

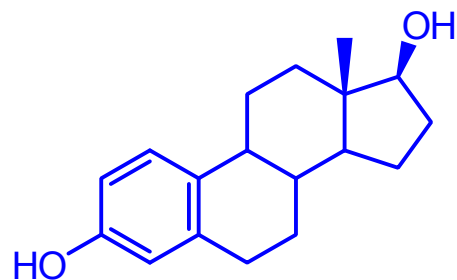
Organic Chem #1: Introduction to Functional Groups

- Because of the larger structure of organic molecules, these notes are provided in landscape format.
- Objectives: by the end of this unit, you should be able to...
 - Convert the Lewis structure of an organic molecule to its condensed structural formula (form), and vice versa
 - Given the condensed form of the structure of an organic molecule, determine its molecular formula, determine the hybridization of each atom in the molecule, and identify the functional groups present in it
 - Recognize the functional groups in a molecule, label all bonds as polar or non-polar, and identify the various types of intermolecular forces (*van der Waals, dipole-dipole and hydrogen-bonding*) that are possible
 - Given a series of organic molecules of similar molecular weight, predict their relative melting and/or boiling points

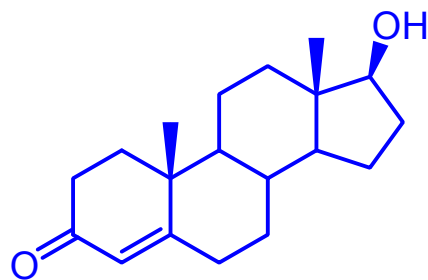
A. What is organic chemistry?

- By definition, it is a branch of chemistry that focuses on carbon compounds.
- While this seems like a very narrow group of compounds, there are over 10 million known molecules, and over 80% of these are classified as organic.
- Organic compounds are ubiquitous and are part of your life.
 - You are a carbon-based life form: DNA, proteins, neurotransmitters, etc.
 - Food is primarily based on organic molecules: starch in toast, orange juice contains vitamins, and coffee contains caffeine and sugar
 - Clothes and shoes that you wear are made of organic molecules and dyes
 - Medications, vitamins, and herbal supplements are organic molecules
 - The paper that is in front of you is made of cellulose
 - Your phone that rings in class contains plastics and other polymers

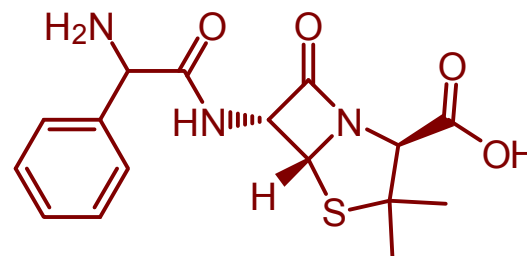
- Examples of organic molecules in your life...



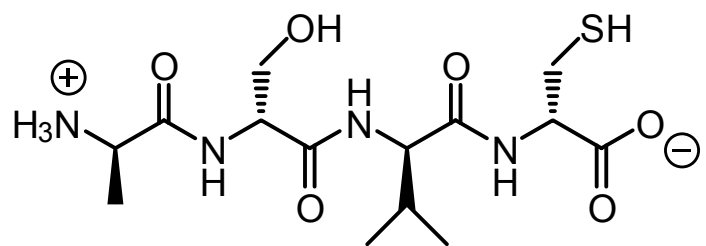
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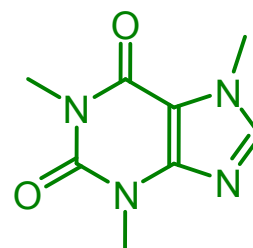
testosterone



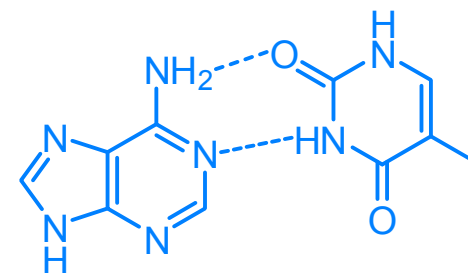
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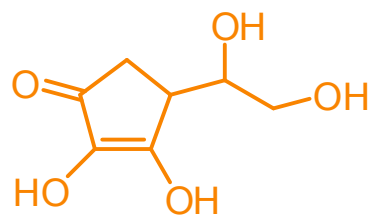
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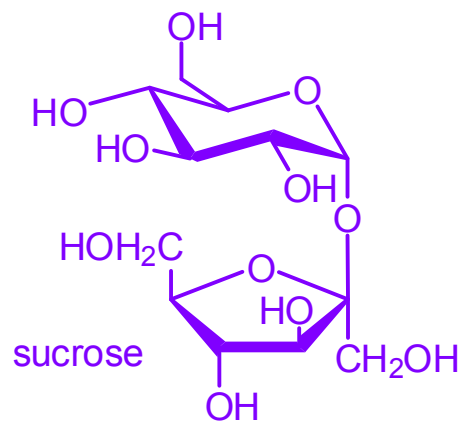
caffeine



