Stoichiometry

• Some minerals contain varying amounts of 2+ elements which substitute for each other

• Solid solution – elements substitute in the mineral structure on a sliding scale, defined in terms of the end members – species which contain 100% of one of the elements
Chemical Formulas

• Subscripts represent relative numbers of elements present

• (Parentheses) separate complexes or substituted elements
  – Fe(OH)$_3$ – Fe bonded to 3 separate OH groups
  – (Mg, Fe)SiO$_4$ – Olivine group – mineral composed of 0-100 % of Mg, 100-Mg% Fe
• $\text{KMg}_3(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$ – phlogopite
• $\text{K(Li,Al)}_{2.3}(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$ – lepidolite
• $\text{KAl}_2(\text{AlSi}_3\text{O}_{10})(\text{OH})_2$ – muscovite

• Amphiboles:
• $\text{Ca}_2\text{Mg}_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ – tremolite
• $\text{Ca}_2(\text{Mg,Fe})_5\text{Si}_8\text{O}_{22}(\text{OH})_2$ – actinolite

• $(\text{K,Na})_{0.1}(\text{Ca,Na,Fe,Mg})_2(\text{Mg,Fe,Al})_5(\text{Si,Al})_8\text{O}_{22}(\text{OH})_2$ – Hornblende

\begin{align*}
\{ & \text{Actinolite series minerals} \\
& \text{minerals} \}
\end{align*}
Compositional diagrams

FeO
wustite

Fe₃O₄ magnetite

Fe₂O₃ hematite

Fe

O

A

B

C

A₁B₁C₁

A₁B₂C₃

X

X
Pyroxene solid solution $\rightarrow$ $\text{MgSiO}_3$ – $\text{FeSiO}_3$

Olivine solid solution $\rightarrow$ $\text{Mg}_2\text{SiO}_4$ – $\text{Fe}_2\text{SiO}_4$
Minor, trace elements

• Because a lot of different ions get into any mineral’s structure as minor or trace impurities, strictly speaking, a formula could look like:
  - Ca$_{0.004}$Mg$_{1.859}$Fe$_{0.158}$Mn$_{0.003}$Al$_{0.006}$Zn$_{0.002}$Cu$_{0.001}$Pb$_{0.00001}$Si$_{0.0985}$Se$_{0.002}$O$_4$

• One of the ions is a determined integer, the other numbers are all reported relative to that one.
Normalization

• Analyses of a mineral or rock can be reported in different ways:
  – Element weight % - Analysis yields x grams element in 100 grams sample
  – Oxide weight % because most analyses of minerals and rocks do not include oxygen, and because oxygen is usually the dominant anion - assume that charge imbalance from all known cations is balanced by some % of oxygen
  – Number of atoms – need to establish in order to get to a mineral’s chemical formula

• Technique of relating all ions to one (often Oxygen) is called normalization
Normalization

• Be able to convert between element weight %, oxide weight %, and # of atoms
• What do you need to know in order convert these?
  – Element’s weight $\rightarrow$ atomic mass (Si=28.09 g/mol; O=15.99 g/mol; SiO$_2$=60.08 g/mol)
  – Original analysis
  – Convention for relative oxides (SiO$_2$, Al$_2$O$_3$, Fe$_2$O$_3$ etc) $\rightarrow$ based on charge neutrality of complex with oxygen (using dominant redox species)
Normalization example

- Start with data from quantitative analysis: weight percent of oxide in the mineral
- Convert this to moles of oxide per 100 g of sample by dividing oxide weight percent by the oxide’s molecular weight
- ‘Fudge factor’ is process called normalization – where we divide the number of moles of one thing by the total moles → all species/oxides then are presented relative to one another
### Feldspar Analysis

\( (\text{Ca, Na, K})_1(\text{Fe, Al, Si})_4\text{O}_8 \)

<table>
<thead>
<tr>
<th>Oxide</th>
<th>Atomic weight of oxide (g/mol)</th>
<th># cations in oxide</th>
<th># of ( \text{O}^{2-} ) in oxide</th>
<th>Oxide wt % in the mineral (determined by analysis)</th>
<th># of moles of oxide in the mineral</th>
<th>mole % of oxides in the mineral</th>
<th>Cation</th>
<th>moles of cations in sample</th>
<th>moles of ( \text{O}^{2-} ) contributed by each cation</th>
<th>Number of moles of ion in the mineral</th>
</tr>
</thead>
<tbody>
<tr>
<td>SiO(_2)</td>
<td>60.08</td>
<td>1</td>
<td>2</td>
<td>65.90</td>
<td>1.09687</td>
<td>73.83</td>
<td>Si(^{4+})</td>
<td>73.83</td>
<td>147.66</td>
<td>2.95</td>
</tr>
<tr>
<td>Al(_2)O(_3)</td>
<td>101.96</td>
<td>2</td>
<td>3</td>
<td>19.45</td>
<td>0.19076</td>
<td>12.84</td>
<td>Al(^{3+})</td>
<td>25.68</td>
<td>38.52</td>
<td>1.03</td>
</tr>
<tr>
<td>Fe(_2)O(_3)</td>
<td>159.68</td>
<td>2</td>
<td>3</td>
<td>1.03</td>
<td>0.00645</td>
<td>0.43</td>
<td>Fe(^{3+})</td>
<td>0.87</td>
<td>1.30</td>
<td>0.03</td>
</tr>
<tr>
<td>CaO</td>
<td>56.08</td>
<td>1</td>
<td>1</td>
<td>0.61</td>
<td>0.01088</td>
<td>0.73</td>
<td>Ca(^{2+})</td>
<td>0.73</td>
<td>0.73</td>
<td>0.03</td>
</tr>
<tr>
<td>Na(_2)O</td>
<td>61.96</td>
<td>2</td>
<td>1</td>
<td>7.12</td>
<td>0.11491</td>
<td>7.73</td>
<td>Na(^+)</td>
<td>15.47</td>
<td>7.73</td>
<td>0.62</td>
</tr>
<tr>
<td>K(_2)O</td>
<td>94.20</td>
<td>2</td>
<td>1</td>
<td>6.20</td>
<td>0.06582</td>
<td>4.43</td>
<td>K(^+)</td>
<td>8.86</td>
<td>4.43</td>
<td>0.35</td>
</tr>
<tr>
<td><strong>SUM</strong></td>
<td></td>
<td></td>
<td></td>
<td><strong>1.48569</strong></td>
<td><strong>100</strong></td>
<td></td>
<td></td>
<td>125.44</td>
<td>200.38</td>
<td></td>
</tr>
</tbody>
</table>

\( \text{Ca}_{0.73}\text{Na}_{15.47}\text{K}_{8.86}\text{Fe}_{0.87}\text{Al}_{25.68}\text{Si}_{73.83}\text{O}_{200.38} \)

\( \text{Ca}_{0.03}\text{Na}_{0.35}\text{K}_{0.35}\text{Al}_{0.03}\text{Si}_{2.95}\text{O}_{8} \)

To get here from formula above, adjust by \( 8 / 200.38 \).