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. Previous versions of this software included basic search and assignment features that were capable of producing a list of probable matches that can be readily evaluated by hand. Since its original release, we have added several new features, including more advanced and automated searching, significant performance increases, multithreading support, and new calculation types. We will discuss the program, improvements, and implementation of its new features.