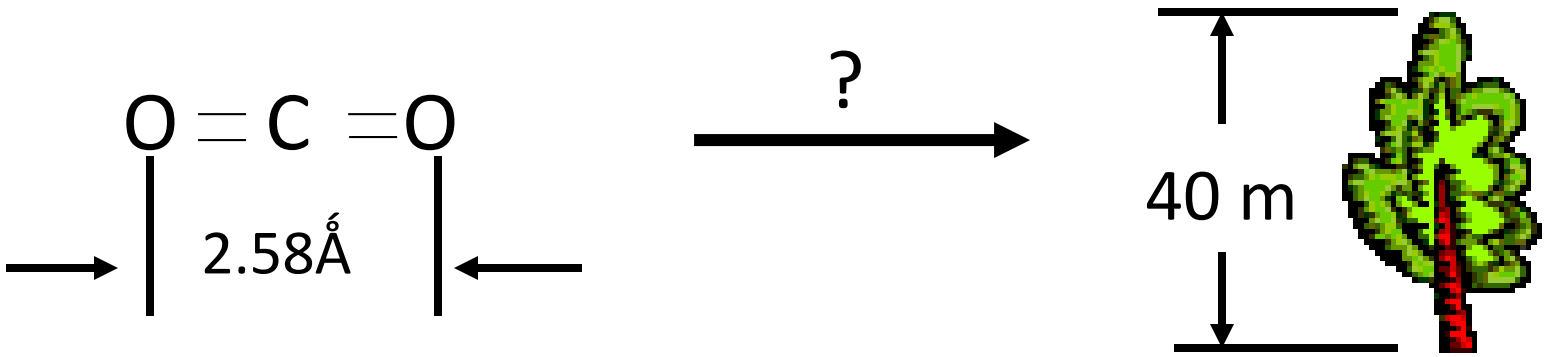
Lecture 2

The framework to build materials and understand properties

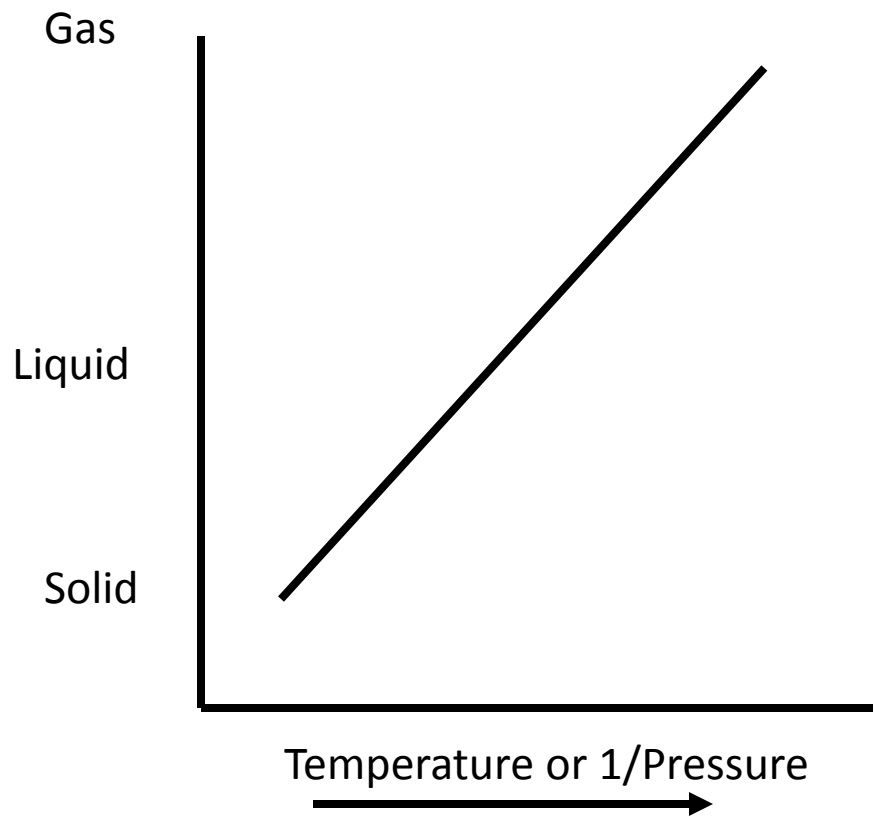
Trees are made into a solid materials/structures in an environment that consists of small molecules: CO_2, N_2, H_20, CH_4

