Welcome to OChem 1

Brent Iverson

At its heart - Organic Chemistry is the science of Carbon-containing molecules

Organic Chemistry is the study of carbon-containing molecules.

This class has two points.

The first point of the class is to understand the organic chemistry of living systems. We will teach you how to think about and understand the most amazing things on the planet!!

Water is essential for life, you will learn why water has such special properties.

You will learn the secret structural reason proteins, the most important molecular machines in our bodies, can support the chemistry of life.

You will learn why when you take Advil for pain, exactly half of what you take works, and the other half does nothing.

You will learn how toothpaste works.

You will learn how a single chlorofluorocarbon refrigerant molecule released into the atmosphere can destroy many, many ozone molecules, leading to an enlargement of the ozone hole.

You will learn how medicines like Benadryl, Seldane, and Lipitor work.

You will learn how Naloxone is an antidote for an opioid overdose.

You will learn why Magic Johnson is still alive, decades after contracting HIV.

You will learn how MRI scans work.

The second point of organic chemistry is the synthesis of complex molecules from simpler ones by making and breaking specific bonds.

You will learn how to understand movies of reaction mechanisms like alkene hydration.

You will learn reactions that once begun, will continue reacting such that each product molecule created starts a new reaction until all the starting material is used up.

You will learn reactions that can make antifreeze from vodka.

You will learn a reaction that can make nail polish remover from rubbing alcohol.

You will learn how to look at a molecule and accurately predict which atoms will react to make new bonds, and which bonds will break during reactions.

You will learn how to analyze a complex molecule’s structure so that you can predict ways to make it via multiple reactions starting with less complex starting molecules.

The ability to rationally synthesize new molecules changed human destiny and drives the economies of the world by enabling:

1. The synthesis of new drugs to cure disease and dramatically increase human life span
2. The development of lubricants and components for virtually all machines
3. The creation of new methods for integrated circuit production enabling faster computation
4. The creation of new materials for millions of uses including 3d printing and biodegradable plastics
5. The synthesis of new pigments for dyes, paints, cosmetics and digital displays
6. The synthesis of all synthetic clothing fibers
7. The production of highly refined and cleaner burning fuels
8. The production of rechargeable batteries
9. …to name just a FEW applications.

In other words, essentially everything that we associate with what makes modern life so incredible.

"You can't stop the waves, but you can learn to surf"

Jon Kabat-Zinn

"Everything should be made
as as possible but
not "

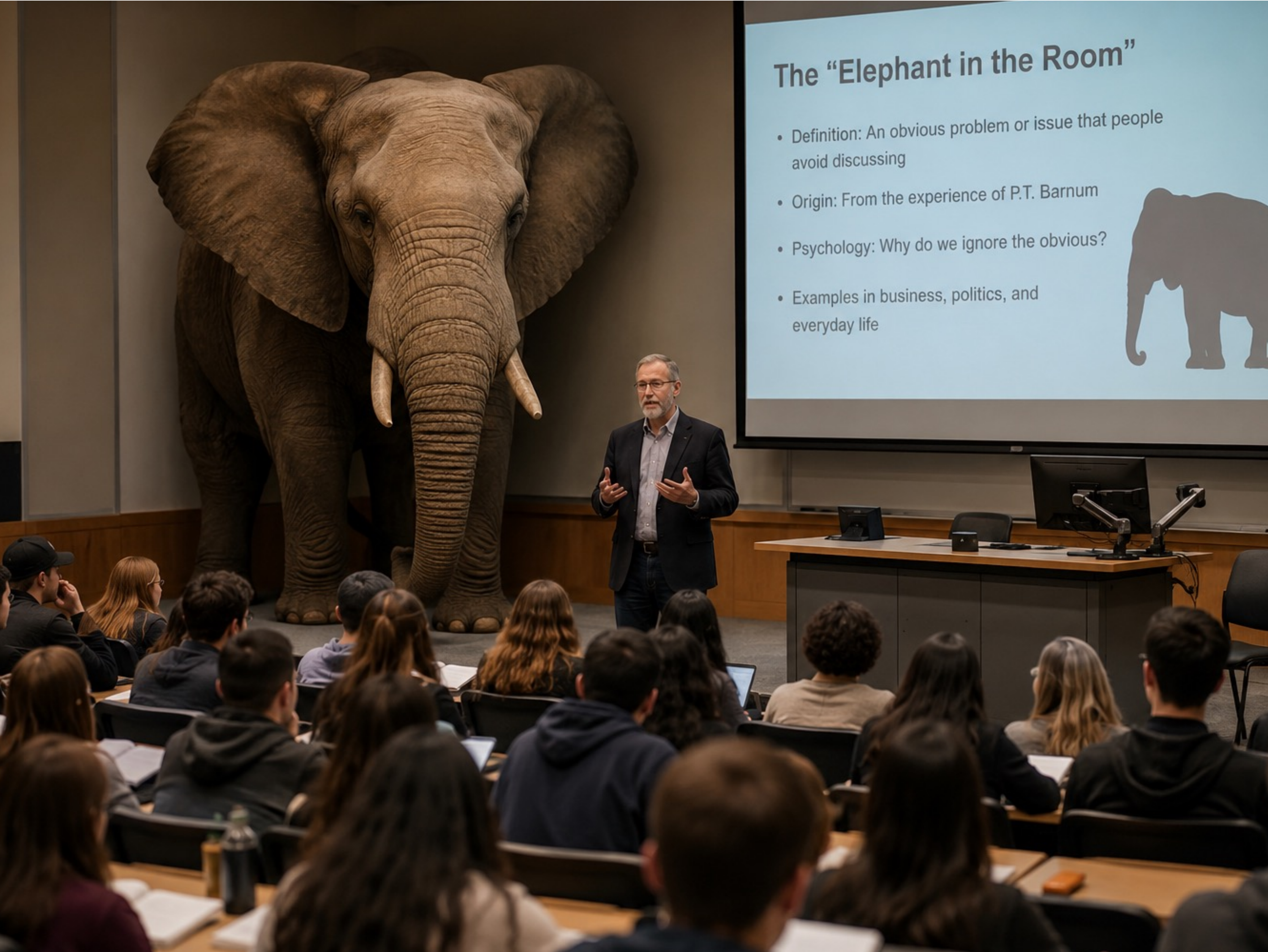
"The only real valuable
thing is "