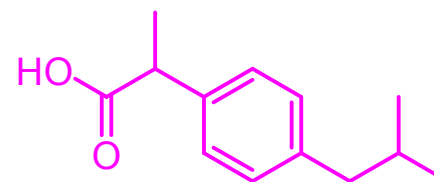
AT base pair



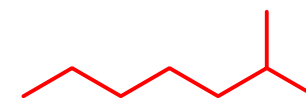
vitamin C



sucrose



ibuprofen

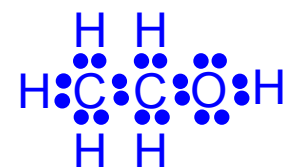


isooctane

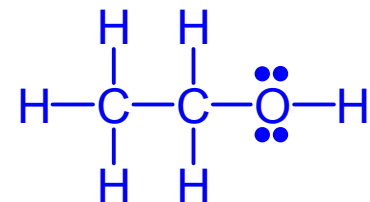
B. Structural Formulas

- Organic chemists use short-hand techniques to show (imply) the locations of electrons and bonds in molecules, as full Lewis structures are messy! The conventions are shown below for ethanol, molecular formula C_2H_6O .

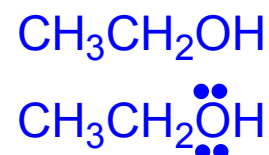
Full Lewis dot structure
(all valence electrons shown)



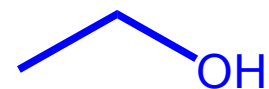
Lewis structure, with covalent bonds represented as lines.



Covalent bonds omitted, but assumed. With or without non-bonding pairs. Used for simple molecules.

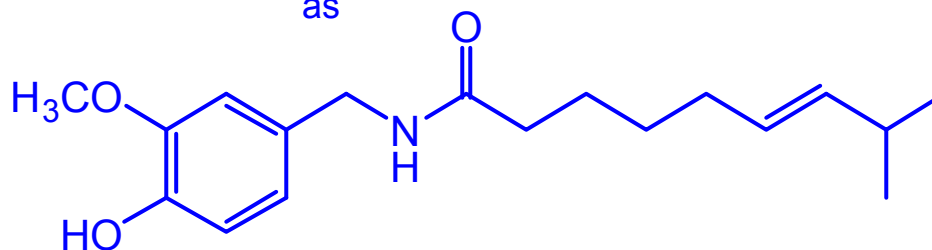
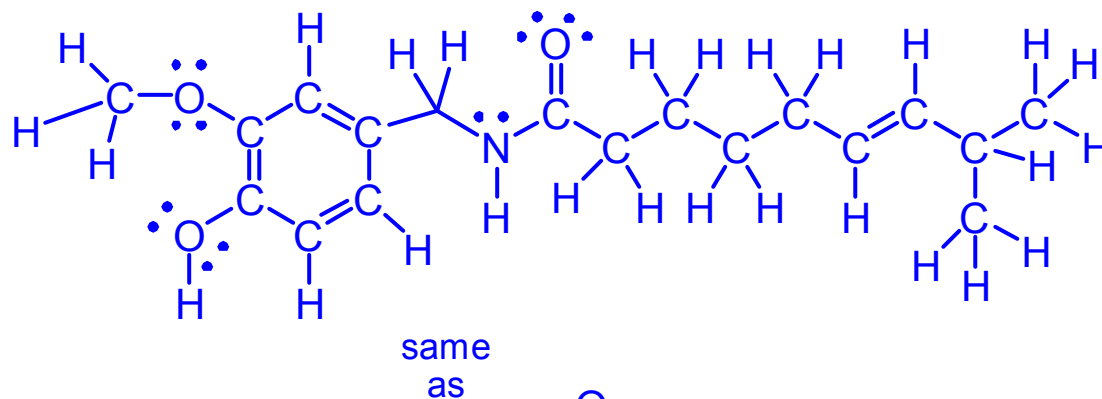


C-C bonds shown only by a line. H atoms bonded to C not shown (implied).



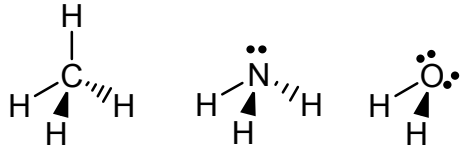
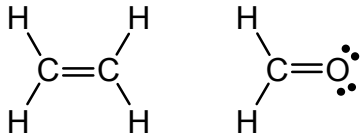

- In these line diagrams:
 - Each solid line represents a two electron covalent bond.
 - When no atom is drawn at the intersection of two covalent bonds (two lines) it is assumed to be a carbon atom, and there are enough hydrogen atoms around each carbon as necessary to make it tetravalent (4 bonds)
 - All non-carbon atoms (heteroatoms) must be drawn with the hydrogen atoms bonded to them.
 - Lone pairs are often not drawn, and are assumed to be there.

- Example: *capsaicin* is the molecule that gives peppers their hot taste.
- For practice, work out the molecular formula of capsaicin and the compounds on page 3.



C. Molecular Shapes

- The basic shapes of organic molecules are well-predicted by VSEPR theory, discussed in the previous section.

Regions of e ⁻ density around central atom	Predicted shape of electrons	Angles	Examples
4	tetrahedral	109.5°	
3	trigonal planar	120°	
2	linear	180°	

- Lone pairs of electrons exert a greater repulsive force than pairs in bonds, causing a reduction in bond angles.
- Double and triple bonds act as single bonds (a single region of electron density) in VSEPR theory.

