# MINERAL FORMULA CALCULATIONS

Sarah Lambart




# RECAP CHAP 7: NON-SILICATE MINERALS

- **Part 1: Native element**
- **Part 2: Sulphides and related minerals**
- **Part 3 : Oxides, Hydroxides and Halides**
- **Part 4: Carbonates, Sulphates and Phosphates**

# RECAP CHAP 7: NON-SILICATE MINERALS

- **Part 1: Native elements**
  - **Rare: 2ppm of Earth's crust**
  - **Close-packing**
  - **Metal, semimetal, non metal**
  - **Metal: gold group, platinum group and iron group**
  - **Occurrences: Au & Ag – hydrothermal; Cu – mafic rock; Pt & Diamond: ultramafic; graphite – sedimentary metamorphic rock; Sulfur – fumaroles & salt domes**

# RECAP CHAP 7: NON-SILICATE MINERALS

- **Part 2: Sulfides and related elements**
  - **Large group: 600 minerals**
  - **Most common source: hydrothermal deposits**
  - most common ore source
  - **$M_pX_r$:** - M is a metal or semimetal
    - X can be: S, As, S+As, Te

# RECAP CHAP 7: NON-SILICATE MINERALS

- **Part3: oxides, hydroxides and halides**
- **Oxides: Metals + oxygen**
  - **$X_2O$ group (X = H or Cu)**
  - **Spinel group: $XY_2O_4$ (Y= Al, Cr or Fe)**
  - **$X_2O_3$ group:** Hematite ($Fe_2O_3$), Ilmenite ($FeTiO_3$), Corundum ($Al_2O_3$)
  - **$XO_2$ group:** rutile ($TiO_2$)

# RECAP CHAP 7: NON-SILICATE MINERALS

- **Hydroxides: Brucite ($Mg(OH)_2$) and gibbsite ($Al(OH)_3$)**
  - $OH^-$: arrange in planes
  - Cation (Mg or Al): octahedral sites between the anion planes

- **Halides:** Halite (NaCl), Fluorite ($CaF_2$), Sylvite (KCl)
  - NaCl and KCl: isostructural – 2 fcc interconnected – found in evaporites
  - $CaF_2$: layer of anions with cations in cubic sites between the layers – found in hydrothermal deposits

# RECAP CHAP 7: NON-SILICATE MINERALS

- **Part 4: Carbonates, phosphates, sulfates**
- **Carbonates:**
  - ~170 minerals
  - 4 Groups: calcite & dolomite (= rhombohedral carbonates), aragonite and hydrated carbonates
- **Sulfates:** Gypsum, anhydrite and barite
- **Phosphates:** Apatite, monazite and xenotime

# MINERAL FORMULA CALCULATIONS

- Chemical analyses are usually reported in weight percent of elements or elemental oxides

- To calculate mineral formula requires transforming weight percent into atomic percent or molecular percent

# ION COMPLEXES OF IMPORTANT CATIONS

*(cation valence in parentheses)*

- $SiO_2$ $TiO_2$ (+4)
- $Al_2O_3$ $Cr_2O_3$ $Fe_2O_3$ (+3)
- MgO MnO FeO CaO(+2)
- $Na_2O$ $K_2O$ $H_2O$ (+1)

# EXAMPLE 1: WEIGHT PERCENT TO FORMULA

| Oxide | wt. % | MolWt oxide | Moles oxide | Moles cation | Mole oxygen |
|---|---|---|---|---|---|
| $SiO_2$ | 59.85 | 60.086 | 0.996* | 0.996 | 2*0.996 = 1.992 |
| MgO | 40.15 | 40.312 | 0.996 | 0.996 | 0.996 |
| Total | 100 | | | | 2.998 |

* 59.85/60.086

- **Mole ratio Mg:Si:O = 1:1:3**
- **Formula: $MgSiO_3$ : enstatite**

# EXAMPLE 2: FORMULA TO WEIGHT PERCENTS

- Kyanite: $Al_2SiO_5$

What are the weight percent of the oxides $SiO_2$ & $Al_2O_3$?

