PROGRAMS FOR TWO-ROTOR PROBLEMS

PETER GRONER, *Department of Chemistry, University of Missouri - Kansas City, Kansas City, MO 64110.*

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, $(CH_3)_2C{=}C{=}CH_2$ [b], and acetone, $(CH_3)_2C{=}O$ [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.

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[b] S. Bell, P. Groner, G. A. Guirgis and J. R. Durig, J. Phys. Chem. A, 104, 514 (2000).
[c] P. Groner, J. Mol. Struct. 550-551, 473 (2000).
[d] P. Groner, J. Chem. Phys. 107, 4483 (1997).
[e] P. Groner, S. Albert, E. Herbst and F. C. De Lucia, Astrophys. J. 500, 1059 (1998).