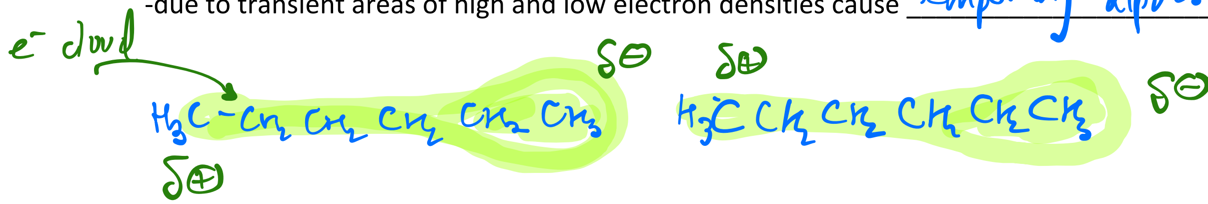
Intermolecular Forces and Organic Compounds
*listed weakest → strongest

Klein 1.12-1.14

1. Important intermolecular forces:

a) induced dipole-induced dipole

-due to transient areas of high and low electron densities cause temporary dipoles



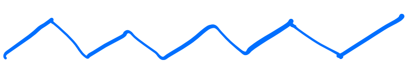
-a.k.a. van der Waals forces or London forces

-weakest of all intermolecular forces: 2-4 kJ/mol

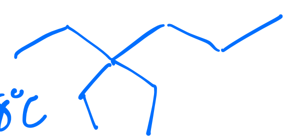
-longer, thinner alkanes (less branching) will have stronger induced dipole-induced dipole interactions (polarizability, the ability to distort an electron cloud, is a characteristic that contributes to stronger intermolecular forces.....analogy: electron flash mobs)

-only intermolecular force with greasy alkanes; will be present in interactions of all alkyl chains as well.

e.g. n-decane vs. 3,3-diethyl-hexane (both 10 C's)



bp = 174 °C



bp = 168 °C

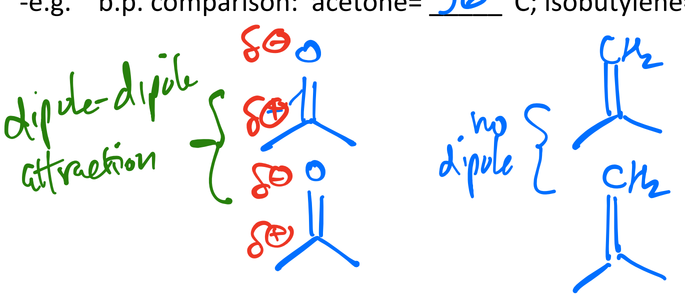
b) dipole-dipole interactions

-slightly stronger at 3-4 kJ/mol

-need bonds with dipole moments, e.g. C–O, C–N, C–Cl, C–Br
electronegativity (eN) difference present

-dipoles align themselves to hold molecules together

-e.g. b.p. comparison: acetone= 56 °C; isobutylene= -7 °C



c) hydrogen bonding (H-bonding)

-stronger still at ~10-40 kJ/mol

-a special kind of dipole-dipole interaction between....

an electron deficient H and an electron rich heteroatom (O, N, F.... S)

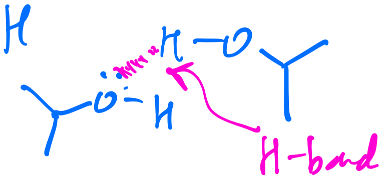
non-carbon

-H-bond acceptors: O's and N's with lone pairs of e⁻'s; F also

e⁻'s

-H-bond donors: primarily N-H and O-H

δ⊖ δ⊕



*Bond strength impacted by:

(1) bond polarity affects H-bond strength:

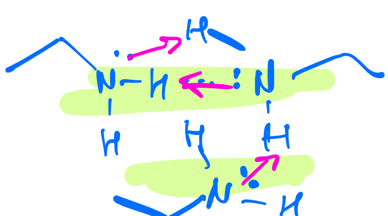
H–O > H–N due to greater eN of O vs. N

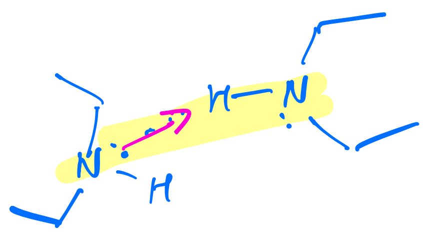
therefore H–O:···H–X > H–N:···H–X

example: CH_3CH_2OH, b.p.= 78 °C vs. $CH_3CH_2NH_2$, b.p.= 17 °C

(2) molecules with more possible H-bonding will have stronger intermolecular forces

-example, intermolecular force strength:





....and this results in a higher b.p.

