TWO-ROTOR CALCULATIONS FOR MOLECULES WITH C_2 OR C_s SYMMETRY

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An effective rotation-internal motion Hamiltonian for molecules with two periodic internal motions [a] has been applied recently to dimethyl ether [b] and acetone [c] whose equilibrium structures have C_{2v} symmetry. The program used to analyze their rotational spectra has been modified to allow treatment of two-rotor molecules with lower symmetry (equivalent rotor problems for molecules with C_s and C_2 symmetry and nonequivalent rotor problems with and without a plane of symmetry). It has been used to analyze the microwave literature data of CH_3SSCH_3 (C_2 symmetry, ground state) [d], CH_3CHFCH_3 (C_s symmetry, ground and two excited states) [e], and CH_3OSiH_3 (nonequivalent, C_s symmetry, ground state) [f]. The experimental data have been fitted to experimental precision by the nonlinear least-squares method to determine spectroscopic parameters (rotational constants, centrifugal distortion constants and tunneling parameters). Applications to other molecules are in progress.

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