



*Geochemistry, Geophysics, Geosystems*

Supporting Information for

**High-pressure and high-temperature single-crystal elasticity of Cr-pyrope:  
implications for the density and seismic velocity of subcontinental lithospheric  
mantle**

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## Text S1

The used third-order Birch-Murnaghan equation of state is described in the following:

$$P = \frac{3K_{T0}}{2} \left[ \left( \frac{V_{T0}}{V} \right)^{\frac{7}{3}} - \left( \frac{V_{T0}}{V} \right)^{\frac{5}{3}} \right] \left\{ 1 + \frac{3}{4} \left( (\partial K_T / \partial P)_T - 4 \right) \left[ \left( \frac{V_{T0}}{V} \right)^{\frac{2}{3}} - 1 \right] \right\} \quad (1),$$

where  $P$ ,  $V_{T0}$ ,  $V$ ,  $K_{T0}$ , and  $(\partial K_T / \partial P)_T$  are pressure, unit-cell volume at temperature and zero-pressure, unit-cell volume at pressure and temperature, zero-pressure bulk modulus, and its pressure derivative, respectively.

The thermal-pressure equation of state is based on the idea of thermal pressure ( $P_{th}$ ; e.g., (Angel et al., 2014). The total pressure ( $P$ ) at a given  $V$  and  $T$  can be expressed as  $P(V, T) = P(V, T_{ref}) + P_{th}$ .  $P(V, T_{ref})$  is the pressure at reference temperature ( $T_{ref}$ ) which is described by the Birch-Murnaghan equation of state (1).  $P_{th}$  used here is proposed by Holland & Powell (2011):

$$P_{th} = \alpha_0 K_{T0} \left( \frac{\theta_E}{\xi_0} \right) \left( \frac{1}{\exp(\theta_E/T) - 1} - \frac{1}{\exp(\theta_E/T_{ref}) - 1} \right) \quad (2),$$

where  $\alpha_0$  is the thermal expansion coefficient at  $T_{ref}$ ,  $\theta_E$  is the Einstein temperature, and  $\xi_0$  is given by the following expression (Kroll et al., 2012):

$$\xi_0 = \frac{(\theta_E/T_{ref})^2 \exp(\theta_E/T_{ref})}{(\exp(\theta_E/T_{ref}) - 1)^2} \quad (3).$$

## Text S2

The adiabatic bulk ( $K_S$ ) and shear ( $G$ ) modulus at high  $P$  and high  $T$  are evaluated by the third- or fourth-order finite-strain equations.

(1) For  $K_S$ :

$$K_S = K_{S0}(T) \times (1 + 2f)^{\left(\frac{5}{2}\right)} \times \left( 1 + \left( 3 \left( \frac{\partial K_S}{\partial P} \right)_T - 5 \right) \times f \right) \text{ or} \\ K_S = K_{S0}(T) \times (1 + 2f)^{\left(\frac{5}{2}\right)} \times \left( 1 + \left( 3 \left( \frac{\partial K_S}{\partial P} \right)_T - 5 \right) \times f + 0.5 \times \left( 9K_{S0}(T) \times \left( \frac{\partial^2 K_S}{\partial P^2} \right)_T + 9 \times \left( \frac{\partial K_S}{\partial P} \right)_T^2 - 36 \times \left( \frac{\partial K_S}{\partial P} \right)_T + 35 \right) \times f^2 \right) \quad (4),$$

$$K_{S0}(T) = K_{S0} + \left( \frac{\partial K_S}{\partial T} \right)_P \times (T - T_{ref}) \quad (5),$$

$$\left( \frac{\partial K_S}{\partial P} \right)_T = \left( \frac{\partial K_S}{\partial P} \right)_{T_{ref}} \times \text{Exp} \int_{T_{ref}}^T \alpha \, dT \quad (6),$$

$$f = 0.5 \times \left( \left( \frac{\rho}{\rho_0(T)} \right)^{\frac{2}{3}} - 1 \right) \quad (7),$$

