AN ANALYSIS OF VIBRATION-TORSION-ROTATION INTERACTIONS AND SPECTRA FOR A MOLECULE WITH AN INTERNAL ROTOR

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Based on the analysis of order of magnitude of the term H_{mln} in a Hamiltonian, a new scheme of the ordering by magnitude is proposed to analyze the vibration-torsion-rotation interactions for molecules with internal rotations, in which the order of the torsional angular momentum term with P_γ^2 is considered to be just between those of the vibrational angular momentum term with p_k^2 and the rotational angular momentum term with P^2 (or P_a^2). Therefore, the importance of torsional problem is emphasized. The sequential contact transformation technique is applied to the vibration-torsion-rotation Hamiltonian for a molecule containing a threefold symmetric internal rotor, which makes it possible to analyze clearly various higher-order vibration-torsion-rotation interactions and their effects in the vibration-torsion-rotation spectra. A reduced torsion-rotation Hamiltonian for the molecule with $C_{3v}(M)$ symmetry is given in the new ordering scheme and is applied to analyze the spectra of CH_3OH and $CH_3{}^{18}OH$. Some new lines are observed for $CH_3{}^{18}OH$.