Learning Organic Chemistry

> 10 million organic compounds exist!

Memorizing the structure, properties, and reactivities of each molecule will severely limit your abilities

Organic chemistry is rational and systematic

Goal:

Learn tools to dissect and analyze organic chemistry that is unfamiliar

Pay attention to detail!

Study Tips

1. **Read** the suggested readings before coming to class and record the main ideas.
2. After each lecture, **summarize** the major ideas and concepts in your notes within 24 hours of class.
3. **Annotate** these summaries from your study of the textbook
4. Work the **problems** independently
5. **Master the material from each lecture before going to the next one.**
6. Spend a few minutes each day on **review** to prevent becoming overwhelmed on the night before an exam.

You cannot CRAM

for an Organic EXAM

Syllabus

- Organic chemistry
- Structure and reactivity
- Resonance
- Acidity and basicity of organic compounds
- Alkanes
- Stereochemistry
- Overview of organic reactions
- Alkenes
- Alkynes
- Alkyl halides
- Benzene and aromatic compounds
- Alcohols and phenols
- Carbonyl compounds
- Synthesis using the chemistry of 5.12

Background Review

1. Atomic Structure
2. Atomic Orbitals
3. Electron Configuration
4. Ionic/Covalent Bonding
5. Lewis Structures
6. Formal Charges
7. Valence Bond Theory
8. VSEPR Theory
9. Hybridization
10. MO Theory

Go the the 5.12 Web Page and work through:

- ❑ **Background Handout (PowerPoint and .pdf)**
- ❑ **Background Knowledge Quiz**

Suggested Readings (McMurry): 1.1-1.12, 2.1-2.3
Suggested Problems (McMurry): 1.1-1.16, 1.21-1.47, 2.1-2.9, 2.29-2.35

Lecture 1: Outline

- ❑ Organic Chemistry
- ❑ Relationship of Structure, Energy, and Reactivity
- ❑ Structure
  - ❑ Atoms
  - ❑ Bonding
    - o How/Why Atoms Bond Together
    - o Bonding Patterns
  - ❑ Representing molecules (putting the atoms together)
    - o Lewis and Kekulé Structures
    - o Line-angle Formula
    - o 3-D
    - o Orbital Drawings
  - ❑ Functional Groups
  - ❑ Resonance

Suggested Readings (McMurry): 2.4-2.12
Suggested Problems (McMurry): 2.36-2.41, 2.43-2.51, 2.53-2.57, 2.59

Organic Chemistry

What: **The study of carbon-containing compounds**

Why: **Pervasive in nature**

Chemical foundation of biology

Improve standard of living (medicines, plastics, pesticides . . .)

How: **Examine structure and analyze how it governs reactivity**

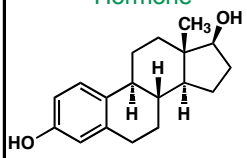
What: Carbon-Containing Compounds

Middle of second row

Can neither accept or give up electrons easily

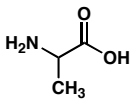
Share e^- with other carbon atoms - incredible structure diversity!

Hormone



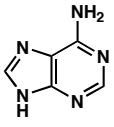
Estradiol

Amino acid



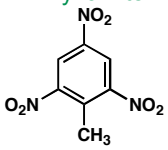
Alanine

DNA base

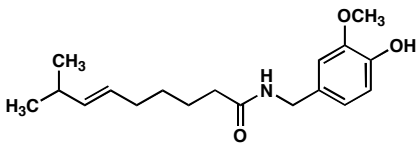


Adenine

Dynamite

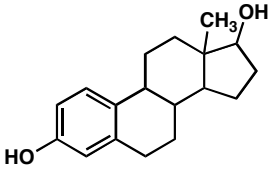


TNT

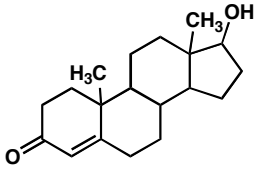


Capsaicin (peppers)

