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GEOLOGY 284: MINERALOGY

Mineral Formulas

- Remember, minerals must have a "well-defined chemical composition" (that can be represented by a formula)
- The composition range of a mineral is conveniently expressed by a **general chemical formula**, e.g.,
  - quartz $SiO_{\mathbf{2}}$
  - feldspar $(Ca,Na,K)_1(Fe,Al,Si)_4O_{\mathbf{8}}$
  - olivine $(Mg,Fe^{2+})_2SiO_{\mathbf{4}}$
  - garnet $(Ca,Mg,Fe^{2+},Mn)_3(Al,Fe^{3+})_2Si_3O_{\mathbf{12}}$

  * **Formulas are written in terms of moles (more later)**

  * **Note: formulas for different minerals are written with different numbers of oxygens!**

  * **Why? So that elements or groups of elements will turn out to be integers (see above).**

Mineral Formulas (cont.)

- If you have a chemical analysis of a particular mineral sample, you can calculate a mineral formula from it or “normalize” it
- The method we will use is a little different than calculating a general empirical formula (like you might have done in Chemistry), because we want to end up with a certain number of oxygens (or sulfurs or something).
- Our method is slightly different than Perkins’ method **(ignore Box 1.5 in textbook)**
  - His method includes an unnecessary and confusing step

Mineral Formulas (cont.)

- Our goal: Calculate a mineral formula from the mineral analysis we're given (the feldspar analysis of Box 1.5)
- Feldspar formulas are written with 8 oxygens
  - All feldspars must fit the general formula: $(Ca,Na,K)_1(Fe^{3+},Al,Si)_4O_{\mathbf{8}}$
  - Ca, Na, and K fit in the same type of position (site) in the mineral structure, that's why they're in parentheses (similarly Fe^{3+}, Al, and Si fit in the same type of position or site)
  - I will always tell you how many oxygens to use
- The first step is to figure out how many moles of each cation go with the 8 moles of oxygen
- The last step is to write your result as a specific (horizontal) chemical formula

What is a mole?

- One mole of an element is the amount of that element whose weight in grams is equal to its atomic weight
- A mole of any element always contains the same number of atoms: 6.022×10^{23} atoms, called Avogadro's number
- Elements combine in integral numbers of moles
- A mole of quartz, which has the chemical formula SiO_2, has
  - 1 mole (6.022×10^{23} atoms) of **Si** 28.086 grams
  - 2 moles ($2 \times 6.022 \times 10^{23}$ atoms) of **O** <u>2 x 15.999 grams</u>
- <u>Molecular</u> weight of quartz (SiO_2) is 60.084 grams/m
- One mole of quartz contains 6.022×10^{23} molecules of SiO_2

Perkins Box 1.5 modified

This is the mineral analysis

How do we get this?

Feldspar Analysis

Oxide	Mol. Wt. of oxide (g/mole)	# cations in oxide	#anions in oxide	Oxide Wt% in mineral (grams)	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.90					
Al_2O_3	101.96	2	3	19.45					
Fe_2O_3	159.68	2	3	1.03					
CaO	56.08	1	1	0.61					
Na_2O	61.96	2	1	7.12					
K_2O	94.20	2	1	6.20					
total				100.31					

Mineral formula?

Perkins Box 1.5 modified

What is the cation for each oxide?

Feldspar Analysis

Oxide	Mol Wt	# cations	#anions	Oxide Wt%	Moles of		Moles of	Moles of	Moles of
	of oxide	in oxide	in oxide	in mineral	Oxide	Cation	Cation	Oxygen	Cation
					in 100 grams				per 8 Ox.
SiO_2	60.08	1	2	65.90	1.097				
Al_2O_3	101.96	2	3	19.45	0.191				
Fe_2O_3	159.68	2	3	1.03	0.006				
CaO	56.08	1	1	0.61	0.011				
Na_2O	61.96	2	1	7.12	0.115				
K_2O	94.20	2	1	6.20	0.066				
total				100.31					

How do we know the Cation?

- Each oxygen has a -2 charge
- Each other element has only a few common ions, each with its own charge (See inside front cover of your textbook)
- Stable compounds are neutral (zero charge)
- The charge of the cation in each oxide is whatever is necessary to make the molecule neutral
- Example: Fe_2O_3 Neg. charge=3x(-2)=-6; charge of the two Fe cations must be +6; so each is Fe^{3+}

Perkins Box 1.5 modified

These are the cations

How do we get this?

