Bonds

Chemistry 30 AP – Ms. Hayduk

Lewis Structures

- Used to show 2D bonding shape of covalent molecules
- Bonds are lines (single —, double =, triple ≡), electron pairs (lone pairs) are two dots

Drawing Lewis Structures

1. Count # valence electrons in all atoms (add for negative ions, subtract for positive).
2. Draw symbol of central atom.
3. Draw single bonds between outer and central atom.
4. Draw lone pairs on outer atoms to fill orbitals. Leftover pairs go on central atom.
5. If central atom does not have four pairs, convert outer lone pairs to single/double bonds (only for C, N, O, P and S)

Examples: Lewis Structures

- F_2
- HCN
- NH_3
- SF_6

Lewis Structure Limitations

- Odd-electron compounds (e.g. NO, NO_2 and ClO_2) don't follow octet rule, but are stable

- Octet rule exceptions
  - Fewer than eight (H, Be, B)
  - More than eight (you've seen this)

Review: Bond Energies

- Bond dissociation energy (D): the amount of energy needed to break a specific bond
- Units kJ/mol
- Amount of energy released when one mole of that bond (e.g. H–H) is broken
- Based on average values, since bonds can vary depending on environment

Bond Energy

$$\Delta H = \sum D_{broken} - \sum D_{formed}$$

E required E released

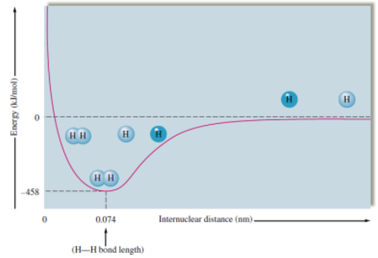
- Reactants → atoms → products
- Multiply D for each bond type by number of bonds (mol)

Example: Bond Energy

Calculate ΔH for this reaction at 25°C.

C_2H_4 (g) + Cl_2 (g) → $C_2H_4Cl_2$ (g)

Bonding: Lowest Energy State



Bond Length

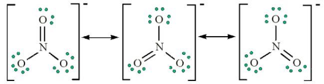
- Lowest energy state results in specific bond length and energy
- Multiple bonds – increase electron density, which <u>decreases</u> repulsion between nuclei
- Nuclei can move closes together, so triple bonds are very short, double bonds are short and single bonds are longer

Resonance Structures

- Occurs when molecule has more than one position where a double or triple bond can be placed
- Multiple bond "resonates" between all possible positions – bond length/strength is somewhere between pure single/multiple bond

Drawing Resonance Structures

- Must have: square brackets, charge (if necessary), double arrows between structures
- Actual structure is an <u>average</u> of all resonance structures; somewhere between single/multiple bond for length and strength



Example: Resonance

Draw resonance structures for O_3.

Formal Charge

- For non-equivalent resonance structures – used to determine most stable option

$$\boxed{\text{Formal charge} = \#\ \text{valence}\ e^- - \#\ \text{lone}\ e^- - \tfrac{1}{2}\ \#\ \text{bonding}\ e^-}$$

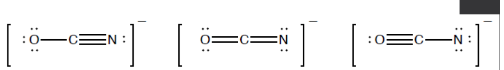
- "Fictitious" number – just for determining stability

Formal Charge Parameters

- Formal charge sum must equal charge on molecule (zero for a neutral atom, charge for a polyatomic ion)
- Smallest formal charge is preferred structure
- Smallest atom should have most negative formal charge (most electronegative – more on this later)

Example: Formal Charge

Determine which structure is most correct for OCN^-.

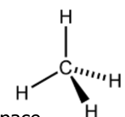


A B C

VSEPR

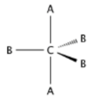
- 3D molecular shapes based on central atom
- Each shape has specific structure and bond angles
- NB: AP expects that you will memorize these shapes and angles

VSEPR



- All bonded atoms/lone pairs space themselves equally around the central atom
- When drawing, solid line is in plane of paper, wedge is forward out of paper, dash is backwards out of paper
- Lone pairs are more repulsive than atoms – <u>decrease</u> all other bond angles slightly when they are asymmetric

Example: VSEPR



1. What electron geometry is shown?
2. A, B and C are atoms.
   a. What is the A-C-B bond angle?
   b. What is the B-C-B bond angle?
3. If there are four atoms and one lone pair:
   a. Would the lone pair be on an A site or a B site? Why?
   b. What does this do to the other angles?
   c. What molecular shape does this form?

