L8: Mineral formula

Wednesday, July 22, 2020 18:02

Time on task: about 1 hour (Material posted on Sept 28th, Office hours: Oct 12th and 14th)

Goals:

Being able to:

- Calculate a mineral formula from weight percent of elements or oxides
- Calculate composition from a mineral
- Calculate the proportion of the end-members in a solid solution
- Being able to say if the stoichiometry of the mineral is respected

This lecture is an introduction to your Problem set #3 (due on Friday Oct 16th).

For a demonstration in Excel, check the associated video. If you are not familiar with Excel, you can start by doing the **Excel tutorial** associated with this lecture.

Chemical analyses are usually reported in weight percent of elements or elemental oxides. Calculate mineral formula requires transforming weight percent into atomic percent or molecular percent.

Ions complexes of important cations (cation valency 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)**
- **P_2O_5 (+5)**

Example 1: weight percent to formula

	(1) given	(2) given	(3) =	(4) Calculated	(5) Calculated
Oxide	**Wt.%**	**MolWt oxide**	**#**	**#moles of cations**	**#moles of oxygen**
SiO2	59.83	60.086	0.9957	1*0.9957=0.9957 ~ 1	2*0.9957=1.9914
MgO	40.49	40.312	1.0044	1*1.0044=1.0044 ~ 1	1*1.0044=1.0044
Total	100.32				2.9958 ~ 3

(1) analysis obtained at the electron probe; (2) molecular weight of the oxide (calculated from the periodic table); (4) number of moles of cations. For instance, in one mole of SiO2, I have one mole of Si => in 0.9957 moles of SiO2, I have 0.9957 moles of Si; (5) number of moles of oxygen. For instance, in one mole of SiO2, I have two mole of O => in 0.9957 moles of SiO2, I have 2*0.9957 moles of O. We then need to add the number of moles of oxygen to get the total.

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

Questions you should ask yourself.

- Why the analytical total is different from 100 wt.%? Because each analysis as an analytical uncertainty (due to the apparatus or to the homogeneity of the sample). Those errors will propagate to the total.
- Which level of precision should I use for the oxide molecular weight? If you don't use enough significant figures, you might introduce additional uncertainty early in the calculations that will

propagate (and become larger) in your final calculations. If you use too much digits, they might not be relevant for the final results, however you would not introduce additional uncertainty. **It is always good practice to keep the maximal level of precision in your input data, use "formula algebra in Excel" and decide only in the final calculations what is the needed significant digits.**

- The number of significant figures of the final calculations. It depends on the type of calculations. **It is usually defined by the input data with the less good precision (e.g., wt.%).** In addition, we are calculating the formula of a pure end-member (no solid solution), so the number of cations (and oxygen) is an integer.

L8: Example 2: Formula to weight percent

Tuesday, August 25, 2020 3:01 PM

Kyanite: Al_2SiO_5

	(1) given	(2) given	(3) = (1)*(2)	(4) = (3)*100/$(3)_{total}$
Oxide	**# of moles***	**MolWt oxide**	**# of grams of oxides**	**wt. %**
SiO2	1	60.086	60.086	37.079
Al_2O_3	1	101.963	101.963	62.921
Total			162.049	100

* Always assume that Oxygen is in excess. At the surface of the Earth and in the mantle, it's true. So you just have to look at the cations.

The number of significant figures is there define by the molecular weight of the oxide you used.

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)
The formula has 8 oxygens: $(Na,K)AlSi_3O_8$ (the parentheses indicate the solid solution)
The alkalis may substitute in any ratio, but total alkalis (Na + K) to Al is 1 to 1.

	(1) given	(2) given	(3) = (1)/(2)	(4) Calculated	(5)	(6) = (4)*8/$(5)_{total}$
Oxide	**Wt.%**	**MolWt**	**# moles oxide**	**#moles cations**	**#moles of**	**#moles cations for 8 oxygens**
SiO2	59.83	60.086	1.1350	1*1.1350=1.1350	2*1.1350=	2.9997 ~ 3
Al_2O_3	40.49	101.963	0.1892	2*0.1892=0.3784	3*0.1892=	1.0001 ~ 1
Na_2O	10.20	61.9796	0.1646	2*0.1646=0.3291	0.1645	0.8699 ~ 0.87
K_2O	2.32	94.204	0.0246	2*0.0246=0.0493	0.0246	0.1311 ~ 0.13
Total	100*				3.0269	

* the true total was probably not equal to one but analyses are often renormalized to 100 in papers to make the comparison between the analyses easier.

