EFFECTIVE ROTATIONAL HAMILTONIAN FOR ETHANOL-TYPE MOLECULES

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The effective rotational Hamiltonian for molecules with one or two periodic large amplitude motions [a] has been applied successfully to the microwave and sub-millimeter wave spectra of a number of molecules with one or two methyl rotors. The latest examples include methyl formate-1-^{13}C [b] and the ν_{17} torsional excited state of acetone [c]. Ethanol-type molecules require some modifications of the theory to account for the presence of two conformers. An isolated vibrational state of the trans conformer can be treated with the current theory and computer program. In contrast, the theory may not be applied to the equivalent gauche conformers because of the tunneling interconversion between them. Moreover, the trans conformer interacts with the gauche conformer even in the ground state.[d] The modifications of the theory are outlined in this presentation. It includes tunneling interactions between the gauche conformers themselves but also between them and the trans conformer. Future applications of this model are envisioned for dimethyl ether-d_1, acetone-d_1, ethylphosphine, but also methanol-C-d_1. It is hoped that the modifications can be implemented in the computer program ERHAM in time to present results at the symposium.

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