High-Pressure and High Temperature Behavior of Datolite

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The mineral datolite, CaBSiO4(OH), crystallizes in the monoclinic space group $P2_1/c$ with $a \sim 4.83$, $b \sim 7.61$, $c \sim 9.63$ Å, $\beta \sim 90.15^\circ$, and $V \sim 354$ Å$^3$. Datolite forms layers of corner sharing SiO$_4$ and BO$_3$(OH) tetrahedra parallel to (001) with Ca sitting between layers. Earlier studies explored the low-temperature (100-300 K) behavior of datolite. This study extends the studies into the high-temperature (300-750 K) and high pressure (0-7.5 GPa) regimes. No phase changes are observed at these temperatures and pressures. The 3rd order Birch-Murnaghan equation of state fit to the P-V data gives a bulk modulus, $K=90.8(7)$ GPa and $dK/dP=5.7(2)$. The axial responses to temperature and pressure and structural changes as a function of pressure will be presented.