A HIGH SPEED FITTING PROGRAM FOR ROTATIONAL SPECTROSCOPY

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The ongoing development of rotational spectroscopy through the growth of broadband capabilities and automated acquisition schemes regularly generates a wealth of data to be analyzed. However, assigning these data is often a bottleneck to obtaining useful chemical information. This is particularly true for unknown carriers for which no initial guess or constraint is available. Development of automated spectral analysis tools is therefore critical to fully utilize rotational spectroscopy data.

We have previously reported the development of a high speed algorithm for the calculation of asymmetric rotor spectra. The initial report demonstrated the efficacy of the program to calculate spectra hundreds of times faster than conventional methods. Building on the underlying engine, we have constructed a set of high speed spectral fitting and analysis tools. These tools include a general spectral line fitter and brute force searching algorithms. We have combined these into a pipeline for automated spectral assignment. An initial version of the pipeline has been successfully used for automated assignment of double resonance data, and has been expanded to analyze data using only rotational spectra as an input. A preliminary version is capable of producing a list of probable matches that can be readily evaluated by hand. We will present this work, and discuss the efficacy and limitations of our approach as well as potential future development.