STUDY OF DISTORTED SPHERICAL TOPS USING SYMMETRY-ADAPTED TENSORIAL FORMALISM: APPLICATION TO SF_5Cl AND SO_2F_2

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The techniques of symmetry-adapted tensorial formalism and of vibrational extrapolation developed since many years have proved their efficiency for the spectroscopy of spherical-top molecules (CH_4, SF_6, ...)[a]. We have recently extended these methods to the case of "distorted spherical-tops", *i.e.* XY_4 or XY_6 type molecules for which one or two of the Y ligands has been substituted by another atom. To do this, we start from the $O(3) \supset T_d$ or $O(3) \supset O_h$ formalism and perform a reorientation into the subgroup C_{2v} or C_{4v}.
We have first considered the case of XY_5Z (C_{4v}) molecules[b,c]. This model has been used to perform the analysis of the ν_1/ν_8 dyad of $SF_5{}^{35}Cl$[d] A set of programs for spectrum calculations and fits using these methods has been developed[e] and is made freely available through the World Wide Web[f]. We also plan to use these programs for the spectroscopy of SF_5Br or IOF_5, for instance.
We have also undertaken the study of XY_2Z_2 (C_{2v}) molecules[g] in the aim of studying the quasi spherical-top SO_2F_2. Our model has already been used to perform the analysis of the ground state of this molecule. These results have been compared to those of the usual asymmetric-top approach[h]. We now intend to use this formalism to treat the strongly interacting pentad of this species.

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