OCHEM 1 REVIEW SHEET: ESSENTIAL INFORMATION ONLY

Chapter 1: Basics

- How bonds form… duh
- Functional groups… also duh
- Lewis structure review
    - Try to minimize formal charge and put charges on appropriate electronegative atoms
    - Resonance
        - Use double sided arrows to show resonance between structures
        - Real structure is some intermediate between the resonance forms, so there may be dispersed partial charges
            - Never break a sigma bond to make a new resonance structure
        - Having an octet takes precedence over minimizing formal charges
- Bonding is the result of electron wave particle theory
    - Energy of electrons differ, proportional to the wave function
        - Greatest probability of location of electron is its orbital
    - Bonds occur when constructive overlap of wave functions occur (additive effect)
        - Antibonding occurs when waves are destructive (not in sync)
        - For every orbital, there is one bonding orbital and one antibonding orbital of higher energy
            - If antibonding orbital is filled, it will cancel any bonding
- To make orbitals of equal energy, we create hybrid orbitals
    - May bump up electron from s orbital to p orbital to create uniform distribution of electron density, then create hydridized orbitals
        - Possible to do so because we can add the wave functions
    - Sp3, sp2, sp orbitals
        - More p means longer bond, weaker bond (more s character is stronger bond, closer to nucleus = greater effective nuclear charge)
        - Also helps minimize electron-electron repulsion
        - Remember geometry (tetra = 109, trig. pyr = 107, bent = 103)
        - Lone pairs will reside in a hybrid orbital if present to minimize repulsion

Chapter 2: Acid Base

- Acid dissociation constant (K_a) is $K_{eq} = ¿¿$
    - H_2O is on both sides of the equation, so it cancels out
    - A large K_a means that it is a strong acid
        - K_a for water is 10^{-16}… = $[10^{-7}]^2$/(density of water = 55.5)
    - pKa is −logKa, a simpler way of communicating constant
        - as pKa increases, acidity decreases
    - Key pKa's to know
        - alkanes = 50
        - alkenes = 42
        - alkyne = 24
        - NH3 = 38

        - Alcohols = 18
        - H_2O = 16
        - HCOOH = 5
        - HCl = -7
- Determining the best conjugate base is easy way to predict reaction direction
    - Should be most electronegative atom with neg. charge, more stable (when going across period)
    - When going down a column, larger polarizable atoms are better as outermost e- shell is large and can easily accept another e-
    - If applicable, more stable base has the most s character in its orbitals (variation on more electronegative because closer to the nucleus)
    - Resonance distributes negative charge, so better
    - Large e- withdrawing groups have inductive effects that also stabilizes negative charge
    - Could also use pKa argument; more stable conjugate base has the acid that has lower pKa (run away from low pKa in reaction)
- Bronsted Lowry acid base
    - Acids donate protons, bases accept protons
- Lewis acid base
    - Acids accept electrons, bases donate electrons

Chapter 3: Alkanes

- Naming alkanes
    - Use base name derived from number of carbon (weird ones are undecane, dodecane, tridecane, tetradecane, pentadecane... icosane(20))
        - Some common names to know: isopropyl, isobutyl, sec-butyl, t-butyl
    - Halogens are put in front of base with #- defining position
    - To name
        - Find largest carbon chain, this is your base
        - Number substituents to minimize total sum and give priority to proper groups
        - add substitutions in alphabetical order to name
            - iso- and cyclo- prefixes are the only ones that count towards naming
- Physical properties
    - Physical state at RT
        - C_1-C_4 are gases
        - C_5-C_{20} are liquids
        - C_{20+} are solids
        - Increased carbons means molecule have greater surface area, resulting in more potential van der waals forces as the result of dipole moments (random dipoles made from e- movement)
    - Combustion
        - Reacts with oxygen when heated to produce carbon dioxide and water
        - State of alkane will alter reaction rate
    - Boiling points
        - To vaporize, must interrupt the van der waals interactions

        - So more surface area = higher boiling point
        - Branched alkanes will have lower boiling point than straight alkanes of the same size
    - Melting point
        - Dependent entirely on how well a molecule can form a crystal lattice
            - More symmetrical and condensed alkanes (branching) allows for tighter packing, so they have a higher melting point
            - Straight alkanes can't really pack together that tightly (think a stack of paper), so have a lower melting point
    - Solubility
        - Highly dependent on the polarity and dipole moments of the molecule
            - Water is polar (has permanent dipole)
            - Alkanes are nonpolar, but have dipole moments
                - Without the dipole, they are not soluble in the polar solvents because there are no attractions between nonpolar and polar molecules
                - The temporary dipoles may result in slight, negligible solubility
- Conformational analysis
    - Looking down an atom's bonds through Newman Projections
    - C-C single bonds allow for free rotation around a bound
        - Therefore attachments can revolve around the carbon in space
        - This allows for different confirmations, called conformers
            - Not seen in double bonds because they lack free rotation
        - Staggering the attached bonds to the carbons (ie they don't overlap) creates the more stable, staggered conformer
            - Minimize e- e- repulsion
            - Overlapping bonds results is less stable eclipsed conformer
                - Of a higher energy state than the staggered conformer
    - Conversion between conformers requires energy
        - Barrier to free rotation caused when 2 sigma bonds try to pass each other is called torsional strain
            - Typically this barrier can be overcome because it is very small and RT provides enough energy (about 17-20 kcals available for use)
    - Larger molecules with lots of large groups cause steric strain
        - This is the e- e- repulsion caused when two large groups (like two methyls) try to occupy the same space (ie overlap)
        - Therefore, the most stable conformer is the anti-conformer, which is staggered to minimize steric crowding
            - This places the two largest substituents in the Newman Projection in opposite positions
            - When the two largest substituents are approaching eclipsed conformer, this is called the gauche conformer (there are two, one for either side of eclipsed)