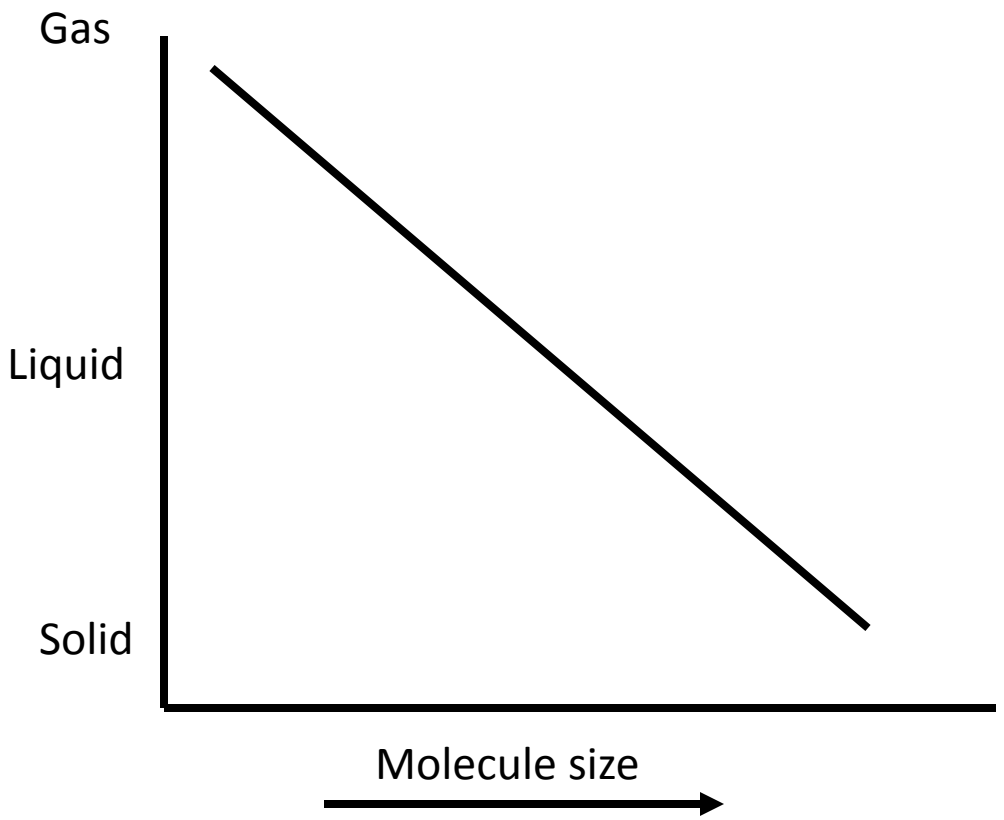


Why do molecules reside in a liquid or solid state at room temperature?

Or what are the “forces” that hold atoms and molecules together?

Methods of developing solid materials





A material's property is dictated by…

- Molecule size
- Chemical composition
- Packing

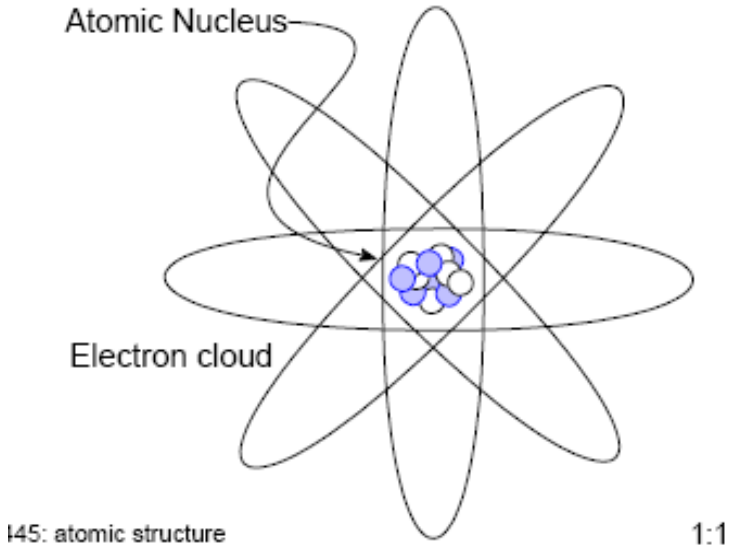
These parameters influence the type of interactions amongst atoms in a molecule and interactions between molecules

Some Basic Information on Condensed Matter

- Atomic structure dictates properties
  Nucleus of protons and neutrons, with electron shell– (atoms are overall neutral)
- Atoms and the Pauli Exclusion principle:
  No two electrons in an atom can have the same set of four quantum numbers.
- Electrostatic interactions cause attraction between particles

Atoms associate due to

- Primary and secondary bonds
  - Ionic and covalent
  - Dipole bonds
  - Hydrogen bonds
  - London dispersion forces
- Metallic bonds



C. Frazier

Covalent bonds form when two atoms of same or similar electronegativities react and share electrons

Nonpolar covalent bond is when the distribution of the electron density is symmetrical– bonding is symmetrical between two nuclei

O=O

Polar covalent bond is when the distribution of the electron density is asymmetrical and there is an electronegativity difference > 0.4

More background info

https://www.youtube.com/watch?v=R2TrrmdGM2A

Electronegativitiy: measure of the ability to attract electrons

Ionic compounds (**salts**) will form from the reaction of atoms of greatly differing **electronegativities**–
(interact by gaining or losing electrons)

			H 2.1			
Li 1.0	Be 1.5	B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2	Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8						Br 2.8

More background info

https://www.youtube.com/watch?v=jjOzgw5nAZk

DIPOLES make polar molecules

- Spatially distinct “poles” on single material (remember asymmetric sharing of electrons)
  - Poles are electronic or magnetic
  - For intermolecular forces we discuss electronic poles

Partial charges, δ^+ and δ^-, that are either **temporary** or **permanent** on the molecule

Electrons are not shared equally

All atoms and molecules can be polarizable (related to size) and bond type

The **induced dipole moment** is based on both a chemical characteristic and the applied field

Examples of polarizabilites (gas phase)

