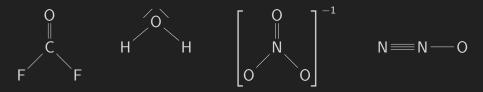
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# 1 General Chemistry Review

### **Electrons, Bonds, and Lewis Structures**

- ▶ Covalent bond: two atoms sharing a pair of electrons.
- ▶ **Octet rule**: *main group elements* that tend to bond in a way that each atom has eight electrons in it's valence shell.
  - Atoms that do not have eight will share electrons with other elements in order to maintain a stable state.
- ▶ Main group elements: sometimes called representative elements, are groups
   1, 2 and 13–18 in periodic table.
  - Some elements in group 3 and 12 share properties between transition metals and the main group.
- ▶ The lowest energy (most stable) state of two atoms is determined both by bond length and bond strength.
- ▶ Valence electrons are determined by the group, 1A–8A, of the periodic table.
- ▶ **Lone pair**: unshared, or nonbonding, electrons.
- ▶ Lewis structures: 2D model that represents covalent bonds as straight lines and lonpairs as dots.
- $\triangleright$  Examples: COF<sub>2</sub>, H<sub>2</sub>O, NO<sub>3</sub>, N<sub>2</sub>O:



▶ **Resonance structures**: a set of two or more Lewis structures that collectively describe the electronic bonding of a single polyatomic species, including fractional bonds.

# **Identifying Formal Charges**

- ▶ **Formal charge**: any atom that does not exhibit the appropriate number of valance electrons.
- > Determing formal charge:

• Formula: 
$$FC = V - N - \frac{B}{2}$$

- V = valance electrons of element
- N = lone pair electrons

- B = bonded electrons
- ▶ Less than expected number of valence electrons results in a positive charge.
- ▶ More than expected number of valence electrons results in a negative charge.
- ▶ The lower the magnitude of formal charge, the greater the stability of the whole molecule.
- Atoms that are more electronegative hold negative formal charges better, which results in greater stability vs when the negative charge is spread on less electronegative elements in a polyatomic species.
  - The dominant resonance structure will be that of the greatest stability.

#### **Induction and Polar Covalent Bonds**

- ▶ Bonds can classified into three categories: covalent, polar covalent, and ionic.
- ▶ The categories emerge from the electronegativity values of the atoms sharing a bond.
- ▶ **Electronegativity**: a measure of the ability of an atom to attract electrons.
  - Electronegativity generally increases left to right, and from the bottom to top of the periodic table.
  - **F, O, N, CI** (Br, I). Most electronegative elements, from left to right, that are often encountered.
- ▶ **Covalent bond**: when the difference in electronegativity is less than 0.5.
- ▶ **Polar covalent bond**: when the difference in electronegativity is between 0.5 and 1.9, then the electrons are not equally shared and become polar.
- ▶ **Induction**: the withdrawl of electrons towards to more electronegative atom.  $\delta^+$  represents partial positive charged gained when electrons are pulled away, while  $\delta^-$  represents the partial negative charge pulled closer.
- ▶ **Ionic bond**: when the difference in electronegativity is greater than 1.9.
  - Electrons are not shared in this case, and attraction is insetsad just the result of oppositely charged ions.

#### **Atomic Orbitals**

- ▶ Atomic orbital (AO): standing quantum wave (excitation in electron field) around an atom.
  - More energy leads to higher orbtails levels.

- Gives principle quantum number, n, as is associated with distance from nucleus.
- o Orbital levels: s(1 pair), p(3 pairs), d(5 pairs), f(7 pairs).
  - Angular momentum quantum number that describes three-dimensional region of space that the electron density occupies.
- Magnetic quantum number descrices orientation in space of electron density.
  - $-m_l=0$ ; s orbital
  - $-m_{l}=-1, 0, 1; p_{x}, p_{y}, p_{z}$  orbitals.
- $\circ$  Locations where  $\psi$  (quantum wave function) is zero are called **nodes**.
  - The more nodes that an orbital has, the greater it's energy.
- Spin: allows an orbital to contain only two electrons,  $\pm \frac{1}{2}$
- Degenerate orbitals: orbitals with the same energy level.
- ▷ Order in which orbitals are filled is determined by three principles:
  - Aufbau principle: lowest energy orbital is filled first.
  - **Pauli exclusion principle**: each orbital can accommodate a maximum of two electrons that have opposite spin.
  - Hund's rule: electrons are placed in each degenerate orbital before being paired up.
- ▷ Describing the nature of atomic orbital is done with two commoly used theories: Valence Bond Theory and Molecular Orbital Theory.
- ▶ The commonly used theories give a deeper understanding of covalent bonds, which is essentially just the overlap of atomic orbitals.
- ▶ Constructive/destructive interference: the result of two waves that approach each other, or overlap.
  - Constructive interference produces a wave with the vector sum of both waves.
  - Destructive interference cancel each other out and produes a node.

