Stoichiometry

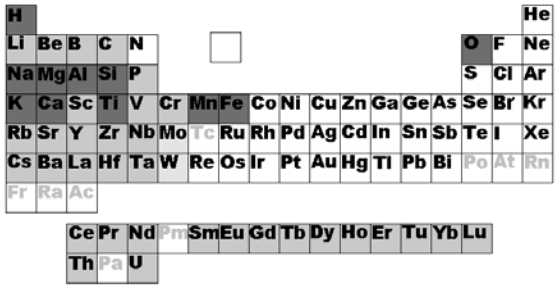
Chemical Analyses and Formulas

Stoichiometry

- *Chemical analyses of oxygen bearing minerals are given as weight percents of oxides.*
- *We need to be able to recalculate oxide analyses to cations per given number of oxygens to derive a chemical formula.*

Oxides of Lithophile Cations

• SiO_2	TiO_2		(4+)
• Al_2O_3	Cr_2O_3	Fe_2O_3	(3+)
• MgO	MnO	FeO	(2+)
• CaO			(2+)
• Na_2O	K_2O	H_2O	(1+)



Example 1
Weight percents to formula

• Oxide	Wt%	MolWt Oxide	Moles Oxide	Moles Cation	Moles Oxygen
• SiO_2	59.85	60.086	.9960	.9960	1.9920
• MgO	40.15	40.312	.9960	.9960	.9960
•	100.0				2.9980

- **Mole ratios Mg : Si : O = 1 : 1 : 3**
- **$MgSiO_3$**

Example 2
Formula to weight percents

- *Kyanite is Al_2SiO_5*
- *Calculate the weight percents of the oxides:*
  - *SiO_2*
  - *Al_2O_3*

Example 2
Formula to weight percents: Kyanite: Al_2SiO_5

Oxide	Moles PFU	MolWt Oxide	Grams Oxide	Wt% Percent
SiO_2	1	60.086	60.086	37.08
Al_2O_3	1	101.963	101.963	62.92
Formula weight			162.049	

Example 3: Solid Solutions
Weight percents to formula

- *Alkali Feldspars may exist with any composition between $NaAlSi_3O_8$ and $KAlSi_3O_8$.*
- *Formula has 8 oxygens: $(Na,K)AlSi_3O_8$*
- *The alkalis may substitute in any ratio, but total alkalis to Al is 1 to 1.*

Example 3: Solid Solutions
Weight percents to formula

Oxide	Wt%	MolWt Oxide	Moles Oxide	Moles Cation	Moles Oxygen
SiO_2	68.20	60.086	1.1350	1.1350	2.2701
Al_2O_3	19.29	101.963	0.1892	0.3784	.5676
Na_2O	10.20	61.9796	0.1646	0.3291	.1646
K_2O	2.32	94.204	0.0246	0.0493	.0246
	100.00				3.0269 x 2.6430=
					8.000

Mole ratios $Na_{0.87}K_{0.13}Al_{1.00}Si_{3.00}O_8$

calculated as cations per 8 oxygens

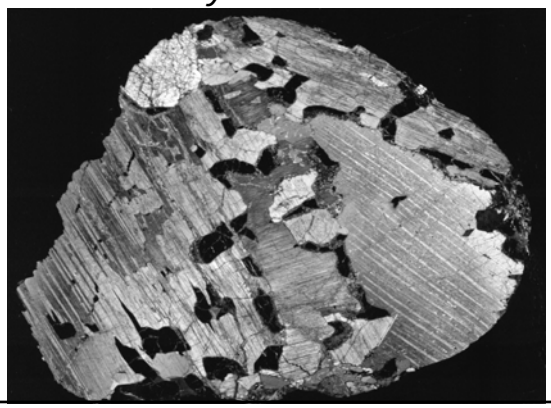
Simple Solid Solutions

- *$NaAlSi_3O_8$ - $KAlSi_3O_8$ Alkali Feldspars*
- *$MgSiO_3$- $FeSiO_3$ Enstatite-Ferrosilite (pyroxene)*
- *$MgCaSi_2O_6$-$FeCaSi_2O_6$ Diopside-Hedenbergite*
- *Mg_2SiO_4- Fe_2SiO_4 Forsterite-Fayalite*
- *$Mg_3Al_2Si_3O_{12}$- $Fe_3Al_2Si_3O_{12}$ Pyrope - Almandine*

Example 4
Weight Percent Oxides from Formula

- *Given the formula $En_{70}Fs_{30}$ for an orthopyroxene, calculate the weight percent oxides.*
- *En = enstatite = $Mg_2Si_2O_6$*
- *Fs = ferrosilite = $Fe_2Si_2O_6$*
- *Formula is $(Mg_{0.7}Fe_{0.3})_2Si_2O_6$ = $(Mg_{1.4}Fe_{0.6})Si_2O_6$*

Pyroxenes



Example 4 $(Mg_{1.4}Fe_{0.6})Si_2O_6$ Weight Percent Oxides from Formula

Oxide	Moles PFU	MolWt Oxide	Grams Oxide	Wt% Percent
SiO_2	2	60.086	120.172	54.69
MgO	1.4	40.312	56.437	25.69
FeO	0.6	71.846	43.108	19.62
Formula weight			219.717	100.00

Example 5 Weight Percent Oxides from Formula

- *A pyroxene is a solid solution of 40% jadeite ($NaAlSi_2O_6$) and 60% acmite ($NaFeSi_2O_6$).*
- *Calculate the weight percent oxides*
- *Formula is $Na(Al_{0.4}Fe_{0.6})Si_2O_6$*

