Wait Lists and Add code requests:
Got you emails, working on it!

Questions? (non chemistry)
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Questions? (chemistry!)
CLAS tutor for this 109A course
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Sign up!
Chapter 1
Electronic Structure and bonding

Ch. 1: Important topics/concepts

Covalent Bonds: polar, or nonpolar (electronegativity)
compare polarity of bonds, such as H-C vs H-N vs H-O vs H-F

Structures: Lewis structures (Kekule, condensed, skeletal)
properly placing lone pairs of e, formal charges

\[
\begin{align*}
\text{H}_2\text{BF}_3 & = \text{H}_2\text{O} \quad \text{H}_2\text{OF} & = ? & \text{Lone pairs?} \\
\text{condensed} & \quad \text{skeletal} & \quad \text{Lewis} \\
\end{align*}
\]

Bonds: \(\sigma\) and \(\pi\) bonds (single bonds, double bonds, triple bonds)

\(\sigma\) formed by orbital overlap, s+s, s+p, p+s, or hybridized
\(\pi\) formed by overlap between p orbitals
double bond = 1 \(\sigma\) bond + 1 \(\pi\) bond
triple bond = 1 \(\sigma\) bond + 2 \(\pi\) bonds
Ch. 1: Important topics/concepts

Hybrid orbitals: s and p orbitals mix to form new hybrid orbitals (comes from valence-shell electron-pair repulsion (VSEPR) theory explains geometry of CH₄ and many other molecules)

Geometry (shape of molecules):
CH₄: tetrahedral, four sp³ orbitals, bond angle 109°,
H₂C=CH₂, ethylene, three sp² orbitals, one p orbital, bond angle ~120°
HC≡CH, acetylene, two sp bonds, 2 p orbitals, bond angle 180°
Bond length and strength: shorter bonds are stronger.

The Distribution of Electrons in an Atom

<table>
<thead>
<tr>
<th>quantum numbers</th>
<th>n</th>
<th>l</th>
<th>m_l</th>
<th>2e per orbital</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td></td>
<td></td>
<td></td>
<td></td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Table 1.1 Distribution of Electrons in the First Four Shells</th>
</tr>
</thead>
<tbody>
<tr>
<td>Atomic orbitals</td>
</tr>
<tr>
<td>--------------------</td>
</tr>
<tr>
<td>s</td>
</tr>
<tr>
<td>Number of atomic orbitals</td>
</tr>
<tr>
<td>Maximum number of electrons</td>
</tr>
</tbody>
</table>

- The first shell is closest to the nucleus.
- The closer the atomic orbital is to the nucleus, the lower its energy.
- Within a shell, s lower in energy than p.
The Distribution of Electrons in an Atom

### Table 1.1 Distribution of Electrons in the First Four Shells

<table>
<thead>
<tr>
<th>n</th>
<th>First shell</th>
<th>Second shell</th>
<th>Third shell</th>
<th>Fourth shell</th>
</tr>
</thead>
<tbody>
<tr>
<td></td>
<td>s</td>
<td>s, p</td>
<td>s, p, d</td>
<td>s, p, d, f</td>
</tr>
<tr>
<td>1</td>
<td>2</td>
<td>5</td>
<td>8</td>
<td>18</td>
</tr>
<tr>
<td>2</td>
<td>8</td>
<td>18</td>
<td>32</td>
<td></td>
</tr>
</tbody>
</table>

- The first shell is closest to the nucleus.
- The closer the atomic orbital is to the nucleus, the lower its energy.
- Within a shell, s lower in energy than p.

2s orbital, presents only one phase for overlap

lobes with opposite phases

Achieving a Filled Outer Shell by Sharing Electrons

\[ \text{H}^\cdot + \cdot\text{Cl}^- \rightarrow \text{H:Cl}^- \quad \text{or} \quad \text{H}–\text{Cl}^- \]

H is surrounded by 2 electrons

Cl is surrounded by 8 electrons
How Many Bonds Does an Atom Form?

Nonpolar and Polar Covalent Bonds

Nonpolar covalent bond = bonded atoms are the same or have similar electronegativities.

\[ \text{H—H} \quad \text{F—F} \quad \text{C—C} \quad \text{C—H} \]

Polar covalent bond = bonded atoms have different electronegativities.

\[ \delta^+ \quad \delta^- \quad \delta^+ \quad \delta^- \quad \delta^- \quad \delta^+ \]

the negative end of the bond
**Nonpolar and Polar Covalent Bonds**

**Nonpolar** covalent bond = bonded atoms are the same 
or have similar electronegativities.

\[ \text{H--H} \quad \text{F--F} \quad \text{C--C} \quad \text{C--H} \]

**Polar** covalent bond = bonded atoms have different electronegativities.

\[ \begin{align*}
\text{H--Cl} & : \quad \delta^+ \quad \delta^- \\
\text{H--O} & : \quad \delta^+ \quad \delta^- \\
\text{H--N} & : \quad \delta^+ \quad \delta^- \\
\text{H--Cl} & : \quad \delta^+ \quad \delta^- \\
\end{align*} \]

[Diagram showing the negative end of the bond]
Differences in electronegativity between atoms lead to polar bonds. The bigger the difference, the more polar the bond.

