

CHIRAL ANALYSIS OF ISOPULEGOL BY FOURIER TRANSFORM MOLECULAR ROTATIONAL SPECTROSCOPY

LUCA EVANGELISTI, *Dipartimento di Chimica G. Ciamician, Università di Bologna, Bologna, Italy*; NATHAN A SEIFERT, *Department of Chemistry, University of Alberta, Edmonton, AB, Canada*; LORENZO SPADA, *Dep. Chemistry 'Giacomo Ciamician', University of Bologna, Bologna, Italy*; BROOKS PATE, *Department of Chemistry, The University of Virginia, Charlottesville, VA, USA*.

Chiral analysis on molecules with multiple chiral centers can be performed using pulsed-jet Fourier transform rotational spectroscopy. This analysis includes quantitative measurement of diastereomer products and, with the three wave mixing methods developed by Patterson, Schnell, and Doyle (Nature 497, 475-477 (2013)), quantitative determination of the enantiomeric excess of each diastereomer. The high resolution features enable to perform the analysis directly on complex samples without the need for chromatographic separation. Isopulegol has been chosen to show the capabilities of Fourier transform rotational spectroscopy for chiral analysis. Broadband rotational spectroscopy produces spectra with signal-to-noise ratio exceeding 1000:1. The ability to identify low-abundance (0.1-1%) diastereomers in the sample will be described. Methods to rapidly identify rotational spectra from isotopologues at natural abundance will be shown and the molecular structures obtained from this analysis will be compared to theory. The role that quantum chemistry calculations play in identifying structural minima and estimating their spectroscopic properties to aid spectral analysis will be described. Finally, the implementation of three wave mixing techniques to measure the enantiomeric excess of each diastereomer and determine the absolute configuration of the enantiomer in excess will be described.