

MILLIMETER-WAVE SPECTROSCOPY OF PHENYL ISOCYANATE

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Phenyl isocyanate (PhNCO) has been studied in the frequency range of 250-360 GHz, improving on rotational and centrifugal distortion constants based on previous spectroscopic studies between 4.7 and 40 GHz.^{ab} Using the rigid rotor/centrifugal distortion model, many transitions have been assigned for the ground state (approximately 2200 transitions) and the fundamental of the -NCO torsional vibration (approximately 1500 transitions) for J values ranging between 140 and 210 and $K_{prolate}$ values from 0 to 42. Beyond these K values, these two spectra show effects of perturbations with other vibrational states. Vibrational energy levels and vibration-rotation interaction constants were predicted using CFOUR at the CCSD(T)/ANO0 level. The two lowest energy excited vibrational modes are predicted to have energies of 47 cm^{-1} (-NCO torsion) and 95 cm^{-1} (in-plane -NCO wag). Fermi resonance between the first overtone of the -NCO torsional vibration (94 cm^{-1}) and the fundamental of the in-plane -NCO wag has been observed in the spectra of these two states. Analysis for vibrationally excited states up to 190 cm^{-1} is in progress.

^aA. Bouchy and G. Roussy, *Journal of Molecular Spectroscopy*, **65** (1977), 395-404.

^bW. Kasten and H. Dreizler, *Z. Naturforsch.* **42a** (1987), 79-82.