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| $SiO_2$ | 1 | 60.086 | 60.086* | 37.08 |
| $Al_2O_3$ | 1 | 101.963 | 101.963 | 62.92 |
| Total | | | 162.049 | |

* 60.086/162.049*100

# PROBLEM 1: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

- Alkali Feldspars may exist with any composition between $NaAlSi_3O_8$ (Albite) and $KAlSi_3O_8$ (Sanidine, Orthoclase and Microcline)

- Formula has 8 oxygens: $(Na,K)AlSi_3O_8$

- The alkalis may substitute in any ratio, but total alkalis (Na + K) to Al is 1 to 1.

# PROBLEM 1: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

| Oxide | wt. % | MolWt oxide | Moles oxide | Moles cation | Mole oxygen |
|---|---|---|---|---|---|
| $SiO_2$ | 68.20 | | | | |
| $Al_2O_3$ | 19.19 | | | | |
| $Na_2O$ | 10.20 | | | | |
| $K_2O$ | 2.32 | | | | |
| Total | 100 | | | | |

# PROBLEM 1: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

| Oxide | wt. % | MolWt oxide | Moles oxide | Moles cation | Mole oxygen | Moles cations for 8O |
|---|---|---|---|---|---|---|
| $SiO_2$ | 68.20 | 60.086 | 1.1350 | 1.1350 | 2.2701 | 2.9997 |
| $Al_2O_3$ | 19.19 | 101.963 | 0.1892 | 0.3784 | 0.5676 | 1.0001 |
| $Na_2O$ | 10.20 | 61.9796 | 0.1646 | 0.3291 | 0.1646 | 0.8699 |
| $K_2O$ | 2.32 | 94.204 | 0.0246 | 0.0493 | 0.0246 | 0.1311 |
| Total | 100 | | | | **3.0269*** | |

- **Mole ratio Si ~3, Al~1, Na~0.87, K~0.13 (Na+K~1)**
- **Formula: $(Na_{.87}K_{.13})AlSi_3O8$**

# PROBLEM 1: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

- **Various simple solid solutions:**
- Alkali Feldspars: $NaAlSi_3O_8$ - $KAlSi_3O_8$
- Orthopyroxenes: $MgSiO_3$- $FeSiO_3$ Enstatite - Ferrosilite (opx)
- $MgCaSi_2O_6$-$FeCaSi_2O_6$ Diopside-Hedenbergite (cpx)
- Olivines: $Mg_2SiO_4$- $Fe_2SiO_4$ Forsterite - Fayalite
- Garnets: $Mg_3Al_2Si_3O_{12}$- $Fe_3Al_2Si_3O_{12}$ Pyrope - Almandine

# EXAMPLE 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Given the formula $En_{70}Fs_{30}$ for an orthopyroxene, calculate the weight percent oxides
  - En = Enstatite = $MgSiO_3$
  - Fs = Ferrosilite = $FeSiO_3$

# EXAMPLE 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Given the formula $En_{70}Fs_{30}$ for an orthopyroxene, calculate the weight percent oxides
  - En = Enstatite = $MgSiO_3$
  - Fs = Ferrosilite = $FeSiO_3$

- Formula is $(Mg_{0.7}Fe_{0.3})SiO_3$

# EXAMPLE 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $(Mg_{0.7}Fe_{0.3})SiO_3$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| MgO | 0.7 | 40.312 | 28.2184 | 25.69 |
| FeO | 0.3 | 71.846 | 21.5538 | 19.62 |
| SiO2 | 1 | 60.086 | 60.086 | 54.69 |
| Total | | | 109.8582 | |

# PROBLEM 2: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Consider a Pyroxene solid solution of 40% Jadeite ($NaAlSi_2O_6$) and 60% Aegirine ($NaFeSi_2O_6$).
- Calculate the weight percent oxides

# PROBLEM 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $Na(Al_{0.4}Fe_{0.6})Si_2O_6$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| | | | | |
| | | | | |
| | | | | |
| | | | | |
| | | | | |

# PROBLEM 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $Na(Al_{0.4}Fe_{0.6})Si_2O_6$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| $Na_2O$ | | | | |
| $Fe_2O_3$ | | | | |
| $Al_2O_3$ | | | | |
| $SiO_2$ | | | | |
| Total | | | | |

