

HIGH PRECISION STRUCTURES OF CELLULOSE POLYMORPHS OBTAINED WITH AN NMR CRYSTALLOGRAPHIC APPROACH. **Darren Brouwer**, Department of Chemistry, Redeemer University, Ancaster ON, Canada. (dbrouwer@redeemer.ca)

Detailed structural characterization of cellulose has presented numerous challenges due to its fibrous nature and multiplicity of crystalline forms. Although determining its structure(s) has been the focus of much effort, there remain outstanding questions, particularly concerning the hydrogen-bonding networks within and between cellulose chains. Fibre neutron and X-ray diffraction (XRD) experiments have provided structures for the various forms of cellulose, however there are intrinsic limitations to the precision that can be achieved with fibre diffraction. ^{13}C solid-state NMR (SSNMR) has played a vital role in detecting the existence of polymorphism in cellulose, but the structural information accessible by ^{13}C SSNMR has not been fully exploited. Here, it is shown that an “NMR crystallography” approach, in which SSNMR results and DFT calculations are combined, provides high precision structures of four of the polymorphs of cellulose.