XTDS: A JAVA-BASED INTERFACE TO ANALYZE AND SIMULATE SPECTRA OF VARIOUS MOLECULES USING TENSORIAL FORMALISM

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The Dijon group has developed powerful techniques based on group theory and tensorial formalism[a] in order to analyze and simulate absorption and Raman spectra of molecules with various symmetries. Software packages and databases[b] implementing these tools have been created. This concerns: XY_4 (tetrahedral, STDS package)[c], XY_6 (octahedral, HTDS package)[d], XY_2Z_2 (C_{2v} symmetry, C_{2v}TDS package)[e], XY_5Z (C_{4v} symmetry, C_{4v}TDS package)[f] and X_2Y_4 (D_{2h} symmetry and D_{2h}TDS package)[g] species. These packages all consist in FORTRAN 77 programs called by UNIX scripts.

We present here a user-friendly java-based interface, called XTDS, which allows to interactively build and launch spectrum calculation or analysis jobs using any of the above-mentioned packages. This software runs on UNIX systems (UNIX, Linux or Mac OS X workstations). It allows the treatment of complex spectroscopic problems, including molecules with complex polyads, like methane for instance. The user can define the polyad scheme for the molecule under consideration. All interaction terms up to a given order of the development are automatically determined for both the Hamiltonian or transition moments (dipole moment or polarizability). Least-square fits of experimental data can also be run interactively.

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[a] V. Boudon, J.-P. Champion, T. Gabard, M. Loëte, F. Michelot, G. Pierre, M. Rotger, Ch. Wenger and M. Rey, *J. Mol. Spectrosc.*, **228**, 620–634 (2003)

[b] http://www.u-bourgogne.fr/shTDS.html

[c] Ch. Wenger and J.-P. Champion, *J. Quant. Spectrosc. Radiat. Transfer*, **59**, 471–480 (1998).

[d] Ch. Wenger, V. Boudon, J.-P. Champion and G. Pierre, *J. Quant. Spectrosc. Radiat. Transfer*, bf 66, 1–16 (2000).

[e] Ch. Wenger, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer*, **93**, 429–446 (2005).

[f] Ch. Wenger, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer*, **74**, 621–636 (2002).

[g] Ch. Wenger, W. Raballand, M. Rotger and V. Boudon, *J. Quant. Spectrosc. Radiat. Transfer*, in press (2005).