TENSORIAL FORMALISM FOR ROVIBRONIC SPECTROSCOPY OF C_{3v} MOLECULES SPECTROSCOPY OF XY_3Z (C_{3v}) MOLECULES WITH AN EVEN OR ODD NUMBER OF ELECTRONS: A TENSORIAL FORMALISM ADAPTED TO THE $SU(2) \otimes C_I \supset C^S_{\infty v} \supset C^S_{3v}$ GROUP CHAIN

A. EL HILALI, *LISA, CNRS/Universités Paris Est et Paris Diderot, 61 Avenue du Général de Gaulle, 94010 Créteil, France*; V. BOUDON, *Laboratoire interdisciplinaire Carnot de Bourgogne, UMR 5209 CNRS–Université de Bourgogne, 9, Avenue Alain Savary, BP 47870, F-21078 Dijon Cedex, France*.

In molecular spectroscopy, it is often considered that sophisticated group theoretical and tensorial formalism methods are only really useful for spherical top (*i.e.* highly symmetrical) molecules, for which they have proven their high efficiency. Consequently, it is usually admitted that symmetric and asymmetric tops (*i.e.* lower symmetry) species should be treated using more "conventional" methods. However, some key elements of the formalism developed in our group for tetrahedral or octahedral molecules can be used with great profit even for less symmetrical systems: the ability of performing systematic developments of all rovibrational interactions in case of complex polyads and the so-called "vibrational extrapolation" which makes global analyses much easier. Firstly, we present the development of a tensorial formalism adapted to the study of XY_3Z type molecules which possess integer angular momenta (*i.e.* in a singlet electronic state) by using the $O(3) \supset C_{\infty v} \supset C_{3v}$ chain[a,b]. We present also the C_{3v}TDS[c](C_{3v} Top Data System) software for spectrum simulation dedicated to the study of symmetric-top molecules belonging to the C_{3v} point group. Secondly, we present the development of a tensorial formalism adapted to the study of XY_3Z type open-shell species which possess half-integer angular momenta by using the $SU(2) \otimes C_I \supset C^S_{\infty v} \supset C^S_{3v}$ group chain[d,e].

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