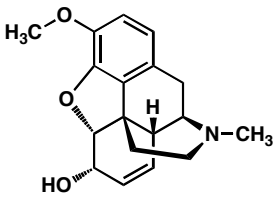
Subtleties in Structure



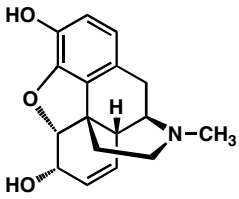
estradiol



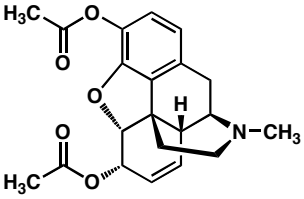
testosterone



codeine

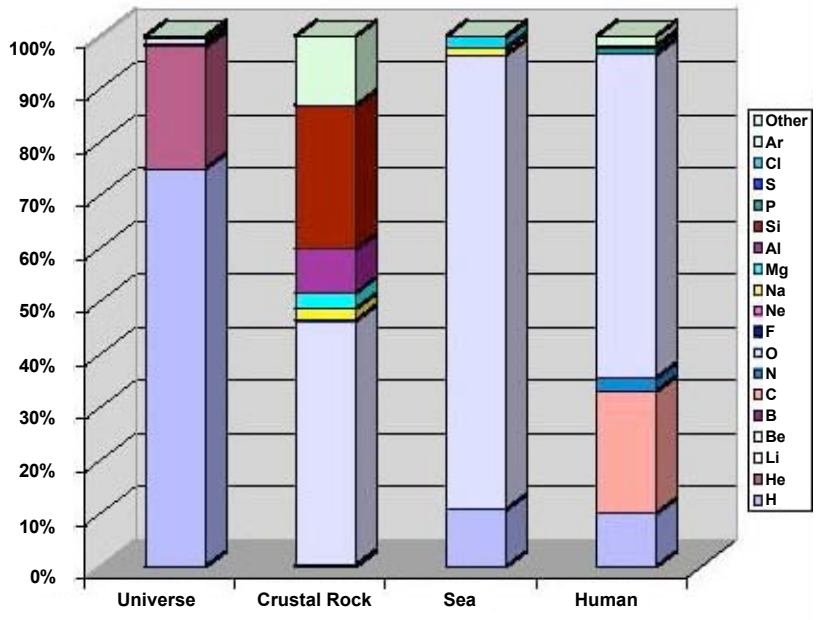


morphine



heroin

Why: Life is Based on Organic Compounds



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How: Structure and Reactivity

Structure - what atoms are present & how they are bonded together

Reactivity - potential of structure to undergo chemical change

If likely - **reactive** (**unstable**)
If unlikely - **unreactive** (**stable**)

Potential Energy:
- function of position or configuration of components
- if low, compound more stable, change less likely
- if high, compound less stable, change more likely

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Structure

Foundation of organic chemistry

1. What atoms (besides carbon) are important?
2. How are these atoms bonded together?

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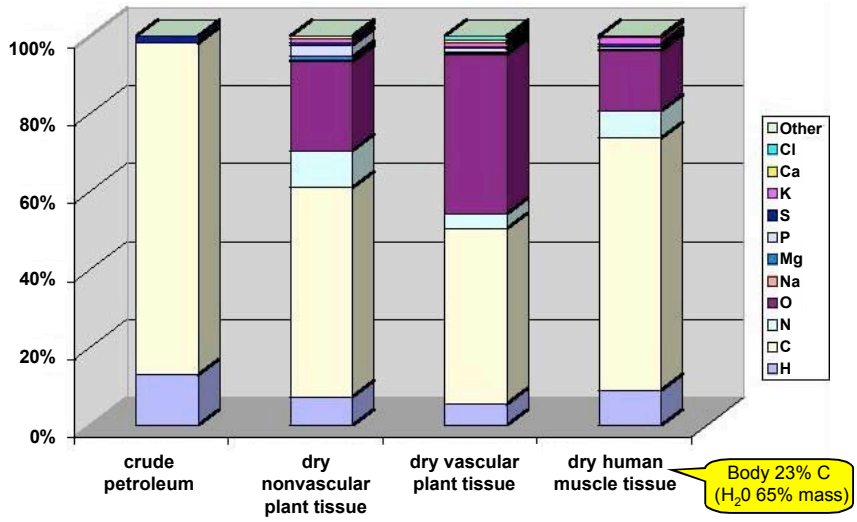
Structure - Atoms of Organic Molecules

