

AUTOMATING SPECTRAL ASSIGNMENT OF ROOM-TEMPERATURE MICROWAVE SPECTRA. Steven T. Shipman, Noah H. Anderson, Ian A. Finneran, Patrick T. McDonald. Division of Natural Sciences, New College of Florida, 5800 Bay Shore Road, Sarasota, FL 34243.

Modern methods for acquiring rotational spectra have improved to the point that data collected in just a few days can easily take weeks to months to fully analyze. We have been developing approaches to automate the initial stages of the spectral assignment process. One method uses genetic algorithms to optimize candidate solutions, and one is a less elegant “brute force” method that simply tries and ranks millions of candidates. These approaches have had some success in the analysis of the rotational spectra of ground and vibrationally-excited molecules and have also been useful at helping undergraduate students make meaningful contributions to research projects in high-resolution spectroscopy without prior exposure to quantum mechanics.