DAPPERS: A NEW PROGRAM FOR THE RAPID ASSIGNMENT AND FITTING OF DENSE ROTATIONAL SPECTRA BASED ON SPECTRAL PROGRESSIONS

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We describe a new interactive program (DAPPERS: Data Analysis Package for Productive and Enthusiastic Rotational Spectroscopists) for the rapid processing of dense and complex rotational spectra of asymmetric rotors. DAPPERS is based on an intelligent algorithm that quickly and accurately locates spectral progressions with user-identified quantum number identities and then seamlessly integrates with Pickett's SPCAT and SPFIT programs to allow complete assignment and fitting. The program has been shown to be proficient across the full range of asymmetry parameters and can produce final fits containing hundreds of transitions of any type (*a*, *b*, or *c*) or branch (P, Q, or R) in just a few minutes. The software interacts with the user through a simple graphical user interface, and includes a peak-finder with adjustable baseline drift compensation, as well as a number of visualization features. It is designed for easy installation and use, with special attention given to the design of a single executable file platform. It is available for download, together with extensive documentation, at www.chem.umn.edu/groups/kleopold.