A windows based, mouse-event driven software program that acts as a graphical user interface to Pickett’s fitting programs has been created and improved. The program, SpecFitter, is aimed at walking users through the process of assigning pure rotational spectra. Rotational spectra, in XY format, may be viewed and inspected and the user is provided with tools for observing and recording repeating, similar patterns of transitions. The structure of these patterns is interpreted into “guesses” at rotational constants which the user may then use to predict a spectrum. Observed transition frequencies may then be assigned quantum number transitions and appended to the .lin file through mouse clicks. Although the thrust of this project is to develop a users ability to assign spectra without knowing the molecule producing the spectra, the program can also read in and display calculated structures of target molecules produced by the Gaussian03/09 software, or alternatively the user can draw their own structures. Structures can be edited allowing users to observe the relationship between molecular structure and (i) the direction of dipole moment components and (ii) the relationships between structure and rotational constants. Users may also easily predict spectra from the molecules structure and further relate rotational constants to observed spectra. Students in CHEM 3510 at Purchase College have been vital in developing the software.