EFFECTS OF CONFORMER EXCHANGE AVERAGING ON THERMAL ROTATIONAL SPECTRA

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The microwave spectrum of ethyl cyanoformate displays three R-branch a-type rotational band series. Two of the band series are easily assigned to two stable conformers but the origin of the third, and most intense, series has remained unexplained for three decades. Spectral simulations demonstrate that this band series arises from thermally populated states which undergo conformational exchange with an average energy specific rate constant, {k(E)}, about 25 GHz. This model can explain anomalies present in rotational spectra of many other compounds composed of mixtures of conformers.