C-H = 0.65

CH_4 = 4 x 0.65 =2.6

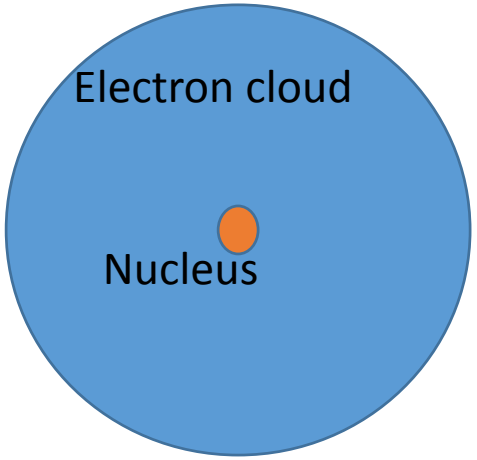
C-C = 0.48

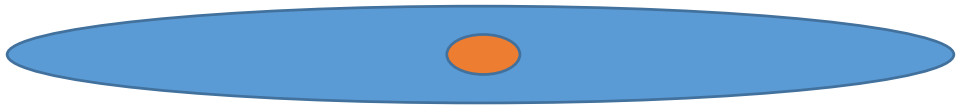
C=C = 1.65

C-OH = 1.28

C-O = 0.60

CH_3OH = 3.2





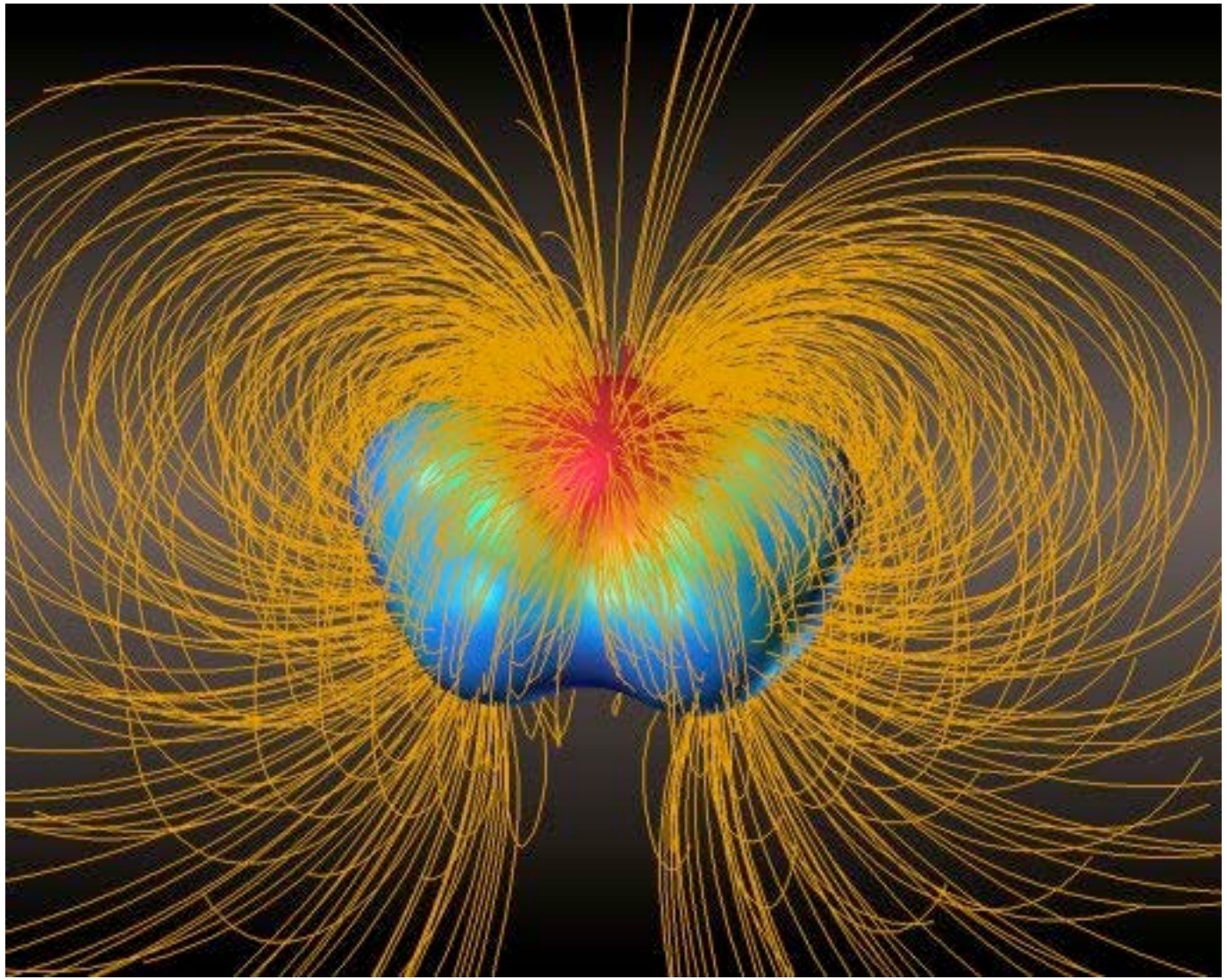
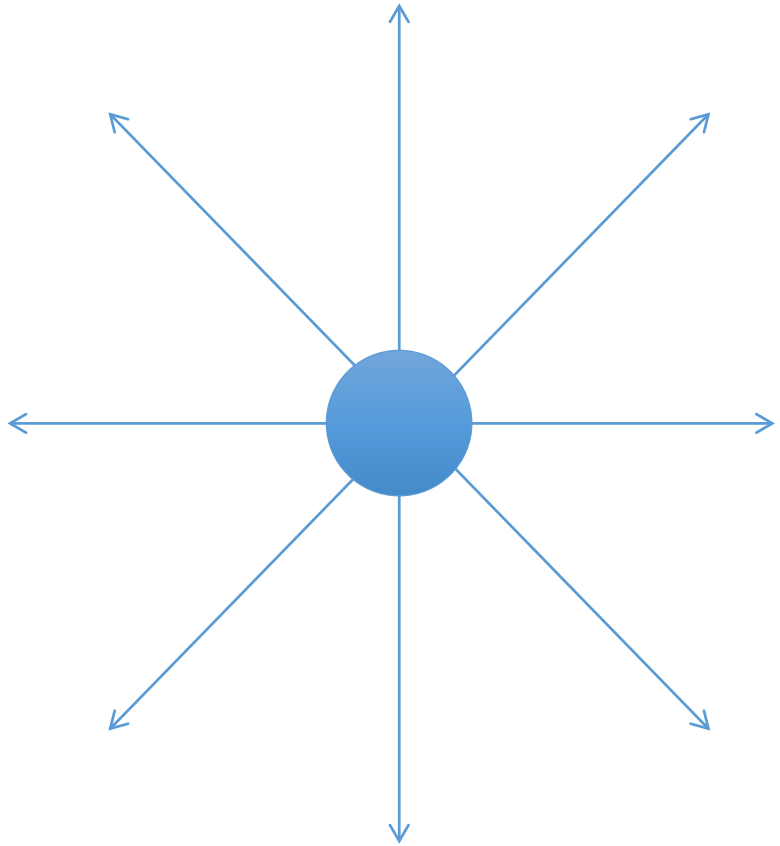
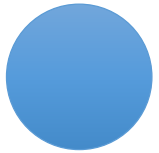


