DETERMINATION OF THE STRUCTURES OF METHYLENE CYCLOBUTANE AND OF THE ARGON METHYLENE CYCLOBUTANE COMPLEX

WEI LIN, JOVAN A. GAYLE, WALLACE C. PRINGLE, and STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*.

The rotation-inversion spectra of five carbon isotopomers of methylene cyclobutane in and between the ground and first vibrational states of the ring-puckering mode have been measured in the frequency range of 5-26 GHz. Ten *c*-type transitions between the v = 0 and v = 1 states of methylene cyclobutane were measured for the first time by pulsed jet Fourier transform microwave spectroscopy. The direct observation of the inversion transitions improves the measurement accuracy of the inversion frequency: ΔE_{01} = 33615.53(4) MHz. The molecular structure of methylene cyclobutane was determined from the rotational constants of the normal and singly-^{13}C substituted isotopomers which were measured for the first time. In addition, the rotational spectrum was measured and assigned for the normal and the four ^{13}C isotopomers of the weakly bound complex, argon methylene cyclobutane. The rotational constants for the all ^{12}C isotopomer of argon methylene cyclobutane, Ar C_5H_8, are A = 3484.0660(4), B = 1308.0501(4), and C = 1127.9153(3) MHz. The structure of Ar C_5H_8 has been determined, and the coordinates of the argon in the C_5H_8 principal axis systems are a = 0.11, b = 0.51, and c = 3.62 Å. The position of the argon atom is shifted $\frac{1}{2}$ Å from the plane of symmetry of methylene cyclobutane due to the large amplitude motion of argon across the ring.