### **Valence Bond Theory**

▶ **Valence bond theory**: the sharing of electron density between two atoms is a result of the constructive interference of their atomic orbitals.

- ▶ Bond axis: the line that can be drawn between two hydrogen atoms.
- $\triangleright$  **Sigma bond** ( $\sigma$ ): a particular type of covalent bond that has circular symmetry with respect to the bond axis.
  - $\circ$  All single bonds are  $\sigma$  bonds.
  - The strongest type of covalent bond.
- $\triangleright$  **Pi bond** ( $\pi$ ): covalent bonds where two lobes of an orbital overlap with two lobes of another atom.
  - Each atomic orbital has zero electron density at a shared nodal plane, passing through the two bonded nuclei.
  - $\circ$   $\pi$  bonds form double  $(\sigma + \pi)$  and triple bonds  $(\pi + \sigma + \pi)$ .
  - $\circ$  Individual  $\pi$  bonds are weaker than  $\sigma$  bonds.

### **Molecular Orbital Theory**

- ▶ **Molecular orbital theory (MO)**: uses linear combinations of atomic orbitals to model and explore the consequences of orbital overlap.
  - The newly described orbitals are called molecular orbitals accroding to MO theory.
- ▶ Atomic orbitals refer to an individual atom, while molecular orbitals is associated with an entire molecular.
- ▶ In other words, MO theory states that atomic orbitals cease to exist when they overlap. Instead they are replaced with multiple molecular orbitals which span the entire molecule.
- ▶ Molecular orbitals are more stable (lower energy) since electrons are attracted by both nuclei.
- $\triangleright$  When there are nodes between the nuclei, then the resulting  $\sigma^*$  orbitals become antibonding, as they destabilize (increase the energy) of a molecular orbital.
- ▶ Best used to produce a quantitative picture of bonding.
  - o Describes strength, order, and polarity of bonds.
  - Allows for the presence of paired or unpaired electrons.
  - Has spectroscopic preperties.

### **Hybridized Atomic Orbitals**

- ▶ **sp³-hybridized orbitals**: produced by averaging one *s* orbital and three *p* orbitals.
  - Hybridized orbitals explains to geomtry of methane, which results form the now four degenerate orbitals pushing apart to achieve tetrahedral geometry.
  - Hybridized orbitals become unsymmetrical, producing a larger front lobe that is more efficient than standard p orbitals in the ability to form bonds.
  - $\circ$  All bonds in are  $\sigma$  bonds, and thus can be individually represented by the overlap of atomic orbitals.
- $\triangleright$  **sp**<sup>2</sup>**-hybridized orbitals**: produced by averaging the *s* orbital with only two of *p* orbitals.
  - The remaining p orbital is unaffected, and free multiple p orbitals results in a  $\pi$  bond.
  - o This is done to expain geometry of compounds bearing a double bond.
  - $\circ$  A double bond if formed from one  $\sigma$  bond and one  $\pi$  bond.
  - Associated with trigonal planar geometry.
- ▶ sp-hybridized orbitals: produced by averaging of one s orbital and one p orbital.
  - Leaves two p orbitals and resulting in two  $\pi$  bonds.
  - A triple bond is formed with the addition of one  $\sigma$  bond due to the overlap of the sp orbitals.
  - o Geometry of a triple bond has linear geometry.
- ▶ Finding the hybridization of any atom can be done simply:
  - 1. Look at the central item.
  - 2. Determin groups (number of bonds,  $\pi$  bonds count as 1, and lone pairs attached) of atom.
    - groups aka regions of electron density.
  - 3. For groups 1-4:  $sp^x$ ; x = groups 1
  - 4. For groups 5-6:  $sp^3d^x$ ; x = groups 4
- ▶ Bond Strength and Bond Length:
  - o Bond length decreases with more bonds.

