Introduction to Organic Chemistry

HSSP 2010

Lecture 1

Slides modified from MIT 5.12 Organic Chemistry lecture notes, Spring 2007

Organic chemistry

What: The study of carbon-containing compounds

Why: Pervasive in nature

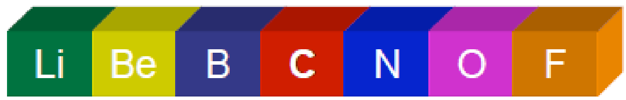
Chemical foundation of biology

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

How: Examine structure and analyze how it governs reactivity

What: Carbon-containing compounds

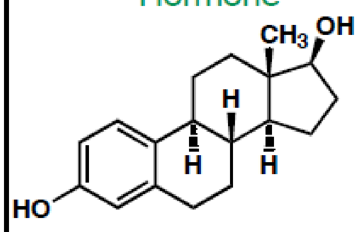
Middle of second row



Can neither accept or give up electrons easily

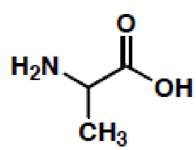
Share e^- with other carbon atoms - incredible structure diversity!

Hormone



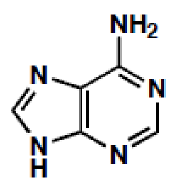
Estradiol

Amino acid



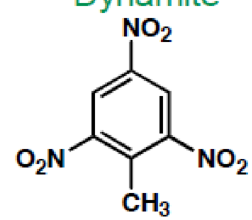
Alanine

DNA base

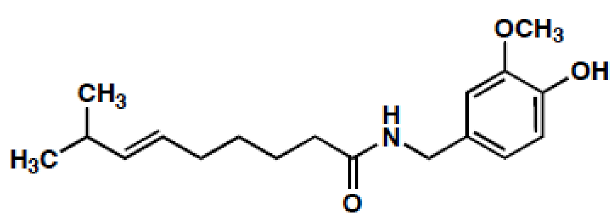


Adenine

Dynamite

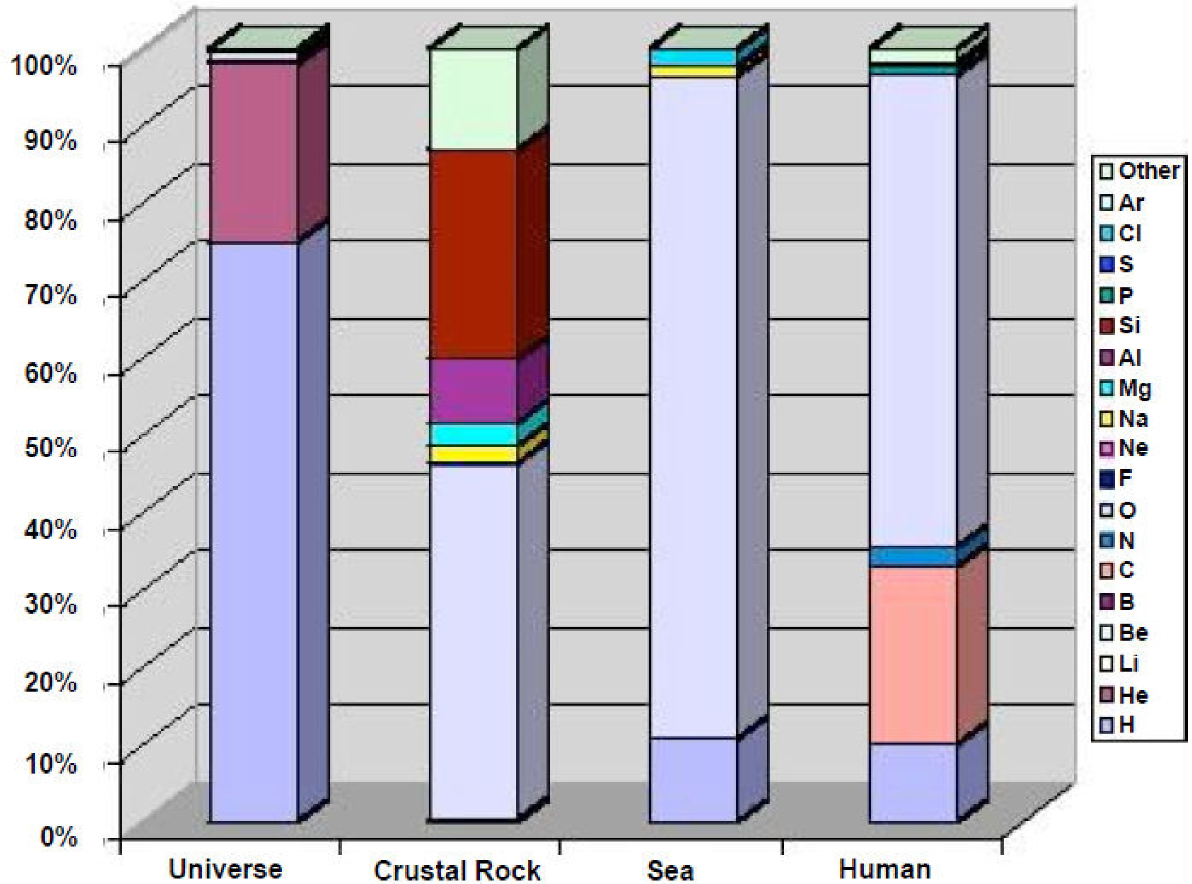


TNT



Capsaicin (peppers)

Why: Life is based on organic compounds



How: structure and reactivity

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

Reactivity - potential of structure to undergo chemical change

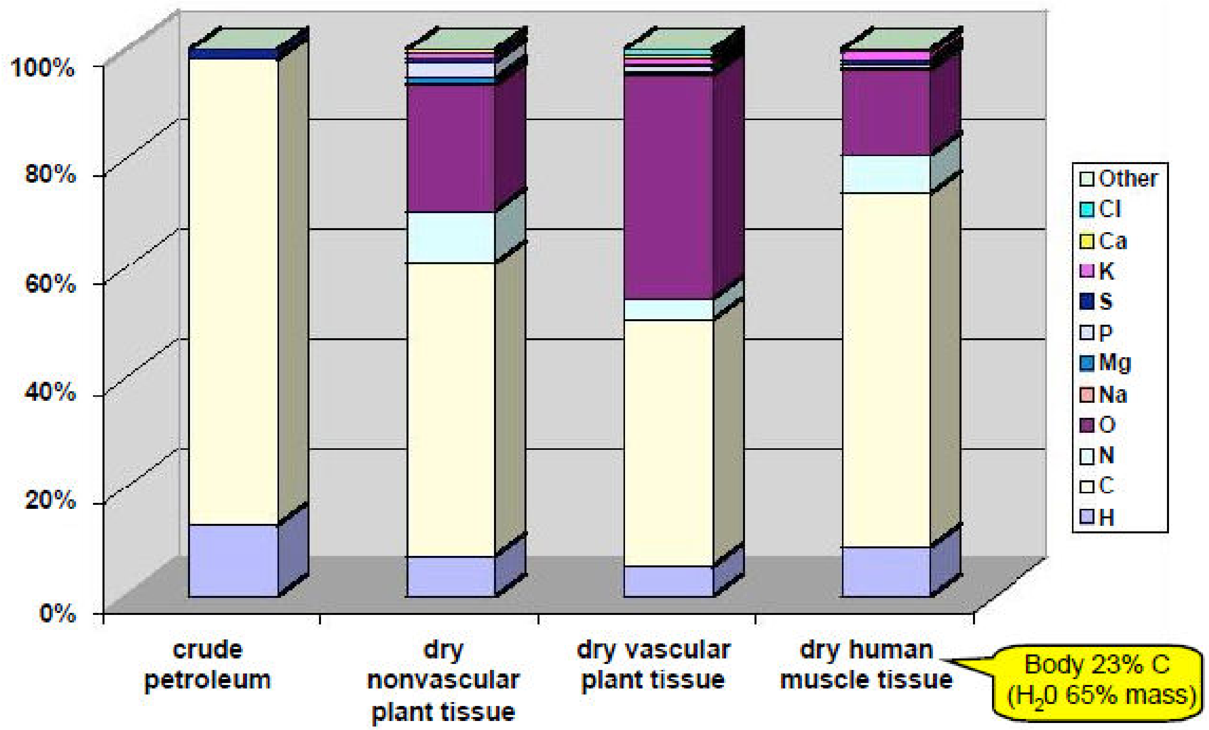
If likely - **reactive** (**unstable**)
If unlikely - **unreactive** (**stable**)

