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Comparative Raman spectroscopic study on ilmenite-type $MgSiO_3$ (akimotoite), $MgGeO_3$, and $MgTiO_3$ (geikielite) at high temperatures and high pressures

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ABSTRACT

The Raman spectra of $MgXO_3$-ilmenites (X = Si, Ge, Ti) were recorded up to 773 K at ambient pressure and up to 20–30 GPa at room temperature. Temperature and pressure dependence of the force constant of X-O stretching bands revealed that the expansion and compression behavior of XO_6 octahedra differed in the three ilmenites. For SiO_6 and GeO_6 octahedra, the shorter Si-O or Ge-O bonds became more lengthened with temperature and more shortened with pressure than did the longer Si-O or Ge-O bonds. In contrast, for TiO_6 octahedra, the longer Ti-O bonds became more lengthened with temperature and more shortened with pressure than did the shorter Ti-O bonds. For SiO_6 and GeO_6 at high temperatures and TiO_6 at high pressures, the cation positions moved in the direction of the **c** axis and tended to approach the center of the octahedra, decreasing the distortion of XO_6. For SiO_6 and GeO_6 at high pressures and TiO_6 at high temperatures, the cations moved away from the center, increasing the distortion of XO_6. One of the anharmonic correction terms on isochoric specific heat was also elucidated. The anharmonic effects were related to the elastic Debye temperature of the three ilmenites.

Keywords: Raman spectroscopy, ilmenite, high temperature, high pressure, crystal structure