- By applying VSEPR shapes to all bonded sites in a molecule, the correct shape of nearly every organic molecule can be predicted and drawn in 3D
- The dot-line-wedge symbolism is the most common way of depicting three-dimensional structures:

Line: represents a bond
in the plane of the paper



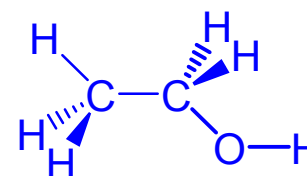
Dotted line: represents a bond directed
behind the plane of the paper



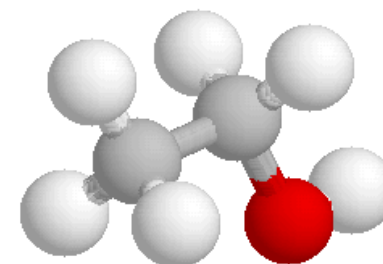
Wedged line: represents a bond directed
in front of the plane of the paper



- The 3D structure of ethanol is therefore represented as:



- The best 3D representation of ethanol is given by molecular models, or drawn as ball-and-stick models.
 - C = grey, H = white, O = red



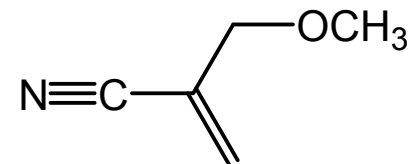
D. Hybridization

- Recall we discussed hybridization in the previous unit. For organic molecules, there are only three types of hybridization we need to worry about.

Regions of e ⁻ density	Atomic orbitals	Hybrid orbitals	Electronic arrangement
2	one s, one p	two sp	linear
3	one s, two p	three sp ²	trigonal planar
4	one s, three p	four sp ³	tetrahedral

- Regions of electron density: an NB pair, a single bond, or a multiple bond each constitutes one region.
- Electronic arrangement may not equate to molecular shape if there is one or more NB pair present.

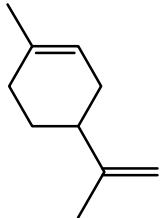

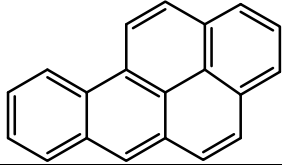
- Example: label the hybridization and give the approximate bond angles for C, N, and O in this molecule.



E. Functional Groups

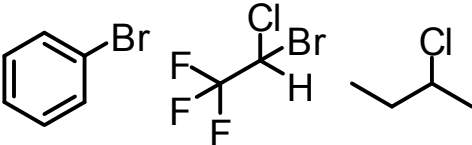
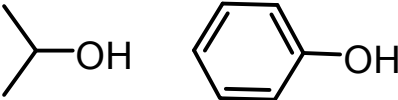
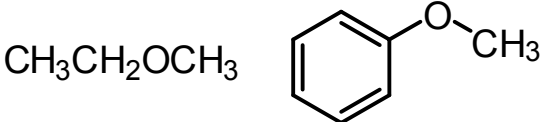
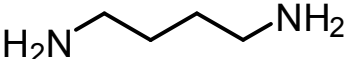
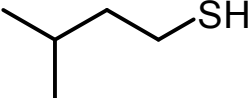
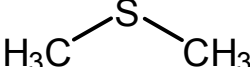
- A **functional group** is an atom or a group of atoms within a molecule that have characteristic physical properties and are often the sites of chemical reactivity. It determines all of the following properties of a molecule:
 - Bonding and shape
 - Type and strength of intermolecular forces
 - Physical properties
 - Chemical reactivity
 - Nomenclature
- In first-year chemistry, we will focus on the first few functional groups. Their reactivity and nomenclature will be left for second-year organic chemistry.

Functional Groups: Hydrocarbons

Type of Compound	General structure	Functional Group	Hybridization	Example
Alkane	R_3C-H C_nH_{2n+2}	-----	sp^3	$CH_3CH_2\overset{CH_3}{CH}CH_3$
Alkene	$R_2C=CR_2$ C_nH_{2n}	Double bond	$C=C$ sp^2	
Alkyne	$RC\equiv CR$ C_nH_{2n-2}	Triple bond	$C\equiv C$ sp	$HC\equiv CCH(CH_3)_2$
Aromatic compounds	contain 	Phenyl group	$C-C$ sp^2	

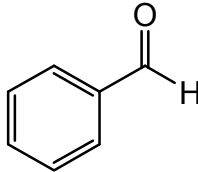
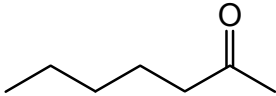
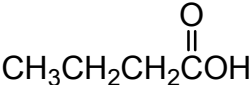
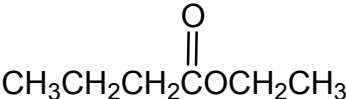
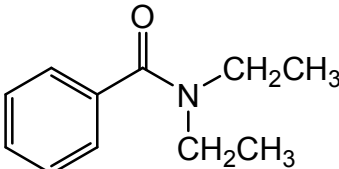
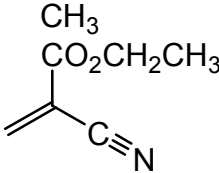
In all functional groups listed above, R = any chain of carbon atoms, or sometimes, an H atom, if H does not result in a different functional group.

