Properties Study Guide

DRAFT

Property	Structural Factors affecting property	Example	Application or biological relevance
Solubility (in water vs. oil)	Interaction between molecules and solvent, based on the following forces in order of decreasing strength: covalent, ionic, hydrogen bonding, ion-dipole, dipole-dipole, London. General principle is like dissolves like, meaning nonpolar repels polar. Rule of thumb: OH solubilizes 3 C's, COOH solubilizes 4 C's	Solubility in water: $CH_3CH_2CH_2CH_2ONa$ > $CH_3CH_2CH_2CH_2OH$ > $CH_3CH_2CH_2CH_3$	Micelle formation in fatty acids, lipid bilayer formation, Protein folding influenced by nonpolar groups and polar groups
Ambiphilic compounds (soluble in water and oil)	*As above, but large molecule with very different polarity*		
Boiling point and volatility	As with solubility, and including stacking of molecules		
Melting point	As with solubility AND symmetry of molecule which improves packing in crystal structures		Cholesterol, cis fats affect membrane fluidity
Absorption of visible and ultraviolet light	Presence of conjugation. More conjugation means lower energy of absorption max moves towards IR (i.e. IR		DNA damage, photosynthesis, color of blood, grass, urine; photobleaching of

	ROYGBIV UV)		paper, pigments
Optical rotation	Presence of chirality, meaning no plane of symmetry in the molecule.		Levo (L) (-) or Dextro (D) (+) in drug names, LCD, bird and fish vision, polarized sunglasses
Interaction with chiral molecules	Presence of chirality		Drug enantiomers, mint vs caraway and other flavors
Viscosity	Very long chains, interchain interaction as with melting and boiling points		Can measure DNA supercoiling by viscosity?
Acidity and Basicity	(Use pKa table to assess relative acidity) Aliphatic amines are more basic than aromatic amines, which are more basic than amides. Acidity of acids increases when electronegative groups are attached close to the COOH		

Molecules that can hydrogen bond to water are more soluble in water than those that can not.
Molecules that can hydrogen bond to each other have a higher boiling point and are less volatile than those that can not..
Charged molecules (i.e. salts) are more soluble in water than neutral molecules.
Charged molecules (i.e. salts) have a higher boiling point and are less volatile than neutral molecules.
The reaction of a base with a carboxylic acid changes a neutral R-COOH into a charged $R\text{-}COO^-$, thereby affecting solubility and volatility.
The reaction of an acid with an amine changes a neutral $R\text{-}NH_2$ into a charged $R\text{-}NH_3^+$ (similar for 2° or 3° amine) thereby affecting solubility and volatility.
If the pH is greater than the pKa of an acid, the acid will be 99+% deprotonated; if the pH is equal to pKa it will be 50% protonated, if the pH is lower than pKa it will be 99+% protonated.
Quaternary amines are always positively charged at any pH.
Aliphatic amines are more basic than aromatic amines, which are much more basic than amides. Amides are only protonated by strong acids. The pKa's of the conjugate acids are: aliphatic 9.5, aromatic 3.5, amide -0.5

Small changes in chemical structure can result in large changes in bioactivity
"Natural" does not mean safe

Amines taste bitter and have pungent or putrid odors
Western medicine looks to traditional "folk" medicine for drug candidates
The dose makes the poison

Structural Theory Study Guide

Items in italics have not been covered as of 9/22/06

Lewis Structures
VSEPR
Formal charge
Degree of hydrogen deficiency
Constitutional isomers
Functional groups
Cis-trans isomers in rings
Cis-trans isomers in double bonds
Newman projections and conformations
Chirality (R/S, D/L, +/-)
Fisher projections
Axial and equatorial positions in cyclohexane
Haworth projections