ROTATIONALLY RESOLVED DIODE LASER JET SPECTRUM OF PROPADIENONE (CH_3CCO) IN THE ν_2 BAND REGION

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The unstable molecule propadienone (methylene ketene) is the third member of the cumolenone series (H_2C_nO). In contrast with the first two members of this series, formaldehyde and ketene, no rotationally resolved infrared spectra have been reported. However, the pioneering work from the Monash microwave group[a] has provided rotational and distortion parameters for the ground state of the molecule. In particular they demonstrated the non-rigidity of the molecule associated with the double minimum potential of the ν_{12} mode. We have generated propadienone by the pulsed thermolysis of acrylic anhydride in quartz or ceramic tubes heated to 1000°C, which were an integral part of a diode laser jet spectrometer. The complete spectrum between 2123cm^{-1} and 2133cm^{-1} was recorded, corresponding to the absorption position for the intense C=O stretching mode reported by Chapman et al[b] in the matrix. This mode should have the appearance of a parallel band of a near prolate top (κ = - 0.998). Several series of lines were identified in the jet spectrum but the spectrum is clearly perturbed. Nevertheless using ground state combination differences it has been possible to assign 73 lines in the spectrum of K_a = 0 and 1 sub-bands. The ground state combination differences give rotational constants in good agreement with the microwave values.

[a] R.D.Brown, P.D.Godfrey, R.Champion, *J. Mol. Spec.* **123**, 93 (1987)
[b] O.L.Chapman, M.D.Miller, S.M.Pitzenberger, *J. Am. Chem. Soc.* **109**, 6867 (1987)