DETERMINATION OF TORSIONAL BARRIER DERIVATIVES WITH RESPECT TO INTERNAL COORDINATES FOR METHANOL

LI WANG, AND KOJIRO TAKAGI, *Department of Physics, Toyama University, Toyama 930-8555, Japan*.

Torsional potential barrier and their derivatives with respect to space coordinates of the nuclei in the methanol molecule are caused by the interactions between the electrons and nuclei of the internal rotor and those of the frame. The straitforward quantum-mechanical calculation is so complex that a satisfied result will not be obtained. Duan ang Takagi represented a theory on the centrifugal distortion effect for a molecule with an internal rotor. [a] In this theory, an effective vibration-torsion-rotational Hamiltonian can be determined from molecular structure, barrier height and its derivatives. Some centrifugal distortion constants in the Hamiltonian are not calculable due to the lack of available torsional barrier derivatives. In the present work, the torsional barrier derivatives along with molecular structure and force constants will be determined by fitting them to microwave and FIR data. The obtained constants are useful to calculate the vibration-torsion-rotational energy levels.

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[a] Y. B. Duan and K. Takagi, Phys. Lett. A 207, 203 (1995).