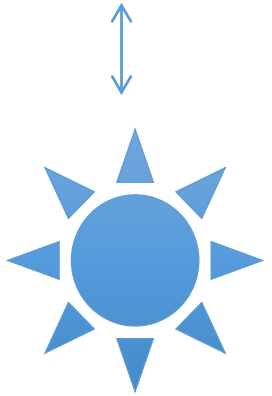
Image is from MOLCAD GmbH
http://www.molcad.de/competence/fieldlines.html.en



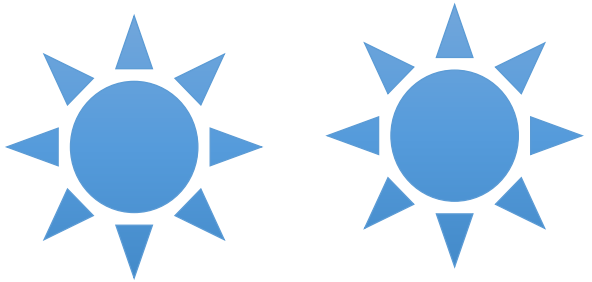
Ion with field



Non-polar molecule

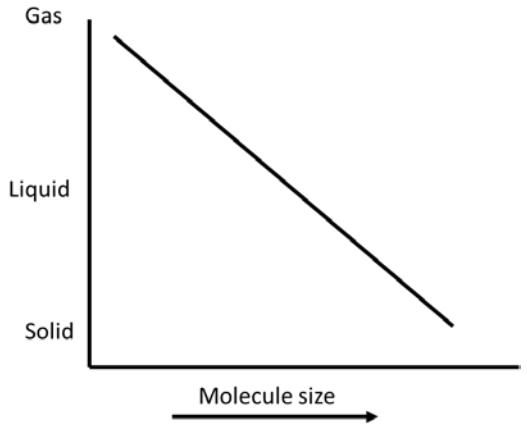


Non-polar molecule with **instantaneous** dipole



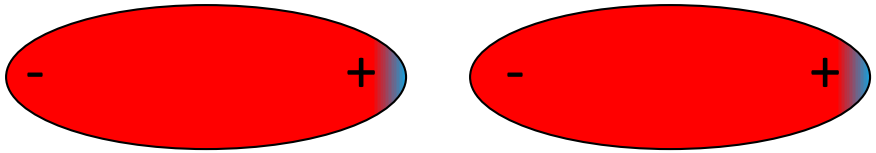
Intermolecular forces limit free motion of molecules in space

Hydrocarbon	Boiling point (˚C)
Methane	-161
Ethane	-88
Propane	-42
Butane	0



Larger molecules undergo increased intermolecular interactions (dispersion forces increase with molar mass size)

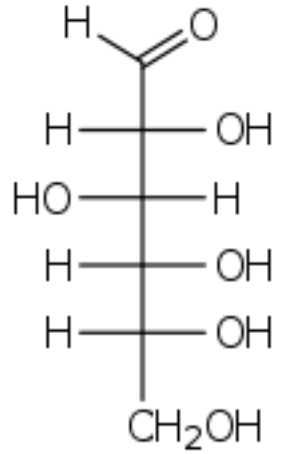
Temporary dipoles



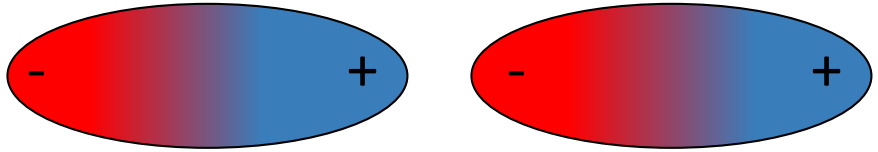
Added permanent dipoles increase interactions

with OH	Boiling point (˚C)
Methanol	65
Ethanol	78
1-Propanol	98
1-Butanol	118
<u>With 2 OH</u>	
Ethylene glycol	196

Plants make glucose via photosynthesis, a carbohydrate C(H2O) that has 5 “free” hydroxyl groups



Permanent dipoles



Hydrogen bonds– A specific type of intermolecular bond

Molecules must have H attached to strongly electronegative atoms such as (O, N, and F*)

-creates a permanent dipole and hydrogen is unique in size and electron content

Oxygen containing compounds, if have accessible lone pair electrons, can be hydrogen bond acceptors

More background info

http://chemwiki.ucdavis.edu/Physical_Chemistry/Physical_Properties_of_Matter/Intermolecular_Forces/Hydrogen_Bonding

Bond Strengths

• Covalent Bonds	60-700 KJ/mole	
• Ionic Bonds	600-1100 KJ/mole	
• Hydrogen bonds	10-25 KJ/mole	
• Dipole-Dipole	4-20 KJ/mole	
• Dipole-induced dipole	<2 KJ/mole	
• London (induced-induced)	0.8-40 KJ/mole	**$1/r^6$**