Food we eat, fragrances we smell, colors we see, clothes we wear



Typical drug contains 20-80 atoms (C, H, N, O, F, S, P, Cl, Br, I)

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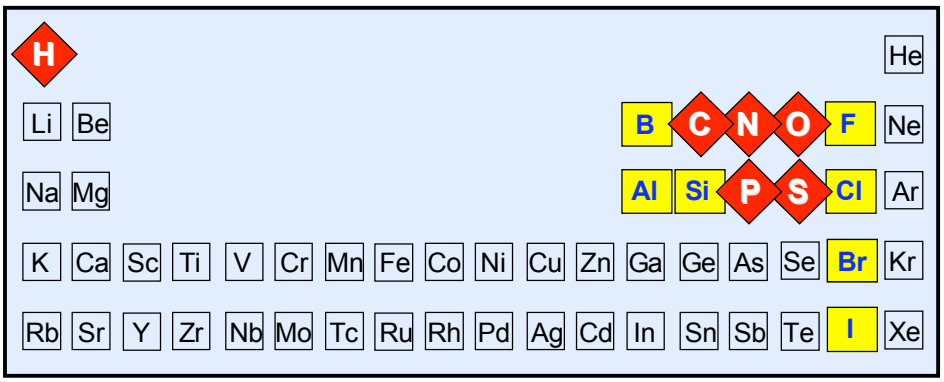
Main Atoms in Organic Chemistry



Electron configuration:

number and arrangement of electrons about an atom

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Electron Configuration of Main Atoms

Element	Ground State Configuration	1s	2s	2p			3s	3p		
H	$1s^1$	↑								
He	$1s^2$	↑↓								
Li	$1s^2 2s^1$	↑↓	↑							
Be	$1s^2 2s^2$	↑↓	↑↓							
B	$1s^2 2s^2 2p^1$	↑↓	↑↓	↑						
C	$1s^2 2s^2 2p^2$	↑↓	↑↓	↑	↑					
N	$1s^2 2s^2 2p^3$	↑↓	↑↓	↑	↑	↑				
O	$1s^2 2s^2 2p^4$	↑↓	↑↓	↑↓	↑	↑				
F	$1s^2 2s^2 2p^5$	↑↓	↑↓	↑↓	↑↓	↑				
Ne	$1s^2 2s^2 2p^6$	↑↓	↑↓	↑↓	↑↓	↑↓				
Na	$1s^2 2s^2 2p^6 3s^1$	↑↓	↑↓	↑↓	↑↓	↑↓	↑			
Mg	$1s^2 2s^2 2p^6 3s^2$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓			
Al	$1s^2 2s^2 2p^6 3s^2 3p^1$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑		
Si	$1s^2 2s^2 2p^6 3s^2 3p^2$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	
P	$1s^2 2s^2 2p^6 3s^2 3p^3$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑	↑
S	$1s^2 2s^2 2p^6 3s^2 3p^4$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑	↑
Cl	$1s^2 2s^2 2p^6 3s^2 3p^5$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑
Ar	$1s^2 2s^2 2p^6 3s^2 3p^6$	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓	↑↓

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Electron Configuration and Valence Electrons

Electron redistribution (change in configuration) is the origin of chemical change

WHY? Attain lower **ENERGY**

(achieved when outer shell is filled - 8 electrons)

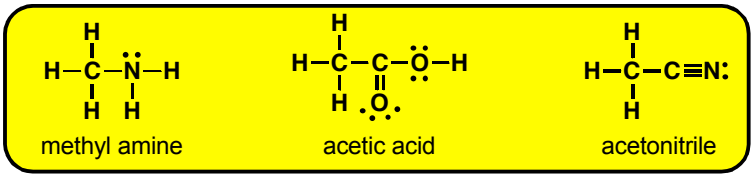
Process of chemical bonding:
adding or taking away outer shell electrons to gain a closed shell configuration

How do atoms maintain 8 electrons as well as participate in chemical bonding?

