CONFORMER DEPENDENCE OF VIBRATIONAL DYNAMICS SEEN IN THE ASYMMETRIC =CH₂ EIGENSTATE RESOLVED INFRARED SPECTRA AND SINGLE EIGENSTATE MICROWAVE SPECTRA OF CIS AND GAUCHE ALLYL FLUORIDE

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The high-resolution (5 MHz) asymmetric =CH₂ hydride stretch infrared spectra of the cis and gauche conformers of allyl fluoride (3-fluoropropene), at 3114 cm⁻¹ and 3100 cm⁻¹ respectively, have been measured in an electric resonance optothermal spectrometer. Infrared-microwave double-resonance was used to assign rotationally homogeneous IVR multiplets. The vibrational dynamics associated with the cis molecule differ greatly from that of the gauche. The average IVR lifetime for the cis conformer is approximately 5 ns whereas for the gauche conformer, the IVR rate is about 90 ps. The experimental state density for the cis conformer is about 100 states/cm⁻¹ and the state density for the gauche conformer is approximately 60 states/cm⁻¹. The microwave spectra of several eigenstates in each band have been obtained in order to detect conformational coupling in the eigenstates. Isomerization following coherent excitation of the =CH₂ stretch of the cis conformer is about 1000 times slower than predicted by RRKM theory.