Geology 284 - Mineralogy, Fall 2009

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Mineral Formula Recalculation

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

• 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 (definite) chemical composition"

• The composition range of a mineral group 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 **specific** 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 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 for a given mineral

• First step is to figure out how many moles of each cation go with the 8 moles of oxygen

• Last step is to write our result as a specific (horizontal) chemical formula

Use the first (blank) page of the handout to follow along in the calculation

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 periodic table on 2nd page of textbook)

• Stable compounds are neutral (zero charge)

• The charge of the cation in each oxide is whatever makes the molecule neutral

• Example: Fe_2O_3 Neg. charge=3x(-2)=-6; charge of 2Fe cations must be +6; each is Fe^{3+}

Follow the calculation on your handout

The **Factor** is the number of oxygens you want (8 for feldspars) divided by the sum of the Moles Oxygen that you have calculated. Write the Factor at the bottom of the page!

Write the final result as a specific (horizontal) formula at the bottom of the page! (Don't forget the Oxygens!)

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

If it doesn't you have almost certainly made a mistake!   Find and correct the mistake!

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

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