Formulation - Explanation & Example

Ex. Pyroxene - (ideal formula: $Ca(Mg,Fe)Si_2O_6$

Calculations:

given		sum of atomic weights for oxide		mol. proportion = wt% ÷ mol. wt.	cation prop. = mol. prop x # of cations in oxide	oxygen prop. = mol. prop x # of oxygens in oxide	cations based on ideal = cation prop x correction factor
Element expressed as oxide	**Weight %**	**Mol. weight**		**Mol. Prop.**	**Cation Prop.**	**Oxygen Prop.**	**Cation prop. based on # of oxygens in ideal formula**
SiO_2	50.38	60.09		0.838	0.838	1.677	1.875
Al_2O_3	3.01	101.96		0.030	0.059	0.089	0.132
TiO_2	0.45	79.90		0.006	0.006	0.011	0.013
Fe_2O_3	1.95	159.70		0.012	0.024	0.037	0.055
FeO	4.53	71.85		0.063	0.063	0.063	0.141
MnO	0.09	70.94		0.001	0.001	0.001	0.003
MgO	14.69	40.31		0.364	0.364	0.364	0.815
CaO	24.32	56.08		0.432	0.432	0.432	0.966
Na_2O	0.46	61.97		0.007	0.015	0.007	0.033
K_2O	0.15	94.19		0.002	0.003	0.002	0.007
total	99.94				sum of oxy. props =	2.683	

← this should be close to the ideal # for Si. If it isn't, check your math

correction factor to bring to ideal 6 oxygens for pyroxene = 6 ÷ sum of oxy. props

correction factor = 6 ÷ 2.683 = 2.235

Ionic Radii for the 10 Major Elements in Common Minerals

	4 CN	6 CN	8 CN
P^{5+}	0.31	0.52	
Si^{4+}	0.40	0.54	
Al^{3+}	0.53	0.68	
Ti^{4+}	0.56	0.75	0.88
Fe^{3+}	0.63	0.69 - 0.79	0.92
Mg^{2+}	0.71	0.86	1.03
Mn^{2+}	0.80	0.81 - 0.97	1.10
Ca^{2+}		1.14	1.26
Na^{1+}	1.13	1.16	1.32
K^{1+}	1.51	1.52	1.65

Guidelines for entering values into actual formula:

1. Fill coordination sites backwards from the oxygen.
2. Start with the lowest coordination site - fill it completely starting with smallest cation, then next biggest cation, and next, etc.
3. Then move to the next biggest coordination site and do the same.
4. If a cation can take more than one coordination, you can divide it between coordination sites to fill them to their ideal #s

Ex. Pyroxene - (ideal formula: $Ca(Mg, Fe)Si_2O_6$

Actual formula based on measured chemistry:

8 CN **6 CN** **4 CN**

$(K_{0.007}\ Na_{0.033}\ Ca_{0.966})\ (Mn_{0.003}\ Mg_{0.815}\ Fe^{2+}_{0.141}\ Fe^{3+}_{0.055})\ (Ti_{0.013}\ Al_{0.132}\ Si_{1.875})\ 0_6$

totals to 1.01 totals to 1.01 totals to 2.02