Materials are influenced by bond type

Thermal Energy (KT) at 25C (J) 4.1E-21

Bond type	Bond energy J/bond (examples)	bond energy/ KT
covalent	3.321E-19	81.00
dipole	2.491E-20	6.08
disper	6.642E-21	1.62

London Dispersion bonds are between non-polar molecules
Dipole and hydrogen bonds are between polar molecules

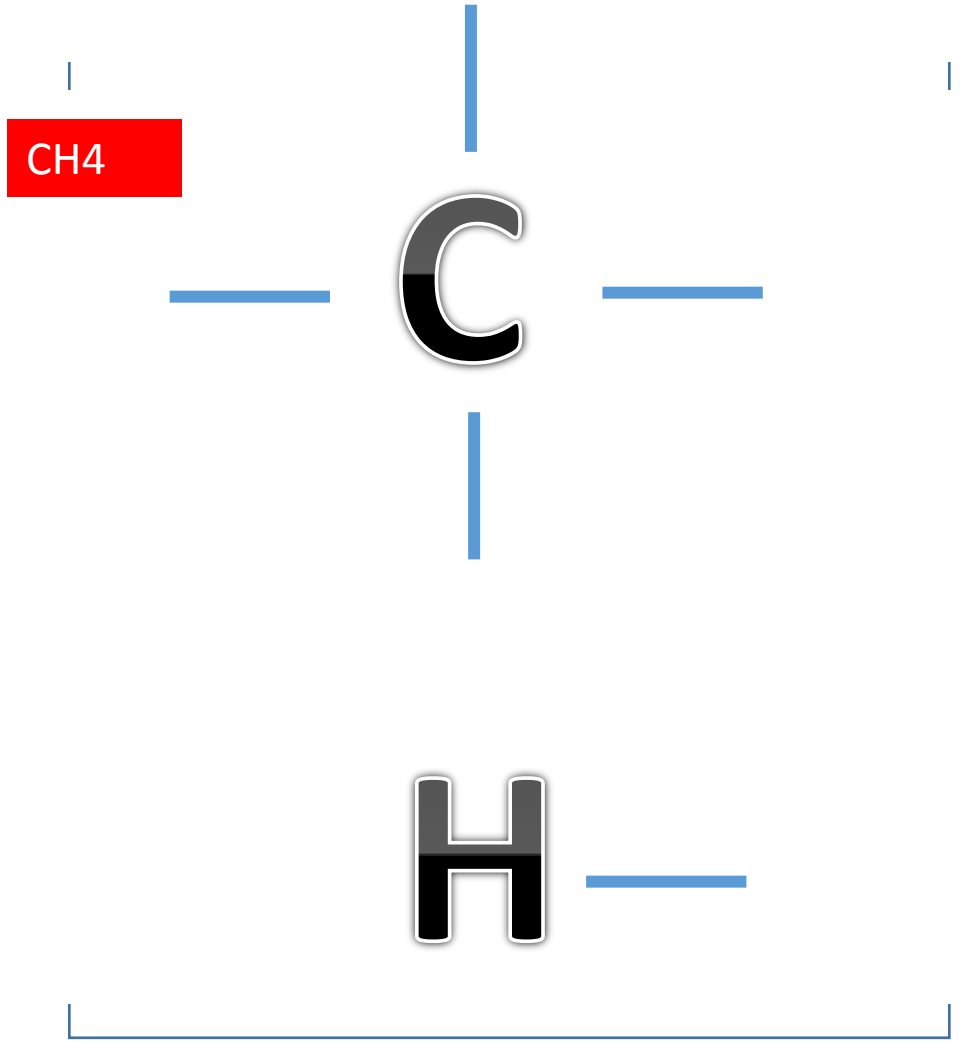
So the ability of a molecule to interact will be dictated by chemical composition

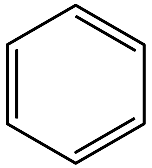
Functional groups can be used to help classify chemical composition

Responsible for chemical reactivity and interactivity

Hydrocarbons

- Alkanes (aliphatics)
  - alkyl groups, drop an H
- Alkenes
- Alkynes
- Aromatics
  - Benzene, phenyl, and benzyl groups



