THE AABS PACKAGE FOR ASSIGNMENT AND ANALYSIS OF BROADBAND SPECTRA

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Analysis of broadband spectra poses a considerable challenge to data reduction and management, The advent of the FASSST technique has brought these issues into the realm of rotational spectroscoy, in which instrumental constraints have generally tended to limit the sizes of data sets. The problem has already been addressed at Ohio State with the CAAARS (Computer Aided Assignment of Asymmetric Rotor Spectra) package, implemented in the Igor Pro software environment, with which the FASSST spectra are recorded and calibrated.

Details of a new software package, called AABS (Assignment and Analysis of Broadband Spectra), are now reported. This package is designed as an alternative to CAAARS in situations where the latter may be difficult to implement. AABS is highly portable in that it does not require a proprietary software package, uses moderate computer resources, and ready to run executable versions are freely available from the PROSPE website.^a AABS provides an extended set of features for navigating broadband spectra and associated predictions, efficient addition of measurements to datafiles, and graphical assignment by means of Loomis-Wood type plots. Integration with SPFIT/SPCAT or ASFIT/ASROT packages for fitting and prediction allows a broad range of spectroscopic problems to be tackled. The general nature of AABS makes it useful also for analysis of other types of high-resolution broadband spectra, such as rotationally resolved vibrational or electronic spectra.

^a available at http://www.ifpan.edu.pl/~kisiel/prospe.htm