PURE ROTATIONAL SPECTROSCOPY OF ASYMMETRIC TOPS IN THE UNDERGRADUATE CLASSROOM OR LABORATORY

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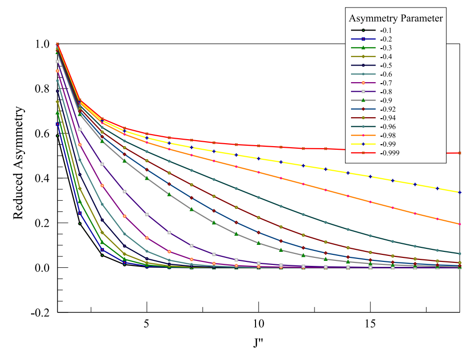

Due to concerns of complexity, the asymmetric top, for which $\kappa = (2B - A - C)/(A - C) \neq \pm 1$, is feared, or at least avoided, by many instructors when explaining the rigid rotor. However, the spectral patterns formed by *cold* asymmetric rigid rotors in the *centimeter-wave* region of the electromagnetic spectrum can be easily identified. We will present some techniques for spectral analyses that we have successfully employed with undergraduate students who are either "pre-quantum mechanics" or are currently enrolled in a chemical quantum mechanics class. The activities are simple, requiring the students to first locate repeating patterns and then apply simple algebraic expressions in order to determine all three rotational constants. The method will be illustrated using the spectra of 2,2,3,3-tetrafluoropropyl trifluoroacetate ($CF_3C(=O)OCH_2CF_2CHF_2$), (E)-1,3,3,3-tetrafluoropropene ($CF_3CH{=}CHF$), 1H,1H,2H-perfluorocyclobutane ($CF_2CF_2CHFCH_2$), and 2H-nonafluorobutane ($CF_3CHFCF_2CF_3$). The first two of these species have predominantly a-type spectra, the third has a predominantly b-type spectrum, the fourth has a predominantly c-type spectrum.