COMPUTER AIDED ASSIGNMENT OF ASYMMETRIC ROTOR SPECTRA (CAAARS)

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The development of a new interactive software package called CAAARS supplements the properties of the FASSST system, enhances its capabilities and significantly speeds up the assignment and the spectroscopic analysis of the calibrated (raw) data. The software package is capable of sorting the output of the fitting program, which is used in the background to fit the assigned transitions to the spectroscopic constants of an asymmetric rotor Hamiltonian. The sorting is done according to an arbitrary, user defined, sequence of up to 7 linear combinations of the quantum numbers. The software is capable of individually displaying and manipulating the various P, Q, R branches and their subsets which occur in an asymmetric rotor spectrum. Furthermore, it can assign a particular transition within a given branch and refine the list of predicted lines by means of using the fitting routine of choice, in our case SPFIT/SPCAT[a]. Following the spectroscopic patterns in the assignment process proved to be extremely efficient in the beginning of the analysis as well as at the later stage. CAAARS is implemented as an external library program which is loaded by IgorPro at the start-up. It requires IgorPro and runs under the Windows operating system. It can be downloaded at http://www.physics.ohio-state.edu/ medvedev/caaars.htm.

[a]H. M. Pickett, J. Mol. Spectrosc., 148, 371 (1991)