APPLICATIONS OF EFFECTIVE ROTATIONAL HAMILTONIANS FOR TWO-ROTOR MOLECULES

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Effective rotational Hamiltonians for molecules with one periodic internal motion have been described a few years ago [a]. The same paper also outlined the extension of the model to molecules with more than one periodic motions. Such a Hamiltonian was recently implemented in a computer program to analyze spectra of two-rotor molecules such as CH_3OCH_3 and CH_3COCH_3. Because the analysis was not completely satisfactory, the theoretical treatment was modified producing a different effective rotational Hamiltonian for such molecules. It was subsequently applied, with better success, to the analysis of the same spectra. For the ground state of CH_3OCH_3, 232 rotational transition frequencies of all symmetry species taken from the literature could be fit to an effective rotational Hamiltonian containing 16 parameters, among them 4 internal rotation or tunneling parameters, to yield a standard deviation of 60 kHz; however, about 20 assigned transition frequencies had to be excluded from the fit. Detailed results for the ground and vibrational excited states of CH_3OCH_3, for the ground state of CH_3COCH_3, and for other examples, will be given in the presentation.

[a] P. Groner, J. Mol. Spectrosc. 156, 164-189 (1992).