

LARGE MOLECULE STRUCTURES BY BROADBAND 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*.

Fourier transform molecular rotational resonance spectroscopy (FT-MRR) using pulsed jet molecular beam sources is a high-resolution spectroscopy technique that can be used for chiral analysis of molecules with multiple chiral centers. The sensitivity of the molecular rotational spectrum pattern to small changes in the three dimensional structure makes it possible to identify diastereomers without prior chemical separation. For larger molecules, there is the additional challenge that different conformations of each diastereomer may be present and these need to be differentiated from the diastereomers in the spectral analysis. Broadband rotational spectra of several larger molecules have been measured using a chirped-pulse FT-MRR spectrometer. Measurements of nootkatone ($C_{15}H_{22}O$), cedrol ($C_{15}H_{26}O$), ambroxide ($C_{16}H_{28}O$) and sclareolide ($C_{16}H_{26}O_2$) are presented. These spectra are measured with high sensitivity (signal-to-noise ratio near 1,000:1) and permit structure determination of the most populated isomers using isotopic analysis of the ^{13}C and ^{18}O isotopologues in natural abundance. The accuracy of quantum chemistry calculations to identify diastereomers and conformers and to predict the dipole moment properties needed for three wave mixing measurements is examined.