Bonding Possibilities of Main Organic Atoms

Each atom has a limited number of possibilities to satisfy octet:

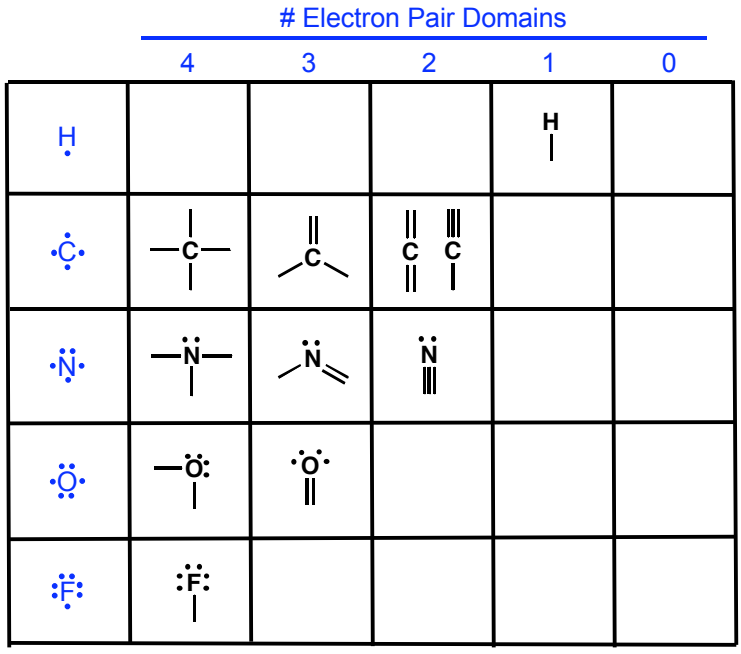
1. Nonbonding (electron pair localized on one atom)
2. Bonding (electron pair shared between two atoms)
   a. Single bond (1 shared pair)
   b. Double bond (2 shared pairs)
   c. Triple bond (3 shared pairs)



(H is exception to octet rule - has 1 electron)

Electron Pair Domain - region of high valence shell electron density (bonding or nonbonding)

Bonding Patterns: Formal Charge 0



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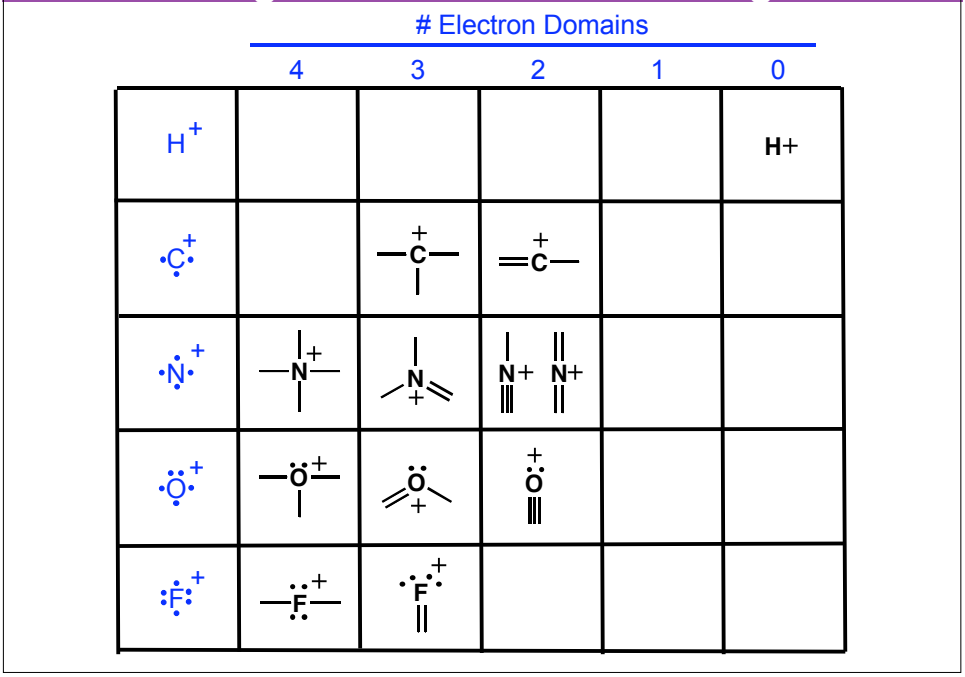
Bonding Patterns: Formal Charge +1



