Chapter 1:
Electronic Structure and Bonding

Or

A Brief Review of General Chemistry

Part 2: Quantum Mechanics and Molecular Orbital Theory

Review ideas from general chemistry:
atoms, bonds, molecular geometry

Finish Chapter 1

What is the electron configuration of an oxygen ion with a single positive charge and what neutral atom shares the same electron configuration?

a. $1s^2 2s^2 2p^3$

b. $1s^2 2s^2 2p^4$

c. $1s^2 2s^2 2p^5$

d. $1s^2 2s^1 2p^4$

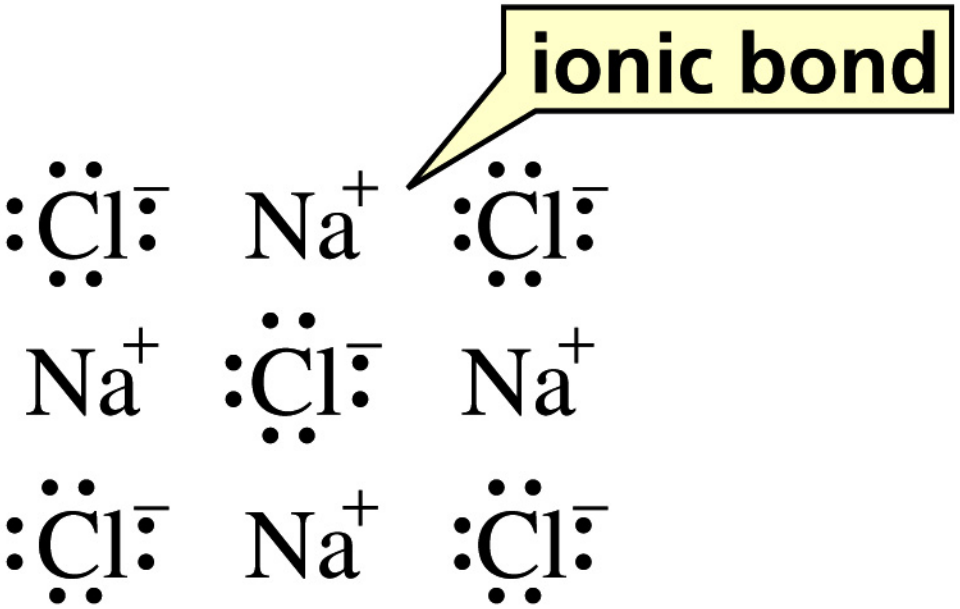
1. Nitrogen

2. Fluorine

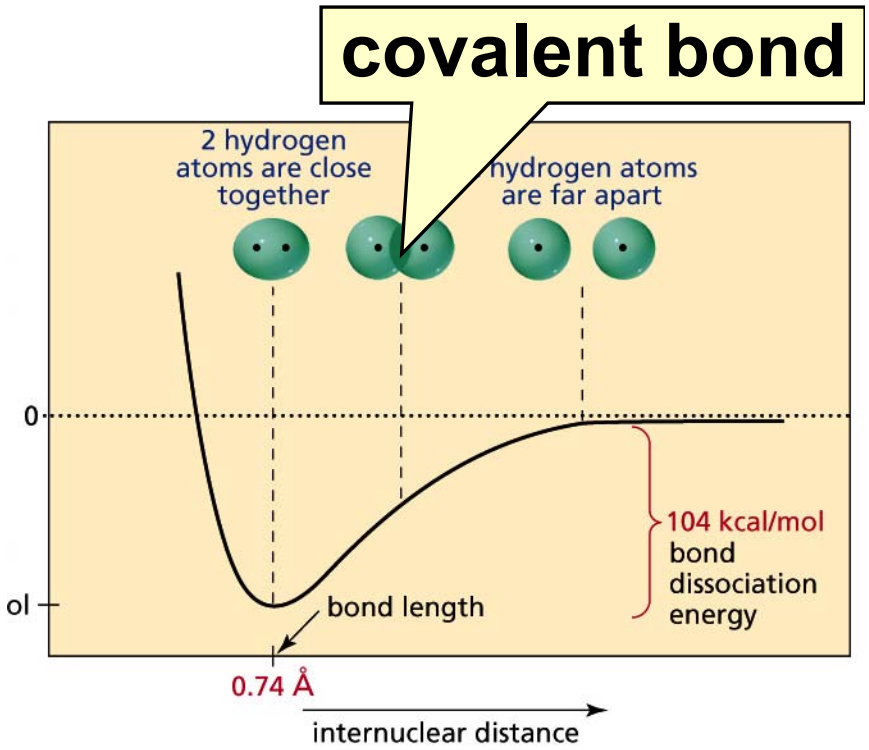
