The Structure of the Atom

Let’s remind ourselves of the basic structure of the atom:

Chemistry is based on changes in the arrangements of electrons around atoms, ions and molecules. For this reason, we need a detailed understanding of the electronic structure of atoms.
Electron shells

To a first, simple approximation, we say that the electrons in an atom are arranged in concentric shells, like the layers in an onion:

<table>
<thead>
<tr>
<th>Shell</th>
<th>Max no. of electrons</th>
</tr>
</thead>
<tbody>
<tr>
<td>1</td>
<td>2</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
</tr>
<tr>
<td>3</td>
<td>8</td>
</tr>
<tr>
<td>4</td>
<td>18</td>
</tr>
<tr>
<td>5</td>
<td>18</td>
</tr>
<tr>
<td>6</td>
<td>32</td>
</tr>
<tr>
<td>7</td>
<td>32</td>
</tr>
</tbody>
</table>
Now we can understand two important features of the periodic table: the **periods** (or rows) correspond to the electron shells (**called principal quantum shells**) and the **groups** (columns) correspond to the number of electrons in the outermost shell.

Note that the principle quantum shells fill consecutively from the innermost shell outwards. The outermost shell with electrons is known as the **valence shell**. It is the electrons in the valence shell that determine the chemistry of an element and we do not usually care much about the electrons in the inner shells.
The Octet ‘Rule’

The basis of the octet rule is that atoms ‘want’ a full outer shell of electrons, i.e. they are most **stable** with a full outer shell. This explains why the Group 8A elements, the noble gases, do not react to make compounds — they are already as stable as they can be (there are different meanings to the word ‘stable’ in chemistry. In this case, we mean the atom does not react easily with other atoms). An atom can get a full outer shell by losing or gaining electrons.

**The octet ‘rule’:** Row 1 elements: Hydrogen will usually lose an electron to gain a full outer shell, helium already has a full outer shell. Row 2 elements on the left will lose electrons to get a full outer shell, elements on the right will gain electrons to get 8 electrons in their outer shell. Row 3 elements on the left lose electrons to gain a full outer shell, elements on the right ***usually*** gain electrons to have 8 electrons in their outer shell.

The **octet rule** is a useful way to understand how and why atoms form molecules and ions. However, it is important to remember that the octet ‘rule’ is not a strict rule but a **rule of thumb**, so do not be surprised when you see exceptions.

H, 1 space, unstable
He, full valence shell, stable
Li, 7 spaces, unstable
F, 1 space, unstable
Ne, full valence shell, stable
Covalent Bonds — The Lewis Approach

One easy way for atoms to achieve a full outer shell is to share electrons in their outside, valence shells. When atoms share their valence electrons, they form a molecule with covalent bonds. One pair of electrons makes one covalent bond. A chemist called Lewis first proposed the following diagrams to explain why elements make certain compounds. Drawing a Lewis diagram is an important basic skill.

Hydrogen atom unstable, hydrogen molecule stable.

Oxygen atom unstable, water molecule stable.

Nitrogen atoms share six electrons to make a nitrogen molecule with a triple bond. N≡N.

Oxygen is a special case.
Electrons do not just form pairs in covalent bonds, they are often most stable in pairs. This means that electrons in a valence shell will often try to form a pair. Pairs of electrons on an atom that do not form a chemical bond are called lone pairs.

Sometimes an atom or molecule will have unpaired electrons, either because it has an uneven number of electrons or because a bond has been broken in half. These particles are called free radicals. Free radicals are usually very unstable and will try to take an electron from another atom or molecule to make pairs. Ultra-violet light damages skin by breaking bonds and making free radicals that react with other molecules in your cells.

The hydroxyl radical is a common and highly reactive radical.
Ions

The octet rule also helps us to understand how and why atoms form ions. If sodium (group 1) loses 1 electron, it gets a full outer shell. Because the sodium ion then has 11 protons but only 10 electrons, it gains a positive charge of $+1$. Calcium, the next atom along, needs to lose 2 electrons to get a full outer shell, giving it a charge of $+2$. Positive ions are called cations.

![Diagram of sodium atom losing an electron to form a sodium cation]

Conversely, chlorine, group 7, needs to gain 1 electron to get a full outer shell. This gives chlorine 17 protons and 18 electrons so it has a negative charge of $–1$. Oxygen, group 6, needs to gain 2 electrons for a full outer shell, giving it a charge of $–2$. Negative ions are called anions.

![Diagram of chlorine atom gaining an electron to form a chloride anion]
Ionic compounds

Now we can understand the formation of salt, NaCl. A sodium atom ‘wants’ to lose one electron and a chlorine atom ‘wants’ to gain one electron. By passing one electron from sodium to chlorine, we can form a pair of ions, Na⁺Cl⁻ (note, we do not usually perform this reaction in real life as it gives off a lot of energy and is very dangerous).

\[
\begin{align*}
2Na + Cl_2 & \rightarrow 2Na^+Cl^- \\
2Na & \rightarrow 2Na^+ + 2e^- \\
Cl_2 + 2e^- & \rightarrow 2Cl^- \\
Ca + Cl_2 & \rightarrow Ca^{2+}Cl^- \\
Ca & \rightarrow Ca^{2+} + 2e^- \\
Cl_2 + 2e^- & \rightarrow 2Cl^- \\
2Ca + O_2 & \rightarrow 2Ca^{2+}O^{2-} \\
2Ca & \rightarrow 2Ca^{2+} + 4e^- \\
O_2 + 4e^- & \rightarrow 2O^{2-}
\end{align*}
\]

(Note that the actual mechanism of the reaction may be more complex than one atom simply giving an electron to another one.)
Molecules or Ions? — Electronegativity

The Pauling electronegativity scale gives us a clue as to whether pairs of elements will form covalent compounds or ionic compounds. The scale goes from 0.8 to 4.