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

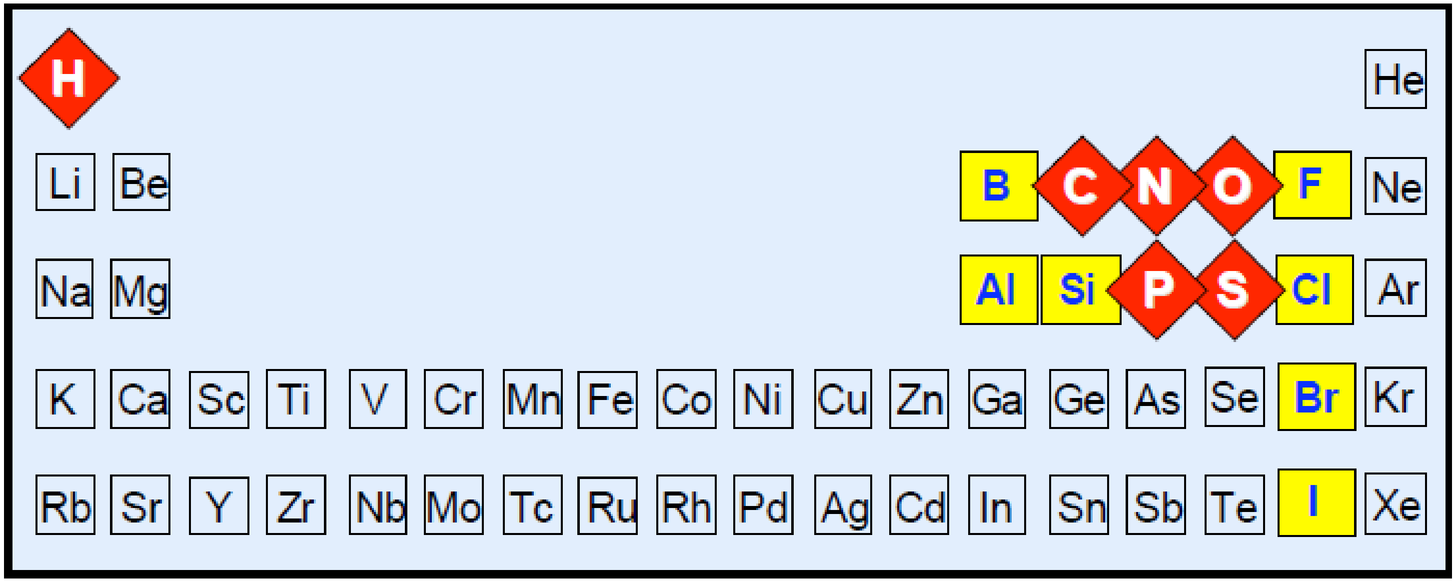
Atoms of organic molecules

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)

Main atoms in organic chemistry



Background review

Chemical bonding

WHY?

Atoms bond together because the resulting molecule is more stable (has less energy) than the individual atoms

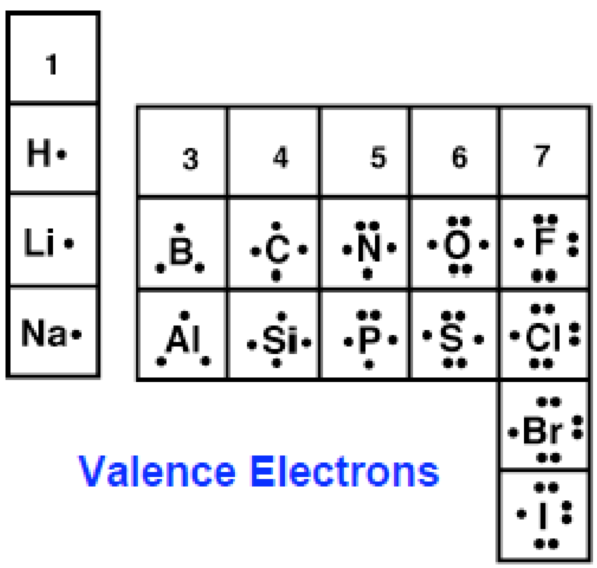
Making bonds - energy is released
Breaking bonds - energy is absorbed