Functional Groups: Compounds containing a C-Z single bond

Type of Compound	General formula	Functional Group	Hybridization	Example
Alkyl (aryl) Halide	R-X (X = F, Cl, Br, I)	-X halo group	Alkyl C-X sp^3 Aryl C sp^2 X = sp^3	
Alcohol	R-OH	-OH hydroxyl group	C sp^3 O sp^3	
Ether	R-O-R	-OR alkoxy group	C sp^3 O sp^3	
Amine	R-NH ₂ R ₂ NH R ₃ N	-NH ₂ amino group	C sp^3 N sp^3	
Thiol	R-SH	-SH mercapto	C sp^3 S sp^3	
Sulfide	R-S-R	-SR alkylthiol	C sp^3 S sp^3	

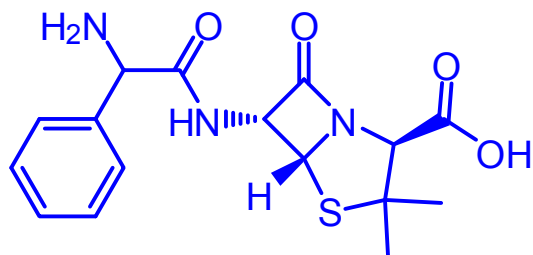
In all functional groups listed above, R = any chain of carbon atoms, phenyl or sometimes, an H atom, if H does not result in a different functional group.

Functional Groups: compounds containing a C=O Group

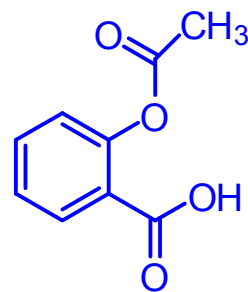
Type of compound	General formula	Functional group	Hybridization	Example
Aldehyde	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCH} \end{array}$	C=O carbonyl	C sp^2 O sp^2	
Ketone	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCR} \end{array}$	C=O carbonyl	C sp^2 O sp^2	$\text{CH}_3\text{C}(=\text{O})\text{CH}_3$ 
Carboxylic acid	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOH} \end{array}$	-COOH carboxyl	C sp^2 O sp^2	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COOH}$ 
Ester	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCOR} \end{array}$	-COOR	C sp^2 O sp^2	$\text{CH}_3\text{CH}_2\text{CH}_2\text{COCH}_2\text{CH}_3$ 
Amide	$\begin{array}{c} \text{O} \\ \parallel \\ \text{RCNR}_2 \end{array}$	-CONH ₂ -CONHR -CONR ₂	C sp^2 O sp^2 N sp^2	
Nitrile	R-C≡N	R-C≡N	C sp N sp	

In all functional groups listed above, R = any chain of carbon atoms, or sometimes, an H atom, if H does not result in a different functional group.

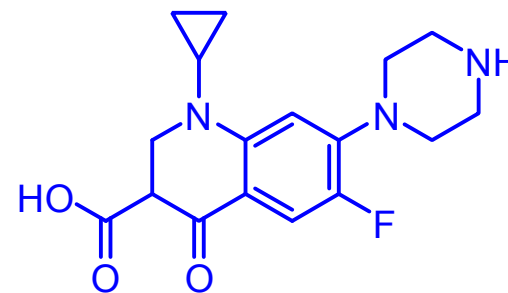
- Practice: identify the functional groups in the molecules below, and assign hybridizations to all the atoms.



