CHEM 109A
Organic Chemistry

Wait Lists and Add code requests:
Got you emails, working on it!

Questions? (non chemistry)
Chika Anyiwo, undergraduate advisor
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CHEM 109A
Organic Chemistry

Questions? (chemistry!)
CLAS tutor for this 109A course
Timothy Ngo: txngo@umail.ucsb.edu
Sign up!

CHEM 109A

Organic Chemistry

https://labs.chem.ucsb.edu/zakarian/armen/courses.html

Chapter 1
Electronic Structure and bonding

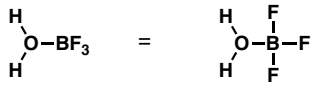
Ch. 1: Important topics/concepts

Covalent Bonds: polar, or nonpolar (electronegativity)

compare polarity of bonds, such as H-C vs H-N vs H-O vs H-F

Structures: Lewis structures (Kekule, condensed, skeletal)

properly placing lone pairs of e, formal charges



Lone pairs?
Formal charges?

condensed skeletal Lewis

Bonds: σ and π bonds (single bonds, double bonds, triple bonds)

σ formed by orbital overlap, s+s, s+p, p+s, or hybridized

π formed by overlap between p orbitals

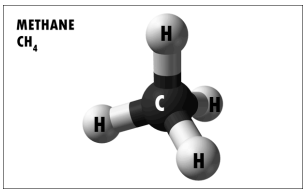
double bond = 1 σ bond + 1 π bond

triple bond = 1 σ bond + 2 π bonds

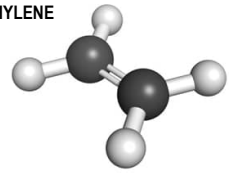
Ch. 1: Important topics/concepts

Hybrid orbitals: **s and p orbitals mix to form new hybrid orbitals**
(comes from valence-shell electron-pair repulsion (VSEPR) theory
explains geometry of CH_4 and many other molecules

Geometry (shape of molecules):
CH_4: tetrahedral, four *sp*^{3} orbitals, bond angle 109°,
$H_2C{=}CH_2$, ethylene, three *sp*^{2} orbitals, one *p* orbital, bond angle ~120°
HC≡CH, acetylene, two sp bonds, 2 p orbitals, bond angle 180°
Bond length and strength: shorter bonds are stronger.



ETHYLENE



ACETYLENE

The Distribution of Electrons in an Atom

quantum numbers

Table 1.1 Distribution of Electrons in the First Four Shells

	First shell	Second shell	Third shell	Fourth shell
Atomic orbitals	*s*	*s, p*	*s, p, d*	*s, p, d, f*
Number of atomic orbitals	1	1, 3	1, 3, 5	1, 3, 5, 7
Maximum number of electrons	2	8	18	32

n

l

m_l

2 e per orbital

- The first shell is closest to the nucleus.
- The closer the atomic orbital is to the nucleus, the lower its energy.
- Within a shell, *s* lower in energy than *p*.

The Distribution of Electrons in an Atom

quantum numbers

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n				
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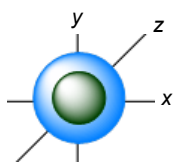
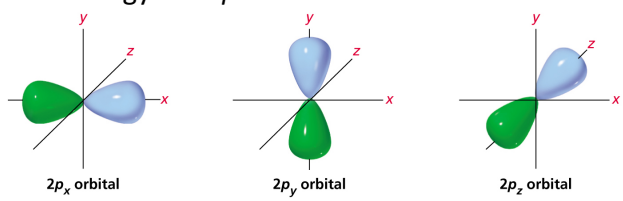
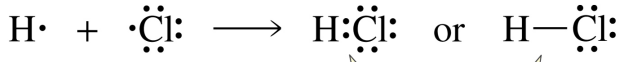


