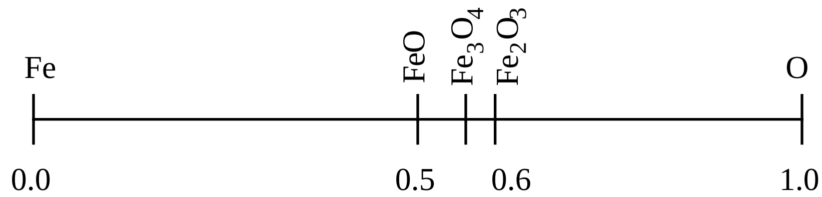
Lecture Notes - Composition Axes

- With chemical data for minerals in hand, we can begin to consider possible variations in chemical composition of minerals. Because rocks contain assemblages of minerals, we will also want to consider relationships among the chemical compositions of minerals that may occur together. These and other tasks are simplified if we can represent the compositions of minerals (and rocks!) on a graph. To make such a graph we must define a **composition axis**, a line that represents all chemical compositions that can be expressed as a linear combination of two **chemical components** (specific compositions). For example, if the components chosen are Fe and O, the composition axis might look like this:



Implicit in this figure are two important assumptions: (a) that the units of quantity of Fe and O used to define the axis are moles of Fe and moles of O; and (b) that the scale of the axis is given by

$$N_O \equiv \frac{n_O}{n_{Fe} + n_O}$$

where n_o is the number of moles of oxygen in one mole of the composition being plotted, n_{Fe} is the number of moles of iron in one mole of the composition being plotted, and N_o is the **mole fraction** of O. Other choices of units of quantity are in common use, *e.g.* mass of Fe and mass of O, but the scale selected is likely to have the same <u>form</u> as the mole fraction scale. A recipe for the graphical representation of simple mineral compositions follows:

Step #1 - Choose two components (chemical compositions) to define the composition axis.

Chemical components are specific chemical compositions: linear combinations of elements. They need not represent the compositions of actual minerals and may even be "negative."

Step #2 - Select a unit of quantity.

Possibilities include mole units (moles of the components), mass units (kilograms of the components), oxygen units (moles of oxygen "contributed" by each component), atom units (moles of atoms "contributed" by the components), cation units, anion units, oxide units, etc. Normally, the same unit of quantity is selected for each component.

Step #3 - Identify the expression that defines the scale of the axis (*e.g.* mole fraction, weight percent) in terms of the chosen components and unit of quantity.

There should be no ambiguity in the definition of the scale; always put the definition on your drawing of the composition axis.

Step #4 - For each composition you wish to plot on the composition axis, write an equation (in mole units) that gives the composition in terms of the chosen components.

Use the same tricks you use to balance chemical reactions. If negative numbers are a problem, remember that you can add the negative terms to both sides of the equation and work only with positive terms.

Step #5 - If the unit of quantity is not mole units, convert the equation of Step #4 to the desired units.

Note that the conversion factor is likely to be different for different compositions. For example, the number of oxygen units in one mole of SiO_2, is different than the number of oxygen units in one mole of MgO.

Step #6 - Substitute the coefficients from the resulting equation into the expression for the scale.

Steps #4 through #6 are repeated if other mineral compositions are to be plotted.

Examples for the system MgO - SiO_2

$1\ Mg_2SiO_4 = 2\ MgO + 1\ SiO_2$ **mole units** $N_{SiO_2} = \dfrac{n_{SiO_2}}{n_{MgO} + n_{SiO_2}} = \dfrac{1}{2+1}$

$1\ MgSiO_3 = 1\ MgO + 1\ SiO_2$ **mole units** $N_{SiO_2} = \dfrac{n_{SiO_2}}{n_{MgO} + n_{SiO_2}} = \dfrac{1}{1+1}$

$140\ Mg_2SiO_4 = 80\ MgO + 60\ SiO_2$ **mass units** $M_{SiO_2} = \dfrac{m_{SiO_2}}{m_{MgO} + m_{SiO_2}} = \dfrac{60}{140}$

$100\ MgSiO_3 = 40\ MgO + 60\ SiO_2$ **mass units** $M_{SiO_2} = \dfrac{m_{SiO_2}}{m_{MgO} + m_{SiO_2}} = \dfrac{60}{100}$

$4\ Mg_2SiO_4 = 2\ MgO + 2\ SiO_2$ **oxygen units** $O_{SiO_2} = \dfrac{o_{SiO_2}}{o_{MgO} + o_{SiO_2}} = \dfrac{2}{4}$

$3\ MgSiO_3 = 1\ MgO + 2\ SiO_2$ **oxygen units** $O_{SiO_2} = \dfrac{o_{SiO_2}}{o_{MgO} + o_{SiO_2}} = \dfrac{2}{3}$

$7\ Mg_2SiO_4 = 4\ MgO + 3\ SiO_2$ **atom units** $A_{SiO_2} = \frac{a_{SiO_2}}{a_{MgO} + a_{SiO_2}} = \frac{3}{7}$

$5\ MgSiO_3 = 2\ MgO + 3\ SiO_2$ **atom units** $A_{SiO_2} = \frac{a_{SiO_2}}{a_{MgO} + a_{SiO_2}} = \frac{3}{5}$

Examples from the system Mg_2SiO_4 - $MgSiO_3$

$1\ MgO = 1\ Mg_2SiO_4 - 1\ MgSiO_3$ **mole units** $N_{SiO_2} = \frac{n_{MgSiO_3}}{n_{Mg_2SiO_4} + n_{MgSiO_3}} = \frac{-1}{0}$

$1\ SiO_2 = -1\ Mg_2SiO_4 + 2\ MgSiO_3$ **mole units** $N_{SiO_2} = \frac{n_{MgSiO_3}}{n_{Mg_2SiO_4} + n_{MgSiO_3}} = \frac{2}{1}$

$40\ MgO = 140\ Mg_2SiO_4 - 100\ MgSiO_3$ **mass units** $M_{SiO_2} = \frac{m_{MgSiO_3}}{m_{Mg_2SiO_4} + m_{MgSiO_3}} = \frac{-100}{40}$

$60\ SiO_2 = -140\ Mg_2SiO_4 + 200\ MgSiO_3$ **mass units** $M_{SiO_2} = \frac{m_{MgSiO_3}}{m_{Mg_2SiO_4} + m_{MgSiO_3}} = \frac{200}{60}$

$1\ MgO = 4\ Mg_2SiO_4 - 3\ MgSiO_3$ **oxygen units** $O_{SiO_2} = \frac{o_{MgSiO_3}}{o_{Mg_2SiO_4} + o_{MgSiO_3}} = \frac{-3}{1}$

$2\ SiO_2 = -4\ Mg_2SiO_4 + 6\ MgSiO_3$ **oxygen units** $O_{SiO_2} = \frac{o_{MgSiO_3}}{o_{Mg_2SiO_4} + o_{MgSiO_3}} = \frac{6}{2}$

$2\ MgO = 7\ Mg_2SiO_4 - 5\ MgSiO_3$ **atom units** $A_{SiO_2} = \frac{a_{MgSiO_3}}{a_{Mg_2SiO_4} + a_{MgSiO_3}} = \frac{-5}{2}$

$3\ SiO_2 = -7\ Mg_2SiO_4 + 10\ MgSiO_3$ **atom units** $A_{SiO_2} = \frac{a_{MgSiO_3}}{a_{Mg_2SiO_4} + a_{MgSiO_3}} = \frac{10}{3}$