Calculation of mineral chemistry

➢ Determination of Weight Percent (Wt%) of elements oxides in a mineral:

- This is very smilar to Lab. No.1 except for an additional step below since the mineral contains O as an important anion in the formula.
- Required chemical formula of mineral.
- Required to determine the molecular weights of each element (cation) oxide.

➢ Breack down chemical formula into balanced cation oxides:

1. Draw anarrow to the right of mineral formula and <u>place an O (oxygen) after each cation</u>; then place the approperiate subscript for each cation below that of the associated oxygen.

$$\mathbf{CaMgSi_2O_6 \longrightarrow CaO + MgO + SiO_2}$$

2. Balance the number of each element <u>on both sides of the arrow</u> by placing a whole number in front of each cation oxide pair and in front of the mineral formula if necessary.

$$\mathbf{CaMgSi_2O_6 \longrightarrow CaO + MgO + 2\ SiO_2}$$

Example: Calculate the weight % of the mineral; Beryl ($\mathbf{Be_3Al_2Si_6O_{18}}$)

Follow steps 1 and 2 above:

From step 1: $\mathbf{Be_3Al_2Si_6O_{18} = BeO + Al_2O_3 + SiO_2}$

From step 2: $\mathbf{Be_3Al_2Si_6O_{18} = 3\ BeO + Al_2O_3 + 6\ SiO_2}$

Element Oxide	Molecular Weight	Atoms	Molecular Weight Contribution	Weight % of oxide
BeO	25	3	75	(75/537) x 100 = 13.97
Al_2O_3	102	1	102	(102/537) x 100 = 19.0
SiO_2	60	6	360	(360/537) x 100 = 67.03
Sum.			537	

There are specific names given to cation oxides in Mineralogy

Know the names below given to some element (cation) oxides:

SiO_2 = Silica	CaO = Lime	Al_2O_3 = Alumina
MgO = Magnesia	Fe_2O_3 = Ferric oxide	MnO = Manganous oxide
FeO = Ferrous oxide	MnO_2 = Manganic oxide	K_2O = Potash
P_2O_5 = Phosphate	Na_2O = Soda	TiO_2 = Titania

- **Determination of the chemical formula of a minerla with oxygen in the formula :**

1. Divide eacd oxide constituent by the formula weight of the oxide. This gives you the **Molar Proportions of each oxide**.

   * Molar Prop. Oxide = Wt % / Mol. Wt. Of Oxide

2. Multiply the molar proportions of each oxide by the number of cations in the oxide. This gives you the **molar prportions of cations** in your mineral.

   ** Molar Prop. Of Cation = Molar Prop. Oxide x No. of cation.

3. Multiply the molar proportions o each oxide by the number of oxygen in each. This gives you the **molar proportions of oxygen** in your mineral.

   *** Molar Prop. of Oxygen = Molar Prop. Oxide x No. of Oxygen

4. **Sum the Molar Proportions of Oxygen**, and divide this sum by the number of oxygen in the mineral's ideal chemical formula (i.e. 4 oxygens for Olivine; 8 oxygens for Feldspar). The value you get is a **Correction factor**.

   ****** Correction factor = No. of Oxygen / ∑ molar prop. of Oxygen**

5. Now, multiply the **Molar Proportion of each Cation by the Correction factor** (multiplication factor). This will give you the **Proportions of each cation with respect to oxygen** in your mineral. At ths point, one can group your cations by valence and calculate the REAL minerla formula.

   ***** Proportion of Cation = Correction Factor x Molar Prop. of Cation

Example: Determine chemical formula for Pyroxene mineral, if you know that number of Oxygen is equal to 6 .

Oxide	Wt %	Mol. Wt. Oxide	* Moles of Oxide	** Moles of Cation	*** Moles of Oxygen	***** Prop. Cations O_6
SiO_2	56.64	60.086	0.9426	0.9426	1.8852	2.00
Na_2O	4.38	61.99	0.0707	0.1414	0.0707	0.30
Al_2O_3	7.21	101.963	0.0707	0.1414	0.2121	0.30
MgO	13.30	40.312	0.3299	0.3299	0.3299	0.7
CaO	18.46	55.96	0.3299	0.3299	0.3299	0.7
					2.8278	

But Pyroxenes here have 6 moles oxygens/mole, not 2.8278

****** Multiply moles cation by: 6 / 2.8278 = 2.121 (multiplication factor)**

$$Na_{0.3}\,Ca_{0.7}\,Mg_{0.7}\,Al_{0.3}\,Si_2O_6$$

Q1/ calculate the percentage composition by weight, in term of constituent oxides, of the Illmenite mineral ($FeTiO_3$)

Note: Atomic weight of Fe = 55.847 ; Ti = 47.90 ; O = 16

Q2/ Determine chemical formula for the follwing minerals:

Oxide	Weight %	Mol. Wt % Oxide
SiO_2	64.28	60.086
Al_2O_3	19.19	101.96
Fe_2O_3	0.09	159.69
MgO	0.10	40.305
BaO	0.11	153.327
CaO	0.11	56.087
K_2O	15.3	94.196
Na_2O	0.92	61.97

If you know that number of Oxygen in Feldspar mineral is equal to 8 .