SPIN ORBIT COUPLING JAHN-TELLER (SOCJT)

TIMOTHY A. BARCKHOLTZ, *ExxonMobil Research and Engineering, Corporate Strategic Research, 1545 Route 22 East, Annandale, NJ 08801*; BRIAN E. APPLEGATE, *University of North Carolina, Dept. of Chemistry, Chapel Hill, NC 27599*; TERRY A. MILLER, *The Ohio State University, Dept. of Chemistry, Laser Spectroscopy Facility, 120 W. 18th Avenue, Columbus, Ohio 43210*.

SOCJT is a PC based program for determining the lowest energy eigenvalues of the Jahn-Teller Hamiltonian including linear and quadratic Jahn-Teller and spin-orbit terms. Calculations may be run for any molecule with non-cubic symmetry, having *n* arbitrary Jahn-Teller active modes, and arbitrary integer or half-integer spin state. In addition to calculating the lowest energy eigenvalues, SOCJT also computes several properties derived from the resulting eigenvectors, including the Coriolis coupling constants and the relative vibronic transition intensities to another electronic state. For the purpose of fitting experimental spectra, a non-linear least squares routine is included which allows for the fitting of the spin orbit coupling constant, $a\zeta$, the *n* linear Jahn-Teller coupling constants D_i, the *n* quadratic Jahn-Teller coupling constants K_i, the *n* unperturbed harmonic vibrational frequencies, $\omega_{e,i}$, and the *n* unperturbed anharmonic corrections $\omega_e x_{e,i}$, to experimentally determined line positions. SOCJT has been used successfully to fit the spectra of several Jahn-Teller active molecules, including CH_3O, CF_3S, C_5H_5, and $C_6H_6^+$.