$$\rho_0(T) = \rho_0(T_{ref}) \times \left( \text{Exp} \int_{T_{ref}}^T \alpha \, dT \right)^{-1} \quad (8),$$

where  $K_{S0}(T)$  is the adiabatic bulk modulus at room  $P$  and temperature ( $T$ ),  $f$  is the Eulerian finite strain,  $\left(\frac{\partial K_S}{\partial P}\right)_T$  is the first-order pressure derivative of  $K_S$  at temperature  $T$ ,  $\left(\frac{\partial^2 K_S}{\partial P^2}\right)_T$  is the second-order pressure derivative of  $K_S$  at  $T$ ,  $K_{S0}$  is the adiabatic bulk modulus at room  $P-T$ ,  $\left(\frac{\partial K_S}{\partial T}\right)_P$  is the temperature derivative of  $K_S$ ,  $\left(\frac{\partial K_S}{\partial P}\right)_{T_{ref}}$  is the first pressure derivative of  $K_S$  at  $T_{ref}$ ,  $\rho$  is the density at high  $P-T$ ,  $\rho_0(T)$  is the density at room  $P$  and  $T$ ,  $\rho_0(T_{ref})$  is the density at room  $P-T$ , and  $\alpha$  is the thermal expansion coefficient.

(2) For  $G$

$$G = (1+2f)^{\frac{5}{2}} \times (G_0(T) + b_1 f) \text{ or}$$

$$G = (1 + 2f)^{\frac{5}{2}} \times (G_0(T) + b_1 f + 0.5b_2 f^2) \quad (9),$$

$$G_0(T) = G_0 + \left(\frac{\partial G}{\partial T}\right)_P \times (T - T_{ref}) \quad (10),$$

$$b_1 = 3K_{T0}(T) \left(\frac{\partial G}{\partial P}\right)_T - 5G_0(T) \quad (11),$$

$$b_2 = 9(K_{T0}^2(T) \left[\left(\frac{\partial^2 G}{\partial P^2}\right)_T + 1/K_{T0}(T) \left(\left(\frac{\partial K_T}{\partial P}\right)_T - 4\right) \left(\frac{\partial G}{\partial P}\right)_T\right] + \frac{35G_0(T)}{9}) \quad (12),$$

$$\left(\frac{\partial G}{\partial P}\right)_T = \left(\frac{\partial G}{\partial P}\right)_{T_{ref}} \times \text{Exp} \int_{T_{ref}}^T \alpha_0 dT \quad (13),$$

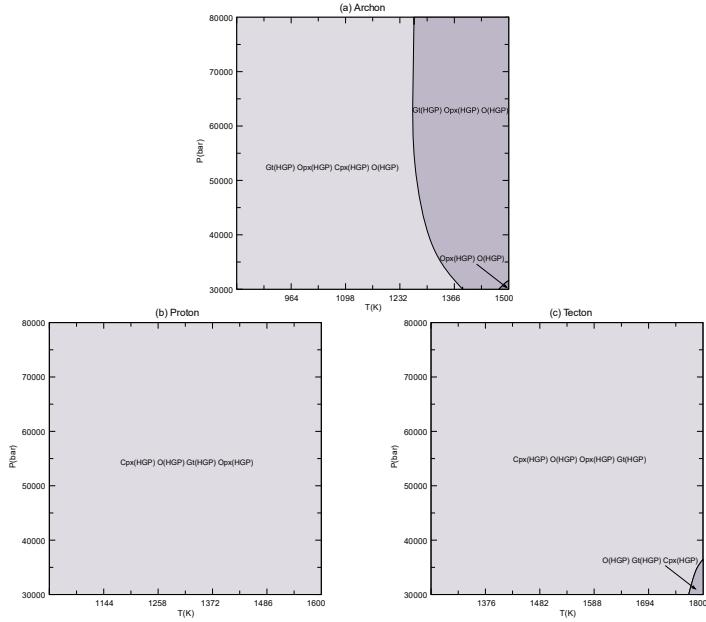
$$K_{T0} = K_{S0}/(1 + \alpha\gamma T) \quad (14),$$

$$\left(\frac{\partial K_T}{\partial P}\right)_T = (1 + \alpha\gamma T)^{-1} \times \left(\left(\frac{\partial K_S}{\partial P}\right)_T - \gamma T/K_{T0}(T) \left(\frac{\partial K_T}{\partial T}\right)_P\right) \quad (15),$$

