ROVIBRONIC ENERGY TOPOGRAPHY I: TENSOR EIGENVALUE STRUCTURE AND TUNNELING EFFECTS IN LOW-SYMMETRY SPECIES-CLUSTERS OF HIGH SYMMETRY MOLECULES

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Centrifugal and Coriolis effects on rovibrational eigensolutions may be analyzed and approximated by rotational-energy-surfaces (RES). This technique is extended to study high rank tensor Hamiltonians that model spectra of symmetric molecules such as CH_4, SF_6 and C_{60}.

Of particular interest here is superfine structure, which was first studied[a] with a fourth order rotational Hamiltonian and experimentally confirmed for SF_6[b] and CH_4[c]. The theoretical framework for this study is reviewed for higher angular momentum and higher order Hamiltonians. Earlier studies show symmetry reduction into clusters of local C_4 and C_3 symmetry. Here we study effects of combinations of fourth, sixth and higher rank tensor Hamiltonians to investigate a reduction to C_2 and C_1 (no symmetry) clusters that involve tunneling between 12 or 24 equivalent local phase-space regions. An understanding of this low symmetry tunneling may prove useful in analysis of internal rotations and provide examples of monodromy.

[a] J.P. Aldridge et. al *J Mol Spec* **58**, 165 (1975)
[b] W.G. Harter, C.W. Patterson, *Phys Rev Lett*, **38**, 244 (1977)
[c] A. Pines, *J. Opt Soc* **66**, 97 (1976)