"The most important thing is to remember the most important thing"

In this class:
The most important thing is

The most important question in Chemistry


Alkanes
Alkenes
Alkynes
Haloalkanes
Vicinal dihaloalkanes
Ketones and Aldehydes
Carboxylic Acids
Alcohols
Where Electrons Are
Mechanisms
Roadmaps
Stereochemistry
Regiochemistry
ROTD
NIRRS
Motive
Opportunity
Carbocation
Radical
Pi-ways
Golden Rules
Make a Bond
Break a Bond
Add a Proton
Take a Proton
Nucleophiles and Electrophiles
Charge Delocalization
Hyperconjugation
Steric strain
Angle and Torsional Strain
Epoxides
Vicinal Diols
Radical Chain
SN2 vs. E2
SN1 and E1
Anti-periplanar
Markovnikov
Zaitsev


The "Elephant in the Room"
• Definition: An obvious problem or issue that people avoid discussing
• Origin: From the experience of P.T. Barnum
• Psychology: Why do we ignore the obvious?
• Examples in business, politics, and everyday life

First Golden Rule of Chenistry:

Lewis Structures → when drawing a Lewis structure it is most helpful to remember

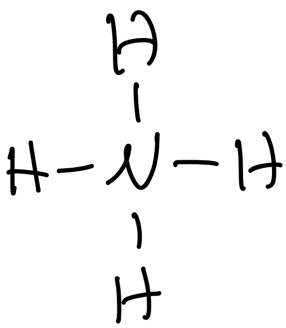
⇒ Make multiple bonds if that avoids unnecessary charges or unpaired electrons

CH_4

CH_2O

Formal Charge → Unequal number of protons and electrons around an atom

→ Always assign half of the electrons in a bond to each atom of the bond



N → atomic #7
so 7 protons

Much better way to calculate formal charge:

*A stepwise approach to perfect Lewis structures**

Step 1: Arrange atoms in space based on connectivity given in molecular formula.

Step 2: Add single bonds to all atoms that are connected to each other.

Step 3: Identify all carbon atoms without a filled valence shell. For each such carbon atom, look for an adjacent atom that is also without a filled valence and connect with one or two multiple bonds.

Step 4: Add lone pairs to fill all remaining unfilled valence shells.

Step 5: Add any formal charges as identified by the table presented during the first lecture.

*This works for all but molecules with a carbocation. Do not worry about those at this time.

