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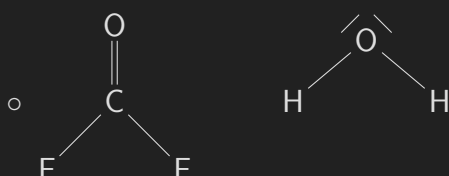
1 General Chemistry Review

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.
- ▷ \ch{x-x} single: -, double: =, triple: +. e.g. $\text{CH}_3\text{--CH}_3$, $\text{CH}_2\text{=CH}_2$, $\text{CH}\equiv\text{CH}$

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.
- ▷ Examples: COF_2 , H_2O , NO_3^- , N_2O



Identifying Formal Charges

- ▷ **Formal charge:** any atom that does not exhibit the appropriate number of valence electrons.
- ▷ **Less** than expected results in **positive** charge.
- ▷ **More** than expected results in **negative** charge.

Induction and Polar Covalent Bonds

- ▷ Bonds are classified into three categories: covalent, polar covalent, 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.
- ▷ If the difference in electronegativity is **less than 0.5**, then the electrons are considered equally shared, which is a **covalent bond**.
- ▷ If the difference in electronegativity is **between 0.5 and 1.7**, then the electrons are not equally shared and thus a **polar covalent bond**.
- ▷ **Induction**: the withdrawal of electrons towards to more electronegative atom. δ^+ represents partial positive charge gained when electrons are pulled away, while δ^- represents the partial negative charge pulled closer.
- ▷ If the difference in electronegativity is **greater than 1.7** then the electrons are not shared and results in an **ionic bond**, which is really just a result of the force between two oppositely charged ions.

Atomic Orbitals

- ▷ **Atomic orbital (AO)**: $s(1)$, $p(3)$, $d(5)$, $f(7)$.
- ▷ Locations where ψ is zero are called **nodes**.
- ▷ The more nodes that an orbital has, the greater its 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 commonly used theories: *Valence Bond Theory* and *Molecular Orbital Theory*.
- ▷ The commonly used theories give a deeper understanding of covalent bonds, which is essentially **overlap of atomic orbitals**.
- ▷ **Constructive/destructive interference**: the result of two waves that approach each other, or overlap.
 - Constructive interference produces a wave with larger amplitude.
 - Destructive interference cancel each other out and produces a node.

Valence Bond Theory

- ▷ **Valence bond theory**: the sharing of electron density between two atoms as a result of the constructive interference of their atomic orbitals.
- ▷ *Bond axis*: the line that can be drawn between two hydrogen atoms.
- ▷ **Sigma bond (σ)**: a particular type of covalent bond that has circular symmetry with respect to the bond axis.
 - All single bonds are σ bonds.
 - The strongest type of covalent bond.
- ▷ **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.
 - 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** according 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

- ▷ **sp^3 -hybridized orbitals**: produced by averaging one s orbital and **three p** orbitals.
 - Hybridized orbitals explains to geometry of methane, which results from 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.

- All bonds in are σ bonds, and thus can be individually represented by the overlap of atomic orbitals.
- ▷ **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.
 - This is done to explain geometry of compounds bearing a double bond.
 - A double bond is 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.
 - 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. Determine 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.
 - Bond strength increases with more bonds.

Molecular Geometry

- ▷ **Valence shell electron pair repulsion (VSEPR) theory:** enables the prediction of molecular geometry due to the presumption 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.
- ▷ **Tetrahedral geometry:** result of four σ bonds and zero lone pairs.
 - produces a tetrahedron with bond angles of 109.5° .

- ▷ **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.
- ▷ **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 H_2O 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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