Formulae of end-members in the 1998 dataset

Ortho & Ring Silicates		
forsterite	fo	Mg_2SiO_4
fayalite	fa	Fe_2SiO_4
tephroite	teph	Mn_2SiO_4
larnite-bredigite	lrn	Ca_2SiO_4
monticellite	mont	$CaMgSiO_4$
clinohumite	chum	$Mg_9Si_4O_{18}H_2$
pyrope	py	$Mg_3Al_2Si_3O_{12}$
almandine	alm	$Fe_3Al_2Si_3O_{12}$
spessartine	spss	$Mn_3Al_2Si_3O_{12}$
grossular	gr	$Ca_3Al_2Si_3O_{12}$
andradite	andr	$Ca_3Fe_2Si_3O_{12}$
osumilite(1)	osm1	$KMg_2Al_5Si_{10}O_{30}$
osumilite(2)	osm2	$KMg_3Al_3Si_{11}O_{30}$
Fe-osumilite	fosm	$KFe_2Al_5Si_{10}O_{30}$
vesuvianite	vsv	$Ca_{19}Mg_2Al_{11}Si_{18}O_{78}H_9$
andalusite	and	Al_2SiO_5
kyanite	ky	Al_2SiO_5
sillimanite	sill	Al_2SiO_5
hydroxy-topaz	tpz	$Al_2SiO_6H_2$
Mg-staurolite	mst	$Mg_4Al_{18}Si_{7.5}O_{48}H_4$
Fe-staurolite	fst	$Fe_4Al_{18}Si_{7.5}O_{48}H_4$
Mn-staurolite	mnst	$Mn_4Al_{18}Si_{7.5}O_{48}H_4$
Mg-chloritoid	mctd	$MgAl_2SiO_7H_2$
Fe-chloritoid	fctd	$FeAl_2SiO_7H_2$
Mn-chloritoid	mnctd	$MnAl_2SiO_7H_2$
merwinite	merw	$Ca_3MgSi_2O_8$
spurrite	spu	$Ca_5Si_2O_{11}C$
zoisite	zo	$Ca_2Al_3Si_3O_{13}H$
clinozoisite	cz	$Ca_2Al_3Si_3O_{13}H$
Fe-epidote	fep	$Ca_2Fe_2AlSi_3O_{13}H$
epidote	ep	$Ca_2FeAl_2Si_3O_{13}H$
lawsonite	law	$CaAl_2Si_2O_{10}H_4$
pumpellyite	pump	$Ca_4MgAl_5Si_6O_{28}H_7$
gehlenite	geh	$Ca_2Al_2SiO_7$
akermanite	ak	$Ca_2MgSi_2O_7$
rankinite	rnk	$Ca_3Si_2O_7$
tilleyite	ty	$Ca_5Si_2O_{13}C_2$
cordierite	crd	$Mg_2Al_4Si_5O_{18}$
hydrous cordierite	hcrd	$Mg_2Al_4Si_5O_{19}H_2$
Fe-cordierite	fcrd	$Fe_2Al_4Si_5O_{18}$
Mn-cordierite	mncrd	$Mn_2Al_4Si_5O_{18}$
phase A	phA	$Mg_7Si_2O_{14}H_6$
sphene	sph	$CaTiSiO_5$
zircon	zrc	$ZrSiO_4$

Chain Silicates		
enstatite	en	$Mg_2Si_2O_6$
ferrosilite	fs	$Fe_2Si_2O_6$
Mg-Tschermak pyroxene	mgts	$MgAl_2SiO_6$