Valence Electrons in Neutral Atoms:

H	C	N	O	F,Cl,Br,I
1	4	5	6	7

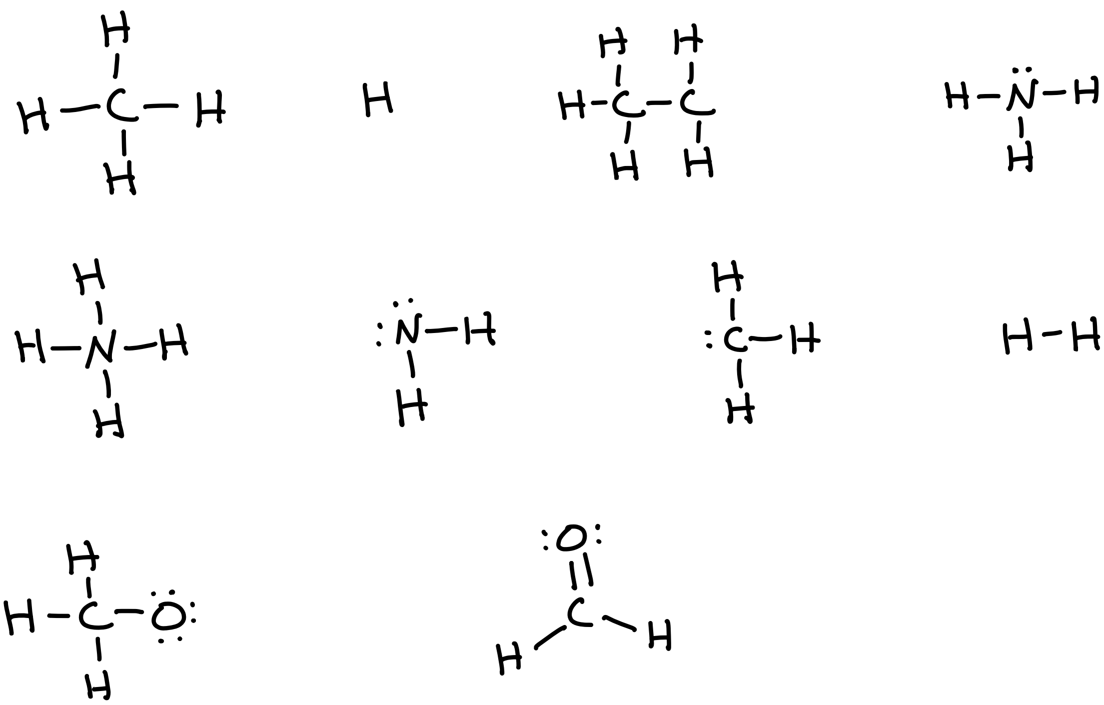
Formal Charge Identification:

		Neutral		Positive Charge		Negative Charge	
Atom	# electrons in the valence shell	Bonds	Lone Pairs	Bonds	Lone Pairs	Bonds	Lone Pairs
H	2	1	0	0	0	0	1 (rare)
C	8	4	0	3	0	3	1
N	8	3	1	4	0	2	2
O	8	2	2	3	1	1	3
F,Cl,Br,I	8	1	3	-	-	0	4

To draw a full Lewis structure, use the stepwise approach (see handout)

$(CH_3)_2CHCH_2NH_3$

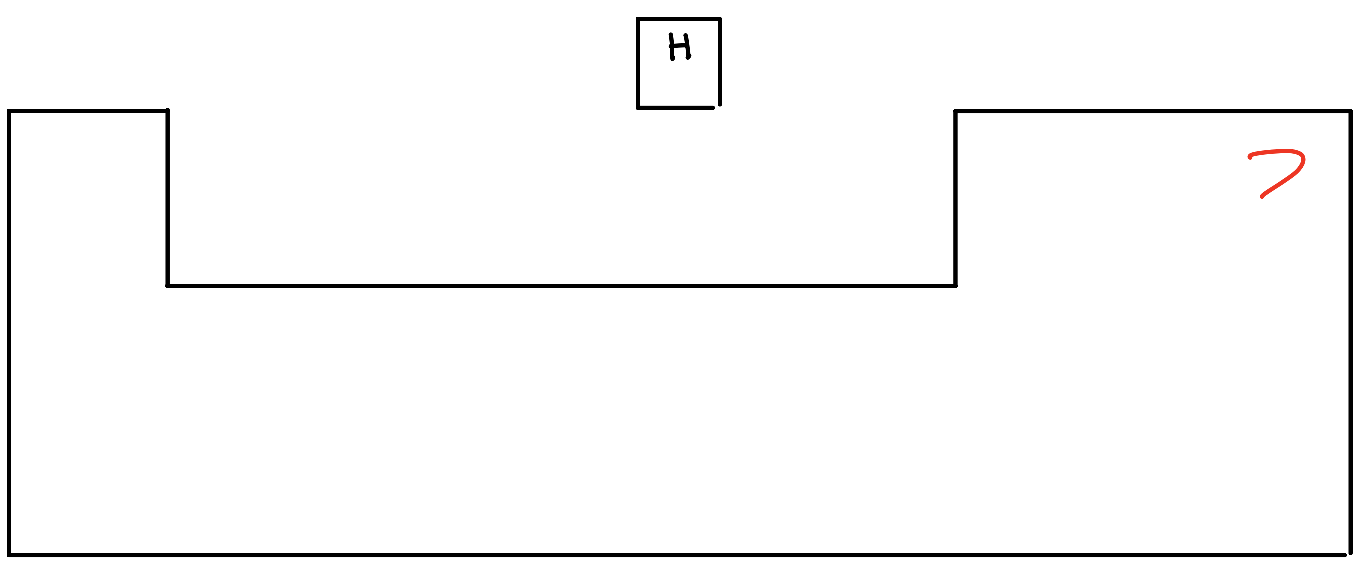
Formal Charge/Lewis Structure Practice:



