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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_2
 - feldspar $(\text{Ca,Na,K})_1(\text{Fe,Al,Si})_4\text{O}_8$
 - olivine $(\text{Mg,Fe}^{2+})_2\text{SiO}_4$
 - garnet $(\text{Ca,Mg,Fe}^{2+},\text{Mn})_3(\text{Al,Fe}^{3+})_2\text{Si}_3\text{O}_{12}$
- * **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:
 $(\text{Ca,Na,K})_1(\text{Fe}^{3+},\text{Al,Si})_4\text{O}_8$
 - 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** 2 x 15.999 grams
- Molecular 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

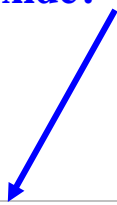
Oxide	Mol. Wt. of oxide (g/mole)	# cations in oxide	#anions in oxide	Oxide Wt% in mineral (grams)	Moles of Oxide	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO ₂	60.08	1	2	65.90					
Al ₂ O ₃	101.96	2	3	19.45					
Fe ₂ O ₃	159.68	2	3	1.03					
CaO	56.08	1	1	0.61					
Na ₂ O	61.96	2	1	7.12					
K ₂ O	94.20	2	1	6.20					
total				100.31					

Mineral formula?

**Perkins Box
1.5 modified**

**Feldspar
Analysis**

What is the
cation for each
oxide?



Oxide	Mol Wt of oxide	# cations in oxide	#anions in oxide	Oxide Wt% in mineral	Moles of Oxide in 100 grams	Cation	Moles of Cation	Moles of Oxygen	Moles of Cation per 8 Ox.
SiO ₂	60.08	1	2	65.90	1.097				
Al ₂ O ₃	101.96	2	3	19.45	0.191				
Fe ₂ O ₃	159.68	2	3	1.03	0.006				
CaO	56.08	1	1	0.61	0.011				
Na ₂ O	61.96	2	1	7.12	0.115				
K ₂ O	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 = $3 \times (-2) = -6$; 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.
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Na ₂ O	61.96	2	1	7.12	0.115	Na ⁺			
K ₂ O	94.20	2	1	6.20	0.066	K ⁺			
total				100.31					

Perkins Box 1.5 modified

How do we
get this?

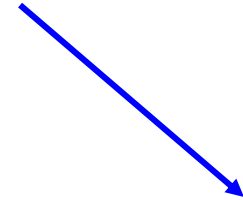


Feldspar Analysis

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Fe ₂ O 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 ₂ O	61.96	2	1	7.12	0.115	Na ⁺	0.230		
K ₂ O	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 ₂ O ₃	101.96	2	3	19.45	0.191	Al ³⁺	0.382	0.572	
Fe ₂ O 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 ₂ O	61.96	2	1	7.12	0.115	Na ⁺	0.230	0.115	
K ₂ O	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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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.

$$\text{Factor} = \frac{\# \text{ox. in formula}}{\Sigma(\text{oxygens})} = \frac{8}{2.977} = 2.687$$

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 ₂ O ₃	101.96	2	3	19.45	0.191	Al ³⁺	0.382	0.572	1.025
Fe ₂ O 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 ₂ O	61.96	2	1	7.12	0.115	Na ⁺	0.230	0.115	0.618
K ₂ O	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

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total				100.31				2.977	5.008

Finally, we can write the formula:



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

Feldspar **General** Formula: $(\text{Ca,Na,K})_1(\text{Fe,Al,Si})_4\text{O}_8$

Our Calculated (**Specific**) Formula:



$$\text{Ca}+\text{Na}+\text{K} = 1.00$$

$$\text{Fe}+\text{Al}+\text{Si} = 4.02$$

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

Do not duplicate the sum of cations as
subscripts in the specific formula!!

General Feldspar Formula: $(\text{Ca,Na,K})_1(\text{Fe,Al,Si})_4\text{O}_8$

Correct **Specific** Formula for our feldspar is this:



Not this:



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 Fe₂O₃; how will that change the calculation?

These columns can be omitted

Perkins Box 1.5 modified

Feldspar Analysis

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total				100.31				2.977	5.008

Specific mineral formula for this feldspar:



Factor =

#ox. in formula/ Σ (oxygens)

$$= 8/2.977=2.687$$