diopside	di	$CaMgSi_2O_6$
hedenbergite	hed	$CaFeSi_2O_6$
jadeite	jd	$NaAlSi_2O_6$
acmite	acm	$NaFeSi_2O_6$
Ca-Tschermak pyroxene	cats	$CaAl_2SiO_6$
rhodonite	rhod	$MnSiO_3$
pyroxmangite	pxmn	$MnSiO_3$
wollastonite	wo	$CaSiO_3$
pseudowollastonite	pswo	$CaSiO_3$
tremolite	tr	$Ca_2Mg_5Si_8O_{24}H_2$
ferroactinolite	fact	$Ca_2Fe_5Si_8O_{24}H_2$
tschermakite	ts	$Ca_2Mg_3Al_4Si_6O_{24}H_2$
pargasite	parg	$NaCa_2Mg_4Al_3Si_6O_{24}H_2$
glaucophane	gl	$Na_2Mg_3Al_2Si_8O_{24}H_2$
Fe-glaucophane	fgl	$Na_2Fe_3Al_2Si_8O_{24}H_2$
riebeckite	rieb	$Na_2Fe_5Si_8O_{24}H_2$
anthophyllite	anth	$Mg_7Si_8O_{24}H_2$
Fe-anthophyllite	fanth	$Fe_7Si_8O_{24}H_2$
cummingtonite	cumm	$Mg_7Si_8O_{24}H_2$
grunerite	grun	$Fe_7Si_8O_{24}H_2$
gedrite	ged	$Mg_5Al_4Si_6O_{24}H_2$
sapphirine (442)	spr4	$Mg_4Al_8Si_2O_{20}$
sapphirine (793)	spr7	$Mg_{3.5}Al_9Si_{1.5}O_{20}$
Fe-sapphirine	fspr	$Fe_{3.5}Al_9Si_{1.5}O_{20}$
Mg-carpholite	mcar	$MgAl_2Si_2O_{10}H_4$
Fe-carpholite	fcar	$FeAl_2Si_2O_{10}H_4$
deerite	deer	$Fe_{18}Si_{12}O_{50}H_{10}$

Sheet Silicates

muscovite	mu	$KAl_3Si_3O_{12}H_2$
celadonite	cel	$KMgAlSi_4O_{12}H_2$
Fe-celadonite	fcel	$KFeAlSi_4O_{12}H_2$
paragonite	pa	$NaAl_3Si_3O_{12}H_2$
margarite	ma	$CaAl_4Si_2O_{12}H_2$
phlogopite	phl	$KMg_3AlSi_3O_{12}H_2$
annite	ann	$KFe_3AlSi_3O_{12}H_2$
Mn-biotite	mnbi	$KMn_3AlSi_3O_{12}H_2$
eastonite	east	$KMg_2Al_3Si_2O_{12}H_2$
Na-phlogopite	naph	$NaMg_3AlSi_3O_{12}H_2$
clinochlore	clin	$Mg_5Al_2Si_3O_{18}H_8$
amesite	ames	$Mg_4Al_4Si_2O_{18}H_8$
Al-free chlorite	afchl	$Mg_6Si_4O_{18}H_8$
daphnite	daph	$Fe_5Al_2Si_3O_{18}H_8$
Mn-chlorite	mnchl	$Mn_5Al_2Si_3O_{18}H_8$
sudoite	sud	$Mg_2Al_4Si_3O_{18}H_8$
Fe-sudoite	fsud	$Fe_2Al_4Si_3O_{18}H_8$
pyrophyllite	prl	$Al_2Si_4O_{12}H_2$
talc	ta	$Mg_3Si_4O_{12}H_2$
Fe-talc	fta	$Fe_3Si_4O_{12}H_2$
tschermak-talc	tats	$Mg_2Al_2Si_3O_{12}H_2$
kaolinite	kao	$Al_2Si_2O_9H_4$
prehnite	pre	$Ca_2Al_2Si_3O_{12}H_2$
chrysotile	chr	$Mg_3Si_2O_9H_4$

