

Overview of the mineral recalculation schemes

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Allanite

Allanite

Description

Allanite formulae are calculated on the basis of 3 atoms.

Synonym names

The programme recognizes the following full names:

allanite,dissakisite

and abbreviations:

Aln,All

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si,Al,Ti,Cr,V,FeIII,FeII,Mg,Mn,Zn,Ca,Pb,Sr,Ba,Na,K,REE.all,Y,Th,F

Sites

The general formula of allanite is $A_2M_3T_3(OH)_{12}$.

Site allocation order is T, M, A, OH.

Site allocation

Site	Sum	Atoms
T	3	Si, Al
M	3	Ti, Al, Cr, V, Mg, Zn, FeIII, FeII, Mn
A	unspecified	Mn, FeII, Ca, Pb, Sr, Ba, Na, K, REE.all, Y, Th, Vc
OH	1	F, OH

Values

In addition are returned extra parameters by a script 'ree.sum.r':

REE,REE + Th

Alumosilicate

Alumosilicate

Description

Alumosilicate formulae are calculated on the basis of 5 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

kyanite,sillimanite,andalusite,mullite,viridine

and abbreviations:

Ky,Sil,Sill,And,ALS,alsi,Sil,Mul

Amphibole

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Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Cr, V, FeIII, Mn, Mg, Ti, Ca, Na, K

Sites

The general formula of aluminosilicate is $Al_2Si_1O_5$.

Site allocation order is Al, Si.

Site allocation

Site	Sum	Atoms
Al	unspecified	Al, Cr, V, FeIII, Mn, Mg, Ti, Ca, Na, K
Si	unspecified	Si

Amphibole

Amphibole

Description

Amphibole formulae are calculated on the basis of 23 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 13-CNK: 13 cations without Ca, Na and K.

Synonym names

The programme recognizes the following full names:

amphibole, actinolite, antigorite, antophyllite, arfvedsonite, anthophyllite, barroisite, cannilloite, clino-holmquistite, cummingtonite, edenite, eckermannite, ferro-actinolite, ferro-edenite, ferro-hornblende, ferro-tschermakite, gedrite, glaucophane, grunerite, hastingsite, holmquistite, hornblende, jeanlouisite, joesmithite, kaersutite, katophorite, leakeite, magnesiohornblende, magnesianriebeckite, obertite, papikeite, pargasite, pedrizite, riebeckite, sadanagaite, suenoite, taramite, tremolite, tschermakite, ungarettiite, winchite

and abbreviations:

Amp, Am, Act, Atg, Arf, Ath, Cum, Ed, Fac, Fed, Fts, Ged, Gln, Gru, Hbl, Hst, Hs, Krs, Mhbl, Mgb, Mg-Hbl, Mrb, Mg-Rbk, Mg-Rbk, Prg, Rbk, Tr, Ts, Amph, Amf, fact, parg, gl, fgl, rieb, anth, fanth, cumm, grun, law

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeII, FeIII, Ti, V, Cr, Mn, Zr, Mg, Zn, Ni, Co, Li, Ca, Sr, Ba, Na, K, F, Cl

Sites

The general formula of amphibole is $A_{0-1}B_2Z_5T_8O_{22}(OH)_2A_{0-1}B_2Z_5T_8O_{22}(OH)_2$.

Site allocation order is T, C, B, A, OH.

Site allocation

Site	Sum	Atoms
T	8	Si, Al, Ti
B	2	Li, Mn, FeII, Co, Ni, Zn, Mg, Zr, Cr, V, FeIII, Ti, Al, Ca, Sr, Ba, Na
A	1	Na, Ba, Sr, Ca, Al, Ti, FeIII, V, Cr, Mn, Zr, Mg, Zn, Ni, Co, FeII, Li, K, Vc
OH	2	F, Cl, OH

Values

In addition are returned extra parameters:

$$Siapfu = Si$$

$$Mg/(Mg + Fe^{II}) = Mg/(Mg + Fe^{II})$$

Apatite	<i>Apatite</i>
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Description

Apatite formulae are calculated on the basis of 12.5 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

apatite, chlorapatite, fluorapatite, hydroxylapatite, francolite

and abbreviations:

Ap, APA

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

P, Ca, FeII, Mn, Mg, As, V, Cr, S, Se, Be, Si, Ge, Sb, B, Sr, Pb, Ba, Ni, Co, Cu, Zn, Sn, Cd,

Na, K, REE.all, Y, Bi, Th, U, F, Cl

Sites

The general formula of apatite is $M_{10}(Z_1O_4)_6(OH)_2$.

