On the Molecular Structure of Ge$_x$Sb$_x$Se$_{1-x}$ glasses$^1$ K. GUNASEKERA, P. BOOLCHAND, University of Cincinnati, A. JACKSON, Central Michigan University — The Ge$_x$Sb$_x$Se$_{100-2x}$ ternary is isovalent to the phase-change material, Ge$_x$Sb$_x$Te$_{100-2x}$, except the Selenides can be prepared as bulk alloy glasses while the Tellurides exist only as amorphous thin-films. Here we report on the Selenides synthesized over a wide composition range, $0 < x < 25\%$, and examined in modulated-DSC, Raman scattering and molar volume experiments. The enthalpy of relaxation at $T_g$ shows the opening of a reversibility window or Intermediate Phase (IP) in the $13\% < x < 18\%$ range, or $2.40 < r < 2.54$ mean coordination number range, where $r = 2 + 3x$. FT- Raman studies reveal frequency of the CS mode of GeSe$_4$ tetrahedra to steadily blue-shift with increasing $x$ as networks stiffen. New vibrational modes are observed near $150 \text{ cm}^{-1}$ and near $220 \text{ cm}^{-1}$ at $x > 18.18\%$, the chemical threshold, and are thought to result from homopolar bonds. Ab-initio cluster calculations place pyramidal SbSe$_3$ units and ethylene-like Sb$_2$Se$_2$ units to reveal Raman activity near $215 \text{ cm}^{-1}$ and $228 \text{ cm}^{-1}$ respectively. Evolution of glass structure with composition $x$ will be discussed.

$^1$Supported by NSF grant DMR- 08-53957