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GEOLOGY 284: MINERALOGY

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

Mineral Formulas

- Remember, minerals must have a "well-defined chemical composition"
- The composition range of a mineral is conveniently expressed by a **general chemical formula**, e.g.,
  - quartz SiO_2
  - feldspar $(Ca,Na,K)_1(Fe,Al,Si)_4O_8$
  - olivine $(Mg,Fe^{2+})_2SiO_4$
  - garnet $(Ca,Mg,Fe^{2+},Mn)_3(Al,Fe^{3+})_2Si_3O_{12}$
  - * **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 Perkin's 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: $(Ca,Na,K)_1(Fe,Al,Si)_4O_8$
  - 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, 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 our result as a specific (horizontal) chemical formula

Perkins Box 1.5 modified

This is the mineral analysis

How do we get this?

Feldspar Analysis

	Mol. Wt.	# cations	#anions	Oxide Wt%	Moles of		Moles of	Moles of	Moles of
Oxide	**of oxide**	**in oxide**	**in oxide**	**in mineral**	**Oxide**	Cation	Cation	Oxygen	Cation
	(g/mole)			(grams)					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 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_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 2Fe cations must be +6; 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

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**		
Al_2O_3	101.96	2	3	19.45	0.191	Al^{3+}	**0.382**		
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**	
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**	

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	**2.937**
Al_2O_3	100.16	2	3	19.45	0.194	Al^{3+}	0.388	0.583	**1.040**
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	**0.615**
K_2O	94.2	2	1	6.2	0.066	K^{+}	0.132	0.066	**0.353**
total				100.31				2.987	**5.009**

Finally, we can write the formula:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.04}Si_{2.94})O_8$$

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:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.04}Si_{2.94})O_8$$

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

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

Do not 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:

$$(Ca_{0.03}Na_{0.62}K_{0.35})(Fe_{0.04}Al_{1.04}Si_{2.94})O_8$$

Not this:

~~$(Ca_{0.03}Na_{0.62}K_{0.35})_1(Fe_{0.04}Al_{1.04}Si_{2.94})_4O_8$~~

that would mean:

4 x 0.04 Fe, 4 x 1.04 Al and 4 x 2.94 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

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**
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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**

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

These columns can be omitted