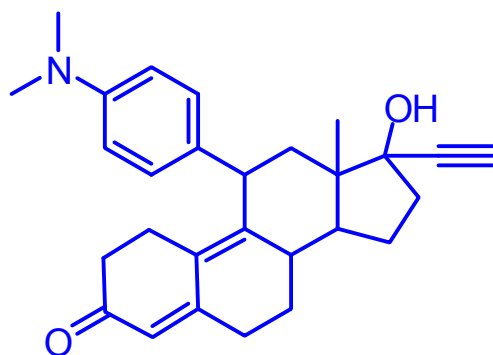
ampicillin



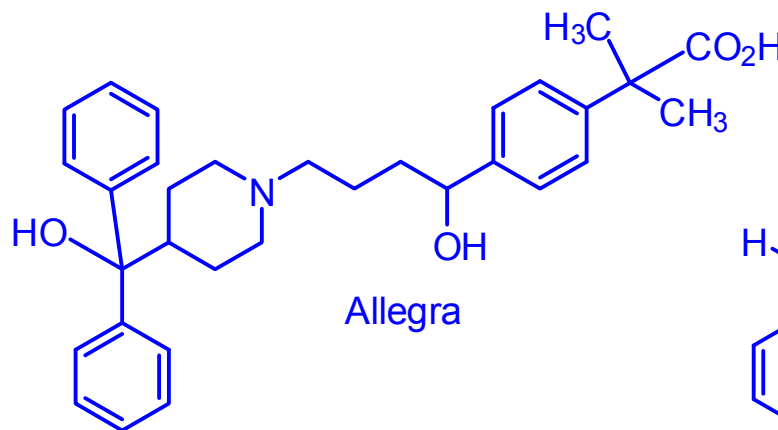
acetylsalicylic acid



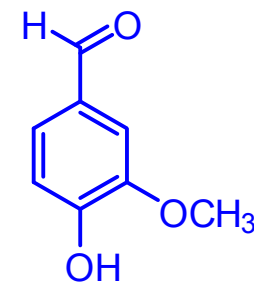
ciprofloxacin



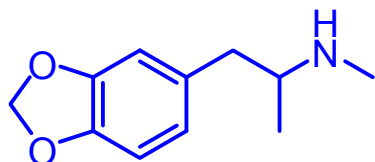
mifepristone



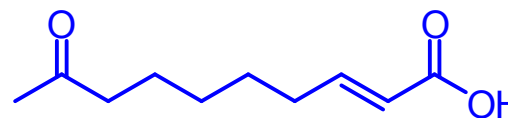
Allegra



vanillin



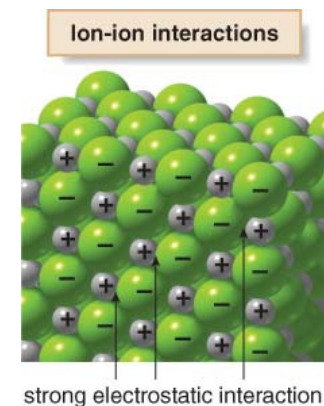
ecstasy: methylenedioxymethamphetamine



honey bee queen pheromone

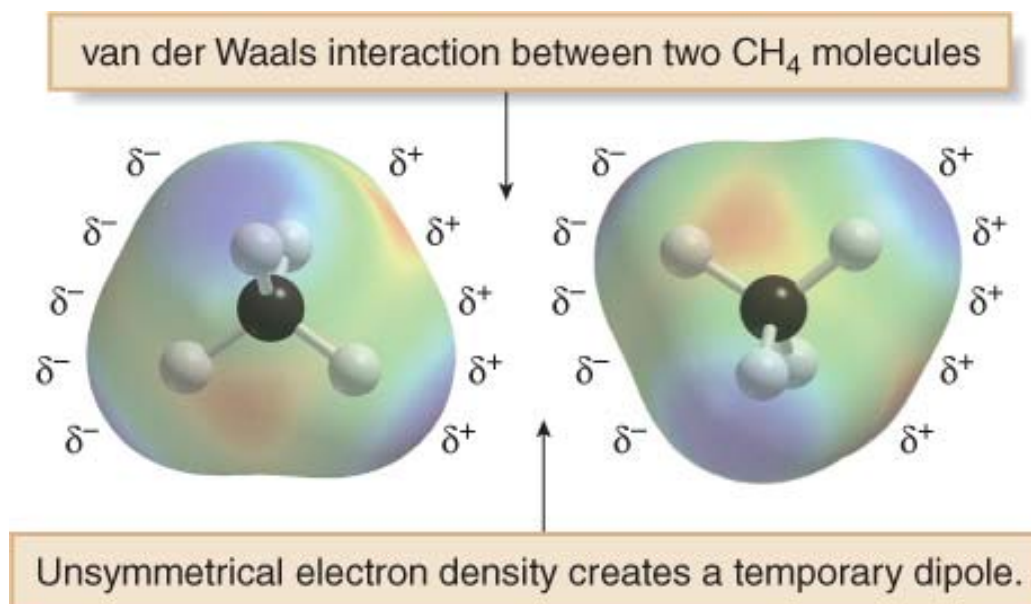
F. Intermolecular Forces

- Intermolecular forces are also referred to as non-covalent interactions or non-bonded interaction. They are weaker interactions than ionic interactions.
- Ionic compounds contain oppositely charged particles held together by extremely strong electrostatic interactions. These ionic interactions are much stronger than the intermolecular forces present between covalent molecules.
- Whereas, covalent compounds are composed of discrete molecules. The nature of the forces between these molecules depends on the functional group(s) present.
- There are three different types of intermolecular interactions, in the order of increasing strength:
 - van der Waals forces
 - Dipole-dipole interactions
 - Hydrogen bonding

