

symbol	meaning
P	pressure
T	temperature
a	activity
x	composition
a_i^j	activity of end-member i in phase j
x_i	composition variable, $\frac{\text{Fe}}{\text{Fe}+\text{Mg}}$, for phase i
y_i	composition variable relating to Tschermak's substitution for phase i
R	gas constant (0.0083144 kJ K ⁻¹)
ΔG_k°	Gibbs energy of reaction for reaction k
n	number of components in a model system
p	number of phases in an equilibrium
s	total number of end-members in the phases in an equilibrium
c	number of composition variables set (i.e. given values) in an equilibrium
v	variance
p_j	modal proportion of phase j in an equilibrium
x_i^j	proportion of end-member i in phase j
c_i^j	number of molecules of component i in end-member j
$x_{i,j}$	site fraction of element i on site j
σ	standard deviation
$[k]$	reaction not involving phase k (i.e. k -out)
x^n	in datafile listings, means x to the power of n

Summary of notation used in Holland & Powell (1998).

T	temperature
P	pressure
R	gas constant (0.0083144 kJ K ⁻¹)
α	thermal expansion
a°	thermal expansion parameter
V	molar volume
G	molar Gibbs free energy
H	molar enthalpy
S	molar entropy
A_T	molar property A at temperature of interest
A_{298}	molar property A at 298 K
ΔA	change in molar property A for a reaction
$\Delta_f H$	molar enthalpy of formation from the elements
$\Delta_f G$	molar Gibbs energy of formation from the elements
σ_i	standard deviation of i
V_{vir}	volume contribution from a virial-like EOS
V_{MRK}	volume contribution from the Modified Redlich Kwong EOS
K	equilibrium constant
κ	bulk modulus
κ'	pressure derivative of the bulk modulus
ρ	density of H ₂ O
β	compressibility of H ₂ O
$f_{\text{H}_2\text{O}}$	fugacity of H ₂ O
C_p	heat capacity at constant pressure
C_v	heat capacity at constant volume
T_c	critical temperature in the Landau model
T_c°	critical temperature in the Landau model at 1 bar
Q	order parameter in the Landau model
S_{max}	maximum entropy of disorder in the Landau model
V_{max}	maximum volume of disorder in the Landau model
G_{excess}	excess Gibbs free energy
G_{equil}	equilibrium Gibbs free energy
h'_{298}	excess enthalpy at 298 K from Landau model disordering
s'_{298}	excess entropy at 298 K from Landau model disordering
v'_T	excess volume from Landau model disordering at the temperature of interest
X_j^k	mole fraction of element i on site k in a crystal
y	compositional parameter for an end-member in a solid solution
p_i	molar proportion of end-member species i in a solid solution
a_i	activity of component i in a solution
a_i^{ideal}	ideal activity of component i in a solution
γ_i	activity coefficient of component i
w_{ij}	macroscopic interaction energy in the ij binary
m_i	molality of component i in an aqueous solution

Summary of mineral abbreviations (*pace* Kretz).

q	quartz
chl	chlorite
ctd	chloritoid
st	staurolite
cd	cordierite
g	garnet
opx	orthopyroxene
sp	hercynitic spinel
bi	biotite
mu	muscovite
ksp	K-feldspar <i>sensu lato</i>
pl	plagioclase
hb	hornblende <i>sensu lato</i>
gl	glaucophane
oa	orthoamphibole
o	omphacite
law	lawsonite
cc	calcite
dol	dolomite <i>sensu lato</i>
liq	silicate melt
H ₂ O	H ₂ O fluid

