spectra of Three Cyanobutadiene Isomers (C_5H_5N) of Relevance to Astrochemistry and Other Harsh Reaction Environments. *J. Am Chem. Soc.* **2021**, *143*, 9551-9564.