INTERNAL ROTATION OF ARGON ACETONE

LU KANG, ALISON R. KEIMOWITZ, MICHAELEEN R. MUNROW, and STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*.

The microwave spectrum of the weakly-bound complex argon acetone was measured by Fourier transform microwave spectroscopy. A preliminary version of this work was reported at this conference in 1997[a]. The torsional state splittings caused by the two internal methyl rotors varies from several kHz to tens of MHz. The spectra was analyzed using a modified *iam* method [b]. More than 200 transitions were recorded between 6 GHz and 20 GHz. Additional fine splittings beyond those caused by the internal rotations have been observed. An approximate "sum rule" for the various torsional splittings was very helpful for the initial assignments[c]. The rotational constants for the complex are A = 4991.808(1), B = 1442.432(1), and C = 1401.040(1) MHz. The argon atom is above the C=O bond, perpendicular to the plane of the acetone, at a distance of $\sim$3.48 $\mathring{A}$. The barrier to internal rotation $V_3 \sim 260$ cm^{-1}, is similar to that of acetone itself ($V_3 = 266$ cm^{-1}) [d].

[a] A. R. Keimowitz, M. R. Munrow, and S. E. Novick, *International Symposium on Molecular Spectroscopy*, talk TB11, (1997)
[b] H. Hartwig, *program XIAM*, private communication
[c] R. Nelson, and L. Pierce, *J. Mol. Spectrosc.* **18**, 344, (1965)
[d] J. M. Vacherand, B. P. Van Eijck, J. Burie, and J. Demaison, *J. Mol. Spectrosc.* **118**, 355, (1986)