DETERMINATION OF THE STRUCTURE OF METHYLENE CYCLOPENTANE AND THE ARGON METHYLENE CYCLOPENTANE VAN DER WAALS COMPLEX

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Rotational spectra of methylene cyclopentane (MCP) and the argon methylene cyclopentane van der Waals complex were studied using pulsed-jet Fabry-Perot Fourier transform microwave spectroscopy. Spectra of the normal isotopologue along with those of the natural abundance ¹³C isotopologues for both the monomer and the complex were observed and assigned in the frequency region of 5-20 GHz. The substitution structure of the monomer has the two methylene carbons on the C₂ axis and the four other ring carbons confirm the twisted conformation. The two ring carbons attached to the ring methylene carbon are 0.14 Å above and 0.14 Å below the methylene plane. The two carbons at the back of the ring are 0.25 Å below and 0.25 Å above the plane of the methylene group. For the argon MCP complex, *a*- and *b*-type transitions were observed and the rotational constants were determined to be *A* = 2472.4022(4), *B* = 1088.2403(2), and *C* = 937.9203(2) MHz. The argon atom is situated 3.6 Å above the methylene group plane and 0.1 Å behind the methylene ring carbon. Additionally, the argon atom is 0.8 Å across the ring from the center of mass of MCP and is above the ring carbon that is 0.14 Å below the plane. An investigation of large amplitude cross ring motion of the argon atom as well as comparison to previous ring complexes studied in this laboratory will be presented.