- o Bond strength increases with more bonds.
- The more s character, the shorter and stronger the bond, and the larger the bond angle.
  - s-character: contribution of the  $\sigma$  bond in a hybridization.
    - e.g. sp = 50%,  $sp^2 = 33\%$ ,  $sp^3 = 25\%$
  - sp-sp bond is the strongest,  $sp^3-sp^3$  is the weakest.

# **Molecular Geometry**

- Valence shell electron pair repulsion (VSEPR) theory: enables the prediction of molecular geometry due to the pressumption that all electron pairs repel each other; resulting in a three-dimensional space that maximizes distance from each other.
- Steric number: the total number of electron pairs in a molecule. Can be bonds or lone pairs.
- $\triangleright$  **Tetrahedral geometry**: result of four  $\sigma$  bonds and zero lone pairs.
  - o produces a tetrahendron with bond angles of 109.5°.
- $\triangleright$  **Trigonal pyramidal geometry**: three  $\sigma$  bonds and one lone pair.
  - The lone pair occupy more space than bonded electron pairs, so the remaining angles are slightly less than a tetrahedral, at 107°.
  - o The lone pair sits atop the base forming a pyramid like structure.
- $\triangleright$  **Bent geometry**: two  $\sigma$  bonds and two lone pairs.
  - VSEPR predicts the lone pairs to be in two corners of the tetrahedral, producing bond angles of 105°.
  - VSEPR predicts geometry H<sub>2</sub>O correctly, but for wrong reasons.
    - The lone pairs in  $H_2O$  have different energy levels, suggesting one pair occupies a p orbital with the other in a lower-energy hybridized orbital.
- ▶ VSEPR theory is best used for a first approximation and is mostly accurate for most small molecules.
- Trigonal planar geometry: three electron pairs forming three bond angles of 120° and lie on the same plan.
- ▶ **Linear geometry**: two electron pairs that oppose each other at 180°, forming a linear structure.
- ▶ General method of determining structure:

- 1. Count steric number—the total number of electron pairs in a molecule. Can be bonds or lone pairs.
- 2. Determine predicted geomterical structure predicted (EDG) by VSEPR using steric number.
  - Octahedral:6, Bipyramid:5, Tetrahedral:4, Trigonal:3, Linear:2
- 3. Determin impact (the MG) of lone pairs; more lone pairs results in less space between bonded pairs. Shape depends on EDG.

### **Dipole Moments and Molecular Polarity**

- ightharpoonup Dipole moment ( $\mu$ ): defined as the amount of partial charge,  $\delta$ , on on either end of the dipole multiplied by the distance separtion, d:
  - $\circ \mu = \delta d$
  - $\circ$   $\mu$  generally has an order of magnitude of  $10^{-18} \, \text{esu} \cdot \text{cm}$  due to general partial charge (esu) and distance (cm) values.
  - $\circ$  1 debye (D) =  $10^{-18}$  esu·cm
- ▶ **Molecular dipole moment**: the vector sum of the individual dipole moments.
  - Lone pairs have significant effect on the molecular dipole moment.
  - o Also called the net dipole moment.

### **Intermolecular Forces and Physical Properties**

- ▶ **Intermolecular forces**: the attractive forces between individual molecules that determed the physical properties of a compound.
- ▶ *Electrostatic*: forces that occur as a result of the attraction between opposite charges.
- ▶ Electrostatic interactions for neutral molecules (no formal charge) are often classified as into the following categories:
  - Dipole-dipole interaction: Compounds with net dipole moments.
    - In solid space these intereactions either repel or attract each other.
    - In liquid space these interactions tend to attract more often, raising melting/boiling point.
    - lon-dipole: electrostatic interaction between an ion and a molecule with a dipole.
  - **Hydrogen bonding**: molecules with a hydrogen attached to an F, O, or N.
    - Not actually a bond, just an interaction.

