SPVIEW AND XTDS: GRAPHICAL TOOLS FOR THE ANALYSIS AND SIMULATION OF HIGH-RESOLUTION MOLECULAR SPECTRA

C. WENGER, V. BOUDON, *Institut Carnot de Bourgogne, UMR 5209 CNRS-Université de Bourgogne, 9. Av. A. Savary, BP 47870, F-21078 Dijon Cedex, France*.

SPVIEW is a multi-platform Java application that allows graphical assignment of high-resolution molecular spectra. It is possible to load, display and manipulate experimental and simulated spectra (XY ASCII format) as well as stick spectra in various formats (including HITRAN format). Lines can be assigned graphically using the mouse. Assignments can also be modified or removed. Local simulations can be performed in order, for instance, to help assignment in partly resolved line clusters. SPVIEW is also able produce peak lists from an experimental spectrum. This tool can be used in conjunction with XTDS, which is a Java front-end to the different programs implementing the tensorial formalism developed in our group[a]. XTDS allows the simulation and analysis of any polyad system for molecules of various symmetries (T_d and O_h spherical tops like CH_4 and SF_6, C_{2v} and C_{4v} quasi-spherical tops like SO_2F_2 and SF_5Cl, D_{2h} molecules like C_2H_4). Its capabilities have been recently augmented and improved.

[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).