Site allocation order is Z, M, OH.

Site allocation

Site	Sum	Atoms
Z	3	P, Si, As, V, S, Se, Be, Ge, Sb, B, Mn, Cr
M	unspecified	Ca, Sr, Pb, Ba, Mn, FeII, Mg, Ni, Co, Cu, Zn, Sn, Cd, Na, K, REE.all, Y, Bi, Cr, Th, U
OH	1	F, Cl, OH

End Members

The end members calculated are:

$$F_{Ap} = F_{OH}$$

$$Cl_{Ap} = Cl_{OH}$$

$$OH_{Ap} = OH_{OH}$$

Biotite	<i>Biotite</i>
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Description

Biotite formulae are calculated on the basis of 7 cations.

Synonym names

The programme recognizes the following full names:

biotite, phlogopite, annite, siderophyllite, eastonite

and abbreviations:

Bt, Phl, Ann, BIO, PHL, bt, east, mnbi, Phg

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Be, FeIII, Mg, Mn, Cr, Ti, FeII, Zn, V, K, Na, Ba, Li, Ca, Rb, Cs, Sr, F, Cl

Sites

The general formula of biotite is $I_1M_3T_4O_{10}(OH)_2$.

Site allocation order is T, M, I, OH.

Site allocation

Site	Sum	Atoms
T	4	Si, Be, Al, FeIII, Ti
M	3	Al, Mg, FeII, Mn, Cr, Ti, Zn, V, Li, FeIII, Vc
I	unspecified	K, Na, Ba, Ca, Rb, Cs, Sr
OH	2	F, Cl, OH

Carbonate	<i>Carbonate</i>
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Description

Carbonate formulae are calculated on the basis of 3 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

carbonate, calcite, dolomite, magnesite, strontianite, rhodochrosite, siderite, witherite,

ankerite, aragonite

and abbreviations:

Cb, Cal, Dol, Mgs, Str, Rds, Sd, Wth, Ank, cal, dol, cc, arag, mag, sid, rhc

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Ca, Mg, FeII, Mn, Sr, Ba, Pb, Zn, La, Ce, C

Sites

The general formula of carbonate is $M_1C_1O_3$.

Site allocation order is M, C.

Site allocation

Site	Sum	Atoms
M	unspecified	Ca, Mg, FeII, Mn, Sr, Ba, Pb, Zn, La, Ce
C	unspecified	C

Chlorite	<i>Chlorite</i>
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Description

Chlorite formulae are calculated on the basis of 28 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

chlorite, clinochlore, chamosite, pennantite, kammererite, baileychlore, nimate

and abbreviations:

Chl, CHL, Clin, Cham, Pnn, Chm, Nim

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeII, FeIII, Mg, Ti, Mn, Zn, Li, Cr, Ni, Co, F, Cl

Sites

The general formula of chlorite is $A_6T_4O_{10}(OH)_8$.

Site allocation order is T, A, OH.

Site allocation

Site	Sum	Atoms
T	8	Si, Al
A	12	Al, FeII, Mg, Ti, FeIII, Mn, Zn, Li, Cr, Ni, Co, Vc
OH	16	F, Cl, OH

End Members

The end members calculated are:

$Clinochlore = Mg / (Ni + Zn + Mg + Mn + Fe)$

Chloritoid

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$$\text{Chamosite} = Fe / (Ni + Zn + Mg + Mn + Fe)$$

$$\text{Pennantite} = Mn / (Ni + Zn + Mg + Mn + Fe)$$

$$\text{Baileychlore} = Zn / (Ni + Zn + Mg + Mn + Fe)$$

$$\text{Nimite} = Ni / (Ni + Zn + Mg + Mn + Fe)$$

Values

In addition are returned extra parameters:

$$Fe = Fe^{II} + Fe^{III}$$

Chloritoid	<i>Chloritoid</i>
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Description

Chloritoid formulae are calculated on the basis of 6 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 4 cations per formula unit (*Droop 1987*).

