SPECDATA: AUTOMATED ANALYSIS SOFTWARE FOR BROADBAND SPECTRA

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With the advancement of chirped-pulse techniques, broadband rotational spectra with a few tens to several hundred GHz of spectral coverage are now routinely recorded. When studying multi-component mixtures that might result, for example, with the use of an electrical discharge, lines of new chemical species are often obscured by those of known compounds, and analysis can be laborious.

To address this issue, we have developed SPECdata, an open source, interactive tool which is designed to simplify and greatly accelerate the spectral analysis and discovery. Our software tool combines both automated and manual components that free the user from computation, while giving him/her considerable flexibility to assign, manipulate, interpret and export their analysis.

The automated – and key – component of the new software is a database query system that rapidly assigns transitions of known species in an experimental spectrum. For each experiment, the software identifies spectral features, and subsequently assigns them to known molecules within an in-house database (Pickett .cat files, list of frequencies...), or those catalogued in Splatalogue (using automatic on-line queries).

With suggested assignments, the control is then handed over to the user who can choose to accept, decline or add additional species. Data visualization, statistical information, and interactive widgets assist the user in making decisions about their data. SPECdata has several other useful features intended to improve the user experience. Exporting a full report of the analysis, or a peak file in which assigned lines are removed are among several options. A user may also save their progress to continue at another time. Additional features of SPECdata help the user to maintain and expand their database for future use. A user-friendly interface allows one to search, upload, edit or update catalog or experiment entries.