Formal Charge →

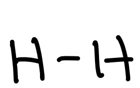
Theory →

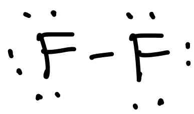
Linus Pauling ⟹

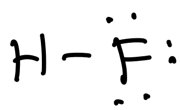


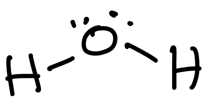
Periodic Table

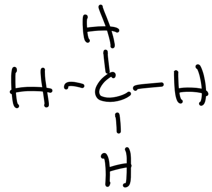
Electronegativity →











b.p

b.p.

<u>Organic Chemistry</u> is the study of carbon-containing molecules.

This class has two points.

The first point of the class is to understand the organic chemistry of living systems. We will teach you how to think about and understand the most amazing things on the planet!!

Water is essential for life, you will learn why water has such special properties.

You will learn the secret structural reason proteins, the most important molecular machines in our bodies, can support the chemistry of life.

You will learn why when you take Advil for pain, exactly half of what you take works, and the other half does nothing.

You will learn how toothpaste works.

You will learn how a single chlorofluorocarbon refrigerant molecule released into the atmosphere can destroy many, many ozone molecules, leading to an enlargement of the ozone hole.

You will learn how medicines like Benadryl, Seldane, and Lipitor work.

You will learn how Naloxone is an antidote for an opioid overdose.

You will learn why Magic Johnson is still alive, decades after contracting HIV.

You will learn how MRI scans work.

The second point of organic chemistry is the synthesis of complex molecules from simpler ones by making and breaking specific bonds.

You will learn how to understand movies of reaction mechanisms like alkene hydration.

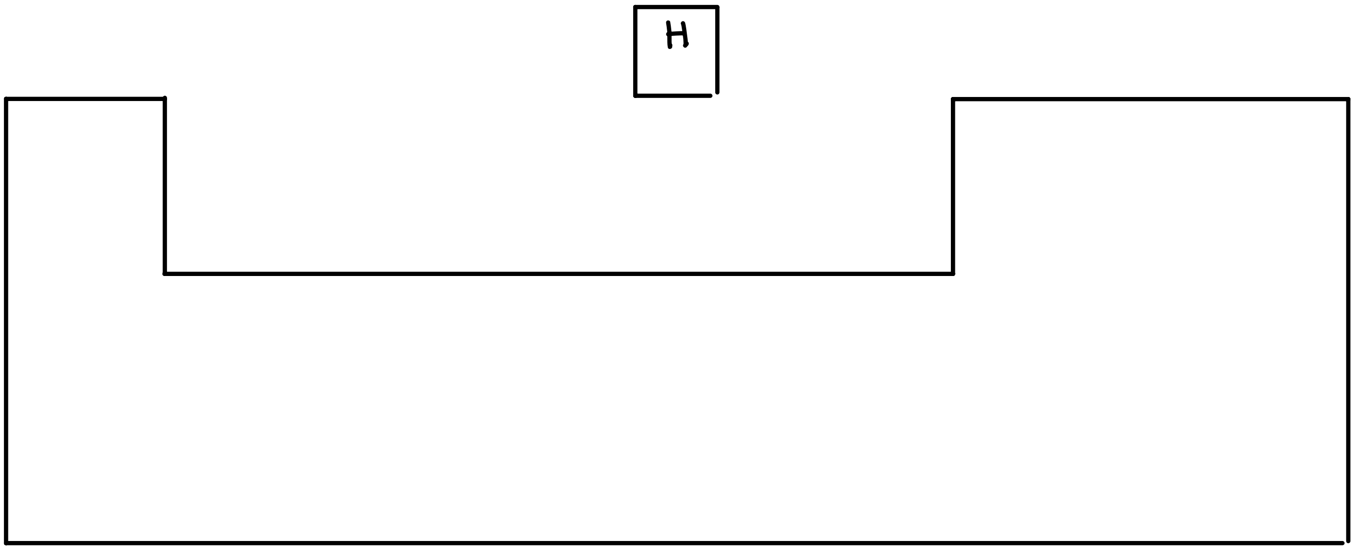
You will learn reactions that once begun, will continue reacting such that each product molecule created starts a new reaction until all the starting material is used up.