3. Sulfur

4. Neon

Ionic Bonds form when an electropositive element transfers electron(s) to an



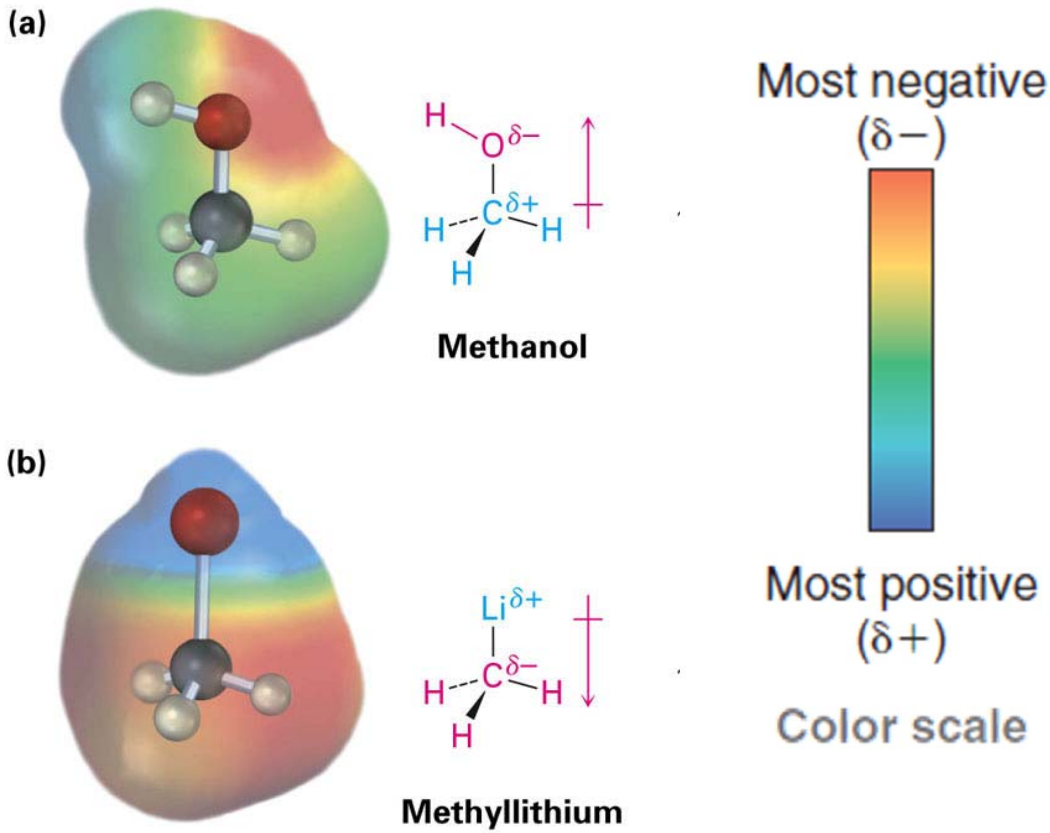
sodium chloride



Covalent Bonds form when electrons are shared between atoms

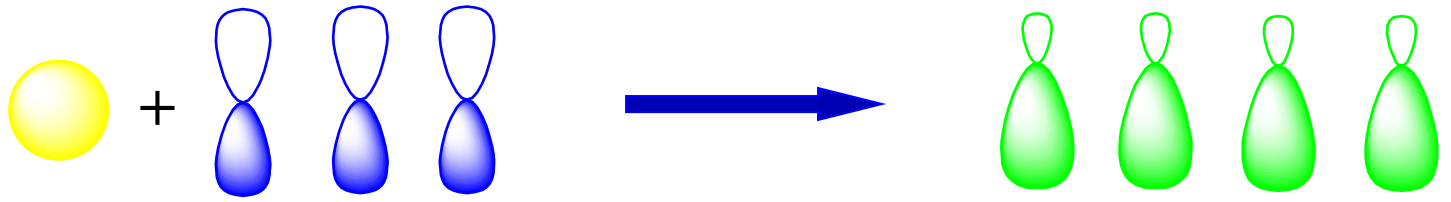
Electrostatic Potential Maps

- **Electrostatic potential maps** show calculated charge distributions
- Colors indicate electron rich (red) and electron-poor (blue) regions
- Used to give a visual depiction of polarity.
- Arrows indicate direction of bond polarity (p.12)

