UPDATES TO AUTOFIT: PROGRESS AND PROSPECTS

ARIANNA T RODRIGUEZ, *Division of Natural Sciences, New College of Florida, Sarasota, FL, USA*;
STEVEN SHIPMAN, *Department of Chemistry, New College of Florida, Sarasota, FL, USA*.

Spectral complexity can prove to be a challenge when investigating the rotational spectra of complicated systems and developments in automated fitting tools can reduce the time spent fitting these spectra. In this talk, we discuss our progress on improving various aspects of Autofit (algorithmic, including incorporating double resonance information, and usability, e.g. improved graphical interface). Our main test cases are spectra collected from our lab of small molecules near room temperature where contributions from multiple vibrational states are present, but we will also discuss results from molecular beam spectra.