You will learn reactions that can make antifreeze from vodka.

You will learn a reaction that can make nail polish remover from rubbing alcohol.

You will learn how to look at a molecule and accurately predict which atoms will react to make new bonds, and which bonds will break during reactions.

You will learn how to analyze a complex molecule's structure so that you can predict ways to make it via multiple reactions starting with less complex starting molecules.

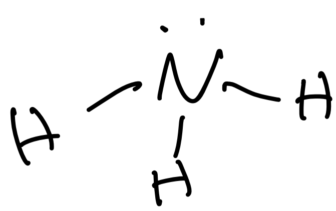


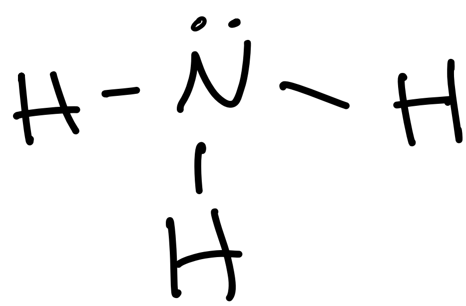
1A	2A	3B	4B	5B	6B	7B	8B			1B	2B	3A	4A	5A	6A	7A
								H 2.1								
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5
Cs 0.7	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Tl 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2

- <1.0
- 1.0 – 1.4
- 1.5 – 1.9
- 2.0 – 2.4
- 2.5 – 2.9
- 3.0 – 4.0

Formal Charge

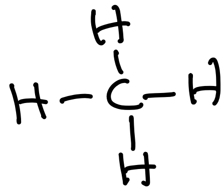
Polar Covalent Bonds

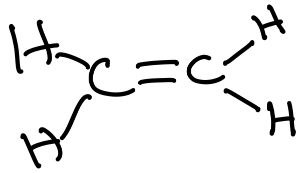


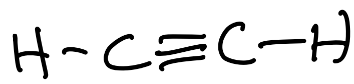


Shapes → VSEPR

↳ 1^{st} approximation →







Putting it all together: Molecular Dipoles

The good news: Lewis structures
accurately
describe
molecules
(most of
the time)

However,

Contributing Structures $\Rightarrow$

Contributing Structures ⇒

⇒ Must be reasonable Lewis structures

→ when deciding which contributing structure makes the major contribution rank according to the following

Classic Example

Solutions to the Schrodinger equation – atomic orbitals

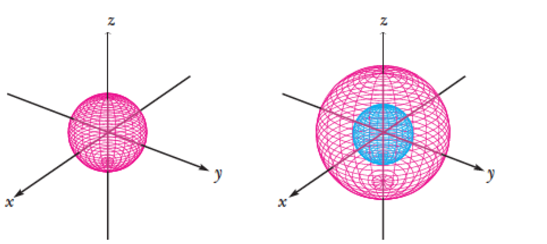
$$\psi_{n\ell m}(r,\theta,\phi) = \sqrt{\left(\frac{2}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]}} e^{-r/na_0} \left(\frac{2r}{na_0}\right)^{\ell} L_{n-\ell-1}^{2\ell+1}\left(\frac{2r}{na_0}\right) \cdot Y_\ell^m(\theta,\phi)$$

where:

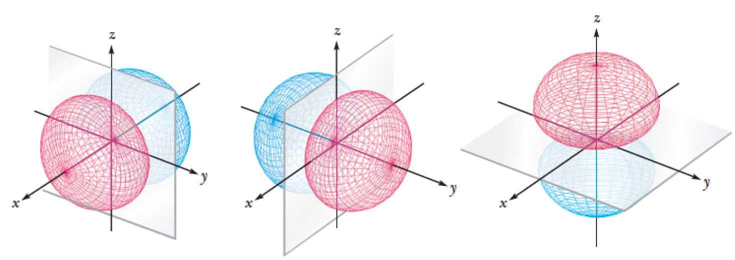
- $a_0 = \dfrac{4\pi\varepsilon_0 \hbar^2}{m_e e^2}$ is the Bohr radius,
- $L_{n-\ell-1}^{2\ell+1}(\cdots)$ are the generalized Laguerre polynomials of degree $n-\ell-1$.
- n, ℓ, m are the principal, azimuthal, and magnetic quantum numbers respectively: which take the values:

$$n = 1, 2, 3, \ldots$$
$$\ell = 0, 1, 2, \ldots, n-1$$
$$m = -\ell, \ldots, \ell$$

