Chem 343  Summer 2002

Lecture 1

Topics

Chemical Bonding
  - octet rule
  - ionic bonding
  - covalent bonding
Lewis Structures (L-formal charges)
Resonance Structures
Shapes of Molecules (VSEPR)

Props/Visuals

Large Molecular Models
  - $\text{Cl}_4^-$
  - $\text{H}_2\text{O}$
Balloon Models for VSEPR

Announcements

- Class format/course organization.
  - Show schedule on overhead.
- Website
  - [WWW, Chem, wisc. edu/courses/343/lass/summer 2002](http://www.chem.wisc.edu/courses/343/lass/summer2002)
- Tips for Success
- Models
Chem 343 Lecture Notes

Chapter 1 - Carbon Compounds and Chemical Bonds

I. Chemical Bonding

⇒ A. Why do elements bond together?

Ans. they can achieve a lower energy state relative to the separate atomic elements.

B. Energy of atoms is largely determined by their electron configuration, that is, if we know the state of the electrons we can account for most of the energy state of atoms or molecules.

1) ground state e- configuration and all possible higher energy configurations were first determined and reported in 1926 by Erwin Schrodinger using a partial differential equation known as eigenfunction.

Wave Equation = Schrodinger Equation
Solutions → Quantum #’s → Orbitals
Quantum It's for H-atom

<table>
<thead>
<tr>
<th>Symbol</th>
<th>Values</th>
<th>Name</th>
<th>Physical Interpret.</th>
</tr>
</thead>
</table>
| n      | 1, 2, 3... | Principal Q# | Principal E-level "Shell" or au.
dist. from nucleus |
| l      | 0, 1, 2...n-1 | Orbital Q# | Shape of Orbital "Subshell" |
|        |        | Momentum Q# | "Subshell" |
| m_e    | -l...-2,-1,0,1,2...l | Magnetic Q# | Orientation of Orbital |
| m_s    | ±1/2, -1/2 | Spin Q# | Direction of Spin |

From n
Total number of states that e- can exist in within each shell:

# microstates = 2n²

From l and m_e we can graph each solution and get shapes and orientations of orbitals

l = 0 \rightarrow 5 - orbital

l = 1 \rightarrow set of 3 - p-orbitals

l = 2 \rightarrow set of 5 d-orbitals

l = 3 \rightarrow set of 7 f-orbitals
2) ground state e- configuration for atoms of higher elements "aufbau" are determined using the "building up" principle starting from the hydrogen atom and filling it up with electrons.

3) With reference to the periodic table, we can determine the order in which orbitals are filled from lowest to highest energy and write an electron configuration for each element.

\[ H = 1s^1 \]
\[ He = 1s^2 \]
\[ Li = 1s^2, 2s^1 \]
\[ Be = 1s^2, 2s^2 \]
\[ B = 1s^2, 2s^2, 2p^1 \]
\[ C = 1s^2, 2s^2, 2p^2 \]
\[ N = 1s^2, 2s^2, 2p^3 \]
\[ O = 1s^2, 2s^2, 2p^4 \]
\[ F = 1s^2, 2s^2, 2p^5 \]
\[ Ne = 1s^2, 2s^2, 2p^6 \]
4. **Hybrid Rule**: when more than one orbital of the same energy is available, electrons will fill different orbitals with spins parallel until each orbital contains 1 electron.

5. **Pauli Exclusion Principle**: When 2 electrons occupy the same orbital, they will have opposite spins, $\uparrow$ and $\downarrow$.

**C. Octet Rule** - atomic elements will form bonds by gaining, losing, or sharing electrons to achieve a full outer shell containing 8 electrons. (e--configuration same as nearest Noble Gas)

**D. Ionic Bonding** - cations formed by losing one or more electrons to achieve Noble Gas config. bond with anions formed by gaining one or more electrons to also achieve noble gas config. The cations and anions combine in ratio to achieve neutral overall charge.