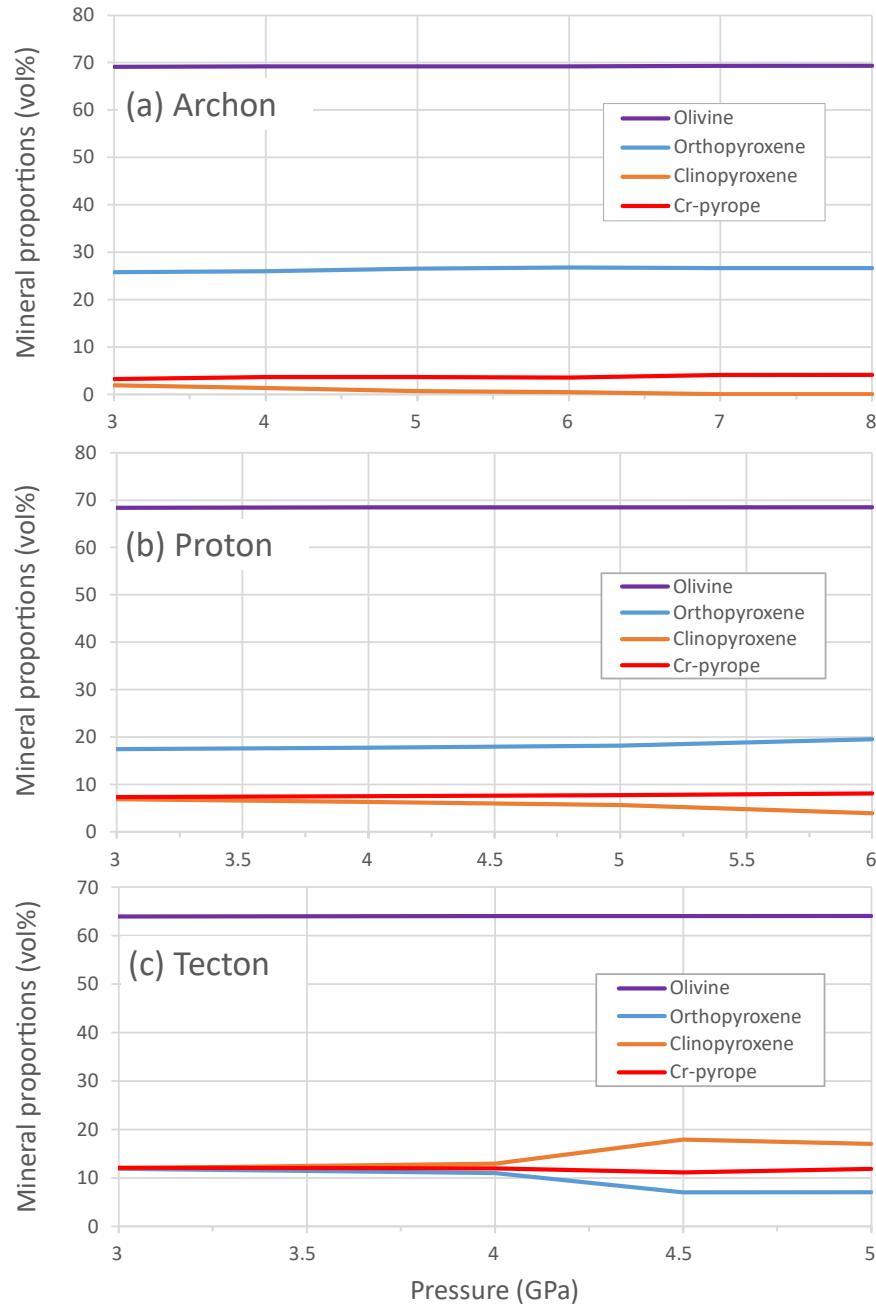
$$\left(\frac{\partial K_T}{\partial T}\right)_P = \left(\frac{\partial K_S}{\partial T}\right)_P - \alpha\gamma T/(1 + \alpha\gamma T) \quad (16),$$