- When hydrogen bonds to a electronegative atom, then the hydrogen will have a  $\delta^+$ .
- Hydrogen bonding is strong due to size of hydrogen atom, resulting in very close partial charge interactions.
- The more hydrogen bonds, the higher the boiling point tends to be.
- Stronger than dipole-dipole interactions.

#### Fleeting dipole-dipole interactions:

- Electrons are considered to be in constant motion, which restult in the center of negative charge to vary.
- London Dispersion Forces (LDFs): On average, the dipole moment is zero, though it can experience transient dipole moments, initiating fleeting attraction/repulsion.
  - · All atoms and molecules have LDFs.
  - · Weakest, but the dominant force in non-polar molecules.
  - · Dispersion forces directly related to molar mass.
- Heavier hydrocarbons generally experience a stronger force due to increased surface area, and thus greater chance for non-zero dipole moments, which results in higher boling points.
- Branched hydrocarbons generally have decreased surface area, decreasing boiling point relative to others of similar weight.
- ▶ When comparing boling points of compounds, look for following factors:
  - Any dipole-dipole interactions? (increases boiling point)
  - Formation of hydrogen bonds? (increase boling point)
  - Number of electrons. (more electrons, higher boiling point)
  - Number of carbon atoms. (more surface area, higher boiling point)
  - Degree of branching of compound. (more branching, more surface area)

## Structural Theory of Matter

- ▶ **Constitutional isomers**: aka structural isomers; same chemical formula, but different in the way the atoms are connect, i.e. their constitution is different.
  - o Consistenet with the octet rule.
  - Each element forms a predictable number of bonds, from one to four.

- The number of possbile constitutional isomers increases as the number of carbon atoms increases
- ▶ **Stereoisomers**: isomers that differ in spatial arrangement of atoms, rather than connectivity.
  - Geometric isomerism: aka cis-trans; locked into spatial positions due to double bonds or a ring structure.
    - Cis indicates functional groups that are on the same side of the carbon chain.
    - Trans indicates functional groups on opposite sides of the carbon chain.
  - **Enantiomers**: aka optical isomers; mirror images of each other that are non-superposable.
    - Human hands are a macroscopic analogy.
- ▶ More detail will be covered in later sections.

# 2 Molecular Representations

### **Types of Molecular Representations**

▶ **Partially condensed structures**: the C−H bonds are not always drawn, saving space.

- ▶ Condensed structures: single bonds are not drawn and groups of atoms are clustered when possbile.
  - CH<sub>3</sub>CH<sub>3</sub>CHOH → (CH<sub>3</sub>)<sub>2</sub>CHOH
- ▶ **Molecular formula**: simply shows number of each type of atom with no structural information.
  - o C<sub>3</sub>H<sub>8</sub>O
- ▶ Example of converting a condensed structure into a partially condensed structure:
  - o (CH<sub>3</sub>)<sub>3</sub>CCH<sub>2</sub>CH(CH<sub>3</sub>)CH(CH<sub>3</sub>)<sub>2</sub>

 This shows just one isomer, more partially condensed structures are possible.

#### **Bond-Line Structures**

- Bond-line structures; aka skeletal structures; simplify drawing process of chemical structures and are easier to read.
- Each corner or endpoint represents a carbon atom.

- All examples have 6 carbon atoms
- Double bonds are shown with two lines, triple with three.

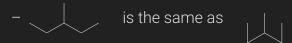
- Triple bonds are drawn linearly due to sp-hybridization

• Hydrogens are not shown; it is assumed that each carbon posses enough to satisfy octet rule.

#### **Notes on Drawing Bond-Line Structrues**

- Carbon atoms in a straight chain should be drawn in zigzag format in order to accurately show each carbon.
- Double bonds should be drawn as far apart as possible:

o Direction of a single bond is irrelevant:



- All heteroatoms (atoms other than carbon and hydrogen) must be drawn.
  - Hydrogens next to heteroatoms must be shown.
- Carbons cannot have more than four bonds.

