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Thermal expansivity of mantle relevant magnesium silicates derived from vibrational spectroscopy at high pressure

ANASTASIA CHOPELAS*

Max Planck Institut für Chemie, Postfach 3060, 55020 Mainz, Germany

ABSTRACT

Thermal expansivities for the $MgSiO_3$ phases of orthoenstatite, high clinoenstatite, ilmenite, and majorite; and for stishovite were estimated using the thermodynamic Maxwell relation $(\partial S/\partial P)_T = -(\partial V/\partial T)_P$ where the entropies at high pressures were derived using a statistical method and spectroscopic data. The spectroscopically determined thermal expansivities for all minerals are in excellent agreement with previously determined volumetric data, where available. A value of $3.25(10) \times 10^{-5}$ K^{-1} for orthoenstatite at room temperature was obtained; this value is situated in the middle of the large spread of reported values and is in excellent agreement with the two latest volumetric determinations. For high clinoenstatite, α at room T is estimated as $2.56(9) \times 10^{-5}$ K^{-1}. This method provides good high temperature estimates of α for the high-pressure polymorphs, where data are scanty or unavailable. Included in this report are previous data for the Mg_2SiO_4 phases and MgO for completeness. The following equations may be used to extrapolate a to higher temperatures at 1 atm in 10^{-5} K^{-1}: α(majorite) = 2.95 + 0.000521x; $\alpha(\gamma\text{-}Mg_2SiO_4)$ = 2.70 + 0.000648x; α(ilmenite) = 2.64+ 0.000537x; α(perovskite) = 2.51 + 0.000805x; and α(stishovite) = 2.19 + 0.000485x, where x is (T/K-750).