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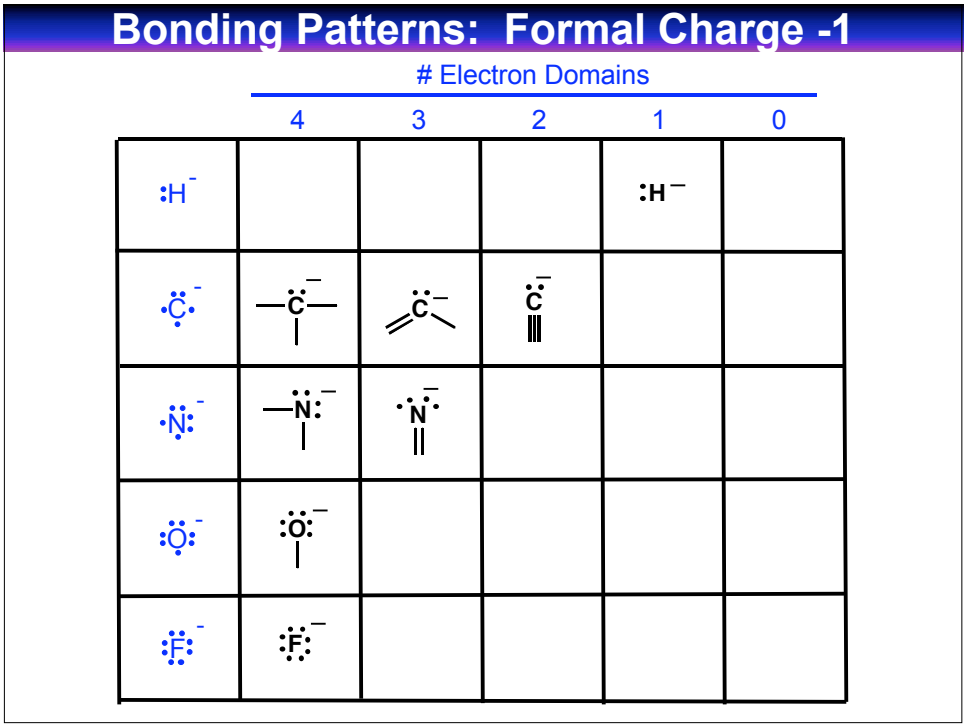
Bonding Patterns: Formal Charge -1



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Boron

Electron configuration

Neutral, but electron deficient

Octet, but charged

can tolerate an incomplete octet better than any other atom in the second row

EN = 2, least suited of all second row elements to carry a negative charge

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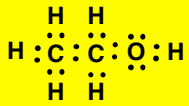
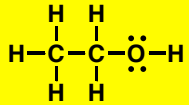
Organic Structures: Summary (so far)

- ✓ Organic Chemistry
- ✓ Relationship of Structure, Energy, and Reactivity
- ❑ Structure
  - ✓ Atoms
  - ✓ Bonding
    - ✓ How/Why Atoms Bond Together
    - ✓ Bonding Patterns
  - ❑ Representing molecules
    - ✓ Lewis and Kekule Structures
    - o Line-angle Formula
    - o 3-D
    - o Orbital Drawings
  - ❑ Functional Groups
  - ❑ Resonance

Ethanol

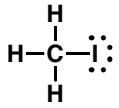


Lewis Structure

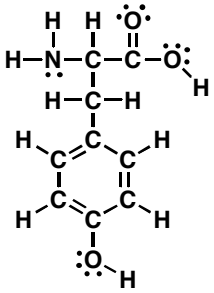


Kekulé Structure

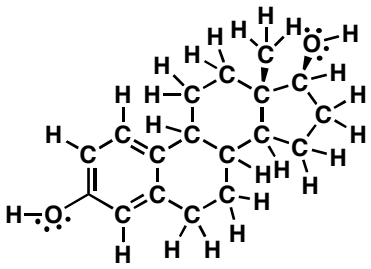
Representing Molecules: Line-Angle Formula