Electronegativity

- Ability of an atom to attract electrons in a chemical bond
- 0 – 4.0 Paulings (0 for noble gases)
- High electronegativity = atom "wants" to gain electrons, low = wants to give away

Thinking Activity

Based on what you know about periodicity:

1. Which element would you expect to have the <u>highest</u> electronegativity?
2. Would noble gases have high or low electronegativity?

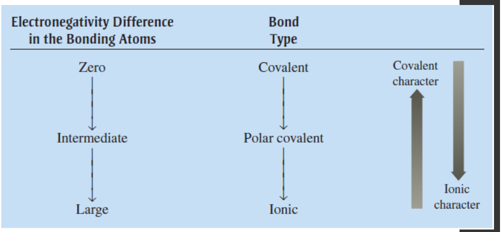
Bond Polarity

- Difference in electronegativity determines **polarity** of a bond
- **Polarity**: unequal sharing of electrons between two atoms
- Determines type of bond within a compound

Bonds and Electronegativity

- Ionic: complete transfer of electrons, EN difference > 2.0
- Covalent:
  - Non-Polar: equal sharing of electrons, EN < 0.5
  - Polar: unequal sharing, 0.5 <EN<1.6
- EN is 1.6-2.0: ionic if a metal is involved, otherwise polar covalent

Bonds and Electronegativity



Example: Bond Polarity

What is the electronegativity difference in a C-F bond? (What type of bond?)

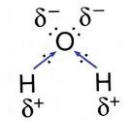
Thinking Activity: Polarity

Write the following bonds in order of increasing polarity:

H-H O-H Cl-H S-H Na-H F-H

Dipoles

- **Dipole**: area of positive or negative charge within a molecule
- Formed when electrons are held closer to one atom in a bond than the other
- Indicated by δ (delta) and the charge



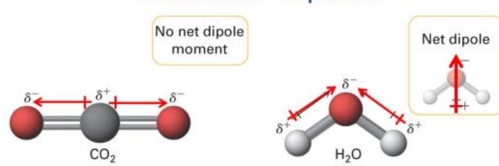
Example: Dipoles

In a C-F bond, identify the dipoles.

Molecular Polarity

- Bond polarity ≠ molecule polarity
- **Dipole moment**: separation of charge in a molecule, based on size of charge and distance of separation
- In plain English: if all polar bonds "cancel", molecule is non-polar (and substance is non-polar)

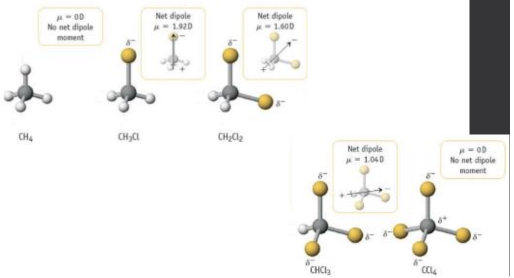
Molecular Dipoles



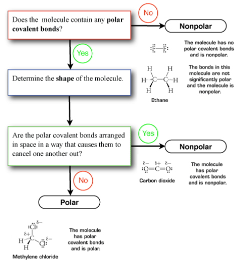
The C=O bonds have dipoles of equal magnitude but opposite direction, so there is no net dipole moment.

The O-H bonds have dipoles of equal magnitude that do not cancel each other, so water has a net dipole moment.

Example: Tetrahedral Structures



Determining Polarity



More on "Shape"

- As a general rule, non-polar molecules are ones that have <u>all the same terminal atoms</u>, and have no lone pairs
- Exceptions are linear and square planar molecules (also non-polar)

Example: Polar… or NOT?

BrF_5

Example: Polar… or NOT?

XeF_4