Basic Concepts of Chemical Bonding

Cover 8.1 to 8.7 EXCEPT

1. Omit Energetics of Ionic Bond Formation
   Omit Born-Haber Cycle
2. Omit Dipole Moments
ELEMENTS & COMPOUNDS

• Why do elements react to form compounds?
• What are the forces that hold atoms together in molecules?
  and ions in ionic compounds?
Electron configuration predict reactivity

<table>
<thead>
<tr>
<th>Element</th>
<th>Electron configurations</th>
<th>Reactivity</th>
</tr>
</thead>
<tbody>
<tr>
<td>Mg (12e)</td>
<td>1S² 2S² 2P⁶ 3S²</td>
<td>Reactive</td>
</tr>
<tr>
<td>Mg²⁺(10e)</td>
<td>[Ne]</td>
<td>Stable</td>
</tr>
<tr>
<td>Cl(17e)</td>
<td>1S² 2S² 2P⁶ 3S² 3P⁵</td>
<td>Reactive</td>
</tr>
<tr>
<td>Cl⁻ (18e)</td>
<td>[Ar]</td>
<td>Stable</td>
</tr>
</tbody>
</table>
**CHEMICAL BONDS**

attractive force holding atoms together

**Single Bond**: involves an electron pair

  e.g. H₂

**Double Bond**: involves two electron pairs

  e.g. O₂

**Triple Bond**: involves three electron pairs

  e.g. N₂
Types of Chemical Bonds

Ionic
Polar Covalent
Covalent

Two Extremes
The Two Extremes

**Ionic Bond** results from the *transfer* of electrons from a metal to a nonmetal.

**Covalent Bond** results from the *sharing* of electrons between the atoms. Usually found between nonmetals.
The polar covalent bond is in-between

• the ionic bond [transfer of electrons]
  and

• the covalent bond [shared electrons]

The pair of electrons in a polar covalent bond are not shared equally.
DESCRIPTION OF ELECTRONS

1. How Many Electrons?
2. Electron Configuration
3. Orbital Diagram
4. Quantum Numbers
5. Lewis Symbols
LEWIS SYMBOLS

1. Electrons are represented as DOTS
2. Only VALENCE electrons are used

Atomic Hydrogen is \( H \cdot \)
Atomic Lithium is \( Li \cdot \)
Atomic Sodium is \( Na \cdot \)

All of Group 1 has only one dot
<table>
<thead>
<tr>
<th>Element</th>
<th>Electron Configuration</th>
<th>Lewis Symbol</th>
<th>Element</th>
<th>Electron Configuration</th>
<th>Lewis Symbol</th>
</tr>
</thead>
<tbody>
<tr>
<td>Li</td>
<td>[He]2s(^1)</td>
<td>Li(^-)</td>
<td>Na</td>
<td>[Ne]3s(^1)</td>
<td>Na(^-)</td>
</tr>
<tr>
<td>Be</td>
<td>[He]2s(^2)</td>
<td>·Be(^-)</td>
<td>Mg</td>
<td>[Ne]3s(^2)</td>
<td>·Mg(^-)</td>
</tr>
<tr>
<td>B</td>
<td>[He]2s(^2)2p(^1)</td>
<td>·B(^-)</td>
<td>Al</td>
<td>[Ne]3s(^2)2p(^1)</td>
<td>·Al(^-)</td>
</tr>
<tr>
<td>C</td>
<td>[He]2s(^2)2p(^2)</td>
<td>·C(^-)</td>
<td>Si</td>
<td>[Ne]3s(^2)2p(^2)</td>
<td>·Si(^-)</td>
</tr>
<tr>
<td>N</td>
<td>[He]2s(^2)2p(^3)</td>
<td>·N(^:)</td>
<td>P</td>
<td>[Ne]3s(^2)2p(^3)</td>
<td>·P(^:)</td>
</tr>
<tr>
<td>O</td>
<td>[He]2s(^2)2p(^4)</td>
<td>·O(^:)</td>
<td>S</td>
<td>[Ne]3s(^2)2p(^4)</td>
<td>·S(^:)</td>
</tr>
<tr>
<td>F</td>
<td>[He]2s(^2)2p(^5)</td>
<td>·F(^:)</td>
<td>Cl</td>
<td>[Ne]3s(^2)2p(^5)</td>
<td>·Cl(^:)</td>
</tr>
<tr>
<td>Ne</td>
<td>[He]2s(^2)2p(^6)</td>
<td>·Ne(^:)</td>
<td>Ar</td>
<td>[Ne]3s(^2)2p(^6)</td>
<td>·Ar(^:)</td>
</tr>
</tbody>
</table>
The Octet Rule

