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Pressure-Volume-Temperature Behavior of Hyperbranched Polyols: Experiment and Modelling MUKUL KAUSHIK, SERGEI NAZARENKO, BRIAN OLSON, School of Polymers and High Performance Materials The University of Southern Mississippi, Hattiesburg, MS 39406 — The pressure volume temperature behavior of two generations of hyperbranched polyesters BoltornTM H40 and H20 was studied by PVT measurements using high pressure dilatometer. Volumetric expansivity, and free volume parameters were determined for both generations in the melt state. The PVT data were fitted to Simha-Somcynsky (SS) equation of state (EOS) and Sanchez–Lacombe (SL) equation of state (EOS) to calculate occupied volume and fractional free volume. The values of occupied volume and fractional free volumes obtained through both the equations of states were similar. Simulated atmospheric pressure V-T data were generated by using Discover module of Accelrys[®]. Quality of equilibrium was confirmed by energy stabilization and closeness of experimental and simulation densities. WAXD and temperature-volume curves obtained by molecular dynamics simulations were comparable to the experimental data. Well relaxed amorphous cell was further utilized to study hydrogen bond network and determination of O-O pair correlation function of terminal hydroxyl groups.

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