The **formulae** of the end-members of the phases in the internally-consistent data set (see Holland & Powell, 1998)

group	end-member	symbol	formula
ortho & ring silicates	akermanite	ak	$\text{Ca}_2\text{MgSi}_2\text{O}_7$
	almandine	alm	$\text{Fe}_3\text{Al}_2\text{Si}_3\text{O}_{12}$
	andalusite	and	Al_2SiO_5
	andradite	andr	$\text{Ca}_3\text{Fe}_2\text{Si}_3\text{O}_{12}$
	clinohumite	chum	$\text{Mg}_9\text{Si}_4\text{O}_{16}(\text{OH})_2$
	clinozoisite	cz	$\text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH})$
	cordierite	crd	$\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}$
	epidote (ordered)	ep	$\text{Ca}_2\text{FeAl}_2\text{Si}_3\text{O}_{12}(\text{OH})$
	fayalite	fa	Fe_2SiO_4
	Fe-chloritoid	fctd	$\text{FeAl}_2\text{SiO}_5(\text{OH})_2$
	Fe-cordierite	ferd	$\text{Fe}_2\text{Al}_4\text{Si}_5\text{O}_{18}$
	Fe-epidote	fep	$\text{Ca}_2\text{Fe}_2\text{AlSi}_3\text{O}_{12}(\text{OH})$
	Fe-osumilite	fosm	$\text{KFe}_2\text{Al}_5\text{Si}_{10}\text{O}_{30}$
	Fe-staurolite	fst	$\text{Fe}_4\text{Al}_{18}\text{Si}_{7.5}\text{O}_{48}\text{H}_4$
	forsterite	fo	Mg_2SiO_4
	gehlenite	geh	$\text{Ca}_2\text{Al}_2\text{SiO}_7$
	grossular	gr	$\text{Ca}_3\text{Al}_2\text{Si}_3\text{O}_{12}$
	hydrous cordierite	hcrd	$\text{Mg}_2\text{Al}_4\text{Si}_5\text{O}_{18}\cdot\text{H}_2\text{O}$
	hydroxy-topaz	tpz	$\text{Al}_2\text{SiO}_4(\text{OH})_2$
	kyanite	ky	Al_2SiO_5
	larnite-bredigite	larn	Ca_2SiO_4
	lawsonite	law	$\text{CaAl}_2\text{Si}_2\text{O}_7(\text{OH})_2\cdot\text{H}_2\text{O}$
	merwinite	merw	$\text{Ca}_3\text{MgSi}_2\text{O}_8$
	Mg-chloritoid	mctd	$\text{MgAl}_2\text{SiO}_5(\text{OH})_2$
	Mg-staurolite	mst	$\text{Mg}_4\text{Al}_{18}\text{Si}_{7.5}\text{O}_{48}\text{H}_4$
	Mn-chloritoid	mnctd	$\text{MnAl}_2\text{SiO}_5(\text{OH})_2$
	Mn-cordierite	mnrd	$\text{Mn}_2\text{Al}_4\text{Si}_5\text{O}_{18}$
	Mn-staurolite	mnst	$\text{Mn}_4\text{Al}_{18}\text{Si}_{7.5}\text{O}_{48}\text{H}_4$
	monticellite	mont	CaMgSiO_4
	osumilite(1)	osm1	$\text{KMg}_2\text{Al}_5\text{Si}_{10}\text{O}_{30}$
	osumilite(2)	osm2	$\text{KMg}_3\text{Al}_3\text{Si}_{11}\text{O}_{30}$
	phase A	phA	$\text{Mg}_7\text{Si}_2\text{O}_8(\text{OH})_6$
	pumpellyite	pump	$\text{Ca}_4\text{MgAl}_5\text{Si}_6\text{O}_{21}(\text{OH})_7$
	pyrope	py	$\text{Mg}_3\text{Al}_2\text{Si}_3\text{O}_{12}$
	rankinite	rnk	$\text{Ca}_3\text{Si}_2\text{O}_7$
	sillimanite	sill	Al_2SiO_5
	spessartine	spss	$\text{Mn}_3\text{Al}_2\text{Si}_3\text{O}_{12}$
	sphene	sph	CaTiSiO_5
	spurrite	spu	$\text{Ca}_5\text{Si}_2\text{O}_8(\text{CO}_3)$
	tephroite	teph	Mn_2SiO_4
	tilleyite	ty	$\text{Ca}_5\text{Si}_2\text{O}_7(\text{CO}_3)_2$
	vesuvianite	vsv	$\text{Ca}_{19}\text{Mg}_2\text{Al}_{11}\text{Si}_{18}\text{O}_{69}(\text{OH})_9$
	zircon	zrc	ZrSiO_4
	zoisite	zo	$\text{Ca}_2\text{Al}_3\text{Si}_3\text{O}_{12}(\text{OH})$

