

ROTATIONAL AND INFRARED SPECTRA OF PYRIMIDINE: VIBRATIONAL GROUND STATE AND NINE VIBRATIONALLY EXCITED STATES

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Pyrimidine is an aromatic heterocycle in which meta C-H units of benzene are replaced by nitrogen atoms. Its detection in the ISM has been sought for decades as it is not only a building block of many biologically relevant molecules, but it could serve as a valuable tracer molecule for other aromatic and polycyclic aromatic compounds. In this work, we collected the millimeter-wave spectrum of pyrimidine from 130-750 GHz. This extended range greatly increases the range of rotational transitions we can observe in the ground and its nine lowest-energy vibrationally excited states. Over 10,000 transitions for the vibrational ground state have been least-squares fit to a A- and S-reduced sextic distorted-rotor Hamiltonians. To supplement the millimeter-wave spectrum, high-resolution infrared spectra were obtained from the Canadian Light Source and provide highly accurate and precise band origins for the vibrationally excited states. The three lowest energy fundamentals (ν_{16} , ν_{11} , and ν_{24}) have been fit to single-state Hamiltonians. The remaining vibrationally excited states presented in this work have perturbed frequencies due to Coriolis, Darling-Dennison, and Fermi coupling. The current progress toward a satisfactory treatment of these interactions will be presented.