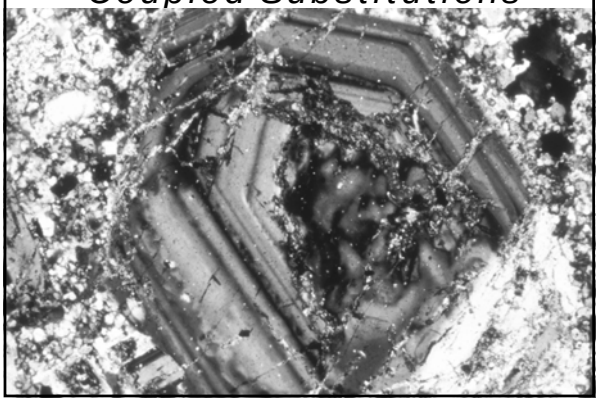
Formula is $Na(Al_{0.4}Fe_{0.6})Si_2O_6$ Calculate Weight Percent Oxides

Oxide	Moles PFU	MolWt Oxide	Grams Oxide	Wt% Percent
SiO_2	2.0	60.086	120.172	54.76
Al_2O_3	0.2	101.963	20.393	9.29
Fe_2O_3	0.3	159.692	47.908	21.83
Na_2O	0.5	61.980	30.990	14.12
Formula weight			219.463	100.00

Coupled Substitutions

- *Plagioclase feldspar $NaAlSi_3O_8$ - $CaAl_2Si_2O_8$*
- *Jadeite-diopside $NaAlSi_2O_6$ - $CaMgSi_2O_6$*

Coupled Substitutions



Coupled Substitution 40% Anorthite; 60% Albite Calculate Weight percent Oxides

- *First write the formula*
- *Anorthite is $CaAl_2Si_2O_8$*
- *Albite is $NaAlSi_3O_8$*
- *An_{40} Ab_{60} is $Ca_{.4}Na_{.6}Al_{1.4}Si_{2.6}O_8$*

$An_{40}\ Ab_{60}$ is $Ca_{.4}Na_{.6}Al_{1.4}Si_{2.6}O_8$

Oxide	Moles PFU	MolWt Oxide	Grams Oxide	Wt% Percent
SiO_2	2.6	60.086	156.22	58.17
Al_2O_3	0.7	101.963	71.37	26.57
CaO	0.4	55.96	22.38	8.33
Na_2O	0.3	61.980	18.59	6.92
Formula weight			268.58	100.00

Example Given Analysis Compute Mole percents of Jadeite and Diopside

- *Jadeite is $NaAlSi_2O_6$*
- *Diopside is $CaMgSi_2O_6$*

Jadeite - Diopside

Oxide	Wt%	MolWt Oxide	Moles Oxide	Moles Cation	Moles Oxygen
SiO_2	56.64	60.086	.9426	.9426	1.8852
Al_2O_3	7.21	101.963	.0707	.1414	.2121
MgO	13.30	40.312	.3299	.3299	.3299
CaO	18.46	55.96	.3299	.3299	.3299
Na_2O	4.38	94.204	.0246	.0493	.0246
	99.99				2.8278 x 2.6430=
Normalize to 8 oxygens					8.000

- $Na_{.3}Ca_{.7}Al_{.3}Mg_{.7}Si_2O_6$ =
- 30% Jadeite 70% Diopside

Unit Cells and Mineral Density

- *Unit cell is basic repeat unit of structure.*
- *Parallel-piped box: **a, b, c** (Å), α, β, γ (°)*
- *Å = 10^{-8}cm*
- *Avogadro's number (# atoms / mole) = 6.02 x 10^{23}*
- *If you know the contents of the box and the size of the box you can calculate the density.*

Cell Volume ($1Å^3 = 10^{-24}\ cm^3$)

- *Cubic* $V = a^3$
- *Tetragonal* $V = a^2c$
- *Hex/Trigonal* $V = a^2c \sin 120°$
- *Orthorhombic* $V = abc$
- *Monoclinic* $V = abc \sin \beta$
- *Triclinic*
- $V = abc\,(1 + 2\cos\alpha\cos\beta\cos\gamma - \cos^2\alpha - \cos^2\beta - \cos^2\gamma)^{1/2}$

Density

- Volume of Avogadro's number of unit cells = AV
- The number of formula units per unit cell = Z
  - Z is a small integer 1 to about 16.
- Weight of Avogadro's number of unit cells = Z* FW

$$\rho = \frac{Z \bullet FW}{A \bullet V}$$

Example Density Calculation

- Calculate the density of ferberite ($FeWO_4$), which is monoclinic with
- a = 4.73; **b** = 5.70; **c** = 4.95; β = 90.01; Z = 2.
- Calculate the gram formula weight:
  - 1 Fe (55.847) = 55.847
  - 1 W (183.85) = 183.85
  - 4 O (15.9995) 63.998
  - FW = 303.695 g

Example Density Calculation: Ferberite $FeWO_4$

- $V = \mathbf{abc} \sin \beta = (4.73)(5.70)(4.95)(\sin 90.01^{o})$
- $V = 133.46\ Å^3$
- $V = 1.335 \times 10^{-22}\ cm^3$
- $\rho = ZFw/AV = 2\ (303.70) / 6.02\ 10^{23} * 1.335\ 10^{-22}$
- $\rho = 7.56\ g/cm^3$