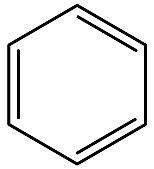


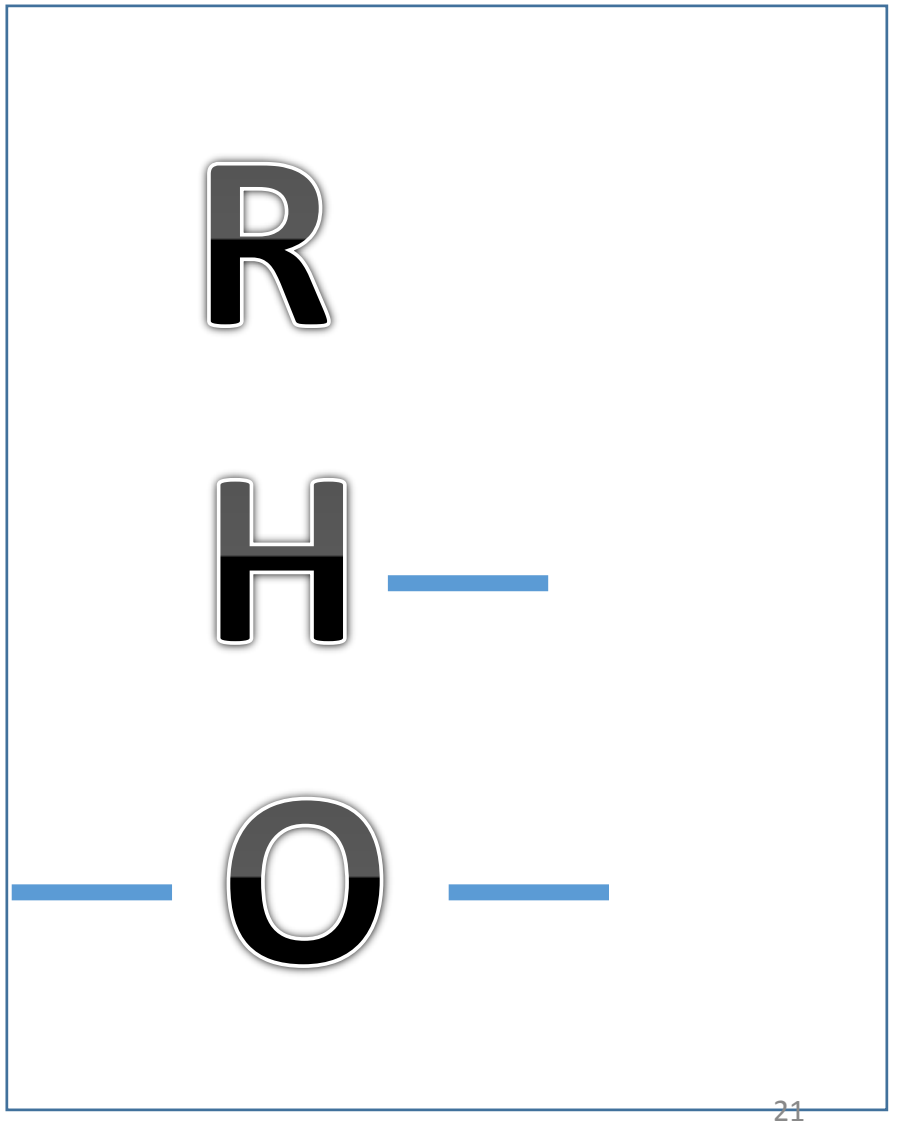
Review octet rules---- https://www.youtube.com/watch?v=TZuRh_epSyI

Alcohols

- Hydroxyl (-OH) vs. alcohols **(R-OH)**
- Hydroxyl derivative of alkane

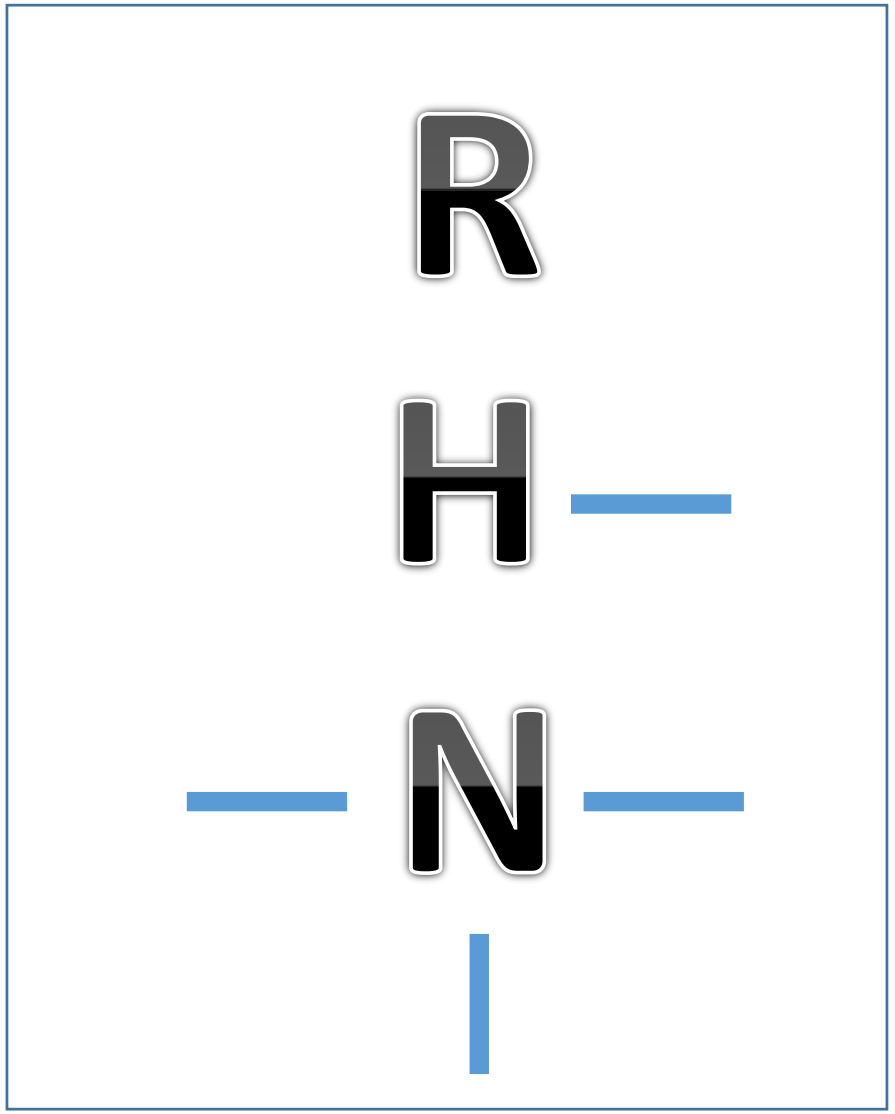
  vs. alkyl derivative of water
- Relatively familiar alcohols
  - Methanol, ethanol, propanol…
- Phenol