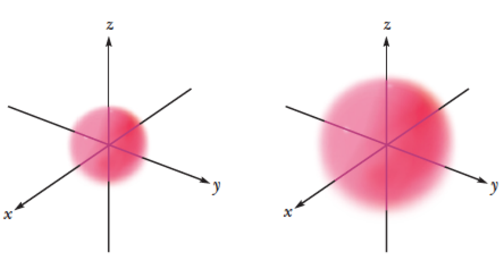
Ψ_{1s} Ψ_{2s} Ψ_{2px} Ψ_{2py} Ψ_{2pz}



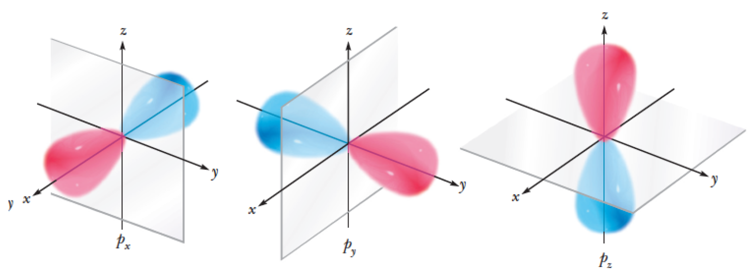
(a) 1*s* and 2*s* orbitals computed using the Schrödinger equation



(a) 2*p* Orbitals computed using the Schrödinger equation



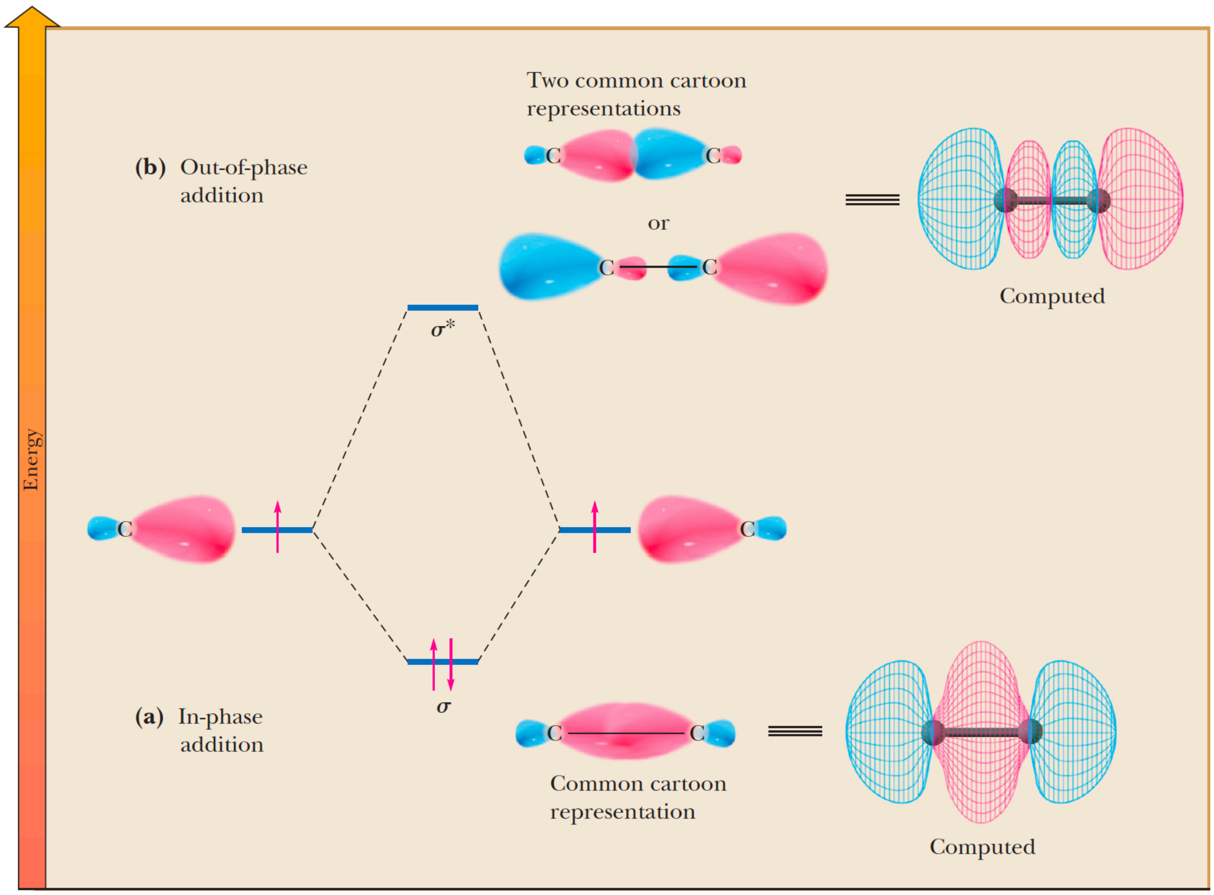
(b) Cartoon representations of 1*s* and 2*s* orbitals