Synonym names

The programme recognizes the following full names:

chloritoid, ottrelite, sismondin

and abbreviations:

Cld, CLD, ctd, mctd, fctd, mnctd

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeIII, FeII, Mg, Mn, Ti, Ca, Na, K, Cl, F

Sites

The general formula of chloritoid is $X_1Y_2Si_1O_5(OH)_2$.

Site allocation order is Y, X, Si, OH.

Site allocation

Site	Sum	Atoms
Y	unspecified	Al, FeIII, Ti
X	unspecified	FeII, Mg, Mn, Ca, Na, K
Si	unspecified	Si
OH	2	F, Cl, OH

Values

In addition are returned extra parameters:

$$XFe^{II} = Fe^{II} / Sum_X$$

$$XMg = Mg / Sum_X$$

$$XMn = Mn / Sum_X$$

Clinopyroxene	<i>Clinopyroxene</i>
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Description

Clinopyroxene formulae are calculated on the basis of 6 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 4 cations per formula unit (*Droop 1987*).

Synonym names

The programme recognizes the following full names:

clinopyroxene, Ca clinopyroxene, aegirine, augite, burnettite, clinoenstatite, clinoferrosilite, colomeraite, davisite, diopside, esseneite, grossmanite, hedenbergite, jadeite, jervisite, johannsenite, kanoite, kosmochlor, kushiroite, namansilite, natalyite, omphacite, petedunnite, pigeonite, ryabchikovite, spodumene, tissintite and abbreviations:

Px, Cpx, Aeg, Ae, Aug, Cen, Cfs, Di, Hd, Jd, Jh, Jhnt, Omp, Pgt, Spd, mgts, hed, acm, cats, PYR

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeIII, FeII, Ti, Cr, V, Zr, Sc, Zn, Ni, Co, Mg, Mn, Li, Ca, Na, K

Sites

The general formula of clinopyroxene is $M2_1M1_1T_2O_6$.

Site allocation order is T, M1, M2.

Site allocation

Site	Sum	Atoms
T	2	Si, Al, FeIII
M1	1	Al, FeIII, Ti, Cr, V, Zr, Sc, Zn, Ni, Co, Mg, FeII, Mn
M2	unspecified	Mg, FeII, Mn, Li, Ca, Na, K

End Members

The end members calculated by a script 'clinopyroxene.end.r' are:

Jd, CaTs, CaTi, CrCaTs, DiHd, EnFs, Sum.end, En, Di

Values

In addition are returned extra parameters by a script 'clinopyroxene.r':

Fe, FeIII/Fetot, XMg, AlIV/AlVI, AlIV, AlVI, aDi

Cordierite

Cordierite

Description

Cordierite formulae are calculated on the basis of 18 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

cordierite, sekaninaite, ferrocordierite, ferro-cordierite, magnesiocordierite, magnesio-cordierite

and abbreviations:

Crd, CRD, cord, Sek, fcrd, mncrd, FeCrd, MgCrd, Cor

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Ti, FeII, Mg, Mn, Zn, Li, Be, Na, K, Ca

Sites

The general formula of cordierite is $A_1B_2T_2T_3T_1O_{18}$.

Site allocation order is A, B, T1, T2.

Site allocation

Site	Sum	Atoms
A	1	K, Na, Ca, Vc
B	unspecified	FeII, Mg, Mn, Zn, Li
T1	6	Si, Be, Al
T2	unspecified	Al, Ti

End Members

The end members calculated are:

$$Crd = Mg / (Mg + Mn + Fe^{II})$$

$$Sek = Fe / (Mg + Mn + Fe^{II})$$

$$Mn - Crd = Mn / (Mg + Mn + Fe^{II})$$

Values

In addition are returned extra parameters:

$$XMg = Mg / (Fe^{II} + Mg + Mn)$$

Dioct_mica

Dioct_mica

Description

Dioct_mica formulae are calculated on the basis of 22 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

muscovite, phengite, margarite, paragonite, celadonite, lepidolite, trilithionite, polyolithionite

and abbreviations:

Ms, Phg, Mrg, Pg, Lpd, Mu, MUS, wm, mu, cel, fcel, pa, ma

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Be, FeIII, Mg, Mn, Cr, Ni, Co, Ti, Sn, FeII, Zn, V, K, Na, Ba, Li, Ca, Rb, Cs, Sr, Pb, F, Cl

Sites

The general formula of dioct_mica is $I_1M_2T_4O_{10}(OH, F)_2$.

