THE MICROWAVE SPECTRUM OF ARGON-TROPOLONE

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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, $F(J_aJ_b+J_bJ_a)$, 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.

^aH. 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).