

## CONFORMATIONAL ANALYSIS OF ALLYLIRONTRICARBONYLBROMIDE FROM THE ROTATIONAL SPECTRUM

B. J. DROUIN, J. J. DANNEMILLER, S. G. KUKOLICH, *Department of Chemistry, University of Arizona, Tucson, AZ 85721.*

Microwave spectra of two structural isomers of allylirontricarboxylbromide were recorded using Fourier transform microwave spectroscopy. Pure rotational transitions for both '*a*' and '*c*' type dipole moments were measured for the '*endo*' isomer, whereas '*a*' and '*b*' type dipole moments were measured for the '*syn*' isomer. Condensed, near symmetric top spectra were obtained for all '*a*' type transitions, but the '*b*' and '*c*' type transitions were spread throughout the spectrum. Quadrupole coupling due to the  $^{79}\text{Br}$  and  $^{81}\text{Br}$  nuclei was observed. Comparison of the quadrupole coupling tensors of the isomers reveals greater anisotropy in the electric field gradient near the Br nucleus in the '*syn*' isomer. The present data allows a partial structure determination and comparison of the properties of the two isomers.