where  $G_0(T)$  is the shear modulus at room  $P$  and temperature  $T$ ,  $G_0$  is the shear modulus at room  $P-T$ ,  $\left(\frac{\partial G}{\partial T}\right)_P$  is the temperature derivative of  $G$ ,  $K_{T0}(T)$  is the isothermal bulk modulus at room- $P$  and  $T$ ,  $\left(\frac{\partial G}{\partial P}\right)_T$  is the first-order pressure derivative of  $G$  at  $T$ ,  $\left(\frac{\partial^2 G}{\partial P^2}\right)_T$  is the second-order pressure derivative of  $G$ ,  $\left(\frac{\partial K_T}{\partial P}\right)_T$  is the pressure derivative of the isothermal bulk modulus at  $T$ ,  $\left(\frac{\partial G}{\partial P}\right)_{T_{ref}}$  is the pressure derivative of  $G$  at  $T_{ref}$ ,  $K_{T0}$  is the isothermal bulk modulus at room  $P-T$ ,  $\gamma$  is the Grüneisen

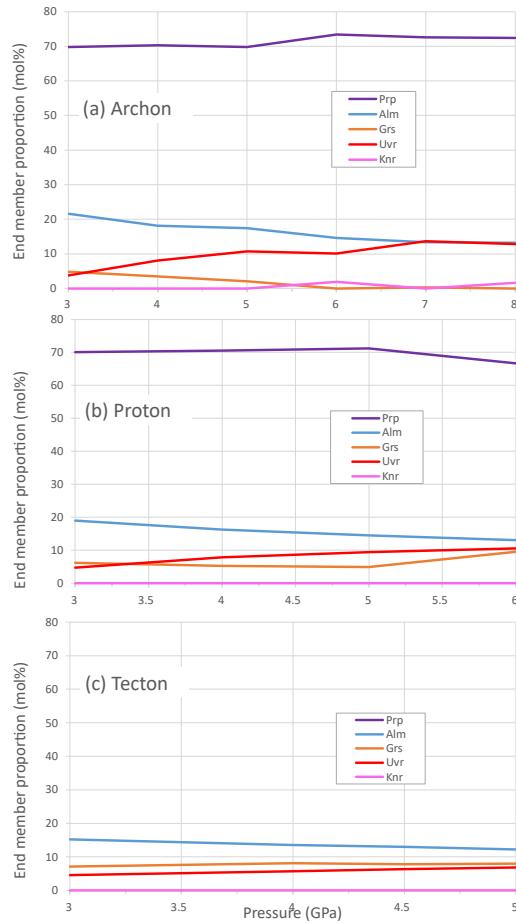
parameter,  $\left(\frac{\partial K_T}{\partial P}\right)_T$  is the pressure derivative of the isothermal bulk modulus at  $T$ , and  $\left(\frac{\partial K_T}{\partial T}\right)_P$  is the temperature derivative of the isothermal bulk modulus.