2s orbital, presents only one phase for overlap



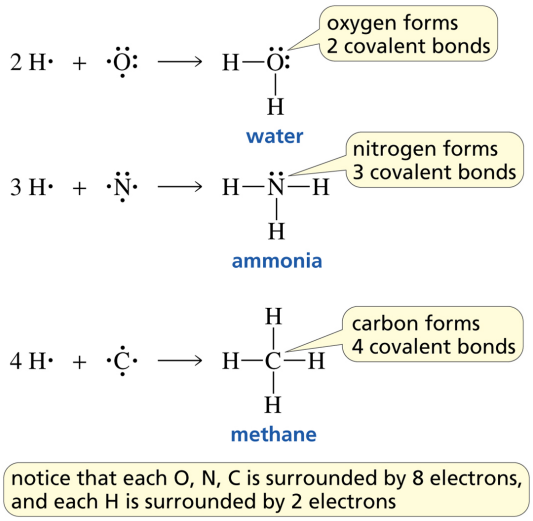
lobes with opposite phases

Achieving a Filled Outer Shell by Sharing Electrons



H is surrounded by 2 electrons
Cl is surrounded by 8 electrons

How Many Bonds Does an Atom Form?



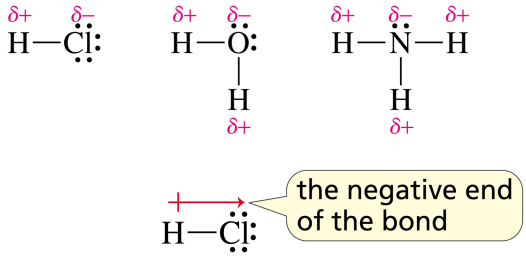
notice that each O, N, C is surrounded by 8 electrons, and each H is surrounded by 2 electrons

Nonpolar and Polar Covalent Bonds

Nonpolar covalent bond = bonded atoms are the same or have similar electronegativities.

H—H F—F C—C C—H

Polar covalent bond = bonded atoms have different electronegativities.



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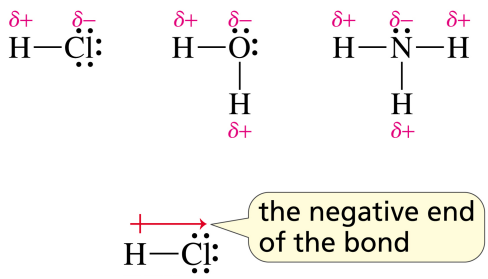

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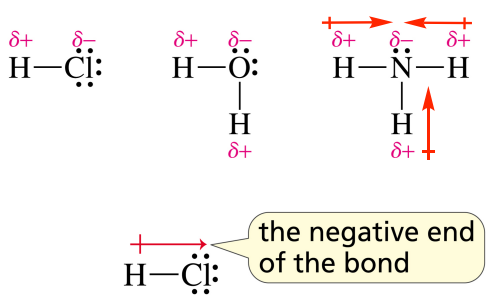


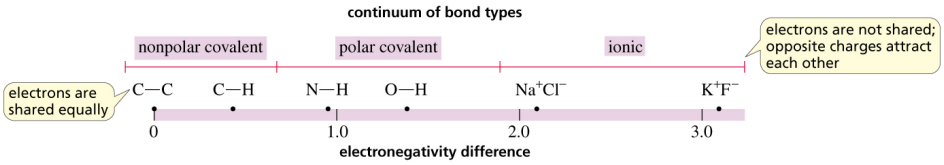
ELECTRONEGATIVITY OF ELEMENTS

Electronegativity increases

Period																		
1	H 2.20																	He
2	Li 0.98	Be 1.57											B 2.04	C 2.55	N 3.04	O 3.44	F 3.98	Ne
3	Na 0.93	Mg 1.31											Al 1.61	Si 1.90	P 2.19	S 2.58	Cl 3.16	Ar
4	K 0.82	Ca 1.00	Sc 1.36	Ti 1.54	V 1.63	Cr 1.66	Mn 1.55	Fe 1.83	Co 1.88	Ni 1.91	Cu 1.90	Zn 1.65	Ga 1.81	Ge 2.01	As 2.18	Se 2.55	Br 2.96	Kr 3.00
5	Rb 0.82	Sr 0.95	Y 1.22	Zr 1.33	Nb 1.6	Mo 2.16	Tc 1.9	Ru 2.2	Rh 2.28	Pd 2.20	Ag 1.93	Cd 1.69	In 1.78	Sn 1.96	Sb 2.05	Te 2.1	I 2.66	Xe 2.6
6	Cs 0.79	Ba 0.89	*	Hf 1.3	Ta 1.5	W 2.36	Re 1.9	Os 2.2	Ir 2.20	Pt 2.28	Au 2.54	Hg 2.00	Tl 1.62	Pb 2.33	Bi 2.02	Po 2.0	At 2.2	Rn
7	Fr 0.7	Ra 0.9	**	Rf	Db	Sg	Bh	Hs	Mt	Ds	Rg	Uub	Uut	Uuq	Uup	Uuh	Uus	Uuo
Lanthanides	*	La 1.1	Ce 1.12	Pr 1.13	Nd 1.14	Pm 1.13	Sm 1.17	Eu 1.2	Gd 1.2	Tb 1.1	Dy 1.22	Ho 1.23	Er 1.24	Tm 1.25	Yb 1.1	Lu 1.27		
Actinides	**	Ac 1.1	Th 1.3	Pa 1.5	U 1.38	Np 1.36	Pu 1.28	Am 1.13	Cm 1.28	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr 1.3		

