DETERMINATION OF THE STRUCTURE OF CYCLOPENTANONE AND OF THE ARGON CYCLOPENTANONE VAN DER WAALS COMPLEX

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A complete heavy-atom substitutional structure has been determined for cyclopentanone, confirming the C_2 twisted structure for this five-membered ring. The rotational constants of seven isotopomers of the argon cyclopentanone van der Waals complex have been determined from the pulsed-jet Fourier transform microwave spectra. An 88-line fit of the all ^{12}C isotopomer gave rotational constants A = 2611.6695(3), B = 1112.3028(1), and C = 971.3195(1) MHz. The molecular structure was determined from the rotational constants of the normal, the five singly-substituted ^{13}C, and the ^{18}O isotopomers. The coordinates of the argon in the principal axis system of C_5H_8O are a = 0.95, b = 0.80, and c = 3.46 Å, where the carbonyl bond lies along the a-axis and the oxygen atom position is a = 2.05 Å.