# PROBLEM 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $Na(Al_{0.4}Fe_{0.6})Si_2O_6$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| $Na_2O$ | 0.5 | 61.9796 | 30.9898 | 14.12 |
| $Fe_2O_3$ | 0.3 | 159.692 | 47.9076 | 21.83 |
| $Al_2O_3$ | 0.2 | 101.963 | 20.3926 | 9.29 |
| $SiO_2$ | 2 | 60.086 | 120.172 | 54.76 |
| Total | | | 219.462 | |

# PROBLEM 4: SOLID SOLUTION WITH COUPLED SUBSTITUTIONS – FORMULA TO WT.%

- Examples:
  - Plagioclase Feldspar $CaAl_2Si_2O_8$ - $NaAlSi_3O_8$
  - Jadeite - Diopside $NaAlSi_2O_6$ - $CaMgSi_2O_6$
- Consider a feldspar composition with 40% Anorthite and 60% Albite. Calculate Weight percent Oxides.

# PROBLEM 4: SOLID SOLUTION WITH COUPLED SUBSTITUTIONS – FORMULA TO WT.%

- 40% Anorthite and 60% Albite.
- 1st step: write the formula
- 40% $CaAl_2Si_2O_8$ – 60% $NaAlSi_3O_8$
- $Ca_{0.4}Na_{0.6}Al_{1.4}Si_{2.6}O_8$

Note: - Silica (0.4 x 2 Silica in Anorthite) + (0.6 x 3 in Albite) = 2.6
- Aluminum (0.4 x 2 Aluminum in Anorthite) + (0.6 x 1 in Albite) = 1.4

# PROBLEM 4: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $Ca_{0.4}Na_{0.6}Al_{1.4}Si_{2.6}O_8$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| $Na_2O$ | 0.3 | | | |
| $CaO$ | 0.4 | | | |
| $Al_2O_3$ | 0.7 | | | |
| $SiO_2$ | 2.6 | | | |
| Total | | | | |

# PROBLEM 3: SOLID SOLUTION - FORMULA TO WEIGHT PERCENTS

- Formula is $Ca_{0.4}Na_{0.6}Al_{1.4}Si_{2.6}O_8$

| Oxide | Mole PFU | MolWt oxide | Gramm oxide | wt. % |
|---|---|---|---|---|
| $Na_2O$ | 0.3 | 61.9796 | 18.5939 | 7.29 |
| CaO | 0.4 | 55.96 | 8.9536 | 3.51 |
| $Al_2O_3$ | 0.7 | 101.963 | 71.3741 | 27.97 |
| $SiO_2$ | 2.6 | 60.086 | 156.2236 | 61.23 |
| Total | | | 255.1452 | 100 |

# PROBLEM 5: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

- We are given the following chemical analysis of a pyroxene. Compute its formula: (Hint: Jadeite $NaAlSi_2O_6$ – Diopside: $CaMgSi_2O_6$)

| Oxide | wt. % | MolWt oxide | Moles oxide | Moles cation | Mole oxygen |
|---|---|---|---|---|---|
| $SiO_2$ | 56.64 | | | | |
| $Na_2O$ | 4.38 | | | | |
| $Al_2O_3$ | 7.21 | | | | |
| MgO | 13.30 | | | | |
| CaO | 18.46 | | | | |
| Total | 100 | | | | |

# PROBLEM 5: SOLID SOLUTION WEIGHT PERCENT TO FORMULA

- We are given the following chemical analysis of a pyroxene. Compute its formula: (Hint: Jadeite $NaAlSi_2O_6$ – Diopside: $CaMgSi_2O_6$)

| Oxide | wt. % | MolWt oxide | Moles oxide | Moles cation | Mole oxygen | Prop cations to O6 |
|---|---|---|---|---|---|---|
| $SiO_2$ | 56.64 | 60.086 | 0.9426 | 0.9426 | 1.8852 | 2 |
| $Na_2O$ | 4.38 | 61.99 | 0.0707 | 0.1414 | 0.707 | 0.3 |
| $Al_2O_3$ | 7.21 | 101.963 | 0.0707 | 0.1414 | 0.2121 | 0.3 |
| MgO | 13.30 | 40.312 | 0.3299 | 0.3299 | 0.3299 | 0.7 |
| CaO | 18.46 | 55.96 | 0.3299 | 0.3299 | 0.3299 | 0.7 |
| Total | 100 | | | | 2.8278 | $Na_{.3}Ca_{.7}Mg_{.7}Al_{.3}Si_2O_6$ |