Iodomethane

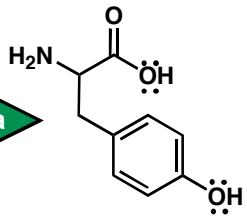


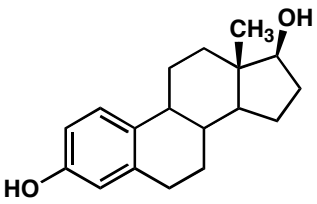
Tyrosine



Estradiol

Line-Angle Formula

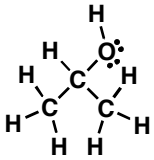


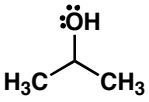


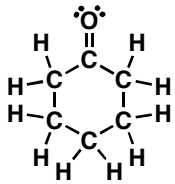
Rules of Drawing Line-Angle Formulas

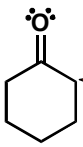
- Bonds are represented by lines
- Assume carbon atoms at the ends of lines and where they meet
- Assume enough C-H bonds to give each carbon atom four bonds (octet)
- Carbon and hydrogen atoms are only drawn at termini for aesthetics
- Draw heteroatoms and attached hydrogen atoms (N, O, P, Cl, Br, F, I, etc.)

(any atom that is not carbon)









HO C CH_3

Incorrect!

(Why?)

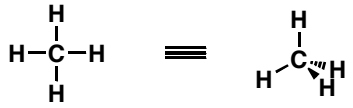
Don't forget about the implied hydrogen atoms!

Always show all lone pairs!
(helps with electron bookkeeping)

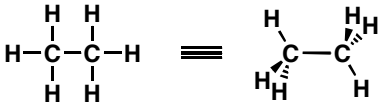
Representing Molecules: 3-D

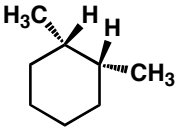
Lewis/Kekulé and Line-Angle structures don't tell the whole story!
Molecules are not flat - use dashes and wedges to show 3-D image

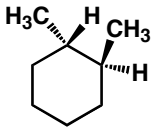
Governed by VSEPR



Line - in plane of paper
Dash - going into the paper
Wedge - coming out of the paper



