



Geochemistry, Geophysics, Geosystems

Supporting Information for

HighPGibbs, a practical tool for fluid-rock thermodynamic simulation in deep earth and its application on calculating nitrogen speciation in subduction zone fluids

Richen Zhong ^{a*}, Yanxia Li ^a, Barbara Etschmann ^b, Joël Brugger ^{b,c}, Chang Yu ^a, Hao Cui ^a

^a Civil and Resource Engineering School, University of Science and Technology Beijing, Beijing 100083, China

^b School of Earth, Atmosphere and the Environment, Monash University, Clayton, Victoria 3800, Australia

^c South Australian Museum, North Terrace, Adelaide, South Australia 5000, Australia

Contents of this file

Text S1 to S2

Introduction

This file contains all the species involved in the simulation (Table S1) and the mixing models of solid solutions (Table S2)

Table S1. Pure minerals and aqueous species included in the modelling.

Species		
Magnetite (Mt)	O ₂ (aq)	FeOH ⁺
Hematite (Hm)	SiO ₂ (aq)	FeO (aq)
Coesite (Coe)	Mg ²⁺	FeOH ²⁺
Quartz (Qt)	MgOH ⁺	FeO ⁺
Sillimanite (Sil)	Mg(HSiO ₃) ⁺	HFeO ₂ (aq)
Kyanite (Ky)	Al ³⁺	FeO ₂ ⁻
Lawsonite (Law)	AlOH ²⁺	N ₂ (aq)
H ₂ O	Al(OH) ₂ ⁺	NH ₄ ⁺
H ⁺	AlO ₂ ⁻	NH ₃ (aq)
OH ⁻	HAIO ₂ (aq)	
H ₂ (aq)	Fe ²⁺	

Table S2. Solid solutions used in the modelling. The thermodynamic properties of end members are from [Holland and Powell \(1998\)](#) and mixing parameters are from [White et al. \(2007\)](#), [Green et al. \(2007\)](#) and [Jennings and Holland \(2015\)](#).

Mineral	End member	Formula	Activity model
Orthopyroxene (Opx)	enstatite	Mg ₂ Si ₂ O ₆	Symmetrical $W_{\text{enstatite}} - W_{\text{ferrosilite}} = 6.8$
	ferrosilite	Fe ₂ Si ₂ O ₆	
Clinopyroxene (Cpx)	diopside	CaMgSi ₂ O ₆	Symmetrical $W_{\text{diopside}} - W_{\text{hedenbergite}} = 4$ $W_{\text{diopside}} - W_{\text{jadeite}} = 26$ $W_{\text{diopside}} - W_{\text{acmite}} = 15$ $W_{\text{jadeite}} - W_{\text{hedenbergite}} = 24$ $W_{\text{acmite}} - W_{\text{hedenbergite}} = 14$ $W_{\text{jadeite}} - W_{\text{acmite}} = 5$
	hedenbergite	CaFeSi ₂ O ₆	
	jadeite	NaAlSi ₂ O ₆	
	acmite	NaFeSi ₂ O ₆	

Garnet (Gt)	almandine	$\text{Fe}_3\text{Al}_2\text{Si}_3\text{O}_{12}$	Symmetrical
	pyrope	$\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$	$W_{\text{almandine}} - W_{\text{pyrope}} = 2.5$
	grossular	$\text{Ca}_3\text{Al}_2\text{Si}_3\text{O}_{12}$	$W_{\text{almandine}} - W_{\text{grossular}} = 10$
	andradite	$\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$	$W_{\text{almandine}} - W_{\text{andradite}} = 75$ $W_{\text{pyrope}} - W_{\text{grossular}} = 45$ $W_{\text{pyrope}} - W_{\text{andradite}} = 90$ $W_{\text{grossular}} - W_{\text{andradite}} = 0$
Chlorite (Chl)	daphnite	$\text{Fe}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_4$	Symmetrical
	Al-free chlorite	$\text{Mg}_6\text{Si}_4\text{O}_{10}(\text{OH})_4$	$W_{\text{daphnite}} - W_{\text{Al-free chlorite}} = 14.5$
	amesite	$\text{Mg}_4\text{Al}_4\text{Si}_2\text{O}_{10}(\text{OH})_4$	$W_{\text{daphnite}} - W_{\text{amesite}} = 13.5$
	clinochlore	$\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_4$	$W_{\text{daphnite}} - W_{\text{clinochlore}} = 2.5$ $W_{\text{Al-free chlorite}} - W_{\text{amesite}} = 20$ $W_{\text{Al-free chlorite}} - W_{\text{clinochlore}} = 18$ $W_{\text{amesite}} - W_{\text{clinochlore}} = 18$
Talc (Tc)	talc	$\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$	Ideal
	Fe-talc	$\text{Fe}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$	
Epidote (Ep)	clinozoisite	$\text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH})$	Symmetrical
	epidote	$\text{Ca}_2\text{FeAl}_2\text{Si}_3\text{O}_{12}(\text{OH})$	$W_{\text{clinozoisite}} - W_{\text{epidote}} = 0$
	Fe-epidote	$\text{Ca}_2\text{Fe}_2\text{AlSi}_3\text{O}_{12}(\text{OH})$	$W_{\text{clinozoisite}} - W_{\text{Fe-epidote}} = 15.4$ $W_{\text{epidote}} - W_{\text{Fe-epidote}} = 3$

References:

- Holland, T. J. B. and Powell, R., 1998. An internally consistent thermodynamic data set for phases of petrological interest. *J Metamorph Geol* 16, 309–343.
- Jennings, E. S. and Holland, T. J. B., 2015. A simple thermodynamic model for melting of peridotite in the system NCFMASOCr. *J Petrol* 56, 869–892.

- White, R. W., Powell, R., and Holland, T. J. B., 2007. Progress relating to calculation of partial melting equilibria for metapelites. *J Metamorph Geol* 25, 511-527.
- Green, E., Holland, T., and Powell, R., 2007. An order-disorder model for omphacitic pyroxenes in the system jadeite-diopside-hedenbergite-acmite, with applications to eclogitic rocks. *Am Mineral* 92, 1181-1189.