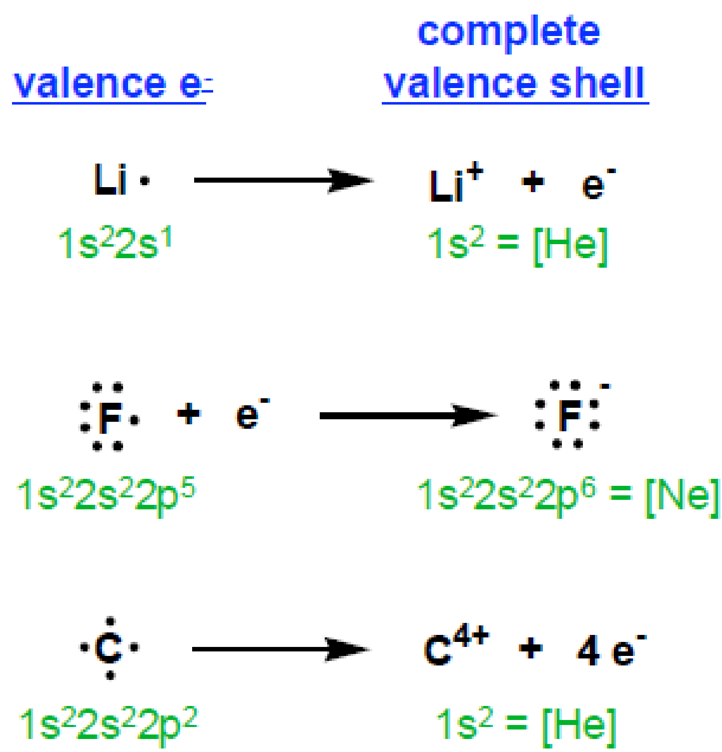
HOW?

Releasing, accepting, or sharing electrons to gain a valence shell octet

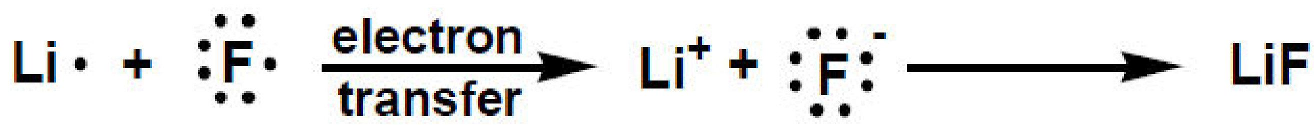
Ionic, covalent, polar covalent

Obtaining valence shell octet





Ionic bonding



Bond Energy ~138 kcal/mol

H 2.2							He
Li 1.0	Be 1.6	B 2.0	C 2.6	N 3.0	O 3.4	F 4.0	Ne
Na 0.93	Mg 1.3	Al 1.6	Si 1.9	P 2.2	S 2.6	Cl 3.2	Ar
K 0.82	Ca 1.3	Ga 1.6	Ge 2.0	As 2.2	Se 2.6	Br 3.0	Kr
Rb 0.82	Sr 0.95	In 1.8	Sn 2.0	Sb 2.1	Te 2.1	I 2.7	Xe
Cs 0.79	Ba 0.89	Tl 2.0	Pb 2.3	Bi 2.0	Po 2.0	At	Rn

Electronegativity Trends

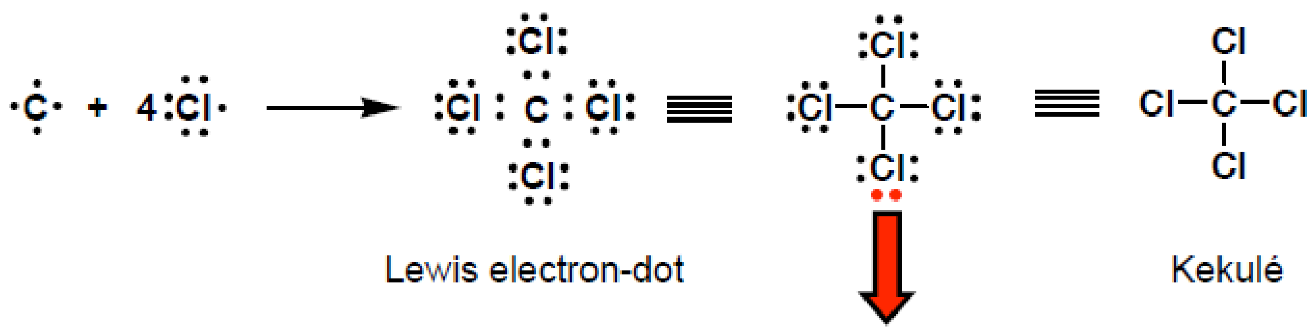
- Δ electronegativity > 2
- between metal and nonmetal
- electron transfer, not sharing

