PROGRAMS FOR TWO-ROTOR PROBLEMS

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The simulation and fitting of spectra of molecules with two periodic large-amplitude motions ("internal rotations") has been a challenging problem for some time. Three Fortran programs (for PC) treat different aspects of the rotation-internal motion Hamiltonian. TACIR (Two Asymmetric Coupled Internal Rotors) solves the internal motion ($J = 0$) Hamiltonian and predicts torsional transitions for equivalent or nonequivalent internal rotors of any periodicity from internal rotation "constants" and potential, each defined as two-dimensional Fourier series. It is a significantly expanded version of a program described earlier \(^a\). The coefficients of the potential and other spectroscopic constants can be adjusted by the least-squares method to fit energy differences (transition frequencies and tunneling splittings). It has been applied recently to 3-methyl-1,2-butadiene, (CH$_3$)$_2$C=C=CH$_2$ \(^b\), and acetone, (CH$_3$)$_2$C=O \(^c\). Program ERHAM (Effective Rotational HAMiltonian) solves the effective rotation-internal motion Hamiltonian for molecules with equivalent internal motions \(^d\). It predicts rotational transitions and intensities and fits spectroscopic constants (by least-squares) simultaneously for several but uncoupled (bound) vibrational states \(^e\). The third program, TWOSER (TWO-dimensional fourier SERies) determines the 2-D Fourier series of the internal rotation "constants" used in TACIR for asymmetric internal rotors from the structural parameters of several conformations.