

Low-pressure clino- to high-pressure clinoenstatite phase transition: A phonon-related mechanism

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ABSTRACT

We have investigated by first principles the compressional behavior of low-pressure (LP) and high-pressure (HP) MgSiO₃ clinoenstatite. We have carefully examined unit-cell shapes, chain angles, and polyhedral volume responses, such as angle variances and quasi-elongations, under pressure at room temperature. We have observed opposite behavior of the tetrahedra in the S-rotated and O-rotated chains with pressure in the LP phase, with a slight increase (decrease) in angle variance and quasi-elongation in the former (latter). Inspection of zone center modes of both phases under pressure reveals a transition path that converts the S-rotated chain in the LP phase into the O-rotated chain in the HP phase. This conversion is related to a slight softening of an A_g “metastable” Raman mode under pressure.

Keywords: Phase transition mechanism, low-pressure clinoenstatite, high-pressure clinoenstatite, Raman, IR, phonon frequency