A COMBINED mm-WAVE AND FAR-INFRARED STUDY OF PYRAZOLE

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Pyrazole ($C_3H_3N_2$, C_s) is an aromatic heterocycle consisting of a 5-membered ring molecule doubly substituted with adjacent nitrogen atoms. Searches for similar heteroaromatic compounds (imidazole, furan, etc.) have been recently conducted in the interstellar medium. This study provides the necessary transition frequencies for a search for pyrazole across the frequency range of available radiotelescopes. We have collected the mm-wave spectrum of pyrazole from 130-750 MHz, which extends the previously published microwave studies from 13 to 35 MHz. The new data greatly expand the range of rotational quantum numbers observed in the ground vibrational state rotational transitions and provide transitions for over a dozen excited vibrational states. These rotational data are simultaneously analyzed with high-resolution rotation-vibration spectra of pyrazole between 500-1300 cm⁻¹ that we have obtained at the Canadian Light Source synchrotron's far-infrared beam line. The considerable benefits of simultaneously analyzing mm-wave and high-res IR transitions that cover the same approximate ranges of J and K will be discussed. The results provide a thorough characterization of all eight vibrationally excited states below 950 cm⁻¹, of which the highest energy states (ν_{16} , ν_{15} , and ν_{14}) form a Coriolis-coupled triad.