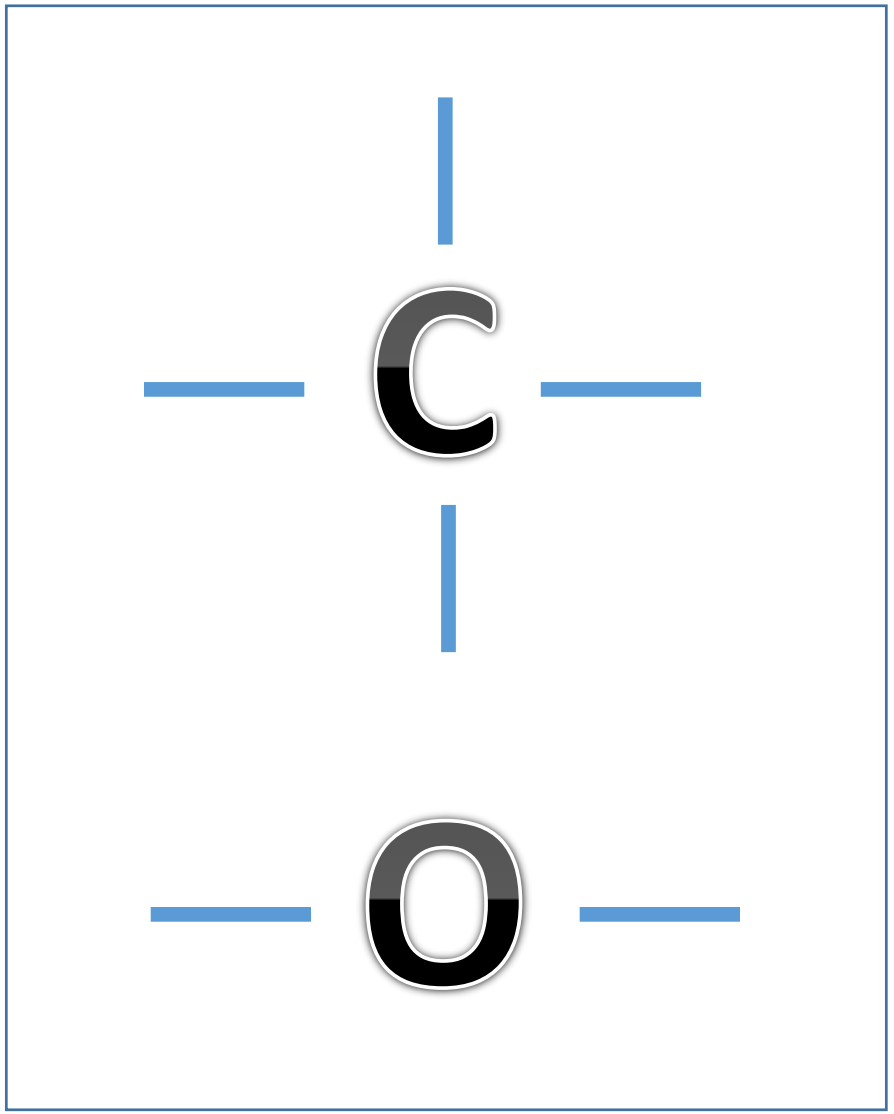
Amines

- Organic derivatives of ammonia
  - Draw ammonia
  - Draw ethylamine



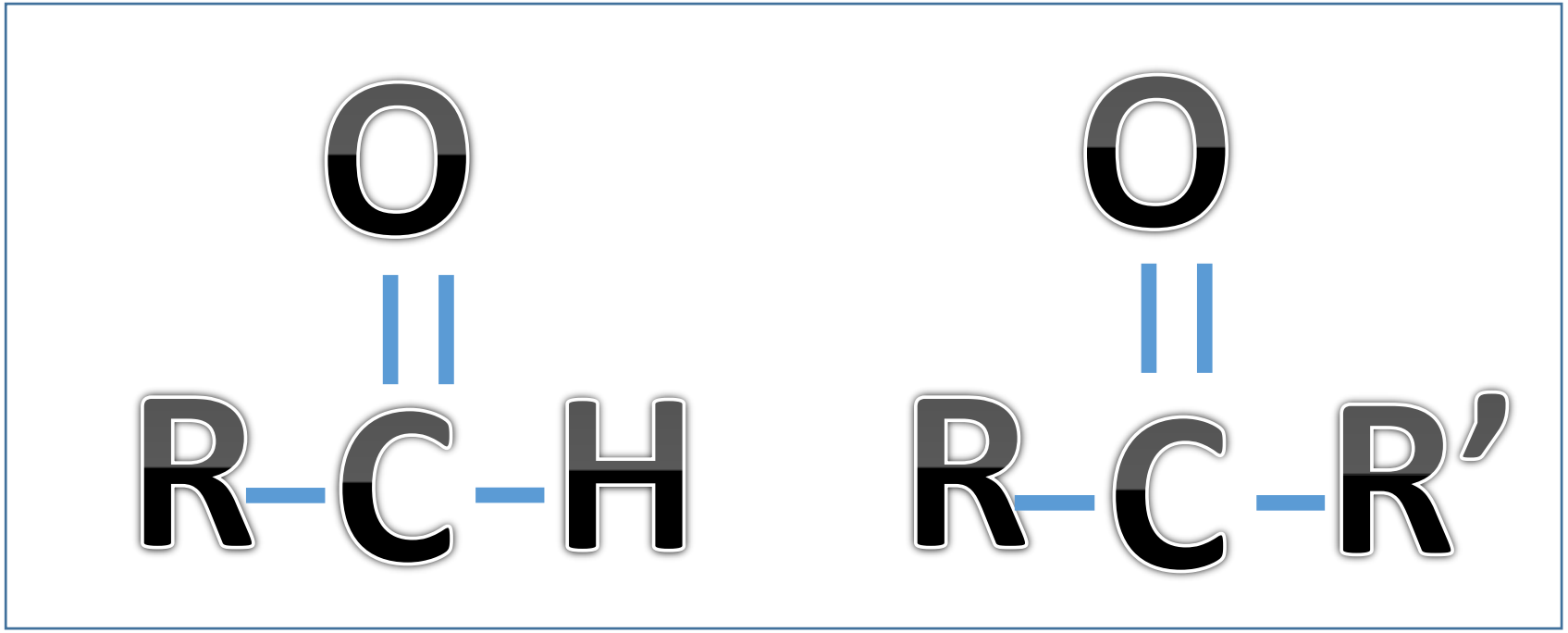
Ethers

- Ethers have an R-O-R or R-O-R’
- Cyclic ethers
  - Oxacyclopropane
  - Oxirane/epoxide
  - Ethylene oxide



