THE CALCULATION OF MOLECULAR PARAMETERS FOR A MOLECULE WITH AN INTERNAL ROTOR

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A detailed description of the numerical calculation of spectroscopic constants from the well-known force constants or conversely the force constants from the spectroscopic ones, based on a recent formulation (Duan and Takagi, Phys. Lett. A, **207**, 203, 1995) of centrifugal distortion effects for a molecule containing a three-fold symmetric internal rotor, is presented to lay down procedures for doing such a calculation. At the present stage, we can only determine the distortion constants which are independent upon the barrier derivatives because we have no method to express the barrier derivative in terms of the molecular geometry and we also have no set of available barrier constants, i.e., the barrier derivatives. In order to check the procedure, some determinable constants in a reduced Hamiltonian are calculated using known force constants for methanol and compared with those obtained from a fitting.