Contents

1	General Chemistry Review	2
	Structural Theory of Matter	2
	Electrons, Bonds, and Lewis Structures	2
	Identifying Formal Charges	2
	Induction and Polar Covalent Bonds	3
	Atomic Orbitals	3
	Valence Bond Theory	4
	Molecular Orbital Theory	4
	Hybridized Atomic Orbitals	5
	Molecular Geometry	6
	Dipole Moments and Molecular Polarity	7
	Intermolecular Forces and Physical Properties	7
	Solubility	7

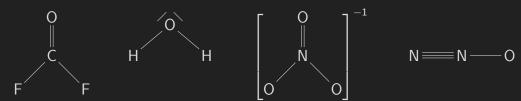
1 General Chemistry Review

Structural Theory of Matter

- ▶ **Constitutional isomers**: same molecular formula, but different in the way the atoms are connect, i.e. their constitution is different.
- ▶ Each element forms a predictable number of bonds, from one to four.

Electrons, Bonds, and Lewis Structures

- ▶ Covalent bond: two atoms sharing a pair of electrons.
- ▶ The lowest energy (most stable) state of two atoms is determined both by bond length and bond strength.
- ▶ **Lewis structures**: drawings that show free electrons.
- ▶ Valence electrons are determined by the group, 1A−8A, of the periodic table.
- ▶ **Lone pair**: unshared, or nonbonding, electrons.
- ▶ **F, O, N, Cl** (Br, I). Most electronegative elements, from left to right; hydrogen needs to bond to these elements.
- \triangleright Examples: COF₂, H₂O, NO₃, N₂O:



▶ **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 result in positive charge.

- ▶ More than expected results in 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.
- ▶ **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 1.7, then the electrons are not equally shared and become polar.
- ▶ **Induction**: the withdrawl of electrons towards to more electronegative atom. δ^+ represents partial positive charged gained when electrons are pulled away, while δ^- represents the partial negative charge pulled closer.
- ▶ **Ionic bond**: when the difference in electronegativity is greater than 1.7.
 - Electrons are not shared in this case, and attraction is insetsad just the result of oppositely charged ions.

Atomic Orbitals

- ▶ **Atomic orbital (AO)**: s(1), p(3), d(5), f(7).
- \triangleright Locations where ψ (quantum wave function) is zero are called **nodes**.
- ▶ The more nodes that an orbital has, the greater it's energy.
- 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.
 - o Constructive interference produces a wave with larger amplitude.
 - 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** (σ): a particular type of covalent bond that has circular symmetry with respect to the bond axis.
 - \circ All single bonds are σ bonds.
 - The strongest type of covalent bond.
- \triangleright **Pi bond (** π **)**: 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 π bonds from double and triple bonds but generally do not form single 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.

Hybridized Atomic Orbitals

- $hd problet sp^3$ -**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 σ bonds, and thus can be individually represented by the overlap of atomic orbitals.
- $\triangleright sp^2$ -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 π bond.
 - o This is done to expain geometry of compounds bearing a double bond.
 - \circ A double bond if formed from one σ bond and one π 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 π bonds.
 - A triple bond is formed with the addition of one σ 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 atoms and lone pairs attached) of atom.
 - 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:
 - Bond length decreases with more bonds.

o Bond strength increases with more bonds.

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 σ bonds and zero lone pairs.
 - o produces a tetrahendron with bond angles of 109.5°.
- \triangleright **Trigonal pyramidal geometry**: three σ 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°.
 - The lone pair sits atop the base forming a pyramid like structure.
- \triangleright **Bent geometry**: two σ 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 H₂O 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 (electron pairs, or the bonds/lonepairs).
 - 2. Determine predicted geometrical structure predicted by VSEPR using steric number (tetrahedral:4, trigonal:3, linear:2).
 - 3. Determin impact of lone pairs; more lone pairs results in less space between bonded pairs.

Dipole Moments and Molecular Polarity

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Intermolecular Forces and Physical Properties

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Solubility

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