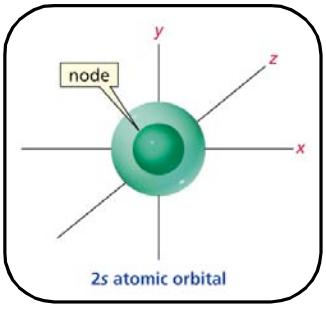


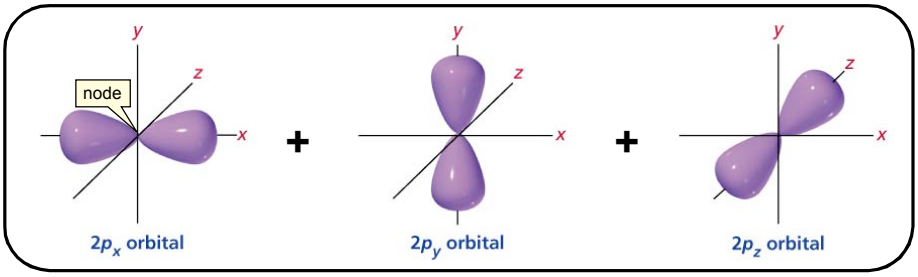


Same atoms, different spatial arrangement

Representing Molecules: Orbital Drawings I

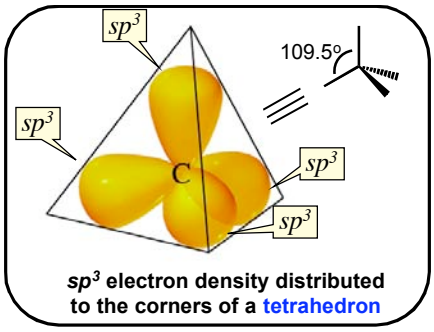
Atomic Orbitals



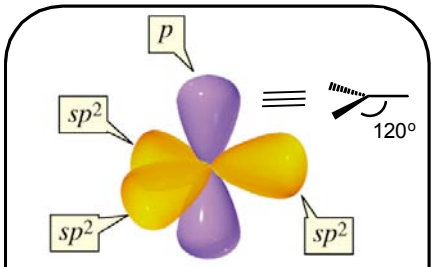


Representing Molecules: Orbital Drawings II

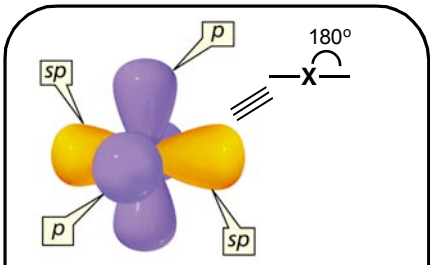
Hybrid Orbitals



sp^3 electron density distributed to the corners of a tetrahedron



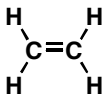
sp^2 electron density distributed to the corners of a triangle (trigonal planar)

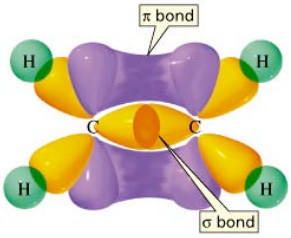


sp electron density distributed linearly

Representing Molecules: Orbital Drawings III

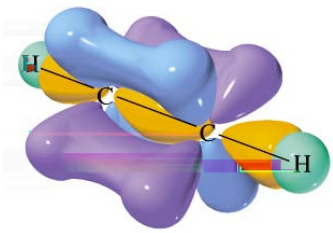
Ethylene

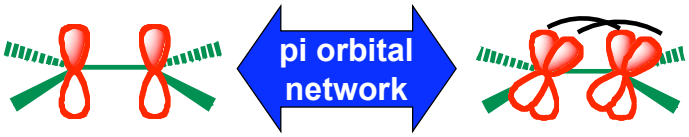




Acetylene

H–C≡C–H





Functional Groups

The atoms of organic molecules exist in common combinations

Each combination:

- unique chemical properties and reactivity
- behaves similarly in every organic molecule

10 million organic compounds exist!

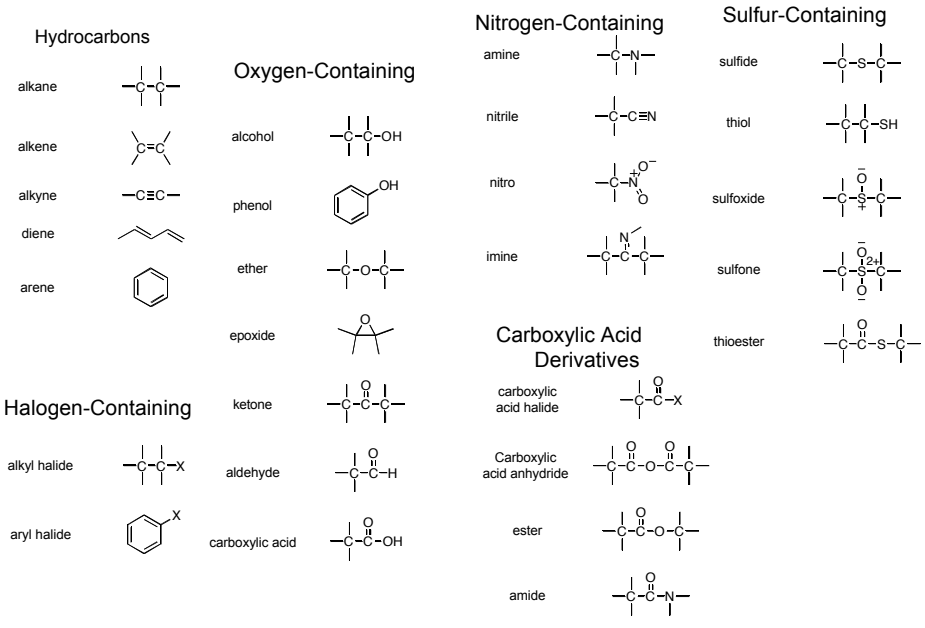
Predict how any one of those compounds reacts by analyzing its

