THE MICROWAVE SPECTRUM OF ARGON-TROPOLONE

WEI LIN, WALLACE C. PRINGLE, STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*; THOMAS A. BLAKE, *Pacific Northwest National Laboratory, P. O. Box 999, Mail Stop K8-88, Richland, WA 99352 (PNNL is operated for the US Department of Energy by the Battelle Memorial Institute under contract DE-AC05-76RLO 1830).*

Using a pulsed jet Fourier transform microwave spectrometer we have recorded the rotational spectrum of the argon-tropolone van der Waals complex between 6 and 17 GHz. Eighty-six transitions were observed (29 a-type and 57 b-type) with J'' values ranging from 2 to 8 and maximum K_a'' and K_c'' values of 5 and 8, respectively. The transitions were fit with a Watson A-reduction Hamiltonian in a I^r representation using the SPFIT program[a]. The fit ground state constants for argon-tropolone are $A = 1080.4365(3)$ MHz, $B = 883.4943(3)$ MHz, $C = 749.0571(2)$ MHz, $\Delta_J = 2.591(2)$ kHz, $\Delta_{JK} = -3.32(1)$ kHz, $\Delta_K = 5.232(9)$ kHz, $\delta_J = 0.944(1)$ kHz, $\delta_K = -0.028(8)$ kHz. The rms error for the transition set in the fit is 4 kHz. When included in the Hamiltonian, the tunneling - rotation interaction term, $F(J_a J_b + J_b J_a)$, did not improve the quality of the fit: proton tunneling in the complex appears to be quenched. The argon coordinates in the principal axis system of tropolone monomer are $a = 0.43$ Å, $b = 0.23$ Å, and $c = 3.48$ Å.

[a] H. M. Pickett, R. L. Poynter, E. A. Cohen, M. L. Delitsky, J. C. Pearson and H. S. P. Muller *J. Quant. Spectrosc. Radiat. Transfer* **60**, 883 (1998).