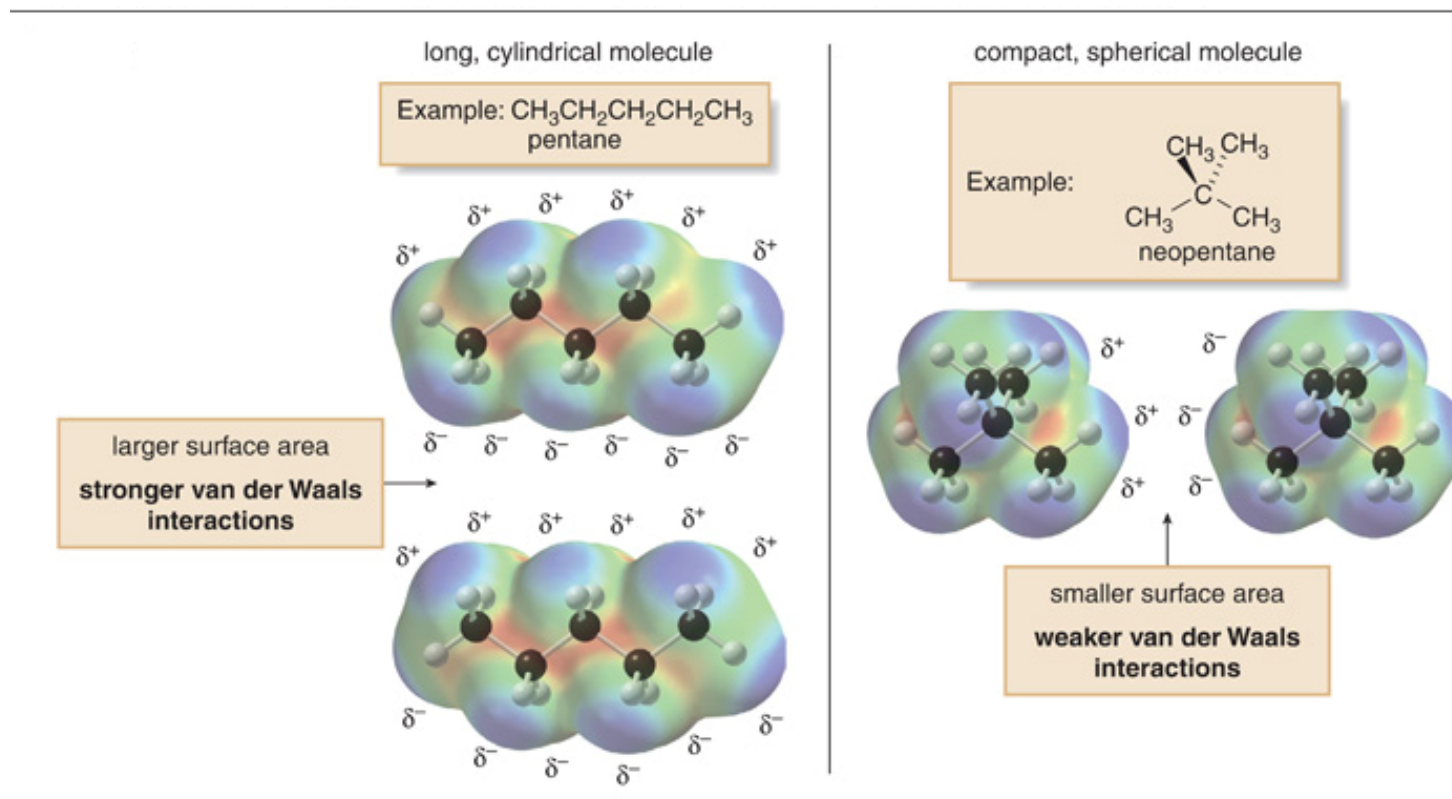


1. *van der Waals forces*

- Also known as London forces, they are weak interactions caused by **momentary changes in electron density** in a molecule.
- While all compounds exhibit these forces, they are the only attractive forces found in non-polar compounds.
- For example, even though CH_4 (or other alkane) has no net dipole, at any one instant, its electron density may not be completely symmetrical, causing a temporary dipole.
- This can induce a temporary dipole in another molecule. The weak interaction of these temporary dipoles is a van der Waals force.

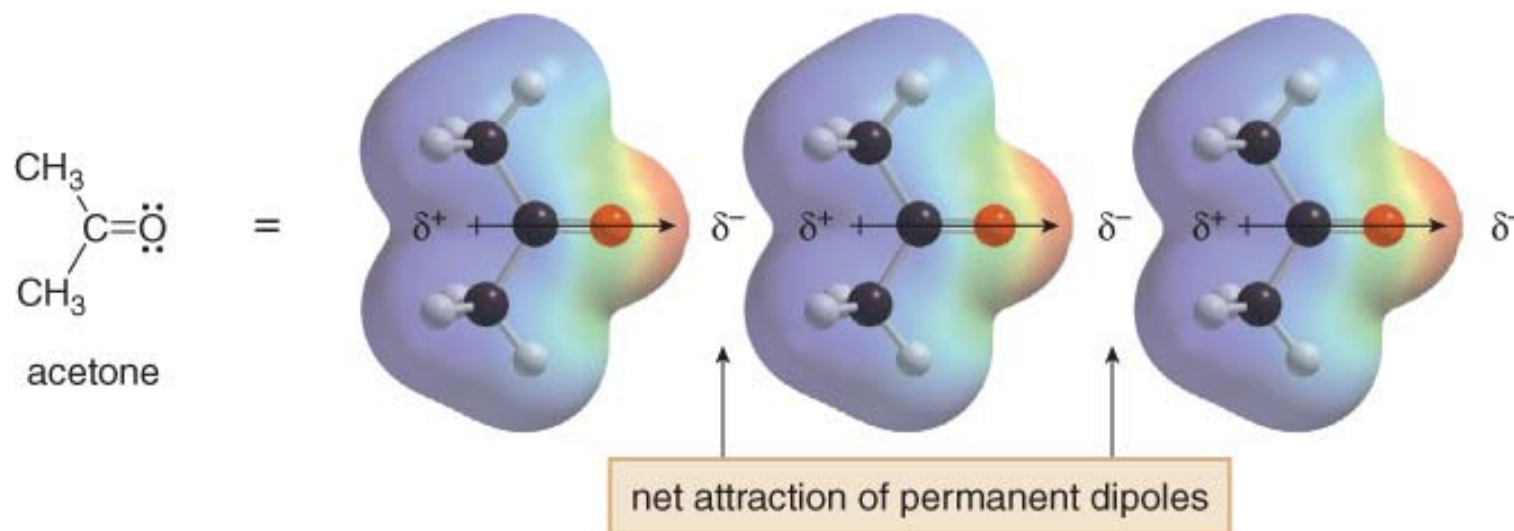


- The surface area of a molecule determines the strength of the van der Waals interactions between molecules. The larger the surface area, the larger the attractive forces, and the stronger the intermolecular forces.