Differences in electronegativity between atoms lead to polar bonds
The bigger the difference, the more polar the bond

The Greater the Difference in Electronegativity, the More Polar the Bond



Nonpolar covalent bond: electonegativity difference < 0.5

Polar covalent bond: electonegativity difference 0.5 – 1.9

Electronegativity difference > 1.9: electrons are not shared;
atoms are held together by
the attraction of opposite charges

Dipole Moment

Dipole moment = size of the charge x the distance between the charges

Table 1.4 The Dipole Moments of Some Common Bonds

Bond	Dipole moment (D)	Bond	Dipole moment (D)
H—C	0.4	C—C	0
H—N	1.3	C—N	0.2
H—O	1.5	C—O	0.7
H—F	1.7	C—F	1.6
H—Cl	1.1	C—Cl	1.5
H—Br	0.8	C—Br	1.4
H—I	0.4	C—I	1.2

The greater the difference in electronegativity,
the greater the dipole moment and the more polar the bond.

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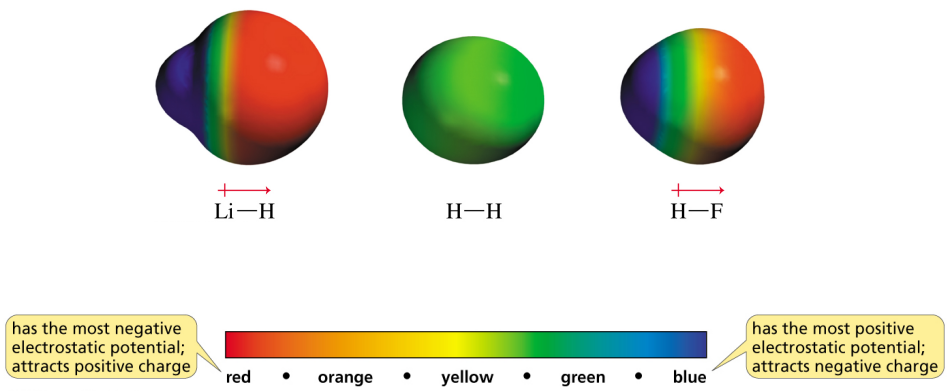
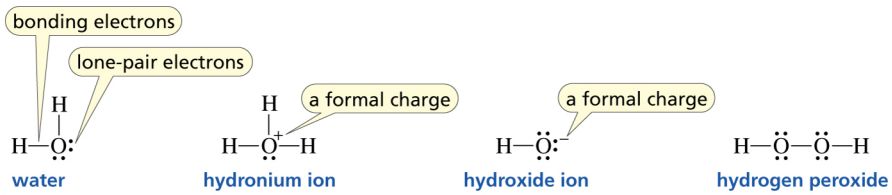
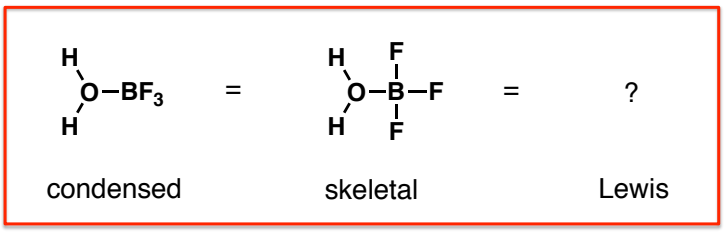
Electrostatic Potential Maps



