OFB Chapter 3
Chemical Periodicity and the Formation of Simple Compounds

3-1 Groups of Elements
3-2 The Periodic Table
3-3 Ions and Ionic Compounds
3-4 Covalent Bonding and Lewis Structures
3-5 Drawing Lewis Structures
3-6 Naming Compounds in which Covalent Bonding Occurs
3-7 the Shapes of Molecules
3-8 Elements Forming More than One Ion
79 - Atomic number
Au - Symbol
196.97 - Relative atomic mass
Modern periodic law

The chemical and physical properties of the elements are periodic functions of their atomic numbers.
<table>
<thead>
<tr>
<th>H</th>
<th>Li</th>
<th>Be</th>
<th>B</th>
<th>C</th>
<th>N</th>
<th>O</th>
<th>F</th>
<th>Ne</th>
</tr>
</thead>
<tbody>
<tr>
<td>Na</td>
<td>Mg</td>
<td>Al</td>
<td>Si</td>
<td>P</td>
<td>S</td>
<td>Cl</td>
<td>Ar</td>
<td></td>
</tr>
<tr>
<td>K</td>
<td>Ca</td>
<td>Sc</td>
<td>Ti</td>
<td>V</td>
<td>Cr</td>
<td>Mn</td>
<td>Fe</td>
<td>Co</td>
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<tr>
<td>Rb</td>
<td>Sr</td>
<td>Y</td>
<td>Zr</td>
<td>Nb</td>
<td>Mo</td>
<td>Tc</td>
<td>Ru</td>
<td>Rh</td>
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<tr>
<td>Cs</td>
<td>Ba</td>
<td>Lu</td>
<td>Hf</td>
<td>Ta</td>
<td>W</td>
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<td>Ir</td>
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<tr>
<td>Fr</td>
<td>Ra</td>
<td>Lr</td>
<td>Rf</td>
<td>Db</td>
<td>Sg</td>
<td>Bh</td>
<td>Hs</td>
<td>Mt</td>
</tr>
<tr>
<td>Ac</td>
<td>Th</td>
<td>Pa</td>
<td>U</td>
<td>Np</td>
<td>Pu</td>
<td>Am</td>
<td>Cm</td>
<td>Bk</td>
</tr>
</tbody>
</table>

1/12/2004   OFP Chapter 3
Elements are classified as metal, non-metals, or semi-metals, and also fall into groups based on similarities in chemical and physical properties.
<table>
<thead>
<tr>
<th>Periodic Table of Elements</th>
</tr>
</thead>
<tbody>
<tr>
<td><strong>Alkali metals</strong></td>
</tr>
<tr>
<td><strong>Alkaline earth metals</strong></td>
</tr>
</tbody>
</table>

- **He**
- **B C N O F Ne**
- **Al Si P S Cl Ar**
- **K Ca Sc Ti V Cr Mn Fe Co Ni Cu Zn Ga Ge As Se Br Kr**
- **Rb Sr Y Zr Nb Mo Tc Ru Rh Pd Ag Cd In Sn Sb Te I Xe**
- **Cs Ba Lu Hf Ta W Re Os Ir Pt Au Hg Tl Pb Bi Po At Rn**
- **Fr Ra Lr Rf Db Sg Bh Hs Mt Uun Uuu Uub**

- **La Ce Pr Nd Pm Sm Eu Gd Tb Dy Ho Er Tm Yb**
- **Ac Th Pa U Np Pu Am Cm Bk Cf Es Fm Md No**
The Electronegativity (the power of an atom when in chemical combination to attract electrons to itself) is a periodic property.

<p>| | | | | | | | | | |</p>
<table>
<thead>
<tr>
<th></th>
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<tr>
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<td>0.98</td>
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<td>0.82</td>
<td>1.00</td>
<td>1.36</td>
<td>1.54</td>
<td>1.63</td>
<td>1.66</td>
<td>1.55</td>
<td>1.90</td>
<td>1.88</td>
<td>1.91</td>
</tr>
<tr>
<td>0.82</td>
<td>0.95</td>
<td>1.22</td>
<td>1.33</td>
<td>1.60</td>
<td>2.24</td>
<td>1.90</td>
<td>2.20</td>
<td>2.28</td>
<td>2.20</td>
</tr>
<tr>
<td>0.79</td>
<td>0.89</td>
<td>1.27</td>
<td>1.30</td>
<td>1.50</td>
<td>2.36</td>
<td>1.90</td>
<td>2.20</td>
<td>2.28</td>
<td>2.54</td>
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</tr>
</tbody>
</table>
Lewis Structures: Ionic compounds

