

## W0034

**Polysaccharide Structures from Powder Diffraction Data.** Srinivas Janaswamy, Rengaswami Chandrasekaran, Whistler Center for Carbohydrate Research, Dept. of Food Science, Purdue Univ., West Lafayette, IN 47907-2009.

Unlike globular molecules which form single crystals, polysaccharide helices tend to align mostly along their molecular axis and may exhibit some lateral ordering. Such specimens contain preferentially oriented micro-crystallites. Although they yield far fewer Bragg reflections than single crystals, their x-ray structure analysis can be conducted to fruition jointly with molecular modeling. However, in some cases, even the best fibers produce merely polycrystalline powder diffraction patterns. Three known examples are arabinan,  $\kappa$ -carrageenan and S-657 originating from beetroot, seaweed and bacteria, respectively. *Ab initio* methods combined with Rietveld technique have led to solving several small molecule structures from powder data. Now we are adapting this approach along with the Linked-Atom Least-Squares procedure in solving the above polysaccharide structures. Preliminary results are reported.