Electrostatic attraction

Covalent bonding

“electron sharing”

between atoms (2 nonmetals) of similar electronegativity

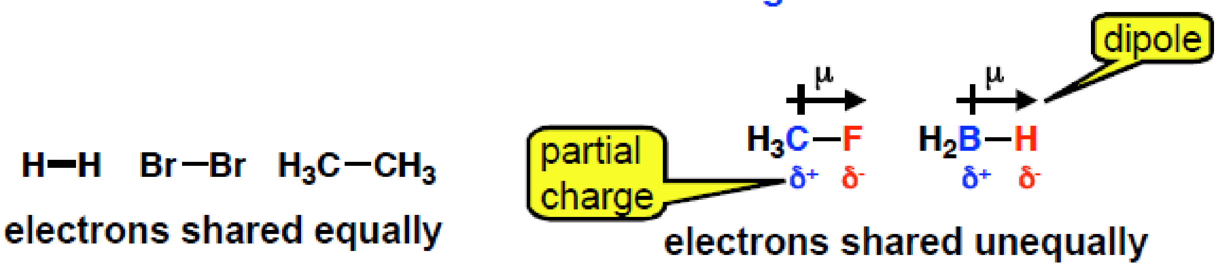


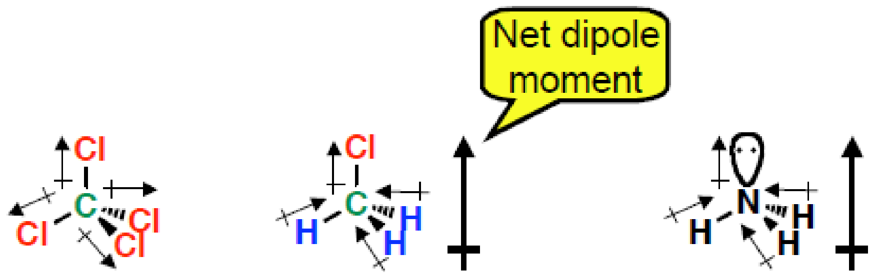
(unshared or non-bonding electron pair)

1 dot = 1 electron
1 bond = 2 electrons

Polar covalent bonding

unequal sharing of electrons between the two atoms in a bond due to a difference in their electronegativities





	EN
B	1.6
H	2.2
C	2.6
Cl	3.2
F	4.0

Electronegativity (EN) - ability of atom to attract the shared electrons in a covalent bond

Inductive effect - shifting of electrons in response to the EN of nearby atoms

Describing covalent bonds

Lewis Structures: represent <u>what</u> covalent bonds are present in a molecule, electron bookkeeping

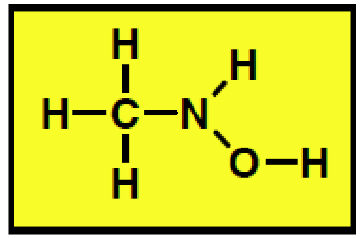
VSEPR Theory: predict relative location of covalent bonds and lone pairs; molecular <u>shape</u>

Lewis dot structures

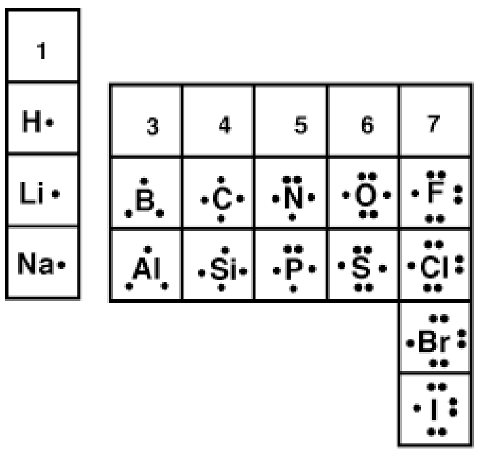
Example: CH_3NHOH

Step 1. Draw the molecular skeleton; connect the atoms with covalent bonds

From periodic table:
H wants 1 bond
C wants 4 bonds
N wants 3 bonds
O wants 2 bonds



Step 2. Count the total valence electrons



5H x 1 = 5

1C x 4 = 4

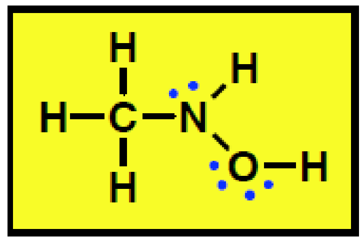
1N x 5 = 5

1O x 6 = 6

Valence e^- = 20

Lewis dot structures

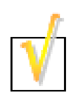
Step 3. Add electrons to each atom to satisfy the octet rule (H requires 2 e^-)



Step 4. Count the e^- in the trial structure and compare to that from Step 2.

