EXTENSION OF THE STDS/HTDS SOFTWARE TO ROVIBRONIC SPECTROSCOPY AND TO LOWER SYMMETRY PROBLEMS

V. BOUDON, M. REY, M. ROTGER, M. LOETE, *Laboratoire de Physique de l'Université de Bourgogne, CNRS UMR 5027, 9 Av. A. Savary, BP 4780, F-21078 DIJON Cedex, FRANCE. E-mail : boudon@jupiter.u-bourgogne.fr.*

We present new softwares using the group-theoretical and tensorial methods developed in the Dijon group. They are based on the Spherical Top Data System (STDS)[a] and the Highly-spherical Top Data System (HTDS)[b] previously written for spherical-top molecules in a singlet electronic state. The two types of problems that can be handled with these new programs are :

- **The case of spherical-top molecules in a degenerate electronic state.** This concerns the rovibronic spectroscopy instead of the rovibrational spectroscopy, for species like ReF_6 or $V(CO)_6$. A new formalism including electronic operators and rovibronic couplings has been developed[c,d] and implemented in a new version of HTDS.
- **The case of "quasi spherical-top" molecules of C_{4v} and C_{2v} symmetry.** This concerns symmetric-top molecules deriving from spherical-tops by substitution of one ligand like SF_5Cl (C_4v symmetry) or asymmetric-tops with ligands having close masses like SO_2F_2 (C_2v symmetry). New formalism using the $O(3) \supset O_h \supset C_{4v}$[e,f] and $O(3) \supset T_d \supset C_{2v}$ group chains have been developed and implemented into two new program suites named C_{4v}TDS and C_{2v}TDS, respectively.

These software packages will be available soon for free download.

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