Atoms gain, lose, or share electrons until they are surrounded by $8$ valence electrons ($s^2 \ p^6$).

All noble gases [EXCEPT HE] have $s^2 \ p^6$ configuration.

Note:
There are exceptions to the octet rule.
I. The Ionic Bond

results from the \textit{transfer} of electrons

\[
\text{Na} \bullet + \bullet \text{Cl} : \rightarrow \text{Na}^+ : \text{Cl}^- \\
\]

Na has lost an electron to become Na\(^+\) and chlorine has gained the electron to become Cl\(^-\).
II. Covalent Bonding

results from the **sharing** of electrons between the atoms.

For example

\[ \text{H} \cdot + \cdot \text{H} \rightarrow \text{H} \cdot\cdot \text{H} \text{ or } \text{H} : \cdot \cdot \text{H} \]

\[
\begin{align*}
: \text{Cl} \cdot & + \cdot \text{Cl}: \\
\end{align*}
\]

Each pair of shared electrons constitutes one chemical bond.
Bonding & Non Bonding Electrons

**Bonding** Electrons: electrons between elements
How many Bonding electrons in
Hydrogen ?  Chlorine ?

**NonBonding** Electrons: those not used in bonding
How many Non Bonding electrons in
Hydrogen ?  Chlorine ?
Multiple Bonds

\[ \text{H–H} \quad \ddot{\text{O}}=\ddot{\text{O}} \quad :\text{N}≡\text{N} : \]

One shared pair of electrons  single bond
  e.g. \( \text{H}_2 \)  \( \text{H} - \text{H} \)

Two shared pairs of electrons  double bond
  e.g. \( \text{O}_2 \)  \( ::\text{O} = \text{O}:: \)

Three shared pairs of electrons  triple bond
  e.g. \( \text{N}_2 \)  \( :\text{N} ≡ \text{N} : \)
Covalent Bonding

When two atoms of the same kind bond, neither of them wants to lose or gain an electron. Therefore, they must share electrons. Each pair of shared electrons constitutes one chemical bond.
Strengths of Covalent Bonds

- We know that multiple bonds are shorter than single bonds.
- We know that multiple bonds are stronger than single bonds.
- As the number of bonds between atoms increases, the atoms are held closer and more tightly together.
III. POLAR COVALENT BONDS

In a Polar Covalent bond, electrons are shared.

But NOT equal sharing of those electrons.

In Polar Covalent bonds, the electrons are located closer to one atom than the other.

Unequal sharing of electrons results in polar bonds.
Polar Covalent Bonds

$H^{\delta+} \rightarrow F^{\delta-}$

There is more electron density on F than on H. Since there are two different “ends” of the molecule, HF has a di pole.
SPECIAL CASE  C- H  Bond

Lewis dot formula  . C .  for carbon

H

Lewis dot formula  . .
H . . C . . H

. .  for methane
H
Electronegativity

The ability of one atoms in a molecule to attract electrons to itself.
Electronegativity 0.7 (Cs) to 4.0 (F)