20

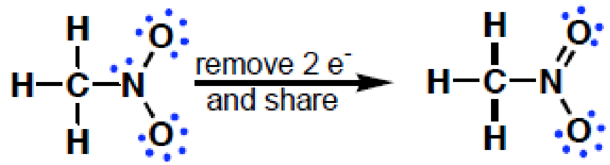
If the numbers are the same, the Lewis e^- configuration is satisfactory (there may be more than one satisfactory structure - we'll discuss this more during class)



Lewis structures & formal charge

Formal charge - expresses surplus and shortage of e^- localized on individual atoms

Example: CH_3NO_2 (24 valence e^-)



Trial structure
26 valence e^- (need 24)

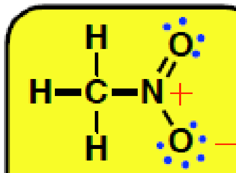
Some of these atoms bear extra e^-
Others are e^- deficient

Remember: 

Must determine the FORMAL CHARGE of each atom in a valid Lewis structure:

Formal charge = (valence e^-) - (nonbonding e^-) - 1/2 (shared e^-)

Formal charges:
C: 4 - 0 - 4 = 0
N: 5 - 0 - 4 = +1
O: 6 - 4 - 2 = 0
O: 6 - 6 - 1 = -1



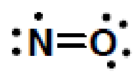
Net charge = 0

Exceptions to the octet rule

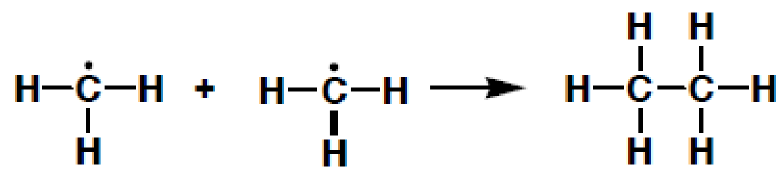
Compounds with a deficiency of valence electrons

(unusually reactive and readily undergo reactions to gain complete octets)

1. Odd number of electrons



Nitric oxide



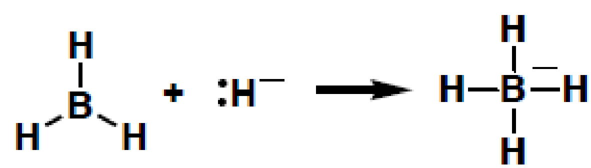
Methyl radical

Ethane

2. Early second-row elements

H−Be−H

Beryllium hydride

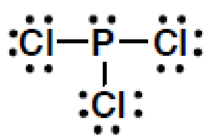
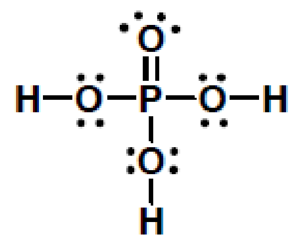
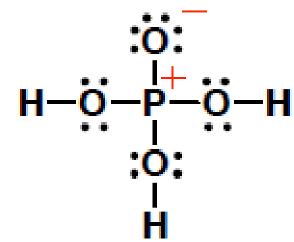
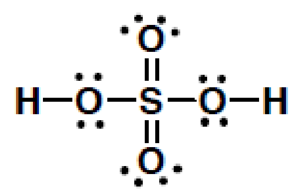
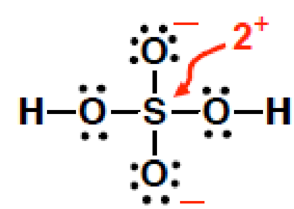


Borane

Borohydride

Exceptions to the octet rule

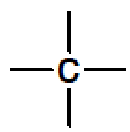
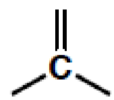
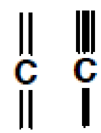
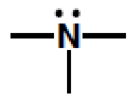
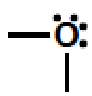
Compounds beyond the second row may have a "valence shell expansion" due to the availability of 3d orbitals

Obeys Octet Rule	Expanded Valence	Dipolar Form (obeys octet)
		
Phosphorus trichloride	Phosphoric acid	
		
Hydrogen disulfide	Sulfuric acid	

Bonding patterns

- All atoms have particular bonding patterns that are dependent on the atom's formal charge.
- All of the important bonding patterns in organic chemistry are contained on the following three slides.
- If you are familiar with these bonding patterns, predicting Lewis structures becomes a much simpler task!