Aldehyde vs. Ketone

- A carbonyl group is a carbon atom that has a double bond to oxygen
- Aldehyde has RCHO and ketone has RCOR’
  - Acetone is a simple ketone CH3-CO-CH3



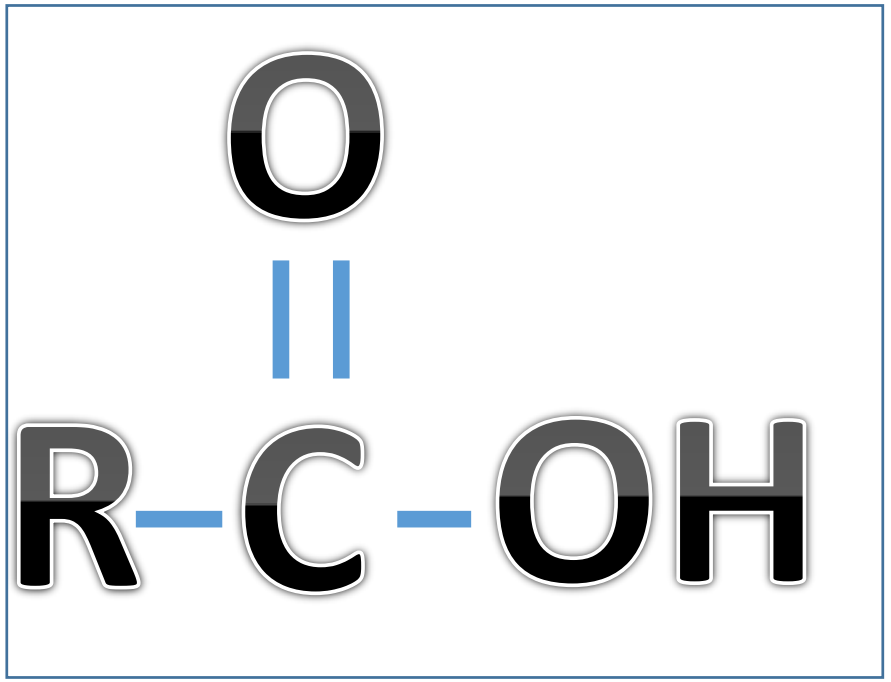
Formaldehyde is the simplest aldehyde -- HCHO

Carbonyls: carboxylic acid

- Carbonyls that are bonded to an

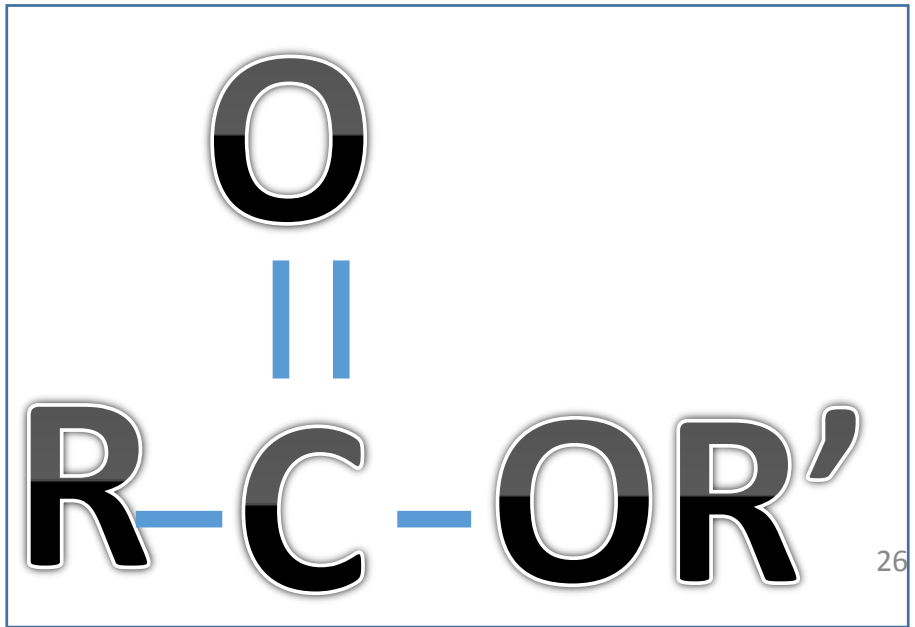
  alcohol (RCO_2H) is a carboxylic acid

- Carbonyl and hydroxyl group together is known as **carboxyl group** (CO_2H or COOH)



Carbonyl: Esters

- Esters are when carbonyl groups are bonded to an alkoxyl group (-OR)
- General formula of **(RCOOR')**
- Based on chain length of **R** common esters are
  - Acetate, propanoate, butyrate



To summarize

- Subatomic particles give rise to interactions amongst atoms and molecules
- Covalent bonds between atoms can be classified as polar or non-polar, depending what atoms are bonded together
- Secondary interaction strength is influenced by chemical composition
- Functional groups dictate the reactivity or interactivity of a molecule and used to classify specific arrangements