SINGLE-CONFORMATION SPECTROSCOPY OF A DIASTEREOMERIC LIGNIN MONOMER: EXPLORING THE HYDROGEN BONDING ARCHITECTURES OF A TRIOL CHAIN

JACOB C. DEAN, EVAN G. BUCHANAN, ANNA GUTBERLET, WILLIAM H. JAMES III, BIDYUT BISWAS, P. V. RAMACHANDRAN, and TIMOTHY S. ZWIER, *Department of Chemistry, Purdue University, West Lafayette, IN 47907*.

The double-resonance methods of UV-UV holeburning and resonant ion-dip infrared (RIDIR) spectroscopy were implemented in this study to obtain conformer-specific UV and IR spectra on the two diastereomers (R,R)/(R,S) 1-(4-hydroxy-3-methoxyphenyl)propane-1,2,3-triol (R,R/R,S-HMPPT). HMPPT is a monomeric unit common to the lignin biopolymer in most plant types, and its spectroscopic signatures as well as conformational preferences yield valuable insight into its structuring in the polymer network. By probing the isolated molecule in the supersonic expansion, the infrared signatures of each OH allow the assessment of unique patterns in the IR spectrum associated with the different types of hydrogen bonded networks sampled in the jet. These observed conformational families are compared between diastereomers to understand the effect of chirality on the conformational minima available to the molecule. A total of nine conformational isomers have been characterized. Examples of three types of H-bonded chains and two H-bonded cycles are observed. Relative populations of the isomers in each diastereomer have also been obtained using a newly developed method, infrared ion gain spectroscopy. Striking differences are observed between the diastereomers, which configure the OH groups in unique positions relative to one another.