SPECTROSCOPIC TREASURE IN FORGOTTEN DATA: ROTATIONAL SPECTRUM ANALYSIS THROUGH AGGREGATED DATABASES

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We present the automated analysis of rotational spectra using archived experimental and ab initio data. Modern rotational spectroscopy techniques have made acquiring experimental data extremely fast, yielding many GHz of information in seconds. This is in contrast to the analysis, which still takes many hours if not weeks of an expert's time to fit. In order to bring rotational spectroscopy to a wider audience, new applications, and enable new science, the effort and time required to analyze a spectrum needs to be reduced.

To reduce the analysis time, we aggregated more than 200 experimental spectra (from local instruments and literature) and more than 16,000 ab initio calculations into a library that is leveraged by automated algorithms to screen for identifications in rotational spectra. Screening with experimental data has been shown to give both highly accurate identification and quantification of a sample within a mixture in under 10 seconds per analysis. Unmatched residual lines are presented to the user for further analysis. Work is in progress to expand the number of matchable spectra inside the database and identify unknown constants using ab initio databases.