



Crack the DAT

Crack Notes [Organic Chem 1] Molecular Structure

Structural formulas

Lewis dot structure:

- 1) Find total # of valence electrons for all atoms
- 2) Use one pair of electrons to form a bond between each atom
- 3) Use other electrons to form double/triple bonds to satisfy octet rule
 - o Exceptions to octet rule: H (2), Be (4), B (6), atoms in 3rd period or higher (up to 12)

Bond-line formula: line intersections/corners/endings are carbons

Fischer projection: horizontal lines are out of page, vertical lines are into page

Newman projection: intersection of 3 lines, big circle are two carbon atoms

Dash-line-wedge formula: dotted wedge going into page, black wedge coming out of page

Formal charge:

$$\# \text{ valence electrons} - \# \text{ lone electrons} - \# \text{ bonds}$$

- Sum of all atom formal charges should be equal to the total charge on the molecule

Index of hydrogen deficiency:

$$\frac{(2 \cdot \# \text{ carbons} + 2) - \# \text{ hydrogens}}{2}$$

- Count halogens as hydrogens, nitrogens as 1/2 hydrogens

Functional groups

- *Alkanes:* all C-C single bonds
- *Alkenes:* C-C double bond
- *Alkynes:* C-C triple bond
- *Alcohol:* R-OH
- *Ether:* R-O-R
- *Amine:* NH_2R (primary), NHR_2 (secondary), NR_3 (tertiary)
- *Aldehyde:* H-C=O
- *Ketone:* C=O with no H
- *Carboxylic acid:* HO-C=O
- *Ester:* RO-C=O
- *Amide:* $\text{NH}_2\text{-C=O}$

Nomenclature

- Meth (1), eth (2), prop (3), but (4), pent (5), hex (6), hept (7), oct (8), non (9), dec (10)
- n-propyl vs. isopropyl, n-butyl vs. sec-butyl vs. isobutyl vs. tert-butyl

Naming

- Longest carbon chain defines base name
- End carbon closest to substituent is labeled #1
- Write carbon#-substituent names, ordered alphabetically (ignore # prefixes, dashed prefixes)



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Bonding

- *Coordinate covalent bond*: one atom donates both electrons
- *Sigma bond*: always makes first bond
- *Pi bond*: second + third bonds, more reactive b/c electrons are farther away from nucleus
triple > double > single in strength/bond energy, single > double > triple in length

Hybridization

- s, p orbitals can combine to form new orbitals
- sp^3 : $1s + 3p$, sp^2 : $1s + 2p$, sp : $1s + 1p$, can tell apart by counting # bonds + # lone pairs
- More % s in orbital = stronger
- Bond angles can be affected by lone pairs, pi electrons, ring strain

Resonance

- When electrons can be spread over more than two atoms, happens when you have alternating double bonds or a lone pair/p orbital next to a double bonded atom
- *Huckel's rule*: rings must have $4n + 2$ pi electrons to be aromatic
- Actual structure will look most like most stable resonance structure that contributes to it

Dipole Moment

- When the charge is not balanced in a molecule
- Most often caused by imbalanced polar bonds
- *Induced dipole*: caused by presence of another polar molecule or electric field
- *Instantaneous dipole*: caused by electrons moving around randomly
- *London dispersion forces*: instantaneous dipole-instantaneous dipole bond

Stereochemistry

- *Conformational isomers/conformers*: different spatial orientation of same molecule
 - Rotation around single bond
 - Staggered vs. eclipsed configurations (Newman projections)
- *Structural isomers*: same molecular formula, different bonding

Chirality - mirror imaged molecules

- *Absolute configuration*: rank atoms by atomic number (count double/triple bonds as 2/3 bonds to same molecule), rotate atom so #4 points into page, then if you go counterclockwise from 1 to 2 it's **S**, clockwise it's **R**
- *Relative configuration*: same when two atoms differ by one substituent but have same orientation (can have different absolute configuration but same relative configuration)
- *Chiral molecules* will rotate plane-polarized light (optically active), but only if there's different % of the two mirror images
 - 50/50 mix of both stereoisomers is optically inactive, and called a *racemic mixture*
- +/d: rotates plane-polarized light clockwise
- -/l: rotates plane-polarized light counterclockwise



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Stereoisomers: same molecular formula, same bond connectivity, but not same compound

- *Enantiomers:* same molecular formula, same bond connectivity, but are mirror images
 - Mirror images will rotate plane-polarized light in opposite directions when they're not a racemic mixture
- *Diastereomers:* same molecular formula, same bond connectivity, but not mirror images
 - Will have different physical/chemical properties
- *Geometric isomer:* diastereomer caused by hindered rotation around a double/triple bond
 - *cis* has substituents on same side, *trans* has on opposite sides
 - *cis* molecules have higher boiling points due to having dipole moments (*trans* can't)
 - *cis* molecules have lower melting points because they can't form crystals as well
 - *cis* molecules can exhibit steric hindrance
 - Can also compare priority of substituents (atomic weight), **E** on opposite sides, **Z** on same side
- Max # optically active isomers $2^{\text{\# chiral centers}}$
- A compound with an even number of chiral centers can be symmetric so optically inactive
 - Called *meso compounds*
- *Epimers:* diastereomers different at one chiral carbon
- *Anomers:* epimers that form rings resulting in two diastereomers