Calculating Oxide Weight Percents from Formulae and Normalizing Chemical Analyses

C:\a-StudioClassroom\minex02.rtf; July 8, 2005 (4:12pm)

The atomic weights of elements tell us how many grams there are per mole. Likewise, the atomic weight of an oxide (or any compound) tells us how many grams there are per mole of the oxide/compound.

For example, the atomic weight of quartz, $SiO_{2,}$ is 60.0843 (=28.0855 + 2*15.9994; make sure you know where these numbers come from). So quartz weighs 60.0843 grams per mole. Each mole contains 6.022×10^{23} (Avagodro's number) of molecules. So each SiO_2 molecule weighs $60.0843 \div 6.022 \times 10^{23}$ = a very small number!

Formulas to Weight percents (wt%)

Suppose I asked you to tell me the wt %s (weight percents) of Li, Al and Si in spodumene, $LiAlSi_2O_6$. The calculation is as follows:

ion	a = # atoms in spod	b = at wt elem	c = a x b	100 x c/d = wt % elem
Li	1	6.941	6.94	3.73
Al	1	26.98154	26.98	14.50
Si	2	28.0855	56.17	30.18
O	6	15.9994	96.00	51.59
TOTAL			d =186.09	100.00

==>Spodumene contains 3.7 wt% Li, 14.5 wt% Al, and 30.2 wt% Si.

For reasons explained in the book, we report chemical analyses in terms of weight percents of the oxides. So, we could redo the above calculation as follows:

ion	oxide	a = at wt oxide	b = # oxides in spod	c = a x b	100 x c/d = wt % oxide in spod
Li	Li_2O	29.8814	0.5	14.94	8.03
Al	Al_2O_3	101.9613	0.5	50.98	27.40
Si	SiO_2	60.0843	2	120.17	64.58
TOTAL				d =186.09	100.00

==>So, spodumene contains 8.0 wt % Li_2O, 27. 4 wt % Al_2O_3 and 64.6 wt % SiO_2.

(Make sure you know where all these numbers came from.)

Wt%s to Formulas

We can also do the reverse calculation. Suppose we have a mineral analysis that is 23.9253wt% FeO, 13.4217 wt% MgO, 22.6359 wt% Al_2O_3 and 40.0170 wt% SiO_2. In the table below I show how to convert an analysis from oxide weight percent to a chemical formula. (See also Box 1.5 in the text for more explanation.)

A	B	C	D	E	F	G	H	I
oxide	at wt of oxide	# cations in oxide	# oxygen in oxide	mineral analysis	=E/B	cation	=F x C =# cations	= F xD = # oxygen
FeO	71.8464	1	1	23.9253	0.3330074	Fe+2	0.333	0.333
MgO	40.3044	1	1	13.4217	0.3330074	Mg+2	0.333	0.333
Al_2O_3	101.9613	2	3	22.6359	0.2220049	Al+2	0.444	0.666
SiO_2	60.0843	1	2	40.0170	0.6660148	Si+4	0.666	1.332
							Oxygen =	2.664

Study the above table and make sure you know where all the numbers come from.

Columns H and I allow us to write the following formula:

$Fe_{0.333}Mg_{0.333}Al_{0.444}Si_{0.666}O_{2.664}$

This is a crummy looking formula because the subscripts are not integers.

After some trial and error, you will find an appropriate fudge factor to multiply everything by, and this formula becomes

$Fe_{1.5}Mg_{1.5}Al_{2.0}Si_{3.0}O_{12}$

If you look this up in a book, after scrounging around for a while you will find that this is the formula of a garnet that is 50 % almandine ($Fe_3Al_{2.0}Si_{3.0}O_{12}$) and 50% pyrope ($Mg_3Al_{2.0}Si_{3.0}O_{12}$).

Note that in real life, the math never comes out as exact as in the above examples (or the problems below). Analytical error introduces some uncertainty and adds difficulties to normalizations, but the approach and principles are still the same.

Your Problems

Be warned - these can be tricky!

1. Consider the mineral orthoclase with formula $KAlSi_3O_8$. What are the weight percents of K_2O, Al_2O_3 and SiO_2 in orthoclase? Show all work, don't just look up the answers.

2. Suppose you conducted an analysis of an unknown mineral and found it contained the following weight percents:

oxide	wt %
Na_2O	15.33079
Al_2O_3	25.22062
SiO_2	59.44859
TOTAL	100

Normalize this analysis by using atomic weights to change it into a formula. You will have to goof around, but if you guess the number of oxygen correctly, all the other subscripts will come out to be integers. Name the mineral!