Nodal plane = *yz* Nodal plane = *xz* Nodal plane = *xy*

Figure 1.18

Molecular orbital mixing diagram for the creation of any C—C σ bond. (a) In-phase addition of two C hybrid orbitals (albeit sp^3, sp^2, or sp orbital) forms a σ orbital that is lower in energy than the two starting orbitals. When the resulting orbital is populated with two electrons, a σ bond results. (b) Addition of the orbitals in an out-of-phase manner (meanin reversing the phasing of one of the starting orbitals) leads to an antibonding σ^* orbital.



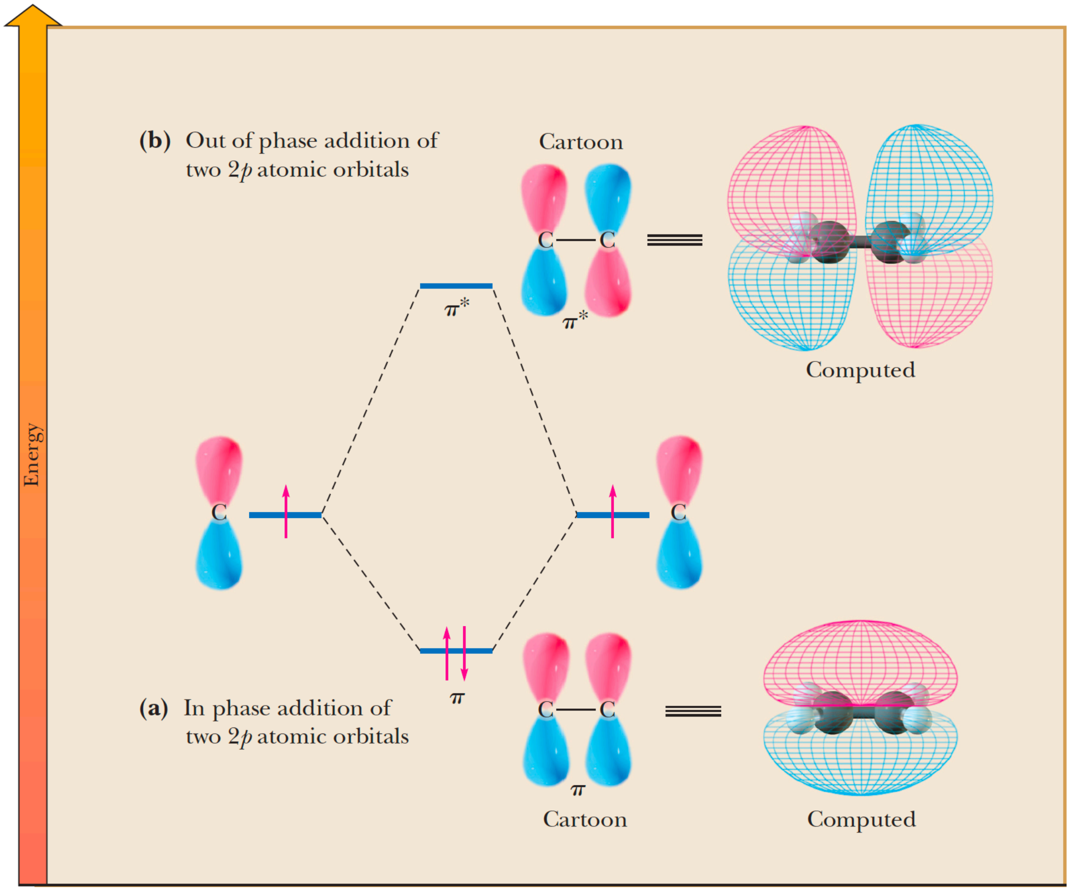
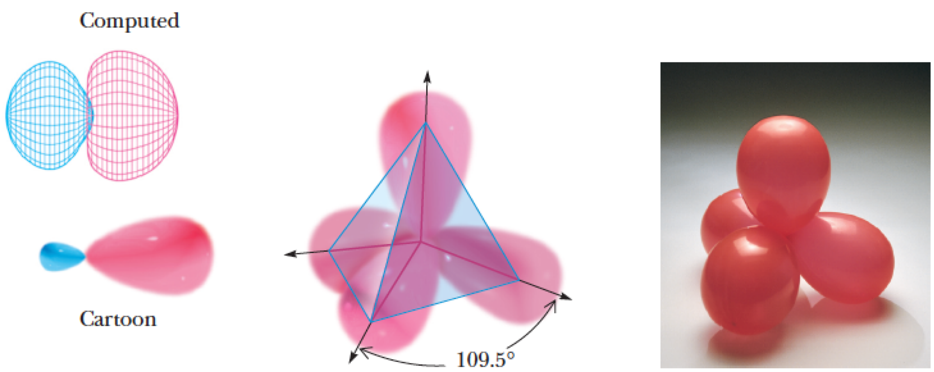