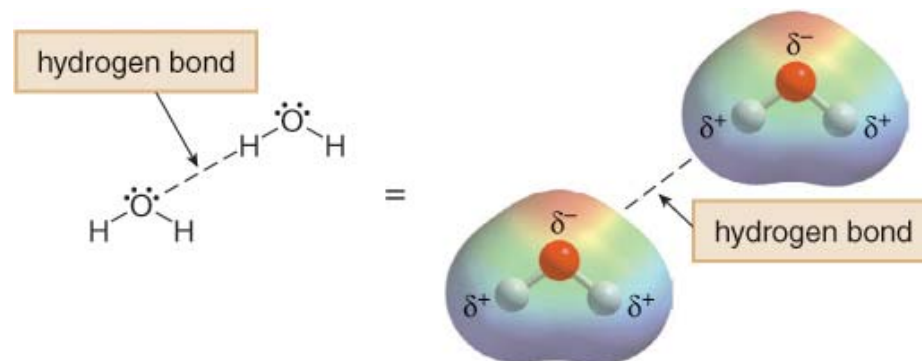
2. Dipole-dipole interactions

- Dipole-dipole interactions are the attractive forces between the **permanent dipoles** of two molecules. These forces between permanent dipoles are much stronger than the relatively weak van der Waals forces.
- The dipoles in adjacent molecules align so that the partial positive and partial negative charges are in close proximity.



3. Hydrogen-bonding interactions

- H-bonding typically occurs when a **hydrogen atom bonded to an O, N, or F** is electrostatically attracted to a lone pair of electrons on an O, N, or F atom in another molecule.

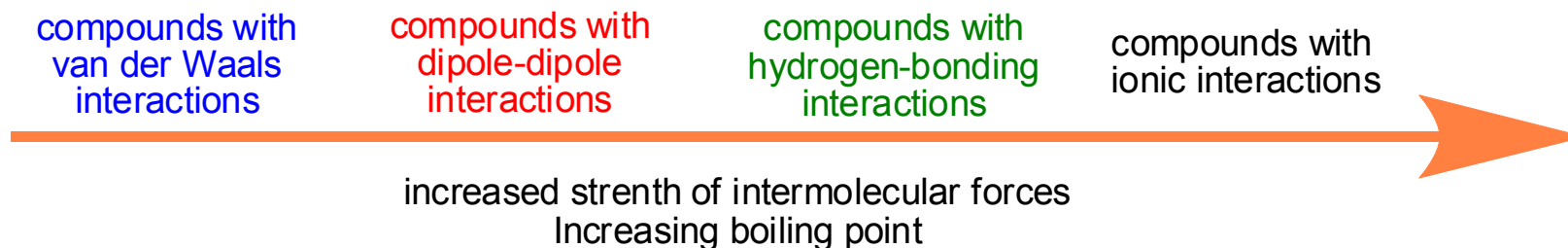


4. Summary of types of forces

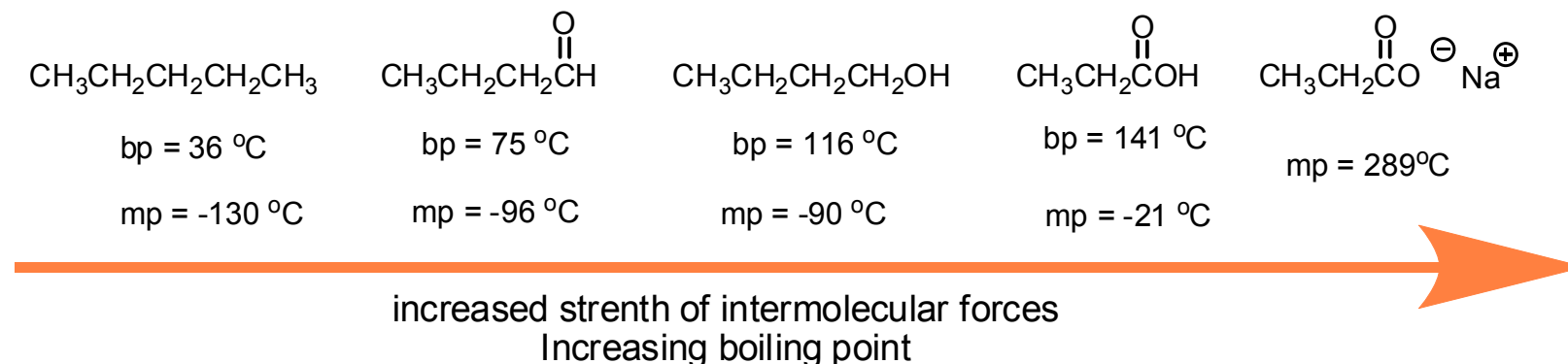
Type of Force	Relative Strength	Exhibited by	Examples
Van der Waals	weak	All molecules	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH}$
Dipole-dipole	moderate	Molecules with a net dipole	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CHO}$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH}$
Hydrogen-bonding	strong	Molecules with N-H, O-H or H-F bonds	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{OH}$ $\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COOH}$
Ion-ion	very strong	Ionic compounds	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{COO}^- \text{Na}^+$ NaCl