### **Hydrogen Deficiency Index: Degrees of Unsaturation**

Excerpt from Chapter 14: Infrared Spectroscopy and Mass Spectrometry

- ▶ Saturated compounds: the maximum number of hydrogen atoms possbile, relative to number of carbon present.
  - o Determining saturation using molecular formula:  $C_nH_{2n+2}$  n= carbon atoms
  - **Halogens**: takes the place of a hydrogen atom; add one H for each halogen.
  - Oxygen: no affect on saturation; ignore.
  - Nitrogen: needs an extra hydrogen; subtract one H for each nitrogen.
- $\triangleright$  **Unsaturated compounds**: a compound that contains at least one  $\pi$  bond, resulting fewer than the maximum number of hydrogen atoms.
  - Compounds with rings also result in an unsaturated compound.
  - Degree of unsaturation: a number that represents half the "missing" number of hydrogen atoms when compared to a saturated compound.
- ▶ **Hydrogen deficiency index (HDI)**: the measure of degrees of unsaturation.
  - e.g. two degrees of unsaturation results in a HDI of 2.

- Degrees of freedom help represent possbile structures, indicating possible double bounds, triple bounds, rings, or various combinations of each.
- o Only helpful when molecular formula is known for certainty.
- Formula: HDI =  $\frac{1}{2}(2C + 2 + N H X)$ 
  - X: halogen atoms.

## **Identifying Functional Groups**

| TABLE 2.1 EXAMP   | LES OF COMMON          | FUNCTIONAL GROUPS  | CHAPTER | FUNCTIONAL GROUP* | CLASSIFICATION     | EXAMPLE                       | CHAPTER |  |  |
|---|------------------------|--------------------|---------|-------------------|--------------------|-------------------------------|---------|--|--|
| R—X:  | Alkyl halide           | CI:                | 7       | ·O·               | Ketone             | ·O·                           | 19      |  |  |
| (X=Cl, Br, or I)  | ,                      | n-Propyl chloride  |         | R R               |                    | 2-Butanone                    |         |  |  |
| R R R   | Alkene                 | 1-Butene           | 7, 8    | R H               | Aldehyde           | Butanal                       | 19      |  |  |
| R <b>−C≡C</b> −R  | Alkyne                 | 1-Butyne           | 9       | R .O. H           | Carboxylic<br>acid | Pentanoic acid                | 20      |  |  |
| R− <mark>Ö</mark> H   | Alcohol                | ÖH<br>1-Butanol    | 12      | R XX:             | Acyl halide        | Ö'.<br>Çİ:<br>Acetyl chloride | 20      |  |  |
| R− <mark>Ö</mark> −R  | Ether                  | Diethyl ether      | 13      | R O               | Anhydride          | O                             | 20      |  |  |
| R— <mark>ÄH</mark>  | Thiol                  | 1-Butanethiol      | 13      | B SO B            | Ester              | .o. Ethyl acetate             | 20      |  |  |
| R− <mark>Š</mark> −R  | Sulfide                | S. Diethyl sulfide | 13      | R R R             | Amide              | NH <sub>2</sub> Butanamide    | 20      |  |  |
|   | Aromatic<br>(or arene) | Methylbenzene      | 17, 18  | R N R             | Amine              | H<br>N<br>N<br>Diethylamine   | 22      |  |  |
| * The "R" refers to the remainder of the compound, usually carbon and hydrogen atoms. |                        |                    |         |                   |                    |                               |         |  |  |

- ▶ **Functional group (R)**: specific substituents or moieties within molecules that may be responsible for the characteristic chemical reactions.
  - **Substituents**: an atom or group of atoms which replaces one or more hydrogen atoms on the parent hydrocarbon chain.
  - Moiety: a part of a molecule which is typically found within other molecules and often given a specific name.

#### **Characterizing Carbon Centers and Functional Groups**

#### Characterizing Carbon Centers

Primary 1°: a carbon with only one carbon-carbon bond.

- Secondary 2°: a carbon with two carbon-carbon bonds.

- Tertiary 3°: a carbon with 3 carbon-carbon bonds.

Quaternary 4°: a carbon with four carbon-carbon bonds.

#### Characterizing Functional Groups

 Certain functional groups can be characters as 1°, 2°, or 3°, based on how many carbon bonds are attached to the carbon with the functional group.

