Abstract Submitted
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Spin-symmetry conversion and internal rotation in high J molecular systems JUSTIN MITCHELL, WILLIAM HARTER, University of Arkansas — Dynamics and spectra of molecules with internal rotation or rovibrational coupling is approximately modeled by rigid or semi-rigid rotors with attached gyroscopes. Using Rotational Energy (RE)[1] surfaces, high resolution molecular spectra for high angular momentum show two distinct but related phenomena; spin-symmetry conversion and internal rotation. For both cases the high total angular momentum allows for transitions that would otherwise be forbidden. Molecular body-frame J-localization effects associated with tight energy level-clusters dominate the rovibronic spectra of high symmetry molecules, particularly spherical tops at J>10. [2] The effects include large and widespread spin-symmetry mixing contrary to conventional wisdom[3] about weak nuclear moments. Such effects are discussed showing how RE surface plots may predict them even at low J. Classical dynamics of axially constrained rotors are approximated by intersecting rotational-energy-surfaces (RES) that have (J-S)·B·(J-S) forms in the limit of constraints that do no work. Semi-classical eigensolutions are compared to those found by direct diagonalization. [1] W.G Hater, in *Handbook of Atomic, Molecular and Optical Physics*, edited by G.W.F Drake (Springer, Germany 2006) [2] *W. G. Harter, Phys. Rev. A24,192-262(1981).* [3] *G. Herzberg, Infrared and Raman Spectra (VanNostrand 1945) pp. 458,463.*

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