G. Physical Properties: Melting and Boiling Points

- The stronger the intermolecular forces, the higher the melting or boiling point.
- Since ionic compounds are held together by extremely strong interactions, they have very high melting points. For example, that of NaCl is 801 °C.
- For compounds with approximately the same molecular weight

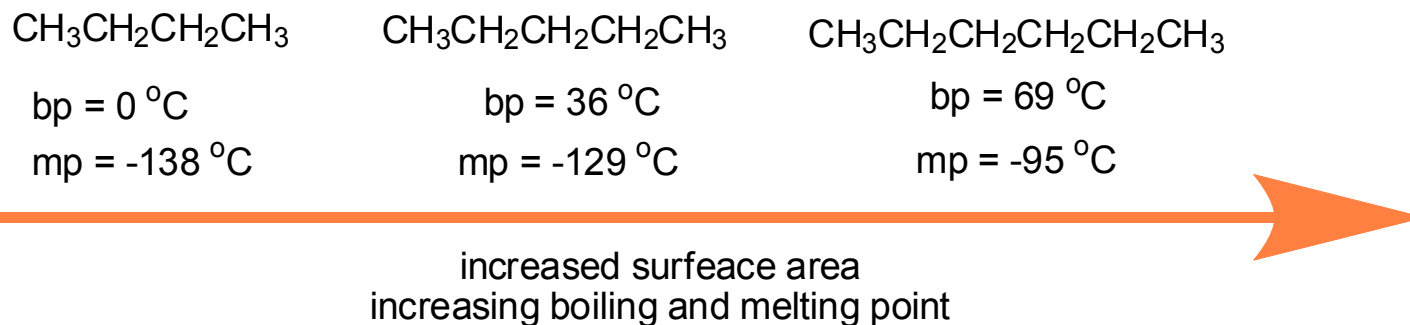


- For example....

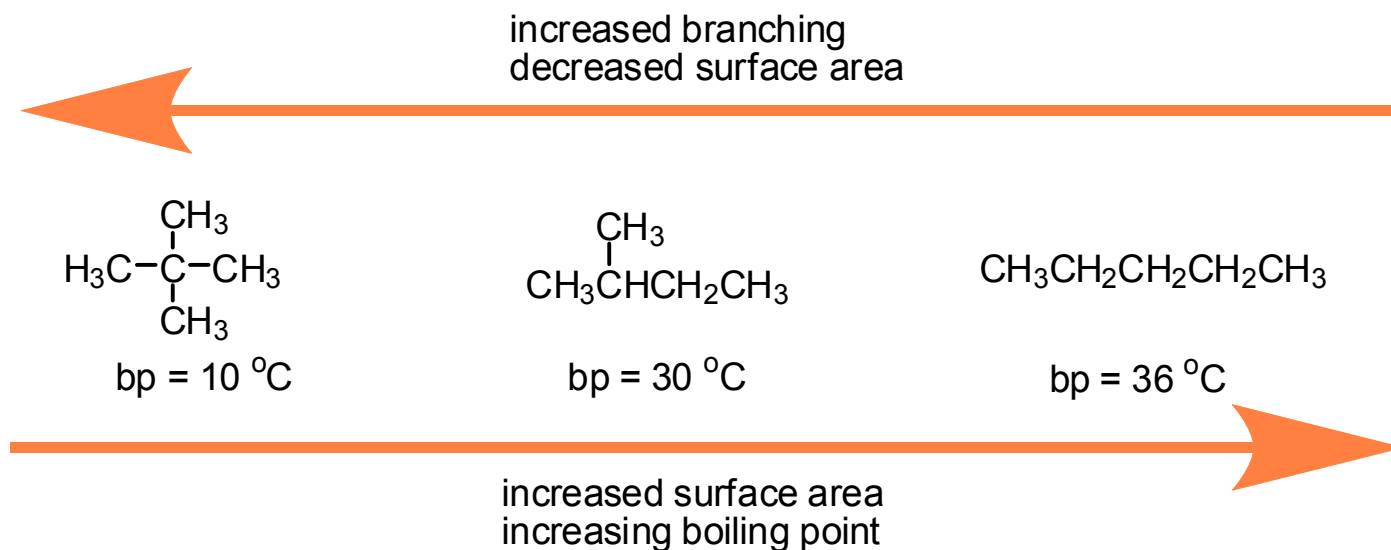


- For compounds with similar functional groups

- The larger the surface area, the higher the melting or boiling point



- The boiling point of isomers (same formula, different structure) increases with branching, because of increasing surface area



- Symmetry also plays a role in determining the melting points of compounds having the same functional group and similar molecular weights, but very different shapes.
- A compact symmetrical molecule like neopentane packs well into a crystalline lattice, whereas isopentane, which has a CH_3 group dangling from a four-carbon chain, does not. So, neopentane has a much higher melting point.

