

## THE LOWEST VIBRATIONAL STATES OF UREA FROM THE ROTATIONAL SPECTRUM

ZBIGNIEW KISIEL, *ON2, Institute of Physics, Polish Academy of Sciences, Warszawa, Poland*; JESSICA THOMAS, IVAN MEDVEDEV, *Department of Physics, Wright State University, Dayton, OH, USA*.

The urea molecule,  $(\text{NH}_2)_2\text{CO}$ , has a complex potential energy surface resulting from a combination of the  $\text{NH}_2$  torsion and  $\text{NH}_2$  inversion motions. This leads to a distribution of lowest vibrational states that is expected to be significantly different from the more familiar picture from simple inversion or normal mode models.<sup>a,b</sup>

The broadband 207-500 GHz spectrum of urea recorded in Dayton has signal to noise sufficient for assignment of rotational transitions in excited vibrational states up to at least  $500\text{ cm}^{-1}$ . In addition to the previously reported analysis of the ground and the lowest excited state we have been able to assign transitions in at least five other excited vibrational states. Strongly perturbed transitions in a close doublet of such states have been fitted to within experimental accuracy with a coupled fit and a splitting in the region of  $1\text{ cm}^{-1}$ . These assignments combined with vibrational energy estimates from relative intensity measurements allow for empirical discrimination between different models for the energy level manifestation of the large amplitude motions in urea.<sup>b</sup>

---

<sup>a</sup>P.D.Godfrey, R.D.Brown, A.N.Hunter *J. Mol. Struct.*, **413-414**, 405-414 (1997).

<sup>b</sup>N.Inostroza, M.L.Senent, *Chem. Phys. Lett.*, **524**, 25 (2012).