

Garnet and spinel in fertile and depleted mantle: insights from thermodynamic modelling

Contributions to Mineralogy and Petrology

Luca Ziberna, Paolo Nimis, Stephan Klemme

Corresponding author: Luca Ziberna

Dipartimento di Geoscienze, Università di Padova, Italy

Bayerisches Geoinstitut, Universität Bayreuth, Germany

luca.ziberna@uni-bayreuth.de

Supplementary Table S1 – Thermodynamic data for Cr-bearing minerals

Data are the same as in Klemme et al. (2009), except for those in *italics*, which were slightly modified in order to improve the agreement of the model with existing experimental data in Cr-bearing systems.

Thermodynamic endmember data:

	S_{298° J mol ⁻¹ K ⁻¹	$\Delta_f H$ J mol ⁻¹	V J bar ⁻¹	a J mol ⁻¹ K ⁻¹	b J mol ⁻¹ K ⁻²	c J K mol ⁻¹	d J mol ⁻¹ K ^{-0.5}
FeCr ₂ O ₄	152.2	-1332863	4.441	139.75	0.294 x 10 ⁻¹	-3359576	474.8
MgCr ₂ O ₄	119.6	-1650534	4.356	221.24	-0.10203 x 10 ⁻²	-1757210	-1247.9
Cr ₂ O ₃	83.1	-1046177	2.9054	227.25	-0.2132 x 10 ⁻¹	3543029	-2567.3
ortho- MgCr ₂ SiO ₆	<i>305</i>	<i>-2352378</i>	<i>5.79</i>	220.0	0.47 x 10 ⁻²	-3780000	-1016.0
clino- MgCr ₂ SiO ₆	<i>305</i>	<i>-2479446</i>	<i>6.31</i>	196.2	0.18 x 10 ⁻²	-5163200	-226.4
Mg ₃ Cr ₂ Si ₃ O ₁₂	357.9	-5275960	11.318	633.5	0	-5196.1	-4375

S_{298° is the standard entropy, $\Delta_f H$ the enthalpy of formation and V the volume at 1 bar. Parameters a, b, c, and d are the coefficients in the heat capacity polynomial $C_p = a + bT + cT^{-2} + dT^{-0.5}$.

Solid solution parameters:

	W ^a	W ^b	W ^c
Al ₂ O ₃ – Cr ₂ O ₃ (corundum–eskolaite)	37484	4.334	0.0386
MgAl ₂ O ₄ – MgCr ₂ O ₄ (spinel–magnesiochromite)	19686	0.463	0.0183
Mg ₃ Al ₂ Si ₃ O ₁₂ – Mg ₃ Cr ₂ Si ₃ O ₁₂ (pyrope–knorringite)	<i>30000</i>	<i>0</i>	<i>0</i>

W^a, W^b and W^c are the terms of the Margules-type excess functions ($W = W^a + W^b T + W^c P$) used for non-ideal solutions. Ideal mixing of Cr and Al was assumed for pyroxenes. Data sources: Oka et al. (1984), Chatterjee et al. (1982).