antigorite	atg	$Mg_{48}Si_{34}O_{147}H_{62}$
Framework Silicates		
albite	ab	$NaAlSi_3O_8$
high albite	abh	$NaAlSi_3O_8$
microcline	mic	$KAlSi_3O_8$
sanidine	san	$KAlSi_3O_8$
anorthite	an	$CaAl_2Si_2O_8$
quartz	q	SiO_2
tridymite	trd	SiO_2
cristobalite	crst	SiO_2
coesite	coe	SiO_2
stishovite	stv	SiO_2
nepheline	ne	$NaAlSiO_4$
kalsilite	kals	$KAlSiO_4$
leucite	lc	$KAlSi_2O_6$
meionite	me	$Ca_4Al_6Si_6O_{27}C$
wairakite	wrk	$CaAl_2Si_4O_{14}H_4$
laumontite	lmt	$CaAl_2Si_4O_{16}H_8$
heulandite	heu	$CaAl_2Si_7O_{24}H_{12}$
stilbite	stlb	$CaAl_2Si_7O_{25}H_{14}$
analcite	anl	$NaAlSi_2O_7H_2$
Oxides & Hydroxides		
lime	lime	CaO
rutile	ru	TiO_2
periclase	per	MgO
manganosite	mang	MnO
corundum	cor	Al_2O_3
hematite	hem	Fe_2O_3
nickel oxide	NiO	NiO
pyrophanite	pnt	$MnTiO_3$
geikielite	geik	$MgTiO_3$
ilmenite	ilm	$FeTiO_3$
baddeleyite	bdy	ZrO_2
spinel	sp	$MgAl_2O_4$
hercynite	herc	$FeAl_2O_4$
magnetite	mt	Fe_3O_4
magnesioferrite	mft	Fe_2MgO_4
ulvospinel	usp	Fe_2TiO_4
brucite	br	MgO_2H_2
diaspore	dsp	AlO_2H
goethite	gth	FeO_2H
Carbonates		
calcite	cc	$CaCO_3$
aragonite	arag	$CaCO_3$
magnesite	mag	$MgCO_3$
siderite	sid	$FeCO_3$
rhodochrosite	rhc	$MnCO_3$
dolomite	dol	$CaMg(CO_3)_2$
ankerite	ank	$CaFe(CO_3)_2$

Elements & Gases

iron	iron	Fe
nickel	Ni	Ni
graphite	gph	C
diamond	diam	C
water fluid	H2O	H_2O
carbon dioxide	CO2	CO_2
carbon monoxide	CO	OC
methane	CH4	CH_4
oxygen	O2	O_2
hydrogen	H2	H_2

Melt species

forsterite liquid	foL	Mg_2SiO_4
fayalite liquid	faL	Fe_2SiO_4
sillimanite liquid	silL	Al_2SiO_5
anorthite liquid	anL	$CaAl_2Si_2O_8$
H2O liquid	h2oL	H_2O
enstatite liquid	enL	$Mg_2Si_2O_6$
K-feldspar liquid	kspL	$KAlSi_3O_8$
Silica liquid	qL	SiO_2
diopside liquid	diL	$CaMgSi_2O_6$
albite liquid	abL	$NaAlSi_3O_8$
Mg-pelitic liquid	mliq	$K_3Mg_{0.5}Al_4Si_{19.5}O_{47}$
Fe-pelitic liquid	fliq	$K_3Fe_{0.5}Al_4Si_{19.5}O_{47}$
H2O pelitic liquid	hliq	H_2O

Aqueous species (e = electron)

hydrogen ion (aq)	H+	H e_{-1}
chloride ion (aq)	Cl-	Cl e
hydroxyl ion (aq)	OH-	OH e
sodium ion (aq)	Na+	Na e_{-1}
potassium ion (aq)	K+	K e_{-1}
calcium ion (aq)	Ca++	Ca e_{-2}
magnesium ion (aq)	Mg++	Mg e_{-2}
ferrous ion (aq)	Fe++	Fe e_{-2}
aluminium ion (aq)	Al+++	Al e_{-3}
carbonate ion (aq)	CO3--	CO_3 e_2
$Al(OH)_3$ (aq)	AlOH3	AlO_3H_3
$Al(OH)_4^-$ ion (aq)	AlOH4-	AlO_4H_4 e
KOH (aq)	KOH	KOH
HCl (aq)	HCl	HCl
KCl (aq)	KCl	KCl
NaCl (aq)	NaCl	NaCl
$CaCl_2$ (aq)	CaCl2	$CaCl_2$
$CaCl^+$ (aq)	CaCl+	CaCl e_{-1}
$MgCl_2$ (aq)	MgCl2	$MgCl_2$
$MgCl^+$ (aq)	MgCl+	MgCl e_{-1}
$FeCl_2$ (aq)	FeCl2	$FeCl_2$
aqueous silica	aqSi	SiO_2