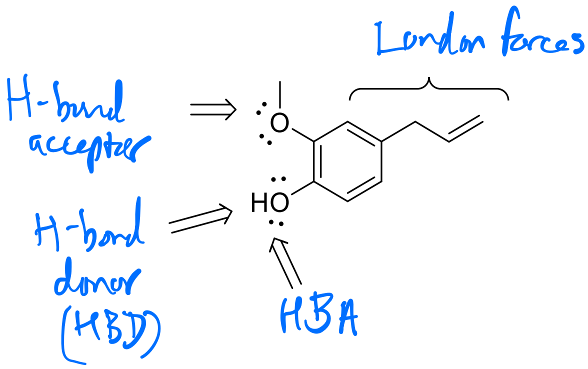
$CH_3CH_2N(H)CH_2CH_3$, bp= 55-6 °C vs. $CH_3CH_2CH_2CH_2NH_2$, bp= 77-9 °C

illustrated....

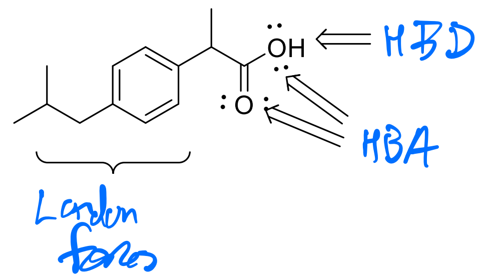
* Also if molecule has both an H-bond donor and H-bond acceptor will have stronger intermolecular forces than molecules with only one or the other

Analyzing intermolecular forces in organic molecules:

eugenol (lab activity in 2013)



ibuprofen



2. Impact of intermolecular forces

a) boiling point: stronger *intermolecular forces* → higher *boiling point* (Same for melting pt.)

b) solubility: "like dissolves like"; that's all you need to know!

-examples

diethyl ether
$CH_3CH_2OCH_2CH_3$ in H_2O? soluble or not? NOT

CH_3CO_2H in H_2O? soluble or not? Soluble

CH_3CH_2OH in H_2O? soluble or not? Soluble

$CH_3CH_2NH_2$ in H_2O? soluble or not? Soluble

$CH_3CH_2CH_2CH_2CH_2CH_3$ (hexane) in H_2O? NOT

General characterization:

-hydrophobic/lipophilic = lots of C's + H's → doesn't dissolve in water

-hydrophilic (lipophobic) = more O's and N's → water soluble

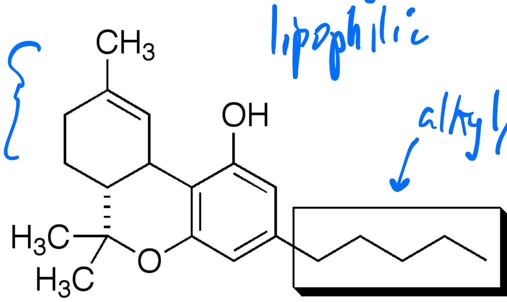
c) intermolecular interactions in biology/biochemistry

(1) Molecules/drugs passing through cell membranes or other barriers and dissolving in aqueous solutions

alkane

lipophilic

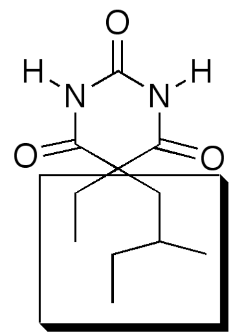
alkyl/alkane



Tetrahydrocannabinol or THC
(Marihuana Active Component)

