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.

---

[a] Ch. Wenger and J.-P. Champion, *J. Quant. Spectrosc. Radiat. Transfer*, **59**, 471–480 (1998).
[b] Ch. Wenger, V. Boudon J.-P. Champion and G. Pierre, *J. Quant. Spectrosc. Radiat. Transfer*, **66**, 1–16 (2000).
[c] M. Rey, V. Boudon, M. Loëte and F. Michelot, *J. Mol. Spectrosc.*, **204**, 106–119 (2000).
[d] M. Rey, V. Boudon and M. Loëte, *J. Mol. Struct.*, in press (2001).
[e] M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.*, **200**, 123–130 (2000).
[f] M. Rotger, V. Boudon and M. Loëte, *J. Mol. Spectrosc.*, **200**, 131–137 (2000).