Site allocation order is T, M, I, OH.

Site allocation

Site	Sum	Atoms
T	8	Si, Be, Al, FeIII, Ti
M	5	Al, Ti, FeIII, FeII, Mn, Mg, Li, Co, Ni, Zn, V, Cr, Sn
I	unspecified	Ca, Na, K, Rb, Cs, Sr, Ba, Pb

Epidote

Epidote

Description

Epidote formulae are calculated on the basis of 8 atoms.

Synonym names

The programme recognizes the following full names:

epidote, clinozoisite, piemontite, hancockite, mukhinite, niigataite, zoisite

and abbreviations:

Ep, Czo, Zo, Pmt, Pie, zoep, cz, fep, EPI, ZOI

Feldspar

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Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Ti, Cr, V, FeIII, FeII, Mg, Mn, Zn, Ca, Pb, Sr, Ba, Na, K, REE.all, Y, Th, F

Sites

The general formula of epidote is $A_2M_3T_3(OH)_{12}$.

Site allocation order is T, M, A, OH.

Site allocation

Site	Sum	Atoms
T	3	Si, Al
M	3	Ti, Al, Cr, V, Mg, Zn, FeIII, FeII, Mn
A	unspecified	Mn, FeII, Ca, Pb, Sr, Ba, Na, K, REE.all, Y, Th, Vc
OH	1	F, OH

Feldspar

Feldspar

Description

Feldspar formulae are calculated on the basis of 8 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

feldspar, K-feldspar, orthoclase, plagioclase, anorthite, albite, oligoclase, andesine, labradorite, bytownite, anorthoclase, sanidine, celsian, microcline, slawsonite, anorthoclase, adularia

and abbreviations:

Fsp, Kfs, Or, Pl, Ab, An, Cln, FEL, kf, plag, Plg, abh, mic, san

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeIII, Ti, Na, K, Ca, Sr, Ba, Rb, Li, Cs, Pb, Eu, Mg, Mn, P

Sites

The general formula of feldspar is $A_1T_2Si_2O_8$.

Site allocation order is Si, T, A.

Site allocation

Site	Sum	Atoms
Si	2	Si
T	2	P, Si, Al, FeIII, Ti
A	unspecified	Na, K, Ca, FeIII, Mg, Mn, Sr, Ba, Rb, Li, Cs, Pb, Eu

End Members

The end members calculated are:

$$Ab = Na / (Na + Ca + K + Ba + Sr)$$

$$An = Ca / (Na + Ca + K + Ba + Sr)$$

$$Or = K / (Na + Ca + K + Ba + Sr)$$

$$Cln = Ba / (Na + Ca + K + Ba + Sr)$$

$$Sl = Sr / (Na + Ca + K + Ba + Sr)$$

Garnet	<i>Garnet</i>
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Description

Garnet formulae are calculated on the basis of 12 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 2 cations in the Y site (iteratively).

Synonym names

The programme recognizes the following full names:

garnet, almandine, pyrope, grossular, spessartine, andradite, uvarovite, majorite
and abbreviations:

Gr_t, Alm, Prp, Grs, Sps, Adr, Uv, Uvt, Maj, Mjt, py, spss, gr, andr, GAR, g

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeIII, Ti, P, Mg, FeII, Ca, Mn, Y, Cr, Zn, V, Zr, Na

Sites

The general formula of garnet is $X_3Y_2Z_3O_{12}$.

Site allocation order is Z, Y, X.

Site allocation

Site	Sum	Atoms
Z	3	Si, P, Al, FeIII, Ti
Y	unspecified	Ti, Al, FeIII, Cr, V, Zr
X	unspecified	Mg, FeII, Ca, Mn, Y, Zn, Na

End Members

The end members calculated by a script 'garnet.end.r' are:

Prp, Alm, Sps, Adr, Uv, Grs, Mjr

Values

In addition are returned extra parameters by a script 'garnet.r':

$XMg, XMg(Fetot), Fe^{II}/Mg, Al^{IV}, Al^{VI}$

Gustavite

Gustavite

Description

Gustavite formulae are calculated on the basis of 11 atoms.

Synonym names

The programme recognizes the following full names:

gustavite

and abbreviations:

Gus

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Cu, Ag, Fe, Pb, Cd, Bi, Sb, Se, S

Sites

The general formula of gustavite is M_5S_6 .

