THE 130 - 360 GHZ ROTATIONAL SPECTRUM OF 2-CYANO-1,3-BUTADIENE IN ITS GROUND VIBRATIONAL STATE AND CORIOLIS-COUPLED DYAD

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Nitriles are of interest to the astrochemical community due to their prevalence in the interstellar medium, their possible link to polyaromatic nitrogen heterocycles and prebiotic molecules, and their frequently strong dipole moments and consequent detectability. We have recently prepared four cyanobutadiene isomers of pyridine, E-1-cyano-1,3-butadiene, Z-1-cyano-1,3-butadiene, 1-cyano-2,3-butadiene, and 2-cyano-1,3-butadiene. Herein, we present the first analysis of the rotational spectrum of 2-cyano-1,3-butadiene (C_5H_5N, μ_a = 3.2 D, μ_b = 2.3 D), including over 4000 transitions from the 130 - 360 GHz frequency region least-squares fit using an octic Hamiltonian. The resulting spectroscopic constants and measured transitions will enable the first radioastronomical search for this species in the interstellar medium. We also present the analysis of the Corioils-coupled dyad of its two lowest-energy fundamental vibrational states (ν_{27} and ν_{19}), which includes over 3200 transitions for each state. The coupling results in remarkably intense a-type and b-type resonances and nominal interstate transitions, and the analysis results in a highly precise determination of the energy separation between the two states.