FOURIER TRANSFORM INFRARED SPECTRAL INVESTIGATION OF THE ν_6 BAND OF CYCLIC-C_3H_2

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The gas phase absorption spectrum of the ν_6 band (out of plane in phase CH bend) of cyclopropenylidene (c-C_3H_2) has been observed using a high-resolution Fourier transform infrared spectrometer for the first time. The molecule was produced by microwave discharge through a flow of allene (25 mTorr) and Ar (30 mTorr) mixture inside a glass cell. The observed spectrum shows c-type ro-vibrational transitions in which the Q-branch lines (J values up to 34 and K_a values up to 8) are strongly and distinctly stand out in the spectrum. A least squares fitting of a total of 357 tranitions (332 ro-vibrational transitions from this work and 25 transitions from the millimeter-wave spectrum with 10^6 times larger statistical weight) results in the determination of the rotational and centrifugal distortion constants in the upper state. The rotational constants agree with those determined by millimter-wave spectrum[a] and thereby confirming the ν_6 band ($\nu_0 = 776.11729(17)$ cm^{-1}) of c-C_3H_2.

[a] R. Mollaaghababa, C. Gottlieb, J. M. Vrtilek, and P. E. Thaddeus, J. Chem. Phys. 99, 890 (1993)