Abstract Submitted
for the MAR09 Meeting of
The American Physical Society

Hydrogen Bonding Structure in Hyperbranched Aliphatic Polyesters Studied by MD Simulations BRIAN OLSON, MUKUL KAUSHIK, SERGEI NAZARENKO, University of Southern Mississippi — Hyperbranched aliphatic polyesters based on dimethoxy propionic acid (bis-MPA) as the repeating unit and ethoxylated pentaerythritol as the tetrafunctional core gained widespread attention due to their unusual structure and properties. These globular macromolecules possess a large number of hydroxyl functional groups in particular on their periphery. These hydroxyl groups interact readily through hydrogen bonding (HB) and form clusters responsible for many physical properties of this system. The structure of these clusters however remains unclear. Therefore MD simulations have been used to elucidate the structure of these clusters. MD simulations revealed that peripheral hydroxyl groups form linear hydrogen bond clusters (strings) similar to those proposed in hydrofluoric acid (HF) but considerably shorter consisting of 4-10 hydroxyl groups per cluster. Simulations also led to prediction of WAXS pattern for these hyperbranched polyesters in the bulk with the characteristic peak at $2\theta = 30^\circ$ due to O-O correlations similar to those in water. The predictions were in excellent agreement with the experimental WAXS data.

Brian Olson
University of Southern Mississippi

Date submitted: 28 Nov 2008 Electronic form version 1.4