Group 1

<p>| | | | |</p>
<table>
<thead>
<tr>
<th></th>
<th></th>
<th></th>
<th></th>
</tr>
</thead>
<tbody>
<tr>
<td>H</td>
<td>EXCEPTION</td>
<td>{HIGH}</td>
<td></td>
</tr>
<tr>
<td>2.1</td>
<td>See Fig 8.6</td>
<td></td>
<td></td>
</tr>
<tr>
<td>Li</td>
<td>page 285</td>
<td></td>
<td></td>
</tr>
<tr>
<td>1.0</td>
<td></td>
<td>3.0</td>
<td>3.5</td>
</tr>
<tr>
<td>Na</td>
<td></td>
<td>4.0</td>
<td>Cl</td>
</tr>
<tr>
<td>0.9</td>
<td></td>
<td></td>
<td>3.0</td>
</tr>
</tbody>
</table>

{LOW}
Dipole

The difference in electronegativity leads to a polar covalent bond.

\[ \text{H}^{\delta+} \rightarrow \text{F}^{\delta-} \]

There is more electron density on F than on H. Since there are two different “ends” of the molecule, HF has a **dipole**.
Resonance Structures

Two or more alternative Lewis structures for a molecule.

The inability to described a molecule with a single Lewis stucture.
In ozone the extreme possibilities have one double and one single bond. The resonance structure has two identical bonds of intermediate character.
Resonance In Nitrate Ion

In Nitrate Ion \([\text{NO}_3^-]\) the extreme possibilities have one double and two single bonds.

The resonance structure has three identical bonds of intermediate character.
Draw the LEWIS STRUCTURE for

HF
NF₃
H₂O
H₂O₂
MgCl₂
CH₄
C₂H₆
Resonance In Nitrite Ion

\[(\text{NO}_2)^-\]

\[(\ O \ - \ N \ - \ O \ )^-\]

Where does the double bond go?

\[
\begin{align*}
\left| \overline{O} = \overline{N - O} \right| & \leftrightarrow \left| \overline{O - N} = \overline{O} \right|
\end{align*}
\]
Formal Charge

The difference between the valence electrons in an isolated atom and the number of electrons assigned to that atom in a Lewis structure.

\[
 \text{FC} = \text{valence electrons} - \text{nonbonding electrons} - \frac{1}{2} \text{bonding electrons}
\]
Formal Charge

Example 1

```
\[ \text{\textasciitilde O = C = O\textasciitilde vs \textasciitilde\textasciitilde\textasciitilde O - C \equiv O} \]
```

<table>
<thead>
<tr>
<th>Valence e⁻</th>
<th>6</th>
<th>4</th>
<th>6</th>
</tr>
</thead>
<tbody>
<tr>
<td>- e⁻ for atom</td>
<td>-\textasciitilde6</td>
<td>-4</td>
<td>-\textasciitilde6</td>
</tr>
<tr>
<td>Formal Charge</td>
<td>0</td>
<td>0</td>
<td>0</td>
</tr>
<tr>
<td></td>
<td>-1</td>
<td>0</td>
<td>+1</td>
</tr>
</tbody>
</table>
Correct formula for \((\text{NCO})^{-1}\) ?

<table>
<thead>
<tr>
<th>Structure 1</th>
<th>Structure 2</th>
<th>Structure 3</th>
</tr>
</thead>
<tbody>
<tr>
<td>::::N - C ≡O::⁻</td>
<td>::::N = C = O::⁻</td>
<td>::N ≡ C –O::⁻</td>
</tr>
<tr>
<td>V e⁻</td>
<td>5  4  6</td>
<td>5  4  6</td>
</tr>
<tr>
<td>- e⁻</td>
<td>-7 -4 -5</td>
<td>-6 -4 -6</td>
</tr>
<tr>
<td>FC</td>
<td>-2 0 +1</td>
<td>-1 0 0</td>
</tr>
</tbody>
</table>

Structure 3 is correct since negative charge is on the oxygen atom (most electronegative)
Formal Charge

1. Neutral molecules: Formal charges add to zero
2. Ions: Formal charges add to charge on ion
3. Smallest formal charge is preferable
4. Negative formal charge placed on most electronegative element