STDS AND HTDS SOFTWARE FOR THE CALCULATION AND ANALYSIS OF SPHERICAL-TOP SPECTRA

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The Spherical Top Data System (STDS)[a] and the Highly-spherical Top Data System (HTDS)[b] software packages for the simulation and analysis of spherical-top spectra are presented. These programs implement the group-theoretical and tensorial methods developed in the Dijon group[c,d]. They allow various types of calculations : rovibrational energy levels, infrared absorption and Raman scattering spectra. STDS is devoted to XY_4 tetrahedral molecules (CH_4, SiH_4, ...) while HTDS handles XY_6 octahedral molecules (SF_6, WF_6, ...). In both cases, numerous parameter files are included for various molecules and band systems that have been analyzed in Dijon. Several job examples for different types of calculations are also provided.
The STDS and HTDS packages are freely downloadable at the URL

`http://www.u-bourgogne.fr/LPUB/shTDS.html`

Both of them are available for Unix, PC-Linux and MacOS™ sytems. A Windows™ version of STDS has also been released. These suites consist of a series of FORTRAN programs called by a script (depending on the operating system).

[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] J.-P. Champion, M. Loëte and G. Pierre, in *Spectroscopy of the Earth's atmosphere and interstellar medium*, edited by K. N. Rao and A. Weber (Academic Press, Inc., San Diego, 1992) pp. 339–422.

[d] N. Cheblal, V. Boudon and M. Loëte, *J. Mol. Spectrosc.*, **66**, 222–231 (1999).