MILLIMETER WAVE SPECTROSCOPY AND EQUILIBRIUM STRUCTURE DETERMINATION OF PYRIMIDINE (*m*-$C_4H_4N_2$)

ZACHARY N. HEIM, BRENT K. AMBERGER, BRIAN J. ESSELMAN, R. CLAUDE WOODS, ROBERT J. McMAHON, *Department of Chemistry, The Univeristy of Wisconsin, Madison, WI, USA*.

Pyrimidine, the *meta* substituted dinitrogen analog of benzene, has been studied in the mm-wave region from 260 – 360 GHz, expanding on previous studies up to 337 GHz.[abc] The spectra of all four of the singly-substituted ^{13}C and ^{15}N isotopologues were observed in natural abundance. Samples of deuterium enriched pyrimidine were synthesized, giving access to several deuterium-substituted isotopologues. The experimental rotational constants have been corrected for vibration-rotation coupling and electron mass. The vibration-rotation corrections were calculated with an anharmonic frequency calculation at the CCSD[T]/ANO1 level using CFOUR. An equilibrium structure determination has been performed using the corrected rotational constants with the xrefit module of CFOUR. Several vibrational satellites of pyrimidine have also been studied. Their rotational constants have been compared to those obtained computationally.

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