

Overview of the mineral recalculation schemes

April 20, 2023

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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

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, magnesioriebeckite, 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

Apatite

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

*Biotite***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

*Carbonate***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

Chlorite

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

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

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

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

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

Values

In addition are returned extra parameters:

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

| | |
|------------|-------------------|
| Chloritoid | <i>Chloritoid</i> |
|------------|-------------------|

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

*Clinopyroxene***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:

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

 Dioc_t_mica

Dioc_t_mica

Description

Dioc_t_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 dioc_t_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

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

Garnet

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 , $XMg(Fe_{tot})$, Fe^{II}/Mg , $AlIV$, $AlVI$

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 |
|------|-----|-------|
|------|-----|-------|

End Members

The end members calculated are:

$$X_{LREE} = La + Ce + Pr + Nd + Sm + Eu$$

$$X_{HREE} = Gd + Tb + Dy + Ho + Er + Tm + Yb + Lu$$

$$X_{Hu} = Th + U + Pb - Ca$$

$$X_{Br} = 2 * Ca$$

$$X_{YPO4} = Y$$

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 $M2_1M1_1T_2O_6$.

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 'orthopyroxene.end.r' are:

NaAl2SiO6, FmTiAlSiO6, CrAl2SiO6, FmAl2SiO6, CaFmSi2O6, Fm2Si2O6, Sum.end, En, Di

Values

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

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

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

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

*Spinel***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:

Spl, 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 *Trioct_mica*

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 *Zircon*

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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