Bonding patterns

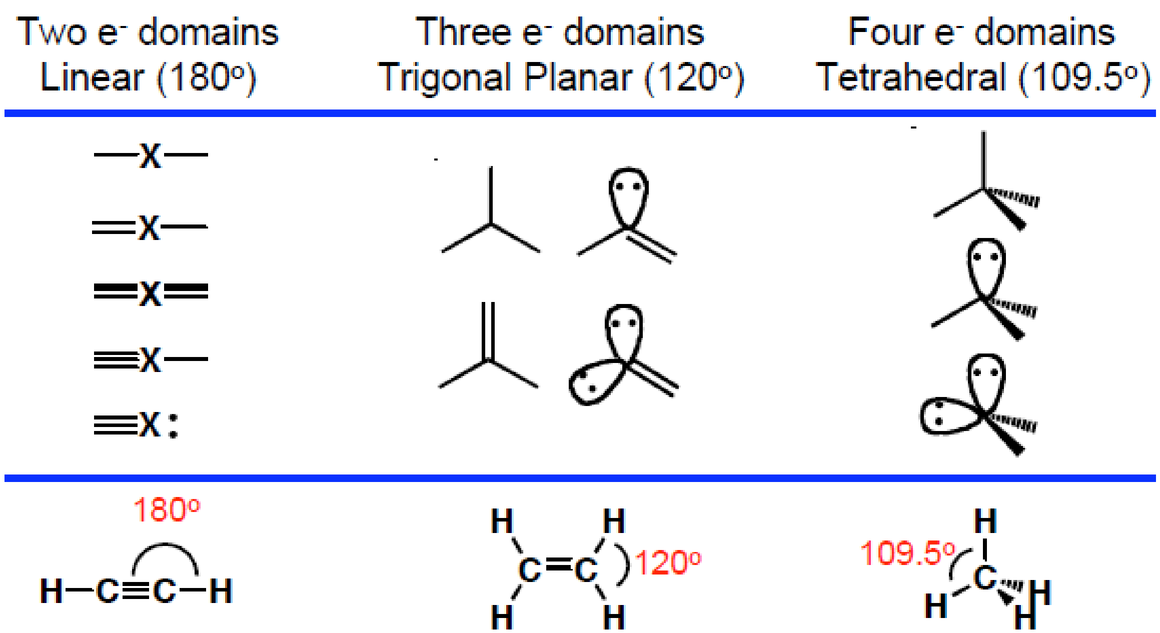
	# Electron Domains				
	4	3	2	1	0
H					
C					
N					
O					
F					

While Lewis structures tell you WHAT covalent bonds are present in molecule, VSEPR theory tells you WHERE these bonds are located in relation to one another . . .

VSEPR theory: molecular geometry

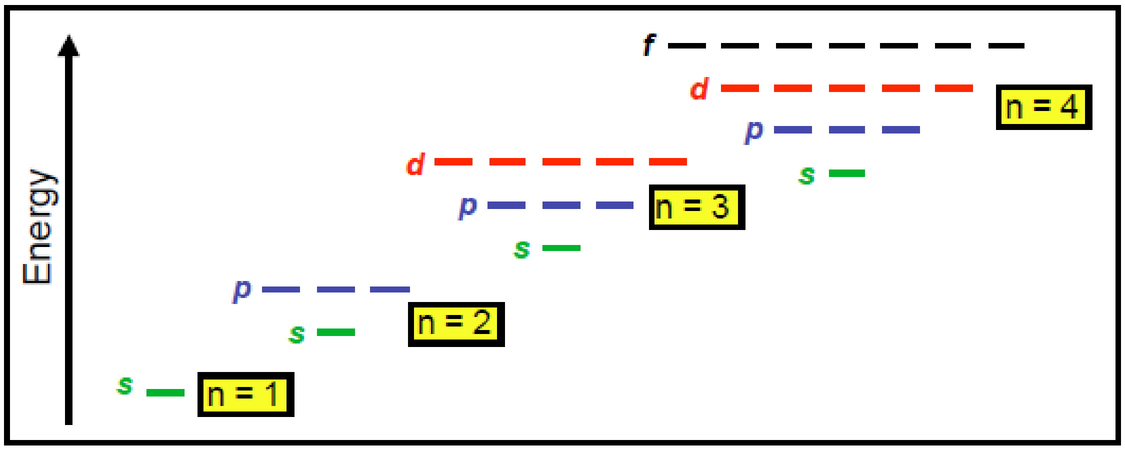
Valence Shell Electron Pair Repulsion Theory (VSEPR)

Electrons repel each other!
Therefore, lone pairs and bonds want to be as far apart as possible.



