ROTOR-ROTOR SPECTRA AND DYNAMICS: COUPLING BETWEEN EXTREMES IN INTERACTION STRENGTH AND SPECTRAL COMPLEXITY

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Examples of rotor-rotor systems which provide models for fluxional or "floppy" molecules have been considered by Ortigoso, Kleiner and Hougen.[a][b] Here we consider a variety of models in which one quantum rotor interacts more or less strongly with another. Weak coupling only slightly perturbs each rotor's spectrum while a strong coupling may "weld" or "constrict" the system into what amounts to a single rotor. Possible component rotors of such models vary in complexity. The simplest component is a rigid uniaxial "pinwheel" (RUP) or else a rigid diatomic rotor (RDR) each able to rotate around one axis at a time. Somewhat more complex components are rigid symmetric tops (RST), either oblate or prolate. Next in line of complexity, is the rigid asymmetric top whose acronym (RAT) aptly describes its distinctly more troublesome nest of possible interaction scenarios. Finally, there are deformable versions DUP, DDR,DST, and DAT of the rigid (RUP, RDR, etc.) rotor models which are more complex but have greater spectroscopic relevancy. The most complex dynamics is that of the deformable spherical rotor (DSR) whose spectra "cluster" into DST-like bands.[c] The 8 or 9 classes of single rotors yield 36 to 45 classes of rotor-rotors beginning with RUP-RUP, RUP-RAT or RAT-RAT and ending with DAT-DAT or DSR-DSR. Each class involves varying theoretical schemes depending on whether the rotors may be treated as concentric (cc) or (more commonly) hetro-centric (hc). A select (and necessarily small) sub-set of this enormous number of possibilities will be discussed, starting with the basic concentric uniaxial pinwheel-on-a-pinwheel(ccRUP-RUP).

[a] J. Ortigoso and J. T. Hougen, J. Chem. Phys. 101, 15 (1994).
[b] [2] J. Ortigoso, I. Kleiner, and J. T. Hougen, J. Chem. Phys. 110, 11688.
[c] W. G. Harter, Princ. of Symmetry, Dynamics & Spectroscopy (Wiley 1993) p. 608.