Site allocation order is M, S.

Site allocation

Site	Sum	Atoms
M	unspecified	Cu, Ag, Fe, Pb, Cd, Bi, Sb, Se
S	unspecified	S

Values

In addition are returned extra parameters:

$Bi/(Bi + Sb) = Bi/(Bi + Sb)$

Ilmenite

Ilmenite

Description

Ilmenite formulae are calculated on the basis of 6 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 4 cations per formula unit (*Droop 1987*).

Synonym names

The programme recognizes the following full names:

ilmenite, pyrophanite, geikielite

and abbreviations:

Ilm, fetiox, Pph, Pyf, Gk, Gkl

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Ti, Si, FeIII, Cr, Al, V, Nb, Ta, FeII, Mg, Mn, Ca, Ni, Zn, Zr, Hf, Sc, Sr

Sites

The general formula of ilmenite is $Fe_1Ti_1O_3$.

Site allocation order is Ti, Fe.

Site allocation

Site	Sum	Atoms
Ti	unspecified	Ti, Si, FeIII, Cr, Ni, V, Al, Zr, Hf, Nb, Ta, Sc
Fe	unspecified	FeII, Mg, Mn, Ca, Zn, Sr

Monazite

Monazite

Description

Monazite formulae are calculated on the basis of 16 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

monazite, xenotime, cheralite, huttonite

and abbreviations:

Mnz, MON, Xen

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

P, Si, Th, U, REE, all, Y, Al, Ca, Mn, Sr, FeII, Mg, Na, Pb, As

Sites

The general formula of monazite is $CaPO_4$.

Site allocation order is P, Ca.

Site allocation

Site	Sum	Atoms
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End Members

The end members calculated are:

$$\begin{aligned}X_{LREE} &= La + Ce + Pr + Nd + Sm + Eu \\X_{HREE} &= Gd + Tb + Dy + Ho + Er + Tm + Yb + Lu \\X_{Hu} &= Th + U + Pb - Ca \\X_{Br} &= 2 * Ca \\X_{YPO4} &= Y\end{aligned}$$

Olivine

Olivine

Description

Olivine formulae are calculated on the basis of 4 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

olivine, forsterite, fayalite, kirschsteinite, glaucochroite, monticellite, gernerite,
tephroite, knebelite, hortonolite

and abbreviations:

Ol, Fo, Fa, Mtc, Tep, teph, mont, OLI

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Mg, FeII, Ni, Cr, Ca, Mn

Sites

The general formula of olivine is $M1_1M2_1Si_1O_4$.

Site allocation order is M1, M2, Si.

Site allocation

Site	Sum	Atoms
M1	1	Mg, FeII, Ni, Cr
M2	unspecified	Ca, Mn, Mg, FeII, Ni, Cr
Si	unspecified	Si

End Members

The end members calculated are:

$$Fo = Mg / (Mg + Mn + Fe^{II})$$

$$Fa = Fe^{II} / (Mg + Mn + Fe^{II})$$

$$Tep = Mn / (Mg + Mn + Fe^{II})$$

Orthopyroxene

Orthopyroxene

Description

Orthopyroxene formulae are calculated on the basis of 6 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming NA

Synonym names

The programme recognizes the following full names:
orthopyroxene, donpeacorite, enstatite, ferrosilite
and abbreviations:
Opx, Don, En, Fs, Fsl

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):
Si, Al, FeIII, FeII, Ti, Cr, V, Zr, Sc, Zn, Ni, Co, Mg, Mn, Li, Ca, Na, K

Sites

The general formula of orthopyroxene is $M_2M_1T_2O_6$.

Site allocation order is T, M1, M2.

Site allocation

Site	Sum	Atoms
T	2	Si, Al, FeIII
M1	1	Al, FeIII, Ti, Cr, V, Zr, Sc, Zn, Ni, Co, Mg, FeII, Mn
M2	unspecified	Mg, FeII, Mn, Li, Ca, Na, K

End Members

The end members calculated by a script 'orthopyroxene.end.r' are:

$NaAl_2SiO_6$, $FmTiAlSiO_6$, $CrAl_2SiO_6$, $FmAl_2SiO_6$, $CaFmSi_2O_6$, $Fm_2Si_2O_6$, *Sum.end*, *En*, *Di*

Values

In addition are returned extra parameters by a script 'orthopyroxene.r':

Fe , Fe^{III}/Fe^{tot} , X_{Mg} , Al^{IV}/Al^{VI} , Al^{IV} , Al^{VI} , aEn

Prehnite

Prehnite

Description

Prehnite formulae are calculated on the basis of 22 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming only trivalent iron

Pumpellyite

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Synonym names

The programme recognizes the following full names:

prehnite

and abbreviations:

Prh

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Ti, FeII, FeIII, Mn, Mg, Ca, Na, K, F

Sites

The general formula of prehnite is $Ca_2Al_2Si_3O_{10}(OH)_2$.