Atomic orbitals

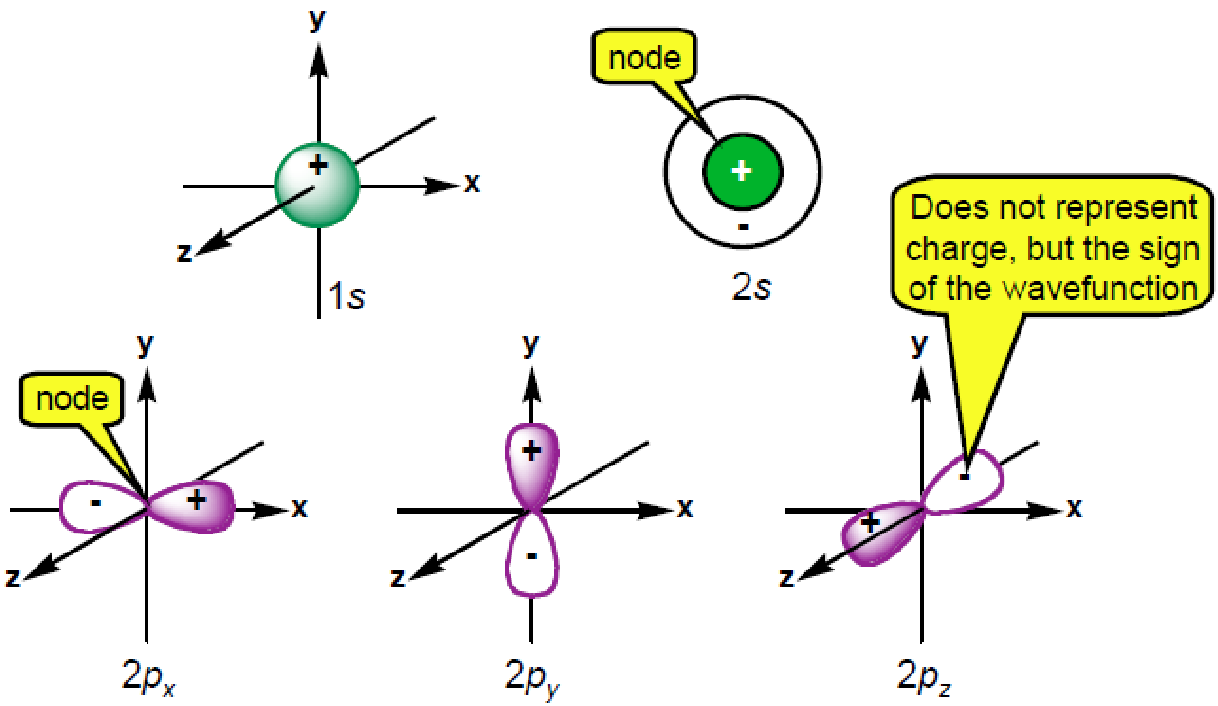
Describes the volume of space where an electron is most likely to be found



Atomic orbitals are described by four quantum numbers

1. Principle, shell (*n*), - orbital energy, size
2. Azimuthal, subshell (*l*), - orbital shape (*s*, *p*, *d*, *f*)
3. Magnetic (m_l)- orbital direction (p_x, p_y, p_z)
4. Spin (m_s) - +1/2, -1/2

Atomic orbital shape



s orbitals - spherical, e- held close to nucleus, one sign

p orbitals - two lobes with opposite signs, e- further from the nucleus,node

node - region of space with zero electron density

Electron configuration

Which orbitals contain electrons? How many electrons does each orbital contain?

Aufbau principle - the lowest energy orbitals fill up first (1*s*, 2*s*, 2*p*, 3*s*, 3*p*, 4*s*, 3*d*, etc.)

Pauli exclusion principle - only two electrons can occupy each orbital, and they must be of opposite spin

Hund's rule - if two or more orbitals of equal energy are available, one e- occupies each will their spins parallel until all orbitals are half-full

Atom	Name of element	Atomic number	1*s*	2*s*	2p_x	2p_y	2p_z	3*s*
H	Hydrogen	1	↑					
He	Helium	2	↑↓					
Li	Lithium	3	↑↓	↑				
Be	Beryllium	4	↑↓	↑↓				
B	Boron	5	↑↓	↑↓	↑			
C	Carbon	6	↑↓	↑↓	↑	↑		
N	Nitrogen	7	↑↓	↑↓	↑	↑	↑	
O	Oxygen	8	↑↓	↑↓	↑↓	↑	↑	
F	Fluorine	9	↑↓	↑↓	↑↓	↑↓	↑	
Ne	Neon	10	↑↓	↑↓	↑↓	↑↓	↑↓	
Na	Sodium	11	↑↓	↑↓	↑↓	↑↓	↑↓	↑