group	end-member	symbol	formula
pyroxenes & pyroxenoids	acmite	acm	$\text{NaFeSi}_2\text{O}_6$
	Ca-Tschermak pyroxene	cats	$\text{CaAl}_2\text{SiO}_6$
	diopside	di	$\text{CaMgSi}_2\text{O}_6$
	enstatite	en	$\text{Mg}_2\text{Si}_2\text{O}_6$
	ferrosilite	fs	$\text{Fe}_2\text{Si}_2\text{O}_6$
	hedenbergite	hed	$\text{CaFeSi}_2\text{O}_6$
	jadeite	jd	$\text{NaAlSi}_2\text{O}_6$
	Mg-Tschermak pyroxene	mgts	$\text{MgAl}_2\text{SiO}_6$
	pseudowollastonite	pswo	CaSiO_3
	pyroxmangite	pxmn	MnSiO_3
	rhodonite	rhod	MnSiO_3
	wollastonite	wo	CaSiO_3
	amphiboles	anthophyllite	anth
cummingtonite		cumm	$\text{Mg}_7\text{Si}_8\text{O}_{22}(\text{OH})_2$
Fe-anthophyllite		fanth	$\text{Fe}_7\text{Si}_8\text{O}_{22}(\text{OH})_2$
Fe-glaucophane		fgl	$\text{Na}_2\text{Fe}_3\text{Al}_2\text{Si}_8\text{O}_{22}(\text{OH})_2$
ferroactinolite		fact	$\text{Ca}_2\text{Fe}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$
gedrite (Na-free)		ged	$\text{Mg}_5\text{Al}_4\text{Si}_6\text{O}_{22}(\text{OH})_2$
glaucophane		gl	$\text{Na}_2\text{Mg}_3\text{Al}_2\text{Si}_8\text{O}_{22}(\text{OH})_2$
grunerite		grun	$\text{Fe}_7\text{Si}_8\text{O}_{22}(\text{OH})_2$
pargasite		parg	$\text{NaCa}_2\text{Mg}_4\text{Al}_3\text{Si}_6\text{O}_{22}(\text{OH})_2$
riebeckite		rieb	$\text{Na}_2\text{Fe}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$
tremolite		tr	$\text{Ca}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$
tschermakite		ts	$\text{Ca}_2\text{Mg}_3\text{Al}_4\text{Si}_6\text{O}_{22}(\text{OH})_2$
other chain silicates		deerite	deer
	Fe-carpholite	fcar	$\text{FeAl}_2\text{Si}_2\text{O}_6(\text{OH})_4$
	Fe-sapphirine (793)	fspr	$\text{Fe}_{3.5}\text{Al}_9\text{Si}_{1.5}\text{O}_{20}$
	Mg-carpholite	mcar	$\text{MgAl}_2\text{Si}_2\text{O}_6(\text{OH})_4$
	sapphirine (442)	spr4	$\text{Mg}_4\text{Al}_8\text{Si}_2\text{O}_{20}$
	sapphirine (793)	spr7	$\text{Mg}_{3.5}\text{Al}_9\text{Si}_{1.5}\text{O}_{20}$