Examples:  

\[ \text{Na}^{+} + \text{Cl}^{-} \rightarrow \text{NaCl} \]  
\[ \text{K}^{+} + \text{Br}^{-} \rightarrow \text{KBr} \]  
\[ \text{Mg}^{2+} + 2\text{Cl}^{-} \rightarrow \text{MgCl}_2 \]  
\[ \text{Ca}^{2+} + \text{O}^{2-} \rightarrow \text{CaO} \]
E. Covalent Bonding - atomic elements form bonds by sharing of e-’s so that each atom attains a full outer shell (or at least a more stable e- config.).

II. Lewis Description of Covalent Bonding and Lewis Dot Structures

A. G.N. Lewis proposed earliest successful description of covalent bonding.

Covalent bond is formed by the sharing of a pair of electrons between two atoms.

B. Lewis Dot Structures

1. must know how atoms are connected together - this can often be determined by applying simple rules of valence.

2. add up total number of valence electrons based on ground state e- config. of each atom.

3. form single bonds to connect all atoms by placing an electron pair between each pair of bonded atoms.
4. add non-bonding pairs around atoms to complete octet as well as possible.

5. form double bonds as necessary to complete octet of all atoms by moving some non-bonded e- pairs into bonding positions.

Example: \( \text{H}_2\text{O} \)

\[
\begin{align*}
\text{H} & : \overset{\text{O}}{\text{O}} : \text{H} \\
\text{or} & \quad \overset{-}\text{H} - \overset{\text{O}}{\text{O}} - \overset{+}{\text{H}}
\end{align*}
\]

Example: \( \text{CO}_2 \)

\[
\overset{\text{\text{-}}}{{\overset{\text{-1}}{\text{C}}} - \overset{\text{\text{-1}}}{\text{O}}}
\]

\[
\left\{ \overset{\text{\text{-}}}{{\overset{\text{\text{-1}}}{\text{O}}} = \overset{\text{\text{-1}}}{\text{C}} = \overset{\text{\text{-1}}}{\text{O}} \right\}
\]

\[\Rightarrow\] C. Formal Charges

The formal charge on each atom in a Lewis structure or VSEPR structure can be determined by counting the non-bonded e-'s around each atom plus le- from each bonding pair and subtracting this total from the number of valence e-’s in the ground state atom.
Example: $HNO_3$

$1 \times N = 5e^-$
$3 \times O = 18e^-$
$1 \times H = 1e^-$

$\frac{24e^-}{\text{Alternate example: } H_2CN_2}$

$\Rightarrow$ D. Exceptions to the Octet Rule

1) Compounds with fewer than 8 $e^-$'s around some atoms

Example: $BH_3$

$\text{These compounds are generally very reactive compared to compounds which fully adhere to the octet rule.}$

2) Atoms below the second row of the periodic table may have more than 8 $e^-$'s in their outer shell.

Examples: $PCl_5$, $SF_6$
3) However, compounds will never have more than 8e- around 2nd row atom or 2e- around H.

E. Resonance

1. Some molecules can be represented by more than one Lewis structure.

Example: Diazomethane

\[
\begin{align*}
\text{H} & \quad \text{C} = \text{N} = \text{N} \quad \leftrightarrow \quad \text{H} \quad \text{C} - \text{N} = \text{N}1 \\
\text{H} & \quad \text{H}
\end{align*}
\]

2. The true molecule is a hybrid of the resonance forms.

\[
\begin{align*}
\text{H} & \quad \text{C} = \text{N} = \text{N}1 \\
\text{H} & \quad \text{H}
\end{align*}
\]

3. When two or more equivalent resonance structures can be drawn, exceptionally good stability is observed compared to that predicted by any one structure.

Example: Acetic acid anion

\[
\begin{align*}
\text{CH}_3 - \text{C} = \text{O} \quad \leftrightarrow \quad \text{CH}_3 - \text{C} = \text{O}^-
\end{align*}
\]