Quantum dynamics of floppy molecular systems with ElVibRot and Tnum

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The description of the dynamics of polyatomic molecules provides a significant challenge to molecular theorists. For floppy molecular systems the use of curvilinear coordinates (z-matrix, polyspherical…) enables one to perform the dynamics more efficiently. The complexity of the kinetic energy operator is hidden behind a numerical and exact description using Tnum. Furthermore, for molecules with a large number of atoms, the number of internal degrees of freedom makes the reduction of dimensionality a requirement that cannot be ignored. Several physical models of increasing accurateness based on a separation between n slow degrees of freedom (active modes) and m fast ones (inactive modes) can be used (constraint models, adiabatic approximation, coupled adiabatic channels or exact models). All those models are implemented in the fortran code ElVibRot without built-in limitation. This program allows simulations of vibrational spectra of floppy molecular systems (nitric acid, methanol, ammonia…) as well as time-dependant simulations (photo-dissociation, optimal control …).