SIGNATURE OF CONFORMATIONAL RELAXATION IN THE MICROWAVE SPECTRUM OF ETHYL TRIFLUOROACETATE, ($CF_3COO\text{-}CH_2CH_3$)

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Ethyl trifluoroacetate is a nearly prolate symmetric top, κ = -0.95, which displays three series of a-type R-branch bands under low resolution conditions in a Stark-modulated spectrometer.[a] Since the molecule exists in only two stable conformers, the origin of the third band series has remained a puzzle for thirty years. We show that the third band series arises from rotational spectra of species undergoing exchange between the two stable forms. This is a purely microwave analog of conformational relaxation which has been observed in NMR spectra under different time, potential energy, and rate regimes.

[a] N. S. True, R. K. Bohn, J. Amer. Chem. Soc. 98, 1188 (1976).