Site allocation order is Si, Al, Ca, OH.

Site allocation

Site	Sum	Atoms
Si	8	Si, Ti, Al
Al	unspecified	Al, FeIII
Ca	unspecified	FeII, Mn, Mg, Ca, Na, K
OH	4	F, OH

Pumpellyite

Pumpellyite

Description

Pumpellyite formulae are calculated on the basis of 12 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 1 cations in the X site (iteratively).

Synonym names

The programme recognizes the following full names:

pumpellyite, julgoldite, okhotskite, poppiite, shuiskite

and abbreviations:

Pmp, pmp

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Ti, Al, FeIII, V, Cr, FeII, Mn, Mg, Ba, Ca, Na, K

Sites

The general formula of pumpellyite is $W_2X_1Y_2Z_3(O, OH)_{14}$.

Site allocation order is Z, Y, X, W.

Site allocation

Site	Sum	Atoms
Z	unspecified	Si
Y	2	Ti, Al, FeIII
X	unspecified	Al, FeIII, V, Cr, FeII, Mg, Mn
W	unspecified	Ca, Ba, Na, K

Rutile

Rutile

Description

Rutile formulae are calculated on the basis of 2 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

rutile

and abbreviations:

Rt, ru

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Ti, Si, Cr, Al, Nb, Ta, FeII, Mg, V, Sn, W, Sb, Mn, Ca, Zr, Hf

Sites

The general formula of rutile is M_1O_2 .

Site allocation order is M.

Site allocation

Site	Sum	Atoms
M	999	Ti, Si, Cr, Al, Nb, Ta, FeII, Mg, V, Sn, W, Sb, Mn, Ca, Zr, Hf

Sphalerite

Sphalerite

Description

Sphalerite formulae are calculated on the basis of 2 atoms.

Synonym names

The programme recognizes the following full names:

sphalerite

and abbreviations:

Sp

Spinel

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Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Zn, Cd, Fe, S

Sites

The general formula of sphalerite is Zn_1S_1 .

No sites allocation is desired.

Values

In addition are returned extra parameters:

$Cd/Fe = Cd/Fe$

Spinel	<i>Spinel</i>
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Description

Spinel formulae are calculated on the basis of 4 oxygen equivalents. The Fe^{II} and Fe^{III} are estimated assuming 3 cations per formula unit (*Droop 1987*).

Synonym names

The programme recognizes the following full names:

spinel, hercynite, gahnite, galaxite, magnetite, maghemite, ulvospinel, franklinite, jacobsonite, trevorite, chromite

and abbreviations:

Sp1, spin, Mt, sp, herc, Hc, Ghn, Glx, Mgt, Mag, Mgh, usp, Usp, Uspl, Frk, Fnk, Jcb, Trv, Chr

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Al, Cr, V, FeIII, FeII, Ni, Co, Ti, Zn, Mg, Mn, Ca, Si, Nb, Ta

Sites

The general formula of spinel is $A_1B_2O_4$.

Site allocation order is B, A.

Site allocation

Site	Sum	Atoms
B	2	FeIII, Al, Cr, V, Si, FeII
A	unspecified	FeII, Ni, Co, Ti, Zn, Mg, Mn, Ca, Nb, Ta

Staurolite

Staurolite

Description

Staurolite formulae are calculated on the basis of 46 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

staurolite, lusakite, ferrostaurolite, magnesiostaurolite, zincianstaurolite

and abbreviations:

St, ST, FeSt, MSt, MgSt, ZnSt, mst, fst, mnst

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Ti, FeIII, FeII, Cr, Mg, Mn, Zn, Co, Ni, V, Na, Li, F, Cl

Sites

The general formula of staurolite is $X_4Y_{18}T_8O_{44}OH_4$.

Site allocation order is T, Y, X, OH.