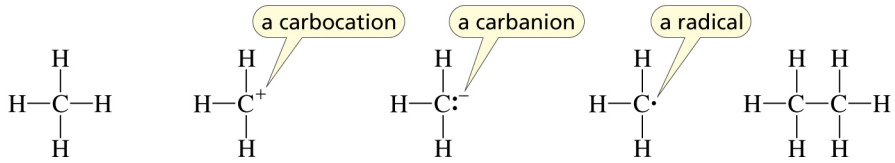
Lewis Structures

Important items: **lone pairs**, **formal charges**





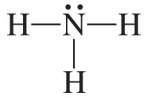
Carbon Forms Four Bonds



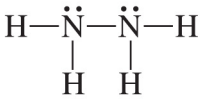
methane | methyl cation | methyl anion | methyl radical | ethane

If carbon does not form four bonds,
it has a charge (or it is a radical).

Nitrogen Forms Three Bonds



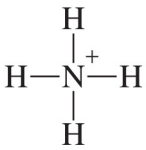
ammonia



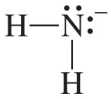
hydrazine

Nitrogen has one lone pair.

If nitrogen does not form three bonds, it is charged.

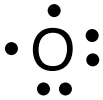


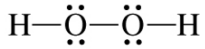
ammonium ion



amide anion

Oxygen Forms Two Bonds

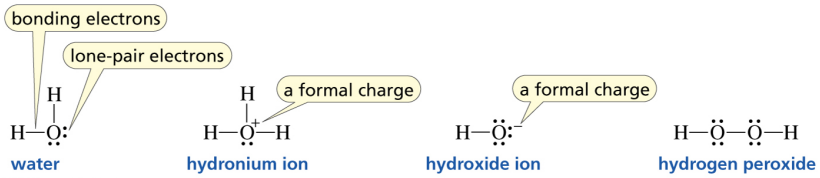




hydrogen peroxide

Oxygen has two lone pairs.

If oxygen does not form two bonds, it is charged.



Hydrogen and the Halogens Form One Bond

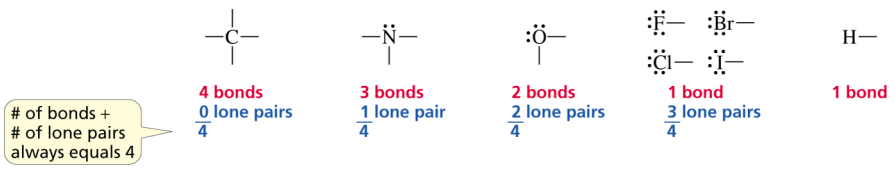
bromine chlorine

A halogen has three lone pairs.

If hydrogen or halogen does not form one bond,
it has a charge (or it is a radical).

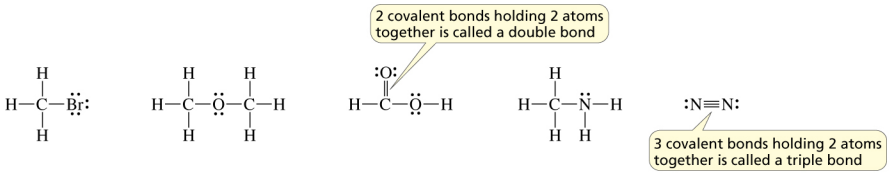
hydrogen ion | hydride ion | hydrogen radical | bromide ion | bromine radical

The Number of Bonds Plus the Number of Lone Pairs Equals Four



# of bonds +
# of lone pairs
always equals 4

Lewis Structures



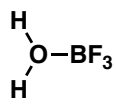
Formal Charge

Important items: **lone pairs**, **formal charges**

Formal Charge =

the # of valence electrons –

(the # of lone-pair electrons + the # of bonds)



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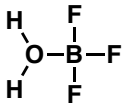

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condensed skeletal Lewis

How to Draw a Lewis Structure

review Gen. Chem. and practice!

