THE SPECTROSCOPIC SOFTWARE UNIVERSE: A "PICKETT 2.0" PROPOSAL

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An important yet often unappreciated aspect of the spectroscopist's workflow is the use of key software packages for data analysis. Spectroscopists young and old alike recall their first experiences with a multitude of packages, such as Herb Pickett's CALPGM for rovibrational spectra, Colin Western's powerful PGOPHER graphical user interface, David Plusquellic's JB95 and its magical B+C/B-C rotational constant sliders, or Kisiel's AABS for speedrunning assignment for large broadband microwave or millimeter wave datasets. There are, of course, many other examples of spectroscopic software, whose existences evoke a wide range of emotions, including passion, apathy, and sometimes even mortal fear.

However, the 21st century has provided a difficult inflection point in the interplay between experiment and software for microwave spectroscopy. Chirped-pulse microwave spectroscopy has ushered in routine acquisition of species- and transition-dense spectroscopic data sets, and the typical workflow for such data is generally split between a series of software packages that each provide only a partial solution to efficient workflow. With the growing promise of high-throughput, library-free spectroscopic analysis using machine learning techniques, there is an increased need for performant and "black box" solutions to interpreting and evaluating spectra. Even worse, with the recent passings of Herb Pickett and Colin Western, the community is left with an issue of sustainability and transparency for continuing use and training in these legacy packages.

In this talk, I propose a new, unified software package for spectroscopic prediction and assignment, the so-called "Pickett 2.0" package, which was introduced as an idea that was informally discussed between a set of concerned microwavers last year at this conference. I will outline the features that modern broadband microwave spectroscopists require from a software package for efficient analysis, as well as those required by an emergent community of chemists who use rotational techniques as merely an analytical tool. I will also present new ideas for features that are more applicable for machine learning and high-throughput applications, as well as a brief discussion about the necessity for long-term software sustainability and methodological transparency.