Whenever possible, the valence electrons in a compound are distributed in such a way that each main-group element in a molecule (except hydrogen) is surrounded by eight electrons (an octet of electrons). Hydrogen should have two electrons in such a structure.
**Lewis Structures:**

<table>
<thead>
<tr>
<th>Na</th>
<th>Na(^+)</th>
<th>Ca</th>
<th>Ca(^{2+})</th>
</tr>
</thead>
<tbody>
<tr>
<td>Sodium atom</td>
<td>Sodium ion</td>
<td>Calcium atom</td>
<td>Calcium ion</td>
</tr>
</tbody>
</table>

- Loss of a valence electron
- Gain of a valence electron
- Combination to form the compound NaCl
<table>
<thead>
<tr>
<th>Anion</th>
<th>Name</th>
<th>Cation</th>
<th>Name</th>
</tr>
</thead>
<tbody>
<tr>
<td>F⁻</td>
<td>fluoride ion</td>
<td>H⁺</td>
<td>hydrogen ion</td>
</tr>
<tr>
<td>Cl⁻</td>
<td>chloride ion</td>
<td>Li⁺</td>
<td>lithium ion</td>
</tr>
<tr>
<td>Br⁻</td>
<td>bromide ion</td>
<td>Na⁺</td>
<td>sodium ion</td>
</tr>
<tr>
<td>I⁻</td>
<td>iodide ion</td>
<td>K⁺</td>
<td>potassium ion</td>
</tr>
<tr>
<td>O²⁻</td>
<td>oxide ion</td>
<td>Rb⁺</td>
<td>rubidium ion</td>
</tr>
<tr>
<td>S²⁻</td>
<td>sulfide ion</td>
<td>Cs⁺</td>
<td>cesium ion</td>
</tr>
<tr>
<td>Se²⁻</td>
<td>selenide ion</td>
<td>Be²⁺</td>
<td>beryllium ion</td>
</tr>
<tr>
<td>Te²⁻</td>
<td>telluride ion</td>
<td>Ca²⁺</td>
<td>calcium ion</td>
</tr>
<tr>
<td>N³⁻</td>
<td>nitride ion</td>
<td>Sr²⁺</td>
<td>strontium ion</td>
</tr>
<tr>
<td>P³⁻</td>
<td>phosphide ion</td>
<td>Ba²⁺</td>
<td>barium ion</td>
</tr>
<tr>
<td>As³⁻</td>
<td>arsenide ion</td>
<td>B³⁺</td>
<td>boron ion</td>
</tr>
<tr>
<td>Sb³⁻</td>
<td>antimonide ion</td>
<td>Al³⁺</td>
<td>aluminum ion</td>
</tr>
<tr>
<td>H⁻</td>
<td>hydride ion</td>
<td>Ga³⁺</td>
<td>gallium ion</td>
</tr>
</tbody>
</table>
Lewis Structures: Covalent Compounds

Whenever possible, the valence electrons in a compound are distributed in such a way that each main-group element in a molecule (except hydrogen) is surrounded by eight electrons (an octet of electrons). Hydrogen should have two electrons in such a structure.
Ammonia and Water have a pair of “lone electrons” called an “lone pairs”
Ammonia (NH₃)

Nitrogen (Group V)

5 valence

+ 2 in 1s = 7 electrons

Lewis Structures
1. Count up the total number of valence electrons available (symbolized by $A$) by first adding the group numbers of all the atoms present. If the species is a negative ion, add the absolute value of the total charge; if it is a positive ion, subtract it.

2. Calculate the total number of electrons needed ($N$) for each atom to have its own noble-gas set of electrons around it (two for hydrogen, eight for the elements from carbon on in the periodic table).

3. Subtract the number in step 1 from the number in step 2. This is the number of shared (or bonding) electrons present ($S$).

4. Assign two bonding electrons (as one shared pair) to each connection between two atoms in the molecule or ion.
Drawing Lewis Structures

5. If any of the electrons earmarked for sharing remain, assign them in pairs by making some of the bonds double or triple bonds. In some cases, there may be more than one way to do this. In general, double bonds form only between atoms of carbon, nitrogen, oxygen, and sulfur.