Figure 1.21 Molecular orbital mixing diagram for the creation of any C—C π bond. (a) Addition of two p atomic orbitals in-phase leads to a π orbital that is lower in energy than the two separate starting orbitals. When populated with two electrons the π orbital gives a π bond. (b) Addition of the p orbitals in an out-of-phase manner (meaning a reversal of phasing in one of the starting orbitals) leads to a π^* orbital. Population of this orbital with one or two electrons leads to weakening or cleavage of the π bond respectively.

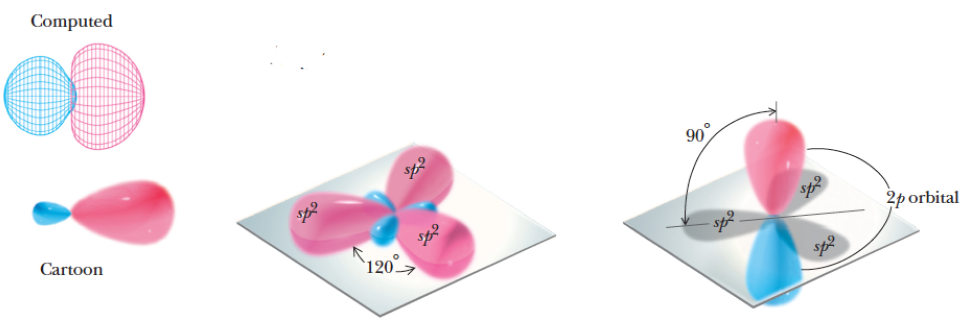
Hybridization – Valence Bond Approach to bonding

sp^3 $(\Psi_{2s} + \Psi_{2px} + \Psi_{2py} + \Psi_{2pz})$



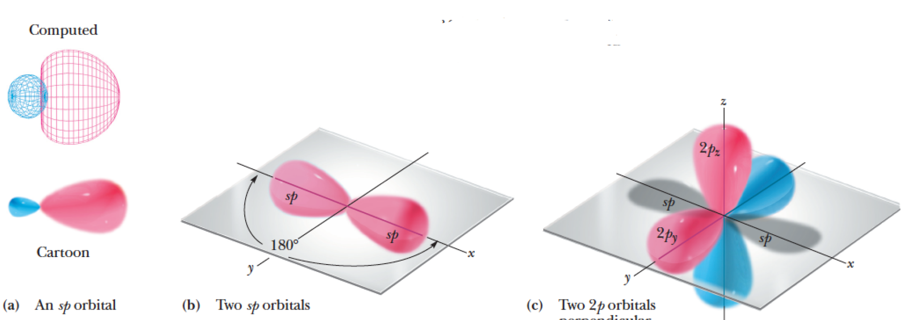
(a) An sp^3 orbital (b) Four sp^3 orbitals in a tetrahedral arrangement (c)

sp^2 $(\Psi_{2s} + \Psi_{2px} + \Psi_{2py}) + \Psi_{2pz}$



(a) An sp^2 orbital (b) Three sp^2 orbitals (c) A $2p$ orbital perpendicular to three sp^2 orbitals.

sp $(\Psi_{2s} + \Psi_{2px}) + \Psi_{2py} + \Psi_{2pz}$



(a) An sp orbital (b) Two sp orbitals (c) Two $2p$ orbitals perpendicular to the sp hybrid orbitals