Feldspar Analysis

Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.90	1.097	Si^{4+}			
Al_2O_3	101.96	2	3	19.45	0.191	Al^{3+}			
Fe_2O_3	159.68	2	3	1.03	0.006	Fe^{3+}			
CaO	56.08	1	1	0.61	0.011	Ca^{2+}			
Na_2O	61.96	2	1	7.12	0.115	Na^{+}			
K_2O	94.20	2	1	6.20	0.066	K^{+}			
total				100.31					

Perkins Box 1.5 modified

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Fe_2O_3	159.68	2	3	1.03	0.006	Fe^{3+}	0.013		
CaO	56.08	1	1	0.61	0.011	Ca^{2+}	0.011		
Na_2O	61.96	2	1	7.12	0.115	Na^{+}	0.230		
K_2O	94.20	2	1	6.20	0.066	K^{+}	0.132		
total				100.31					

Perkins Box 1.5 modified

How do we get this?

Feldspar Analysis

Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.90	1.097	Si^{4+}	1.097	**2.194**	
Al_2O_3	101.96	2	3	19.45	0.191	Al^{3+}	0.382	**0.572**	
Fe_2O_3	159.68	2	3	1.03	0.006	Fe^{3+}	0.013	**0.019**	
CaO	56.08	1	1	0.61	0.011	Ca^{2+}	0.011	**0.011**	
Na_2O	61.96	2	1	7.12	0.115	Na^{+}	0.230	**0.115**	
K_2O	94.2	2	1	6.20	0.066	K^{+}	0.132	**0.066**	
total				100.31				**2.977**	

Perkins Box 1.5 modified

Multiply Moles Cation x Factor to get this.

Feldspar Analysis

Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.90	1.097	Si^{4+}	1.097	**2.194**	
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CaO	56.08	1	1	0.61	0.011	Ca^{2+}	0.011	**0.011**	
Na_2O	61.96	2	1	7.12	0.115	Na^{+}	0.230	**0.115**	
K_2O	94.2	2	1	6.20	0.066	K^{+}	0.132	**0.066**	
total				100.31				**2.977**	

This is the total moles oxygen we have. We want 8 oxygens, so we need a normalization or "fudge" factor to get to 8 oxygens.

Factor = #ox. in formula/Σ(oxygens) = 8/2.977=2.687

Perkins Box 1.5 modified

Feldspar Analysis

Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.9	1.097	Si^{4+}	1.097	2.194	**2.948**
Al_2O_3	101.96	2	3	19.45	0.191	Al^{3+}	0.382	0.572	**1.025**
Fe_2O_3	159.68	2	3	1.03	0.006	Fe^{3+}	0.013	0.019	**0.035**
CaO	56.08	1	1	0.61	0.011	Ca^{2+}	0.011	0.011	**0.029**
Na_2O	61.96	2	1	7.12	0.115	Na^{+}	0.230	0.115	**0.618**
K_2O	94.2	2	1	6.2	0.066	K^{+}	0.132	0.066	**0.354**
total				100.31				2.977	**5.008**

Mineral formula?

Perkins Box 1.5 modified

Feldspar Analysis

Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO_2	60.08	1	2	65.9	1.097	Si^{4+}	1.097	2.194	**2.948**
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total				100.31				2.977	**5.008**

Finally, we can write the formula:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.03}Si_{2.95})O_8$$

Always check to see that your formula fits the general formula for that mineral!!

Feldspar General Formula: $(Ca,Na,K)_1(Fe,Al,Si)_4O_8$

Our Calculated (Specific) Formula:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.03}Si_{2.95})O_8$$

Ca+Na+K = 1.00
Fe+Al+Si = 4.02

If it fits, calculation is probably OK; if not, review calculation to find the error!

<u>Do</u> <u>not</u> duplicate the sum of cations as subscripts in the specific formula!!

General Feldspar Formula: $(Ca,Na,K)_1(Fe,Al,Si)_4O_8$

Correct Specific Formula for our feldspar is this:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.03}Si_{2.95})O_8$$

Not this:

$$\xcancel{(Ca_{0.03}Na_{0.62}K_{0.35})_1(Fe_{0.04}Al_{1.03}Si_{2.95})_4O_8}$$

that would mean:

4 x 0.04 Fe, 4 x 1.03 Al and 4 x 2.95 Si

Important points to remember

- Keep three decimal places throughout the calculation; you can round off at the end.
- Remember to multiply the Mole% oxide by the number of **cations** in the oxide to get Moles Cation
- Remember to multiply the Mole% oxide (not Moles Cation) times the number of **oxygens** in the oxide to get the Moles Oxygen

Perkins Box 1.5 modified

Feldspar Analysis

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total				100.31				2.977	**5.008**

Iron is often reported as FeO, not Fe_2O_3; how will that change the calculation?

These columns can be omitted

Perkins Box 1.5 modified

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K_2O	94.2	2	1	6.2	0.066	K^{+}	0.132	0.066	**0.354**
total				100.31				2.977	**5.008**

Specific mineral formula for this feldspar:

$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.03}Si_{2.95})O_8$

Factor =
#ox. in formula/Σ(oxygens)
= 8/2.977=2.687