**Acid-base reactions & equilibria** [Daley & Daley ch 5]

*This presentation of the material covered within a topic or chapter is meant to give students a clear vision of the central concepts or big picture concepts that all other information expands upon, relates to or serves.
Super concepts are the big picture, central concepts that should be completely obvious to you as we begin to cover them and when you reflect on the topic once we’ve covered it. Everyone who takes the course should be able to remember or recognize the super concepts years after having taken the course.*

*Each concept is an important “chunk” of a super concept. Each concept is a large enough idea to stand on its own. Good (B) students will remember and understand these concepts after taking the course.*

*The details are ideas, methods, or facts that you need to understand to solve problems and actually do chemistry. It’s likely that only the best (A) students will be able to remember and use the details years after taking the course.*

**Superconcepts:**

1. Nucleophilic attack is the mechanism of most acid-base reactions: a free electron pair of the Nu: (LB) attacks the E+ (LA), forming a dative bond to a hydrogen of the LA.
2. The equilibrium state of an acid-base reaction is determined by comparing the pKa values of the Lewis acid (reactant) and the conjugate acid (product). The lower pKa pushes the reaction away from it.

**Concepts:**

1. Lewis acids accept electron pairs while Lewis bases donate electron pairs.
2. Conjugate pairs are pairs of molecules that differ by only a single hydrogen atom. When an acid loses its proton it becomes the acid’s conjugate base.
3. Nucleophiles (Nu: or Nu:-) are electron rich molecules seeking positive electrophiles (LB), while electrophiles (E+) are positively charged, electron-lovers seeking electron-rich nucleophiles (LA).
4. Nu: can act as bases when they steal a hydrogen atom, or as a nucleophile when they are added to the electrophile.
5. Strong acids are weak bases. In other words, the conjugate base of a strong acid will be a weak base. And vice versa.
6. Solvents can ‘level’ (or hijack) an acid base reaction when the solvent reacts with one of the reactants, using it up. In essence, the solvent can compete with the second reactant. Leveling is not an issue if the equilibrium between a reactant and solvent favors reactants.
7. pKa can be estimated from a molecule’s structure using a number of criteria.

 **Details:**

1. Lewis acids don’t have to be hydrogen atoms. For example, iron can act as an acceptor of electron pairs.
2. Dative bonds are formed when the free electron pair of a Nu: attacks an E+ like a polar hydrogen, forming a new bond.
3. Charged nucleophiles (Nu:-) are stronger than neutral nucleophiles (Nu:).
4. Some molecules, like water or alcohols, can act either as LB (Nu:) or LA (E+).
5. Carbonyl groups often have a dipolar positive carbon that acts as an E+.
6. Acidity: sp (alkyne) > sp2 (alkene) > sp3 (alkane). Free electron pairs are closer to their nucleus in sp orbitals, polarizing covalent bonds to hydrogen atoms and thus making that hydrogen atom more acidic.
7. pKa is a measure of acid strength. pKa = -log(Ka). Strong acids have low pKa values or high Ka values.
8. Water has a pKa value of 15.7 and can act either as an acid or as a base, depending on the nature of the other reactant.
9. Difference in acidity can be calculated. Subtract the two pKa values. Raise 10 to the power of the difference.
10. Acid-base equilibrium can be quantitated using the difference in pKa values of the Lewis acid (reactant) and the conjugate acid (product). Calculate the difference in pKa and raise ten to the power of that difference to calculate Keq.
11. When water is used as a solvent, no acid will be stronger than hydronium and no base will be stronger than hydroxide.
12. Estimating pKa looks for: 1) similar functional groups with known pKa; 2) inductive effects; 3) positive charge; 4) stability of the anion (aka conjugate base) formed when the acid reacts; 5) size of the anion or conjugate base; 6) orbital hybridization of the conjugate base; and 7) delocalization of an acid’s positive charge.
13. Acid strength increases: alcohol < phenol < carboxylic acid.
14. Base strength increases as the electronegativity of the atom with the : decreases, because we want the atom to give up, donate, the :.
15. Carbocations & carbanions are very unstable and therefore powerful LA and LB, respectively.