

THE ROTATIONAL ANALYSIS OF 2-CYANOPYRIMIDINE ($C_5H_3N_3$) IN ITS GROUND VIBRATIONAL STATE AND THE DYAD OF ITS LOWEST-ENERGY VIBRATIONALLY EXCITED STATES, ν_{18} AND ν_{27}

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2-Cyanopyrimidine is an attractive molecule for interstellar detection via radioastronomy because it is the pyrimidine analog of the detected interstellar molecule, benzonitrile, and has a substantial dipole moment ($\mu_a = 6.47$ D). In the present work, we have analyzed and assigned the rotational spectrum of 2-cyanopyrimidine ($C_5H_3N_3$) for the first time. Using data in the 130 – 360 GHz frequency region, the vibrational ground state of 2-cyanopyrimidine has been least-squares fit to a partial octic, distorted-rotor Hamiltonian ($N_{lines} \sim 3400$, $\sigma = 40$ kHz). The resulting spectroscopic constants are sufficient for spectral prediction outside of the studied frequency range and enable, for the first time, radioastronomical search for this molecule. Work currently continues on the Coriolis-coupled dyad of the two lowest-energy vibrationally excited states, ν_{18} and ν_{27} . In the present least-squares fit, approximately 2,500 transitions have been assigned for each state. The complete analysis of these states is expected to yield a highly precise energy separation between ν_{18} and ν_{27} , along with interesting comparison to the analogous dyads of benzonitrile and the cyanopyridines.