group	end-member	symbol	formula
micas	annite	ann	$\text{KFe}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2$
	celadonite	cel	$\text{KMgAlSi}_4\text{O}_{10}(\text{OH})_2$
	eastonite	east	$\text{KMg}_2\text{Al}_3\text{Si}_2\text{O}_{10}(\text{OH})_2$
	Fe-celadonite	fcel	$\text{KFeAlSi}_4\text{O}_{10}(\text{OH})_2$
	margarite	ma	$\text{CaAl}_4\text{Si}_2\text{O}_{10}(\text{OH})_2$
	Mn-biotite	mnbi	$\text{KMn}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2$
	muscovite	mu	$\text{KAl}_3\text{Si}_3\text{O}_{10}(\text{OH})_2$
	Na-phlogopite	naph	$\text{NaMg}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2$
	paragonite	pa	$\text{NaAl}_3\text{Si}_3\text{O}_{10}(\text{OH})_2$
	phlogopite	phl	$\text{KMg}_3\text{AlSi}_3\text{O}_{10}(\text{OH})_2$
	chlorites	Al-free chlorite	afchl
amesite (14 Ang)		ames	$\text{Mg}_4\text{Al}_4\text{Si}_2\text{O}_{10}(\text{OH})_4$
clinocllore (ordered)		clin	$\text{Mg}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_4$
daphnite		daph	$\text{Fe}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_4$
Fe-sudoite		fsud	$\text{Fe}_2\text{Al}_4\text{Si}_3\text{O}_{10}(\text{OH})_4$
Mn-chlorite		mnchl	$\text{Mn}_5\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_4$
sudoite		sud	$\text{Mg}_2\text{Al}_4\text{Si}_3\text{O}_{10}(\text{OH})_4$
other sheet silicates	antigorite	atg	$\text{Mg}_{48}\text{Si}_{34}\text{O}_{85}(\text{OH})_{62}$
	chrysotile	chr	$\text{Mg}_3\text{Si}_2\text{O}_5(\text{OH})_2$
	Fe-talc	fta	$\text{Fe}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$
	kaolinite	kao	$\text{Al}_2\text{Si}_2\text{O}_5(\text{OH})_4$
	prehnite	pre	$\text{Ca}_2\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_2$
	pyrophyllite	prl	$\text{Al}_2\text{Si}_4\text{O}_{10}(\text{OH})_2$
	talc	ta	$\text{Mg}_3\text{Si}_4\text{O}_{10}(\text{OH})_2$
	tschermak-talc	tats	$\text{Mg}_2\text{Al}_2\text{Si}_3\text{O}_{10}(\text{OH})_2$
framework silicates	albite	ab	$\text{NaAlSi}_3\text{O}_8$
	analcite	anl	$\text{NaAlSi}_2\text{O}_6 \cdot \text{H}_2\text{O}$
	anorthite	an	$\text{CaAl}_2\text{Si}_2\text{O}_8$
	coesite	coe	SiO_2
	cristobalite	crst	SiO_2
	heulandite	heu	$\text{CaAl}_2\text{Si}_7\text{O}_{18} \cdot 6\text{H}_2\text{O}$
	high albite	abh	$\text{NaAlSi}_3\text{O}_8$
	kalsilite	kals	KAlSiO_4
	laumontite	lmt	$\text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot 4\text{H}_2\text{O}$
	leucite	lc	KAlSi_2O_6
	meionite	me	$\text{Ca}_4\text{Al}_6\text{Si}_6\text{O}_{24}(\text{CO}_3)$
	microcline	mic	KAlSi_3O_8
	nepheline	ne	NaAlSiO_4
	quartz	q	SiO_2
	sanidine	san	KAlSi_3O_8
	stilbite	stlb	$\text{CaAl}_2\text{Si}_7\text{O}_{18} \cdot 7\text{H}_2\text{O}$
	stishovite	stv	SiO_2
	tridymite	trd	SiO_2
wairakite	wrk	$\text{CaAl}_2\text{Si}_4\text{O}_{12} \cdot \text{H}_2\text{O}$	