6. Assign the remaining electrons as lone pairs to the atoms, giving octets to all atoms except hydrogen.

7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.

\[
\text{Formal charge} = \text{group number} - \text{lone-pair electrons} - \frac{1}{2} (\text{number of electrons in bonding pairs})
\]
Drawing Lewis Structures

1. Count up the total number of valence electrons available (symbolized by $A$) by first adding the group numbers of all the atoms present. If the species is a negative ion, add the absolute value of the total charge; if it is a positive ion, subtract it.
Drawing Lewis Structures

2. Calculate the total number of electrons needed \((N)\) for each atom to have its own noble-gas set of electrons around it (two for hydrogen, eight for the elements from carbon on in the periodic table).

\[
\begin{align*}
\text{H} & \quad \text{H} \\
\text{H} & \quad \text{C} \quad \text{H} \\
\text{H} & \\
\text{H} &
\end{align*}
\]
Drawing Lewis Structures

3. Subtract the number in step 1 from the number in step 2. This is the number of \textit{shared} (or bonding) electrons present (S).

\begin{center}
\begin{tikzpicture}
  \node (H1) at (0,0) {H};
  \node (C) at (1,0) {C};
  \node (H2) at (2,0) {H};
  \node (H3) at (1,-1) {H};
  \draw (H1) -- (C);
  \draw (C) -- (H2);
  \draw (C) -- (H3);
\end{tikzpicture}
\end{center}
Drawing Lewis Structures

4. Assign two bonding electrons (as one shared pair) to each connection between two atoms in the molecule or ion.
Drawing Lewis Structures

1. Count up the total number of valence electrons *available* (symbolized by $A$) by first adding the group numbers of all the atoms present. If the species is a negative ion, *add* the absolute value of the total charge; if it is a positive ion, *subtract* it.
Drawing Lewis Structures

2. Calculate the total number of electrons needed \( N \) for each atom to have its own noble-gas set of electrons around it (two for hydrogen, eight for the elements from carbon on in the periodic table).

\[
\text{H} \quad \text{C} = \text{C} \quad \text{H}
\]

\[
\text{H} \quad \text{H}
\]
3. Subtract the number in step 1 from the number in step 2. This is the number of shared (or bonding) electrons present ($S$).
Drawing Lewis Structures

4. Assign two bonding electrons (as one shared pair) to each connection between two atoms in the molecule or ion.

\[ \text{H} \quad \text{C} \quad \text{H} \]
\[ \text{H} \quad \text{C} \equiv \text{C} \quad \text{H} \]
\[ \text{H} \quad \text{H} \]
Drawing Lewis Structures

5. If any of the electrons earmarked for sharing remain, assign them in pairs by making some of the bonds double or triple bonds. In some cases, there may be more than one way to do this. In general, double bonds form only between atoms of carbon, nitrogen, oxygen, and sulfur.

\[
\begin{array}{c}
\text{H} \\
\text{C} \\
\text{H} \\
\text{H} \\
\text{H} \\
\end{array}
\]
Drawing Lewis Structures

1. Count up the total number of valence electrons available (symbolized by $A$) by first adding the group numbers of all the atoms present. If the species is a negative ion, add the absolute value of the total charge; if it is a positive ion, subtract it.

\[\text{C}≡\equiv\text{O}\]
Drawing Lewis Structures

2. Calculate the total number of electrons needed \( (N) \) for each atom to have its own noble-gas set of electrons around it (two for hydrogen, eight for the elements from carbon on in the periodic table).

\[
\text{C≡≡O}
\]
3. Subtract the number in step 1 from the number in step 2. This is the number of \textit{shared} (or bonding) electrons present (S).

\[
\text{C} \equiv \equiv \text{O}
\]
Drawing Lewis Structures

4. Assign two bonding electrons (as one shared pair) to each connection between two atoms in the molecule or ion.

\[ \text{C} \equiv \equiv \text{O} \]
5. If any of the electrons earmarked for sharing remain, assign them in pairs by making some of the bonds double or triple bonds. In some cases, there may be more than one way to do this. In general, double bonds form only between atoms of carbon, nitrogen, oxygen, and sulfur.

\[
\text{C} \equiv \equiv \text{O}
\]
Drawing Lewis Structures

6. Assign the remaining electrons as lone pairs to the atoms, giving octets to all atoms except hydrogen.

\[
\text{C} \equiv \equiv \text{O}
\]
Drawing Lewis Structures

Steps 1.-6.

7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.

Methane $\text{CH}_4$

Formal charge = group number - lone-pair electrons - $\frac{1}{2}$ (number of electrons in bonding pairs)
7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.
7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.

