ASYMMETRY IN THE ARGON CYCLOBUTANONE VAN DER WAALS COMPLEX AS DETERMINED BY CARBON-13 ISOTOPIC SUBSTITUTION

MICHAELEEN R. MUNROW, WALLACE C. PRINGLE, and STEWART E. NOVICK, *Department of Chemistry, Wesleyan University, Middletown, CT 06459*.

We previously showed (OSU 1996 Mol. Spect. Sym. Talk – TD 10) that the position of argon in the van der Waals complex of argon cyclobutanone has coordinates of a = 0.2 A, b = 0.5 A, c = 3.5 A, measured in the principle axis system of the monomer, cyclobutanone. Since the "a" axis of the monomer lies along the carbonyl bond, the argon is 0.5 A to the side of the monomer symmetry plane, which is perpendicular to the ring plane. This non-zero coordinate could be the result of large amplitude motion of the argon above the ring or could be a potential minimum with a barrier to argon being in that plane. If the former were true, there would be only three monosubstituted isotopomers with the isotopomer for the carbon adjacent to the carbonyl having a 2 percent abundance. We report here the Fourier transform microwave spectra and assignment of the four different mono-carbon-13 isotopomers which were observed in natural abundance. The fact that two isotopomers exist with different moments of inertia for the substitution of the carbon closer to and farther away from the argon shows that there is a potential barrier for the argon in the plane perpendicular to the ring plane. The ring is also no longer planar in the van der Waals complex.