ASSIGNING THE VIBRATION-ROTATION SPECTRA USING THE LWW PROGRAM PACKAGE

WIESŁAW ŁODYGA, MAREK KREGLEWSKI, *Faculty of Chemistry, Adam Mickiewicz University, Poznan, Poland*.

The LWW program package is based on traditional methods used in assigning rotationally resolved IR molecular spectra. The Loomis-Wood diagrams, which are used to visualize spectral branches and facilitate their identification, are combined with the power of interactive lower state combination difference (LSCD) checking, which provides immediate verification of correct assignments of quantum numbers to spectral lines. The traditional Giessen/Cologne type Loomis-Wood algorithm is also implemented. Predictions of vibration-rotation wavenumbers are calculated from a table of vibration-rotation energies, which can be imported from any external fitting program. Program includes many additional tools like simulation of a spectrum from a catalog file (list of transitions with intensities), build-up of a vibration-rotation band from individual branches and simultaneous displaying of two IR spectra - active one used for assignments and a reference one, both with full link to their peak-list files. Importing energies as well as exporting assigned data for fitting in an external program is made easy and flexible by a user-programmed import/export interface, which facilitates iterative refining of energy levels and gives a possibility of using directly exact vibration-rotation energies. Program is available in tree versions: for symmetric top, asymmetric top and molecules with large amplitude motions. The program is designed for the Windows operating systems and is available with full documentation on www.lww.amu.edu.pl .