FT MICROWAVE STRUCTURE AND NUCLEAR QUADRUPOLE COUPLING ANALYSIS OF SIX ISOTOPOMERS OF THE ARGON-CHLOROCYCLOBUTANE VAN DER WAALS COMPLEX

RANGA SUBRAMANIAN, STEWART E. NOVICK AND W. C. PRINGLE, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*; J. M. SZARKO, *Department of Chemistry and Biochemistry, University of Colorado, Boulder CO 80309*.

The Fourier Transform Pulsed Jet Microwave spectra of the argon-chlorocyclobutane van der Waals complex has been assigned for six isotopomers including the ^{35}Cl and ^{37}Cl all ^{12}C plus each of the four ^{13}C for the ^{35}Cl. The spectroscopic constants for the ^{35}Cl all ^{12}C complex are A = 2675.264, B = 977. 830, C = 764.938 MHz, Δ_J = 1.73, Δ_{JK} = 7.18, Δ_K = 15.3, δ_J = 0.41, δ_K = 6.6 kHz, χ_{aa} = 28.0, (χ_{bb} - χ_{cc}) = -80.4, χ_{ab} = -22.9, χ_{ac} = 5.3 and χ_{bc} = 26.4 MHz. The structure of the complex has an equatorial chlorine as in the non-complexed ring and the argon coordinates are a = 1.3, b = 2.8 and c = 2.5 Å in the principal axis system of the monomer ring. The chlorine coordinates in this axis system are 1.66, 0.00 and .092 Å respectively. The quadrupole tensor for the chlorine in the complex was fit including all 3 off diagonal moments and this is approximately equal to the tensor generated by projection of the chlorine quadrupole moment that is axially symmetric about the C-Cl bond onto the complex axis system. The argon position is also consistent with the observation and intensities of a, b, and c-type rotational transitions. Large amplitude motion of the argon across the ring that was observed in the cyclobutanone complex is not observed in this complex and is reflected in these smaller centrifugal distortion constants.