hydrophilic

alkyl makes it lipophilic



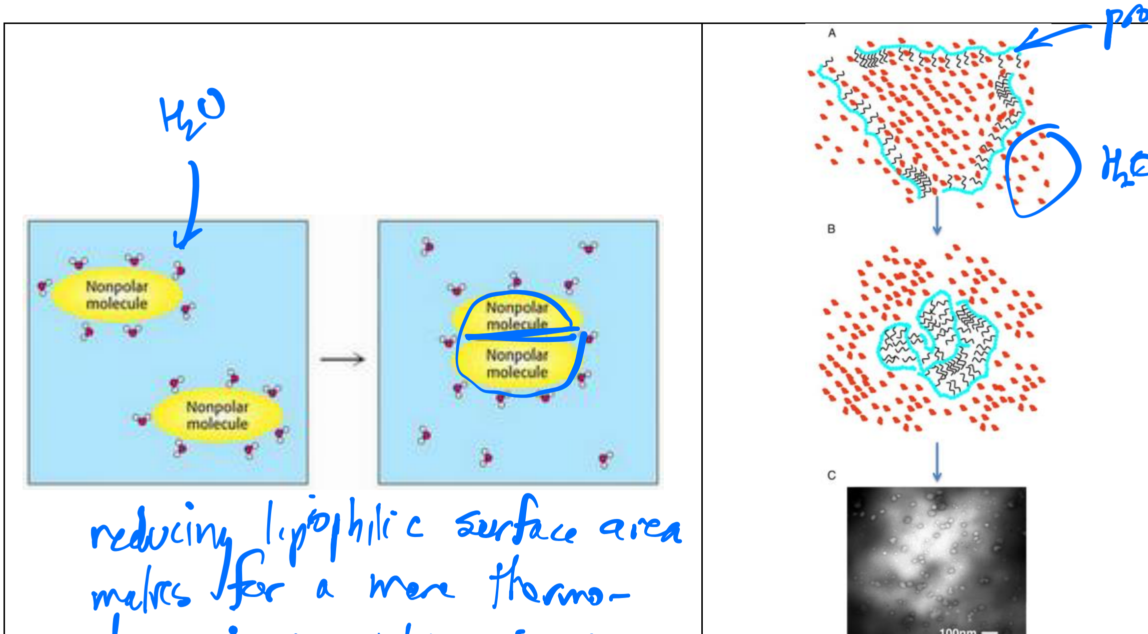
Pentothal
(Barbiturate)

(2) Enzymes + substrates or ligand + receptor

enzymes + receptor = proteins
substrates + liquids are small molecules

**Key interaction: hydrophobic effect

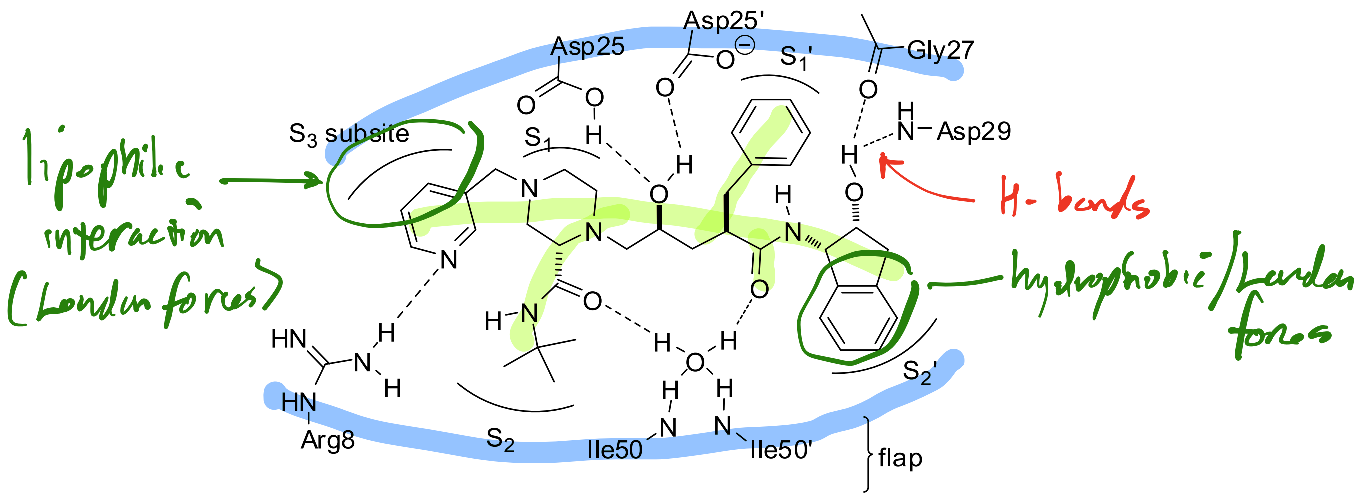
protein



reducing lipophilic surface area makes for a more thermodynamically stable solution (due to increase in entropy of H_2O) → H_2O doesn't need to organize itself on lipid surface

-indinavir (Crixivan), Merck, 1996

-PDB crystal structure: 2R5P



Crixivan's Interactions in HIV-2 proteases active site