Site allocation

Site	Sum	Atoms
T	8	Si, Al
Y	18	Si, Al, Ti, FeIII, Cr, V, Mg
X	4	Mg, FeII, Mn, Zn, Co, Ni, Li, Na, Vc
OH	4	F, Cl, OH

End Members

The end members calculated are:

$$FeSt = Fe^{II}/Sum_X$$

$$MgSt = Mg/Sum_X$$

$$lusakite = Co/Sum_X$$

$$ZnSt = Zn/Sum_X$$

Titanite

Titanite

Description

Titanite formulae are calculated on the basis of 4 atoms.

Synonym names

The programme recognizes the following full names:

titanite, sphene, grothite, keilhauite, yttrotitanite

and abbreviations:

Ttn, TTn, Spn, SPN, SPH

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Ti, Ca, FeIII, FeII, Mg, Nb, Ta, V, Cr, Zr, Na, K, REE.all, Mn, Sr, Ba, Sn, Y, F

Sites

The general formula of titanite is $Ca_1Ti_1Si_1O_4(OH)_1$.

Site allocation order is Si, Ti, Ca, OH.

Site allocation

Site	Sum	Atoms
Si	unspecified	Si
Ti	unspecified	Ti, Al, FeIII, Ta, Sn
Ca	unspecified	Ca, Mg, Na, K, REE.all, Mn, Sr, Ba, FeII, V, Cr, Zr, Nb, Y
OH	1	F, OH

Tourmaline

Tourmaline

Description

Tourmaline formulae are calculated on the basis of 15 atoms.

Synonym names

The programme recognizes the following full names:

tourmaline, dravite, schorl, elbaite, povondraite, buergerite, olenite, foitite, uvite, feruvite, rossmanite

and abbreviations:

Tur, Tour, Drv, Srl, Elb, Pov, Ole, Foi, Uvt, Utv, Fuvt, Fer, Rsm

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, FeIII, Mg, Ti, Li, FeII, Mn, Na, Ca, K, Zn, Ni, Co, Cu, Cr, V, F, Cl

Sites

The general formula of tourmaline is $X_1Y_3Z_6(T_6O_{18})(BO_3)_3V_3OH_1$.

Site allocation order is T, Z, Y, X, OH.

Site allocation

Site	Sum	Atoms
T	3	Si, Al
Z	6	Al, Cr, V, Mg, FeIII, FeII
Y	unspecified	Li, Ti, Zn, Ni, Co, Cu, Mn, FeII, Mg, FeIII, Cr, V, Al
X	1	Ca, Na, K, Vc
OH	1	F, Cl, OH

Trioct_mica	<i>Trioct_mica</i>
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Description

Trioct_mica formulae are calculated on the basis of

Synonym names

The programme recognizes the following full names:

zinnwaldite, lepidomelane, clintonite

and abbreviations:

Znw, Stp, naph

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Si, Al, Be, FeIII, Mg, Mn, Cr, Ti, FeII, Zn, V, K, Na, Ba, Li, Ca, Rb, Cs, Sr, F, Cl

Sites

The general formula of trioct_mica is $I_1M_3T_4O_{10}(OH)_2$.

Site allocation order is T, M, I, OH.

Site allocation

Site	Sum	Atoms
T	4	Si, Be, Al, FeIII, Ti
M	3	Al, Mg, FeII, Mn, Cr, Ti, Zn, V, Li, FeIII, Vc
I	unspecified	K, Na, Ba, Ca, Rb, Cs, Sr
OH	2	F, Cl, OH

Zircon	<i>Zircon</i>
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Description

Zircon formulae are calculated on the basis of 4 oxygen equivalents.

Synonym names

The programme recognizes the following full names:

zircon

and abbreviations:

Zrn, Zrc, ZIR

Formula

The procedure returns the following atoms (if the corresponding oxide is present in the data file):

Zr, Al, Hf, FeIII, Mg, Ti, Nb, Th, Ca, Cu, Na, U, Mn, K, Y, Si, P

Sites

The general formula of zircon is $Si_1M_1O_4$.

Site allocation order is M, Si.

Site allocation

Site	Sum	Atoms
M	unspecified	Zr, Al, Hf, FeIII, Mg, Ti, Nb, Th, Ca, Cu, Na, U, Mn, K, Y
Si	unspecified	Si, P

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