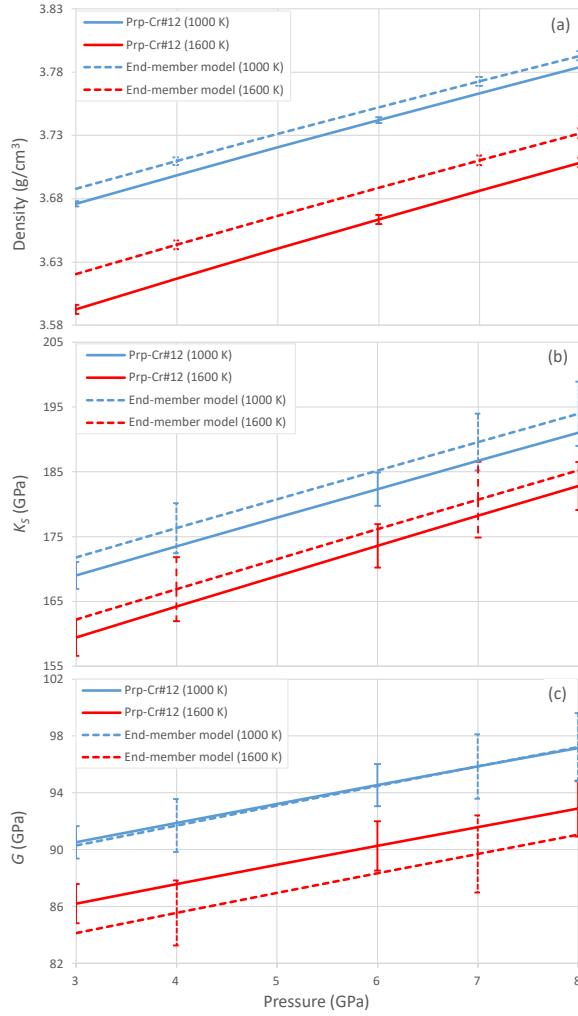
**Figure S1.** The calculated phase diagrams using Perple\_X for the Archon (a), Proton (b), and Tecton (c) SCLM. O-olivine; Opx-orthopyroxene; Cpx-clinopyroxene; Gt-garnet. HGP means the used solution model.



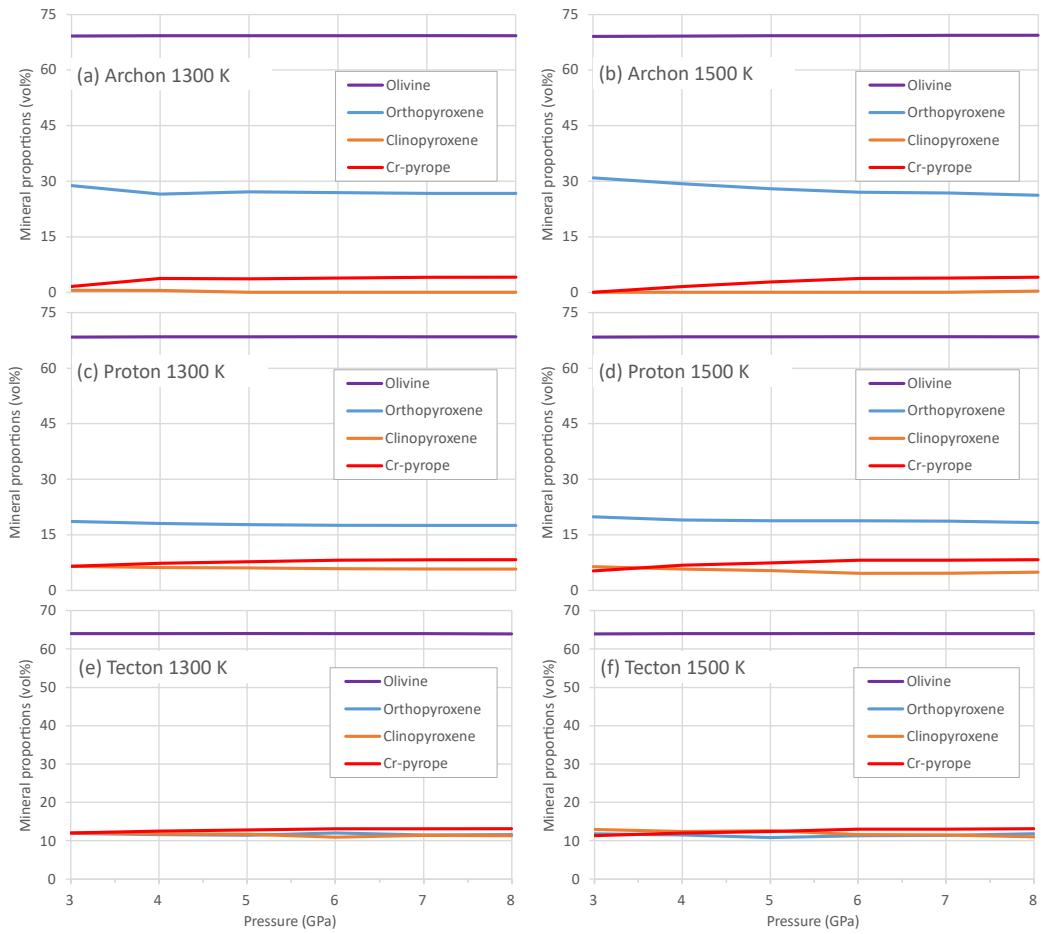
**Figure S2.** Calculated mineral proportions of three SCLMs, (a) Archon (3-8 GPa), (b) Proton (3-6 GPa), and (c) Tecton (3-5 GPa). The used bulk compositions of the SCLMs are extracted from Griffin et al. (2009), and the used geotherms are taken from Deen et al. (2006).