Mole ratio Si:Al:(Na+K) = 3:1:1 - the stoichiometry of the alkali feldspars is respected

We usually don't use more than 2 digits in the mineral formula: **$(K_{.013}Na_{.87})AlSi_3O_8$**

L8: Example 3 - Solid solution: formula to wt. %

Tuesday, August 25, 2020 3:02 PM

Rule to write the formula:

- anions are always at the end of the formula
- cations are in croissant order of charges 1+ (e.g., Na, K), 2+ (Fe, Mg, Mn, Cu), 3+(Cr, Al), 4+ (Si, Ti)
- If two cations have the same charge, the one in the highest molar abundance goes first

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

Given the formula **$En_{70}Fs_{30}$** for an **orthopyroxene**, calculate the weight percent oxides
En = Enstatite = $MgSiO_3$
Fs = Ferrosilite = $FeSiO_3$
The formula is **$(Mg_{.7}Fe_{.3})SiO_3$**

	(1) given	(2) given	(3) = (1)*(2)	(4) = (3)*100/$(3)_{total}$
Oxide	**# of moles**	**MolWt oxide**	**# of grams of oxides**	**wt. %**
MgO	0.7	40.312	28.2184	25.686
FeO	0.3	71.846	21.5538	19.620
SiO2	1	60.086	60.086	54.694
Total			109.8582	100

Problem 2: Solid-solution - formula to weight percent

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

The formula of this pyroxene is: $Na(Fe_{.6}Al_{.4})Si_2O_6$.

Which oxides do you need to describe this pyroxene?
Check the video for calculations in excel - keys are on the next page

Problem 3: Solid-solution with coupled substitutions- formula to wt.%

Consider a plagioclase composition with 40% Anorthite and 60% Albite. Calculate Weight percent Oxides.

The first step is to write the formula of this plagioclase
Check the video for calculations in excel - keys are on the next page

L8: Keys - Problems #2&3

Tuesday, August 25, 2020 3:27 PM

- **Problem #2**

The formula is $Na(Fe_{.6}Al_{.4})Si_2O_6$.
Fe and Al are present in the same sites and have the same valency as it's a simple substitution. Hence, the cation is Fe^{3+}

	(1) given	(2) given	(3) = (1)*(2)	(4) = (3)*100/$(3)_{total}$
Oxide	**# of moles**	**MolWt oxide**	**# of grams of oxides**	**wt. %**
Na2O	0.5	61.9796	30.9898	14.121
Fe2O3	0.3	159.692	47.9076	21.830
Al2O3	0.2	101.963	20.3926	9.247
SiO2	2	60.086	120.172	54.802
Total			219.462	100

- **Problem #3**

1st step, calculate the formula 40% anorthite, 60% albite = 40%CaAl2Si2O3 + 60% NaAlSi3O8
= $(Na_{.6}Ca_{.4})(Al_{1.4}Si_{2.6})o_8$

	(1) given	(2) given	(3) = (1)*(2)	(4) = (3)*100/$(3)_{total}$
Oxide	**# of moles**	**MolWt oxide**	**# of grams of oxides**	**wt. %**
Na2O	0.6	61.9796	18.5936	7.29
CaO	0.4	55.96	8.9536	3.51
Al2O3	0.7	101.963	71.3741	27.97
SiO2	2.6	60.086	156.2236	61.23
Total			255.1452	100

L8: Example 4: Solid solution: wt.% to formula

Example 4: 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: $CaMgSi_2O_6$)

	(1) given	(2) given	(3) = (1)/(2)	(4) Calculated	(5) Calculated	(6) = (4)*6/(5)$_{total}$
Oxide	**Wt.%**	**MolWt**	**# moles oxide**	**#moles cations**	**#moles of**	**#moles cations for 6 oxygens**
SiO2	56.64	60.086	0.9426	0.9426	1.8852	2
Al_2O_3	7.21	101.963	0.0707	0.1414	0.2121	0.30
Na_2O	4.38	61.9796	0.0707	0.1414	0.0707	0.30
CaO	18.46	55.96	0.3299	0.3299	0.3299	0.70
MgO	13.30	40.312	0.3299	0.3299	0.3299	0.70
Total	100				2.8278	

We have substitution between Na, Al, Ca and Mg.

The formula is: $(Na_{.3}Ca_{.7})(Mg_{.7}Al_{.3})Si_2O_6$