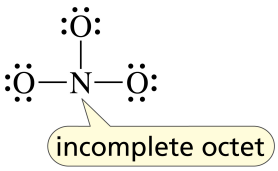
Homework: problems 49, 54, 55

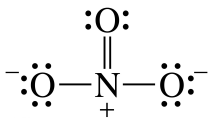
NO_3^- (anion of nitric acid HNO_3)

Determine the total number of valence electrons (5 + 6 + 6 + 6 = 23). Because they are negatively charged, add another electron = 24.

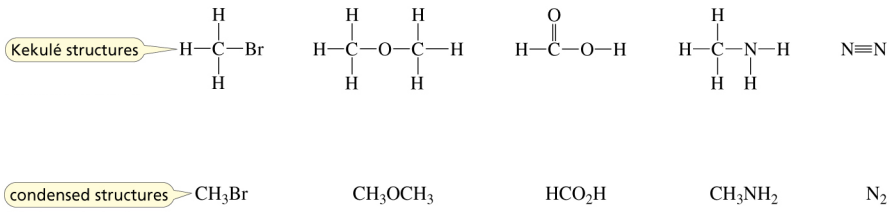
Avoid O—O bonds.

Check for formal charges.



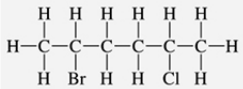
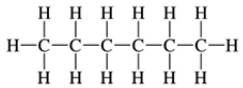
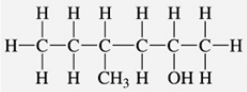
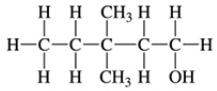


Kekulé Structures and Condensed Structures

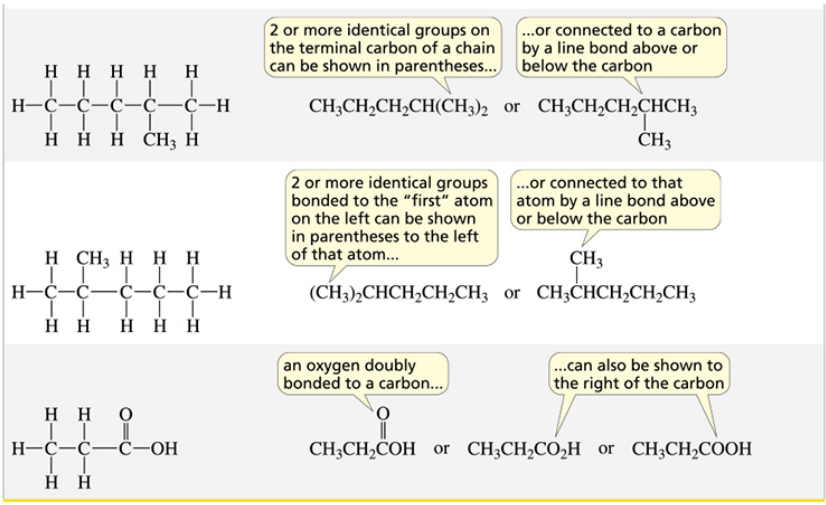


Kekulé Structures and Condensed Structures

Table 1.5 Kekulé Structures and Condensed Structures

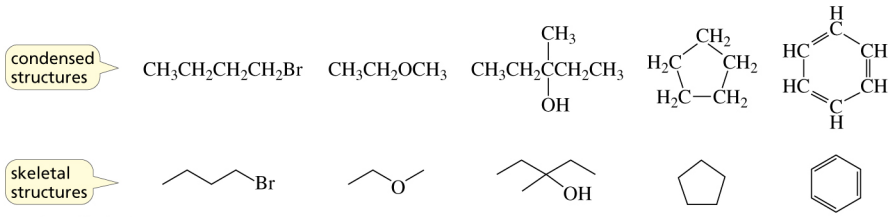
Kekulé Structures	Condensed Structures
	atoms bonded to a carbon are shown to the right of the carbon... $CH_3CHBrCH_2CH_2CHClCH_3$ or ...or connected to a carbon by a line bond above or below the carbon $CH_3CH(Br)CH_2CH_2CH(Cl)CH_3$
	repeating CH_2 groups can be shown in parentheses $CH_3CH_2CH_2CH_2CH_2CH_3$ or $CH_3(CH_2)_4CH_3$
	groups bonded to a carbon can be shown in parentheses to the right of the carbon... $CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$ or ...or connected to the carbon by a line bond above or below the carbon $CH_3CH_2CH(CH_3)CH_2CH(OH)CH_3$
	a single group bonded to the terminal carbon of a chain is not put in parentheses $CH_3CH_2C(CH_3)_2CH_2CH_2OH$ or $CH_3CH_2C(CH_3)CH_2CH_2OH$

