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 $C'_2$ 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$_3$SSCH$_3$ ($C_2$ symmetry, ground state) $^d$, CH$_3$CHFCH$_3$ ($C_4$ symmetry, ground and two excited states) $^e$, and CH$_3$OSiH$_3$ (nonequivalent, $C_4$ 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.