**Figure S3.** End-member proportions of Cr-pyrope in the Archon (a; 3-8 GPa), Proton (b; 3-6 GPa) and Tecton (c; 3-5 GPa). Prp, Alm, Grs, Uvr and Knr represent pyrope, almandine, grossular, uvarovite and knorringite, respectively.



**Figure S4.** Density  $\rho$  (a), bulk modulus  $K_S$  (b) and shear modulus  $G$  (c) of Prp-Cr#12 along isotherms at 1000 K and 1600 K over 3-8 GPa. The solid curves represent values calculated using the elastic parameters (Table S3) fitted to the Prp-Cr#12 data. The dashed curves represent values calculated using the end-member model (linear average of garnet end-member parameters; Table S4) elastic parameters determined for the Prp-Cr#12 composition. Error bars are shown at selected pressures.



**Figure S5.** Calculated mineral proportions of three SCLMs, (a) Archon, (b) Proton, and (c) Tecton at 3–8 GPa along isotherms at 1300 K and 1500 K. The major-element compositions of the SCLMs are extracted from Griffin et al. (2009).

**Table S1.** Average compositions of the Archon, Proton, and Tecton SCLM adopted from Griffin et al. (2009), which are used for the Perple\_X calculation

Oxide (wt.%)	Archon	Proton	Tecton
SiO <sub>2</sub>	45.7	44.7	44.5
Al <sub>2</sub> O <sub>3</sub>	0.99	2.1	3.5
FeO	6.4	7.9	8.0
MgO	45.5	42.4	39.8
CaO	0.59	1.9	3.1
Na <sub>2</sub> O	0.07	0.15	0.24
Cr <sub>2</sub> O <sub>3</sub>	0.28	0.42	0.40

**Note:** other minor components (e.g., TiO<sub>2</sub>, MnO) are not considered in the Perple\_X calculation.



**Table S3.** Chemical Composition of the Cr-pyrope in this study

Oxide (wt.%)	Prp-Cr#12
SiO <sub>2</sub>	41.77(58)
TiO <sub>2</sub>	0.09(3)
Al <sub>2</sub> O <sub>3</sub>	19.91(23)
FeO <sup>a</sup>	6.39(4)
MnO	0.33(3)
MgO	20.15(24)
CaO	6.18(4)
Na <sub>2</sub> O	0.01(1)
K <sub>2</sub> O	0.00(0)
Cr <sub>2</sub> O <sub>3</sub>	4.33(6)
NiO	0.01(2)
Total	99.20(100)

Numbers in parenthesis represent standard deviations

<sup>a</sup> All Fe as FeO







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