group	end-member	symbol	formula
oxides	baddeleyite	bdy	ZrO ₂
	corundum	cor	Al ₂ O ₃
	geikielite	geik	MgTiO ₃
	hematite	hem	Fe ₂ O ₃
	hercynite	herc	FeAl ₂ O ₄
	ilmenite	ilm	FeTiO ₃
	lime	lime	CaO
	magnesioferrite	mft	MgFe ₂ O ₄
	magnetite	mt	Fe ₃ O ₄
	manganosite	mang	MnO
	nickel oxide	NiO	NiO
	periclase	per	MgO
	pyrophanite	pnt	MnTiO ₃
	rutile	ru	TiO ₂
	spinel	sp	MgAl ₂ O ₄
	ulvospinel	usp	Fe ₂ TiO ₄
hydroxides	brucite	br	Mg(OH) ₂
	diaspore	dsp	AlO(OH)
	goethite	gth	FeO(OH)
carbonates	ankerite	ank	CaFe(CO ₃) ₂
	aragonite	arag	CaCO ₃
	calcite	cc	CaCO ₃
	dolomite	dol	CaMg(CO ₃) ₂
	magnesite	mag	MgCO ₃
	rhodochrosite	rhc	MnCO ₃
	siderite	sid	FeCO ₃
elements	diamond	diam	C
	graphite	gph	C
	iron	iron	Fe
	nickel	Ni	Ni
gas species	carbon dioxide	CO2	CO ₂
	carbon monoxide	CO	CO
	hydrogen	H2	H ₂
	methane	CH4	CH ₄
	oxygen	O2	O ₂
	water fluid	H2O	H ₂ O

group	end-member	symbol	formula	
melt species	albite liquid	abL	NaAlSi ₃ O ₈	
	anorthite liquid	anL	CaAl ₂ Si ₂ O ₈	
	diopside liquid	diL	CaMgSi ₂ O ₆	
	enstatite liquid	enL	Mg ₂ Si ₂ O ₆	
	fayalite liquid	faL	Fe ₂ SiO ₄	
	Fe-liquid (in KFMASH)	fliq	K ₃ Fe _{0.5} Al ₄ Si _{19.5} O ₄₇	
	forsterite liquid	foL	Mg ₂ SiO ₄	
	H ₂ O liquid	h2oL	H ₂ O	
	H ₂ O liquid (in KFMASH)	hliq	H ₂ O	
	K-feldspar liquid	kspL	KAlSi ₃ O ₈	
	Mg-liquid (in KFMASH)	mliq	K ₃ Mg _{0.5} Al ₄ Si _{19.5} O ₄₇	
	silica liquid	qL	SiO ₂	
	sillimanite liquid	silL	Al ₂ SiO ₅	
	aqueous species	H ⁺ (aq)	H+	H ⁺
		Cl ⁻ (aq)	Cl-	Cl ⁻
OH ⁻ (aq)		OH-	OH ⁻	
Na ⁺ (aq)		Na+	Na ⁺	
K ⁺ (aq)		K+	K ⁺	
Ca ²⁺ (aq)		Ca++	Ca ²⁺	
Mg ²⁺ (aq)		Mg++	Mg ²⁺	
Fe ²⁺ (aq)		Fe++	Fe ²⁺	
Al ³⁺ (aq)		Al+++	Al ³⁺	
CO ₃ ²⁻ (aq)		CO3-	CO ₃ ²⁻	
Al(OH) ₃ ^o (aq)		AlOH3	Al(OH) ₃	
Al(OH) ₄ ⁻ (aq)		AlOH4-	Al(OH) ₄ ⁻	
KOH ^o (aq)		KOH	KOH	
HCl ^o (aq)		HCl	HCl	
KCl ^o (aq)		KCl	KCl	
NaCl ^o (aq)		NaCl	NaCl	
CaCl ₂ ^o (aq)		CaCl2	CaCl ₂	
CaCl ⁺ (aq)		CaCl+	CaCl ⁺	
MgCl ₂ ^o (aq)		MgCl2	MgCl ₂	
MgCl ⁺ (aq)		MgCl+	MgCl ⁺	
FeCl ₂ ^o (aq)		FeCl2	FeCl ₂	
aqueous silica		aqSi	SiO ₂	

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