**Ethylene** $\text{C}_2\text{H}_4$

Formal charge = group number - lone-pair electrons - $\frac{1}{2}$ (number of electrons in bonding pairs)
Drawing Lewis Structures

7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.
Drawing Lewis Structures

7. Determine the formal charge on each atom, and write it next to that atom. Check that the formal charges add to give a correct total charge on the molecule or molecular ion.

Carbon monoxide

Formal charge = group number - lone-pair electrons - \( \frac{1}{2} \) (number of electrons in bonding pairs)

\[ \text{C} \equiv \equiv \text{O} \]
3-7 the Shapes of Molecules

The VESPR theory

The Valence Shell Electron-Pair Repulsion Theory

**Steric Number**

\[ SN = (\text{number of atoms bonded to a central atom}) + (\text{number of lone pairs on central atom}) \]
3-7 The Shapes of Molecules

The VESPR theory

Text Error OFB 4th Edition

Page 123

Exercise 3-12

SeOF$_4$

The steric number for the Se atom is 5, not 4

See website for other corrections in the text and solutions manual.
The VSEPR Theory

The Valence Shell Electron-Pair Repulsion Theory

Electron pairs in the valence shell of an atom repel each other on a spherical surface formed by the underlying core of the atom.

The geometry which applies to a particular arrangement is determined by the steric number (SN) of the central atom.

“Steric” means “having to do with space.” The steric number of an atom in a molecule can be determined by drawing the Lewis structure of the molecule and adding the number of atoms that are bonded to it and the number of lone pairs that it has.
Geometry and Steric Number

• SN = 2 Linear 180°
• SN = 3 Trigonal planar 120°
• SN = 4 Tetrahedral 109.5°
• SN = 5 Trigonal bipyramidal
  – 90° (equatorial - axial or
  – 120° (equatorial – equatorial)
• SN = 6 Octahedral 90°
• SN for Double and triple bonds count the same as single bonded atoms
• SN = 5 Lone pairs occupy equatorial positions in preference to axial positions.
• When lone pairs are present, the situation is more complicated due to repulsive forces
  – Lone pr. vs lone pair >
  – Lone pr vs. bonding pair >
  – Bonding pr. Vs. bonding pair
Examples with no Lone Pairs on the central Atom

- $XY_2$ (example: $CO_2$)
- $XY_3$ (example: $BF_3$)
- $XY_4$ (example: $CH_4$)
- $XY_5$ (example: $PCl_5$)
- $XY_6$ (example: $SF_6$)
The VSEPR Theory

\[ XY_2 \]
(example: \( CO_2 \))
The VSEPR Theory

$XY_3$
(example: $BF_3$)
The VSEPR Theory

\[ XY_4 \]
(example: CH₄)
The VSEPR Theory

$XY_5$
(example: $PCl_5$)
The VSEPR Theory

$XY_6$
(example: $SF_6$)
The VSEPR Theory
Lone pairs
(a) PF$_5$  
Trigonal bipyramid

(b) SF$_4$  
Seesaw (low-energy, favored)

(c) SF$_4$  
Distorted pyramid (high-energy, not favored)

(d) ClF$_3$  
Distorted T

(e) XeF$_2$  
Linear
(a) $\text{PF}_5$

Trigonal bipyramid
(b) $\text{SF}_4$
Seesaw
(low-energy, favored)

(c) $\text{SF}_4$
Distorted pyramid
(high-energy, not favored)
(d) $\text{ClF}_3$

Distorted T
(e) XeF₂

Linear
Dipole Moments

- Bonded atoms share electrons unequally, whenever they differ in Electronegativity.

- E.g., HCl. The Cl atom carries a slightly negative electric charge and the H atom a slightly positive charge of equal magnitude. Aligns itself in an electric field.

- Dipolar or polar molecules posses a dipole moment, $\mu$.

- To find $\mu$,
  - first draw the VESPR molecular geometry.
  - Next assign a dipole moment to each bond,
  - then vectorially add the dipole moments for each bond.
3-8 Elements Forming more than One Ion

- Oxidation State (Oxidation Number)
  - Ionic vs Covalent bonding
  - *Not* formal electric charges, rather what the charge would be if the compound were ionic
  - Range from -3 to +7

- Examples
  1. CrO$_3$
  2. TlCl$_3$
  3. Mn$_3$N$_2$
  4. VCl$_4$
  5. Mn$_2$O$_7$
Chapter 3
Chemical Periodicity and the Formation of Simple Compounds

• Examples / exercises
  – All (3-1 to 3-16)

• HW Problems
  – 8, 9, 18, 34, 45, 57, 59, 60, 69, 70