Atom pairs with a difference in electronegativity of around 2 or more (e.g. Na and Cl) form ions. Atom pairs with a difference of less than one (e.g. C and H) form molecular compounds. Atom pairs with a difference between 1 and 2 form compounds somewhere between covalent and ionic compounds. Electronegativity only applies to atoms in molecules or ionic compounds.
Compound/Molecular ions

Molecules can also make ions if the total number of electrons is not the same as the total number of protons.
Calculating Formal Charges

Because valence electrons are so important in chemistry, it is important to keep track of the number of electrons ‘owned’ by each atom in a molecule.

To calculate how many electrons are owned by each atom, we first make a Lewis diagram. Unshared electrons belong wholly to the atom they are connected to but shared electrons count only as ½. We then subtract the number of valence electrons the atom has in its elemental form from the number it owns in the molecule to calculate the formal charge.

In water, oxygen owns six electrons \([4 + (4 \times \frac{1}{2}) = 6]\). Oxygen has six valence electrons in its elemental form so its formal charge is \(6 - 6 = 0\). Each hydrogen atom owns one electron \([(2 \times \frac{1}{2}) = 1]\). Hydrogen has 1 electron in its elemental form so its formal charge is \(1 - 1 = 0\). The net charge (net charges are explained below) on the water molecule is therefore \(0 + 0 = 0\), which is what we expect for water.

If we count the electrons for the hydroxide ion (OH\(^-\)), however, we see that oxygen owns \(6 + (2 \times \frac{1}{2}) = 7\) electrons. Oxygen has 6 electrons in its elemental form so its formal charge is \(6 - 7 = -1\). The formal charge on the hydrogen atom is \((2 \times \frac{1}{2}) - 1 = 0\). The total charge on the hydroxide ion is therefore \((-1) + 0 = -1\), i.e. the net charge of the hydroxide ion is \(-1\).
Formal Charges and Net Charges

It is important to understand that formal charges are not really the same as net charges.

Formal charges are only used to calculate how many electrons we have in our molecule and where they are most likely to be. In reality, the electrons do not stick to one atom but are scattered all around the molecule, so even though we calculate a formal charge of $-1$ for the oxygen atom in hydroxide ions, it does not really have this charge all to itself. Even so, formal charges are a very simple way to estimate where the electrons are mostly likely to be and the electrons spend more time on the oxygen atom than on the hydrogen atoms. The most important use for formal charges, however, is to help us make sure we have written our molecules and chemical reactions with the right number of electrons.

Net charges are real. If we calculate a net charge of zero for a molecule, such as water, then it has no electrical charge (the number of protons and electrons balance exactly). If we calculate a positive or negative net charge for a molecule then it really has that charge, i.e. the hydroxide ion ($\text{OH}^-$) has one more electron than protons and so it has a total electrical charge of $-1$. 
Reading and Problems

Reading:
Chapter 7: 7-1, (7-2), 7-3, 7-5, 7-6, 7-7, (7-8), (7-12)

Problems:
Chapter 7: 4, 14, 24, 30, 43
Past exam problems

A) i) Can we easily make O$^{3-}$ ions? Explain why.

ii) How does the arrangement of elements in the periodic table, according to periods (rows) and groups (columns) correspond to the arrangement of electrons in their atoms.

B) Draw simple Lewis diagrams of the following compounds/ions:

i) CO$_3^{2-}$

ii) PH$_3$

iii) AlCl$_3$

iv) I$^-$

C) i) Write the formal charges of the indicated atoms next to the arrows. ii) calculate the net charges of those molecules.

Net charge: Net charge:
A) i) Can we easily make O\(^{3-}\) ions? Explain why.
No. An O\(^{3-}\) ion would have 9 valence electrons and this is not possible.

ii) How does the arrangement of elements in the periodic table, according to periods (rows) and groups (columns) correspond to the arrangement of electrons in their atoms.
The periods correspond to which principal quantum shell an element’s valence electrons belong to. The groups correspond to how many valence electrons an element has.

B) Draw simple Lewis diagrams of the following compounds/ions:
i) CO\(_3^{2-}\)  
\[
\begin{array}{c}
O^-\\
\vdots
\end{array}
\begin{array}{c}
C
\end{array}
\begin{array}{c}
O^-
\vdots
\end{array}
\]

ii) PH\(_3\)  
\[
\begin{array}{c}
H
\end{array}
\begin{array}{c}
P
\end{array}
\begin{array}{c}
H
\end{array}
\]

iii) AlCl\(_3\)  
\[
\begin{array}{c}
Cl
\end{array}
\begin{array}{c}
Al
\end{array}
\begin{array}{c}
Cl
\end{array}
\]

iv) I\(^-\)  
\[
\begin{array}{c}
I^-
\end{array}
\]
(Note, variations such as using circles for orbits or dots, are acceptable. Always check your net charges to be sure your diagrams are correct.)