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

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Buckminsterfullerene (C_{60}) is the roundest commercially available deformable spherical rotors (DSR),[a]. The "Buckyballs" are unique in that they have tri-axial rotation even in the fullerite solid-state above 140K; a box of frictionless ball bearings! Also, the C_{60} cage is large enough to hold atoms and maybe even small molecules. In gas-phase this opens the possibility of a fully triaxial concentric DSR-DST rotor-rotor as well as many of the other more theoretically tractable cases like DSR-RDR or RST-RUP listed in the preceding talk. (C_{60} solid-phase is a hetrocentric $(\mathrm{DSR})^N$ fcc crystal.) Finally, C_{60} is practically unique in that it comes in distinct isotopic varieties, most notably a "Bose-ball" $^{12}C_{60}$, a "mixed-ball" $^{13}C_{59}$ and a "Fermi-ball" of ($^{13}C_{60}$).[b], [c] Differences in symmetry between these casesis enormous. Bose-exclusion kills all but the Ag rovibrational species of $^{12}C_{60}$ and reduces spectral congestion by a factor of 60. In contrast, Pauli-Fermi-exclusion assigns 2^{60} 1.5E18 hyperfine levels to each rovibrational level of $^{13}C_{60}$. Mixed symmetry fullerenes $^{13}C_m$-$^{12}C_{60-m}$[3] lie between the two extremes. The first "mixed-ball" $^{13}C_{60}$ - $^{12}C_{59}$ corresponds to a strong-coupling limit of an hcDSR-RDR model. This observation helps to clarify the enormous symmetry-exclusion diversity. At the bottom of the rotor-rotor symmetry hierarchy are the hetrocentric hcRDR-RDR or hcRAT-RAT arrangements of elongated molecules connected more or less loosely end-to-end, that is, links of folding polymer chains. Such chains and links are nano-sized quantum mechanical analogs of ancient slings, whips, and trebuchets with a devilish dynamics to match! And, biological systems cannot live without them.

[a] H. W. Kroto, J. R. Heath, S. C. O'Brien, R. F. Curl, and R. E. Smalley,Nature 318, 162(1985), W. Kratschmer, et. al. Molecules (cf. SiF_4)
[b] W. G. Harter and D. E. Weeks, Chem. Phys. Letters 132, 387 (1986), J. Chem. Phys. 90, 4744 (1989).
[c] W. G. Harter and T. C. Reimer,Chem. Phys. Letters 194, 230 (1992), J. Chem. Phys. 106, 1326 (1997).