# **Identifying Lone Pairs**

- ▶ Formal charges must always be drawn on bond line structures, otherwise the resulting bond line structures would be inferred incorrectly.
- ▶ Lone pairs do not have to be drawn and usually are omitted.
- ▶ The formal charge allows you to determin lone pairs.

• Formula: 
$$FC = V - N - \frac{B}{2}$$

- V = valance electrons of element
- N = lone pair electrons
- B = bonded electrons

• Solve for lone pairs: 
$$N = V - FC - \frac{B}{2}$$

▶ Frequent usage will allow for intuition for lone pairs.

#### **Common Patterns Between Formal Charge and Lone Pairs**

- Associated Patterns for Oxygen
  - A negative (๑) charge corresponds with 1 bond and 3 lone pairs.
  - The absence of charge corresponds with 2 bonds and 2 lone pairs.
  - A positive (⊕) charge corresponds with 3 bonds and 1 lone pair.

#### Associated Patterns for Nitrogen

- A negative charge corresponds with 2 bonds and 2 lone pairs.
- The absence of charge corresponds with 3 bonds and 1 lone pair.
- A positive charge corresponds with 4 bonds and 0 lone pairs.

#### Resonance

- ▶ **Resonance**: description of bonding in molecules or ions by the combination of multiple contributing streutres.
  - Resonance structures: each contributing structure of the resonance hybrid.
    - Formal charges are important to include when drawing resonance structures as it clarifies where locations of lone pairs and movement of electrons.
    - Total charge must remain the same between structures.
- ▷ Resonance does not describe any real process, rather it's a method to overcome inadequacy of bond-line drawings.
- ▶ Different from isomerism, which differs in arrangements of atomic nuclei in space, rather than how the electrons are assigned to the depictions.

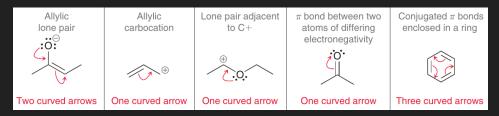
#### **Resonance: Curved Arrows**

- Curved arrows: a tool used to help draw resonance strcutres by representing electrons as if they were moving.
  - Somwhat different from curved arrow notation in reactions, which actually represent the flow of electron density.
  - Can help shows how to change the formal charge:
    - · Formal charges at the tail become more positive, since it's losing an electron.
    - · Formal charges at the head more negative, since it's gaining an electron.

- Avoid breaking a single bond.
  - Structures must have atoms connected in same order, though there are minor exceptions that will be discussed later.
  - This rule affects the placement of the tail of the arrow, as it represents distribution of previous electrons.
- Never exceed an octet for second-row elements.
  - Not a violation to have less than an octet.
  - This rule affects the placement of the head of the arrow, as it represents sharing of new electrons.
- Can only be used on adjcent atoms, though the electrons can be pushed multiple times.
- "Legal" moves:
  - $-\pi$  bond  $\rightarrow$  lone pair.
  - Lone pair  $\rightarrow \pi$  bond.
  - $\pi$  bond  $\rightarrow$   $\pi$  bond.
  - Every resonance structure can be built through a combination of above three moves.

#### **Common Patterns of Resonance Structures**

- Vinylic: the two carbon atoms bearing the double bond of a carbon-carbon double bond.
- Allylic: atoms connected directly to vinylic positions.



#### **Resonance Hybrid**

- Resonance hybrid: respresents the average of the contributing structures, with bond lengths and partial charges taking on intermediate values.
- No matter how many resonance structures are drawn, they collectively represent one entity.

 Drawn partial bonds and charges to illustrate the delocalization of electrons

#### **Delocalization**

- Delocalization: the spreading of electrons between multiple atoms or covalent bonds.
  - Resonance stabilization: molecules and ions that are stabalized by the delocalization of electrons.
  - Plays a major role in the outcome of many reactions.
- When a lone pair participates in resonance, it will occupy a *p* orbtail rather than hybridized; important for 3d shapes of proteins.
- **Localized lone pair**: when a lone pair is not allylic to a  $\pi$  bond.
  - Whenever an atom posses both a  $\pi$  bond and a lone pair, they will not both participate in resonance.
  - Usually  $\pi$  bonds participate first.

