ROTATIONAL ENERGY SURFACES OF DEFORMABLE ROTORS: EASY WAYS TO VISUALIZE AND APPROXIMATE QUANTUM FRAME DYANMICS AND SPECTRA

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While classical Eckart frames serve well for semi-rigid molecules, they become problematic for molecules with loose parts. Molecules carrying spins or other rotors have classical and quantum rotational properties that are more difficult to calculate and visualize than those of a more conventional semi-rigid molecule particularly if the complex has high symmetry. The analogy with a gyro-stabilized spacecraft is a classical starting point, but the quantum mechanics of angular momentum and particle permutation may involve a rich state space with many resonances. To help unravel complex dynamical and spectral possibilities, a semi-classical analysis involving rotational energy surfaces RES[1-2] helps to elucidate both classical and quantum modeling. A simple (and cheap) program to show RES phase space geometry of semi- rigid or resonating molecules [3-4] is compared to not-so-simple quantum spectral models. At the fundamental theoretical level the concept of a molecular frame touches on deep issues of relativity and quantum wave mechanics connected with how matter and optics relate. The 2005 Einstein Centennial provides an impetus for speculation on such connections.
[1] J. Ortigoso and J. T. Hougen, J. Chem. Phys. 101, 15 (1994). [2] W. G. Harter, Princ. of Symmetry, Dynamics & Spectroscopy (Wiley 1993) p. 608. [3] W. G. Harter, Atomic Mol. and Opt. Phys 35, 377#393 (2004). [4] H.T. Crogman and W. G. Harter, J. Chem. Phys. 121, 9297#9312 (2004).