Kekulé Structures and Condensed Structures

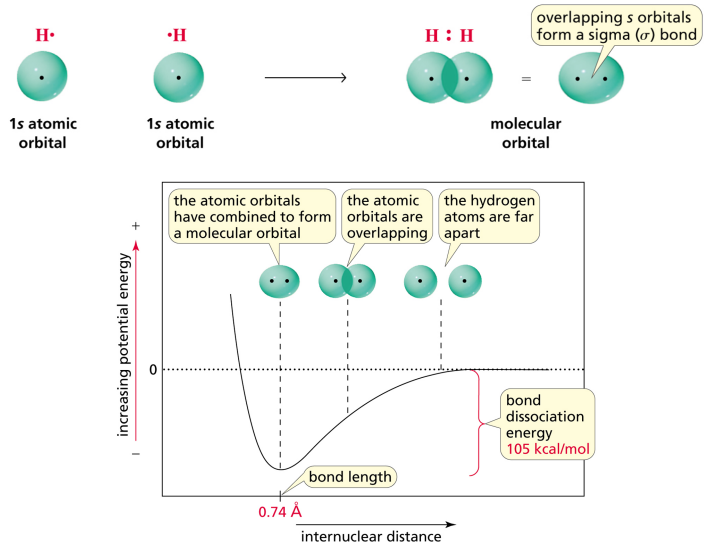


Skeletal Structures

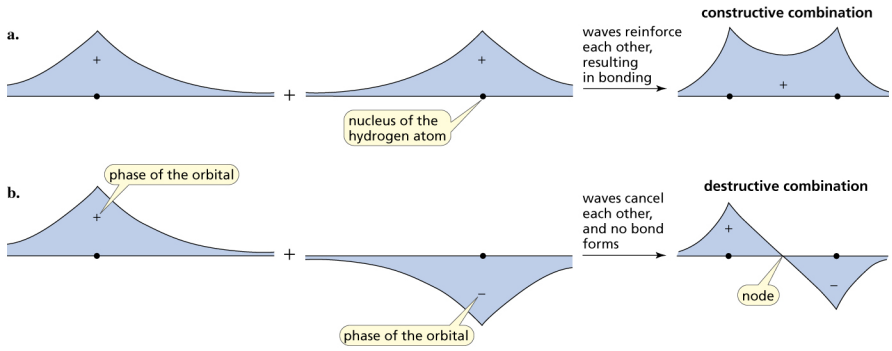
Skeletal structures show the carbon-carbon bonds as lines,
but do not show the carbons
or the hydrogens that are bonded to the carbons.



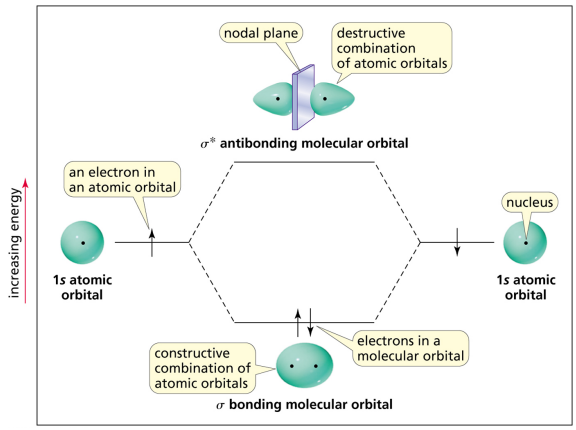
Back to Bonding: Forming a Sigma Bond



Waves Can Reinforce Each Other
Waves Can Cancel Each Other



Atomic Orbitals Combine to Form Molecular Orbitals



Orbitals are Conserved

<u># of Molecular Orbitals = # of Atomic Orbitals Combined</u>

Side-to-Side Overlap of In-Phase *p* Orbitals Forms a *π* Bond