"functional groups"

Functional Group - group of atoms with characteristic chemical behavior no matter what molecule it's in

Chemistry of every organic molecule, regardless of size or complexity, governed by functional groups

Functional Groups to Learn



On to Resonance . . .

- ✓ Organic Chemistry
- ✓ Relationship of Structure, Energy, and Reactivity
- ❑ Structure
  - ✓ Atoms
  - ✓ Bonding
    - ✓ How/Why Atoms Bond Together
    - ✓ Bonding Patterns
  - ✓ Representing molecules
    - ✓ Lewis and Kekule Structures
    - ✓ Line-angle Formula
    - ✓ 3-D
    - ✓ Orbital Drawings
  - ✓ Functional Groups
  - ❑ **Resonance**

Resonance

IF YOU DO NOT UNDERSTAND RESONANCE, YOU WILL NOT PASS 5.12!

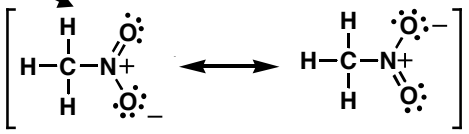
Resonance is like riding a bike. Once you learn, you never forget . . .

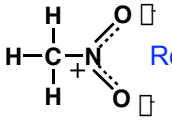
When one Lewis structure just isn't enough…

Lewis structure for CH_3NO_2 = 24 valence e^-

Resonance contributor

Resonance contributor





Resonance Hybrid

Electrons are DELOCALIZED

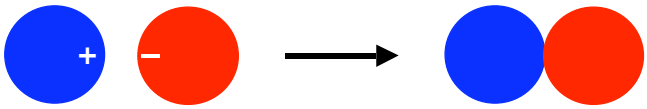
- A molecule can't always be accurately represented by one Lewis structure
- These molecules are weighted average, or hybrids, of two or more Lewis structures (electrons do not move to either one of the oxygen atoms or the other)

A Resonance Metaphor

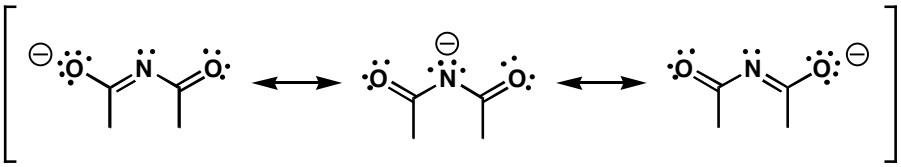
Figure removed due to copyright reasons.

Why is Resonance So *Very* Important?

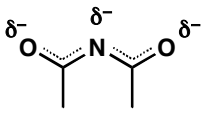
>95% of the reactions in 5.12 occur because of the attraction of one molecule containing a region of high electron density to a second molecule containing a region of low electron density



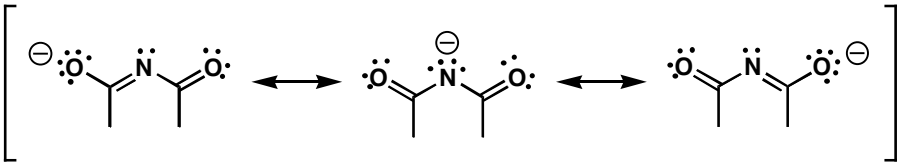
To predict how and when two molecules will react, need to be able to predict the regions of low and high electron density



Resonance hybrid
(lone pairs not depicted in resonance hybrids)



Tracking Changes in e Configuration



Need a way to keep track of the changes in electron configuration between resonance contributors

Curved Arrow Notation

Courtesy of Jeffrey S. Moore, Department of Chemistry, University of Illinois at Urbana-Champaign. Used with permission. Adapted by Kimberly Berkowski.