The Greater the Difference in Electronegativity, the More Polar the Bond

Nonpolar covalent bond: electronegativity difference < 0.5

Polar covalent bond: electronegativity difference 0.5 – 1.9

Electronegativity difference > 1.9: electrons are not shared; atoms are held together by the attraction of opposite charges
Dipole Moment

Dipole moment = size of the charge \times the distance between the charges

<table>
<thead>
<tr>
<th>Bond</th>
<th>Dipole moment (D)</th>
<th>Bond</th>
<th>Dipole moment (D)</th>
</tr>
</thead>
<tbody>
<tr>
<td>H—C</td>
<td>0.4</td>
<td>C—C</td>
<td>0</td>
</tr>
<tr>
<td>H—N</td>
<td>1.3</td>
<td>C—N</td>
<td>0.2</td>
</tr>
<tr>
<td>H—O</td>
<td>1.5</td>
<td>C—O</td>
<td>0.7</td>
</tr>
<tr>
<td>H—F</td>
<td>1.7</td>
<td>C—F</td>
<td>1.6</td>
</tr>
<tr>
<td>H—Cl</td>
<td>1.1</td>
<td>C—Cl</td>
<td>1.5</td>
</tr>
<tr>
<td>H—Br</td>
<td>0.8</td>
<td>C—Br</td>
<td>1.4</td>
</tr>
<tr>
<td>H—I</td>
<td>0.4</td>
<td>C—I</td>
<td>1.2</td>
</tr>
</tbody>
</table>

The greater the difference in electronegativity, the greater the dipole moment and the more polar the bond.
Electrostatic Potential Maps

- Li–H: Has the most negative electrostatic potential; attracts positive charge.
- H–F: Has the most positive electrostatic potential; attracts negative charge.

Lewis Structures

Important items: lone pairs, formal charges

- Water: H–O–H
- Hydronium ion: H–O–H
- Hydroxide ion: H–O–H
- Hydrogen peroxide: H–O–O–H

H→O→BF₃ = H→O→B→F = ?

Condensed, skeletal, Lewis
Carbon Forms Four Bonds

If carbon does not form four bonds, it has a charge (or it is a radical).

Nitrogen Forms Three Bonds

Nitrogen has one lone pair.

If nitrogen does not form three bonds, it is charged.
Oxygen Forms Two Bonds

Oxygen has two lone pairs.

If oxygen does not form two bonds, it is charged.

Hydrogen and the Halogens Form One Bond

A halogen has three lone pairs.

If hydrogen or halogen does not form one bond, it has a charge (or it is a radical).
The Number of Bonds Plus the Number of Lone Pairs Equals Four

Lewis Structures
Formal Charge

Important items: lone pairs, formal charges

Formal Charge =
the # of valence electrons –
(the # of lone-pair electrons + the # of bonds)

\[ \text{Formal Charge} = \text{the # of valence electrons} - (\text{the # of lone-pair electrons} + \text{the # of bonds}) \]

\[
\begin{align*}
\text{BF}_3 & = \text{O} - & \text{H} & \text{O} - & \text{B} - & \text{F} & = & ? \\
\text{condensed} & & \text{skeletal} & & \text{Lewis}
\end{align*}
\]

How to Draw a Lewis Structure

review Gen. Chem. and practice!

Homework: problems 49, 54, 55

\[ \text{NO}_3^- \quad \text{(anion of nitric acid HNO}_3\text{)} \]

Determine the total number of valence electrons \((5 + 6 + 6 + 6 = 23)\). Because they are negatively charged, add another electron = 24.
Avoid \(O-O\) bonds.
Check for formal charges.

\[
\begin{align*}
\text{incomplete octet}
\end{align*}
\]
Kekulé Structures and Condensed Structures

<table>
<thead>
<tr>
<th>Kekulé Structures</th>
<th>Condensed Structures</th>
</tr>
</thead>
<tbody>
<tr>
<td>H–C–Br</td>
<td>CH₃Br</td>
</tr>
<tr>
<td>H</td>
<td>CH₃OCH₃</td>
</tr>
<tr>
<td>H</td>
<td>HCO₂H</td>
</tr>
<tr>
<td>H–C–N–H</td>
<td>CH₃NH₂</td>
</tr>
<tr>
<td>H</td>
<td>N₂</td>
</tr>
</tbody>
</table>

atom bonded to a carbon are shown to the right of the carbon
...or connected to a carbon by a line bond above or below the carbon
repeating CH₂ groups can be shown in parentheses
whether bonded to a carbon can be shown in parentheses to the right of the carbon
...or connected to the carbon by a line bond above or below the carbon
the terminal carbon of a chain is not put in parentheses
### Kekulé Structures and Condensed Structures

**Skeletal Structures**

Skeletal structures show the carbon-carbon bonds as lines, but do not show the carbons or the hydrogens that are bonded to the carbons.
Back to Bonding: Forming a Sigma Bond

Waves Can Reinforce Each Other
Waves Can Cancel Each Other
Atomic Orbitals Combine to Form Molecular Orbitals

Orbitals are Conserved
\[ \text{# of Molecular Orbitals} = \text{# of Atomic Orbitals Combined} \]

Side-to-Side Overlap of In-Phase p Orbitals Forms a π Bond