CLASSICAL, SEMI-CLASSICAL, AND QUANTUM DYNAMICS OF UNI-AXIAL AND MULTI-AXIAL FLOPPY ROTORS

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Molecules carrying more or less freely turning rotors have classical and quantum rotational properties that are more difficult to calculate and visualize than those of a more conventional semi-rigid molecule.[a] The analogy with a gyro-stabilized spacecraft provides a starting point for discussion, but the quantum mechanics of angular momentum provides a far richer state space than the corresponding classical model. To help unravel the many dynamical and spectral possibilities, a semi-classical analysis involving rotational energy surfaces RES[b] may be used to elucidate both classical and quantum modeling. We consider the simplest models of a single uniaxial rotor, such as a methyl group, attached to a larger rigid or semi-rigid molecule, and compare RES geometry to quantum eigenvalue solutions. The possibility emerges for more easily analyzing multi-axial species that are connected in series or parallel to a central rotor.

[a] J. Ortigoso and J. T. Hougen, J. Chem. Phys. 101, 15 (1994).

[b] W. G. Harter, Princ. of Symmetry, Dynamics & Spectroscopy (Wiley 1993) p. 608.