#### **Contributor Significance**

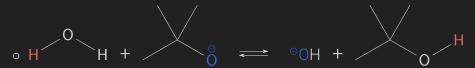
- Some resonance structures may resemble the actual molecule more than another, in regards to energy and stability.
- Strcures with low potential energy are more stable compared to those of higher values and resemble the actual structure more.
- Major contributors: the most stable contributing structures.
- Minor contributors: less favorable contributing strcutres.
- Rules for contributing significance, descending:
  - The greatest number of filled octets.
  - The greatest number of covalent bonds.
  - Minimize formally charged atoms.
  - Separation of unlike and like charges, minimized and maximized respectively.
  - Negative charges placed on the most electronegativity atoms, positive charges placed on the less electronegative atoms.
  - Do not deviate substantially from idealized bond lengths and angles.
  - Maintain aromatic substructures locally while avoiding anti-aromatic ones.

Midterm 1 3 Acids and Bases

### 3 Acids and Bases

### **Introduction to Bønsted-Lowry Acids and Bases**

- ▶ Acid: a proton donor; i.e., a H<sup>+</sup> donor.
- ▶ **Base**: a proton acceptor; i.e., a  $OH^-$  (hydroxide ion), which wants a  $H^+$  to form the more stable  $H_2O$ .
- Symbolically: HA + B ➡ A⁻ + HB⁺
- ▷ Example using bond-line structures:



#### **Lewis Acids and Bases**

- ▶ The lewis definition is more broad than the Brønsted-Lowry definition.
- ▶ Lewis describes acidity in terms of electrons, rather than protons.
- ▶ Lewis acid: electron-pair acceptor.
- Lewis base: electron-pair donor.
- ▶ Most reactions are described in terms of lewis base and acids, since Molecules without donatable protons are unable to be described by the Brønsted-Lowry definition.

### **Nucleophiles and Electrophiles**

Excerpt from Chapter 6: Chemical Reactivity and Mechanisms  $\mapsto$ 

- ▶ **Ionic reactions**, aka polar reactions: reactions that involve the participation of ions as reactants, intermediates, or products.
  - Most cases ions act as intermediates.
  - Radical reactions and pericyclic reactions are also major categories, but are typically not discussed in undergraduate courses.
  - Ionic reactions occur when one reactant has a site of high electron density and the other reactant has a site of low electron density.
- ▶ **Nucleophiles**: an electron rich atom that is capable of donating a pair of electrons.
  - Nucleophiles are Lewis bases.

Midterm 1 3 Acids and Bases

• Any atom that possesses a localized lone pair can be nucleophilic.

- $\circ$   $\pi$  bonds can also function as nucleophiles due to their region of space having high electron density.
- Polarizability: the ability of an atom to distribute its electron density unevenly in response to external influences.
  - Correlated with size of the atom, which increases the number electrons that are distant from the nucleus.
- ▶ **Electrophiles**: an electron-deficient atom that is capable of accepting a pair of electrons.
  - Electrophiles are Lewis acids.

### Flow of Electron Density: Curved-Arrow Notation

- ▶ All reactions are accomplished via a flow of electron density.
- ▶ Electron density flow is illustrated with curved arrows.
  - **Reaction mechanism**: how the reaction occurs in terms of the motion
  - All ionic meachanisms, regardless of complexity, are combinations of four characteristic patterns of electron flow (discussed later).

#### **Notes on Drawing Curved Arrows**

- Tails must be placed on either a bond or a lone pair.
  - Shows the source, i.e., the electron donor (base).
  - Electrons can only be found in lone pairs or bonds, so never place the tail of a curved arrow on a positive charge.
- Heads must be placed so that it shows either the formation of a bond or the formation of a lone pair.
  - Shows the destination, i.e., the electron acceptor (acid).
  - Avoid drawing an arrow that violates the octet rule, so never draw an arrow that gives more than four orbitals to a second-row element.

# 4 Alkanes and Cycloalkanes

# **Introduction to Alkanes**

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# **Nomenclature of Alkanes**

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