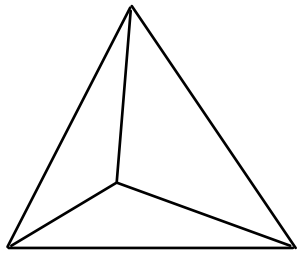


sp^3 Orbitals and the Structure of Methane

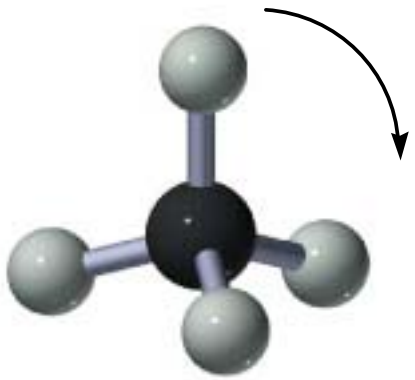
- Carbon has 4 valence electrons ($2s^2\ 2p^2$)
- In CH_4, all C–H bonds are identical



2s 2p sp^3



(tetrahedral)



109.5

1.08Å

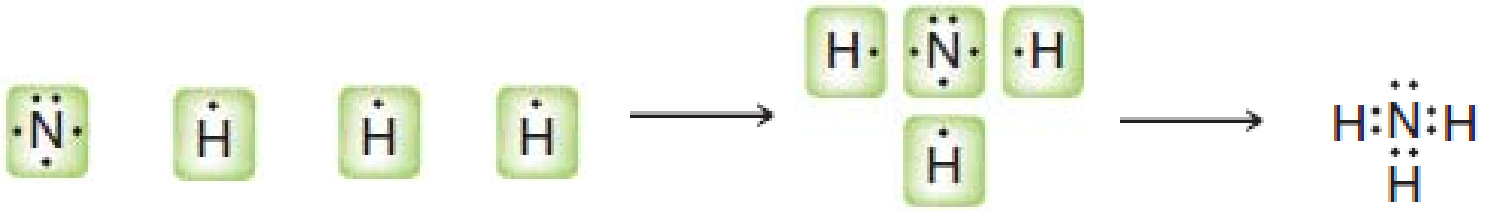
438 kJ/mol

- ***sp*³ hybrid orbitals**: *s* orbital and three *p* orbitals combine to form four equivalent, unsymmetrical, orbitals (sppp = sp^3), Linus Pauling (1931)

Electronic Structure and Bonding

- For simple Lewis Dot structures:
  1. Draw the individual atoms using dots to represent the valence electrons.
  2. Put the atoms together so they share PAIRS of electrons to make complete octets.

- Take NH_3, for example:

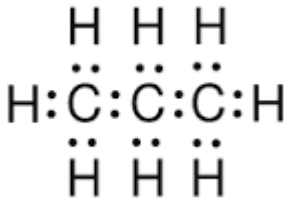


Electronic Structure and Bonding

Lewis Dot Structures

- Each valence electron is indicated by a dot.
- Hydrogen wants to have 2 electrons.

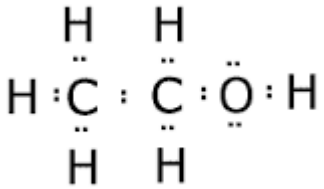
- Propane – C_3H_8



Electronic Structure and Bonding

Lewis Dot Structures

- What about non-bonding electrons?
- Ethanol – C_2H_6O

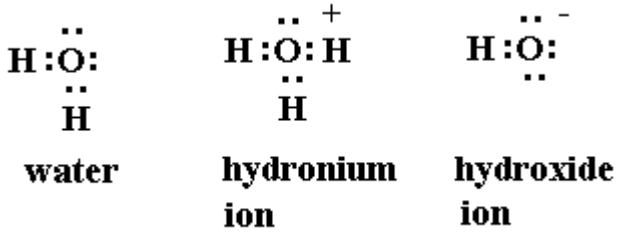


- These are called lone pairs.
- In a neutral compound - one without a formal charge – nitrogen has 1 lone pair, oxygen has 2, the halides have 3.

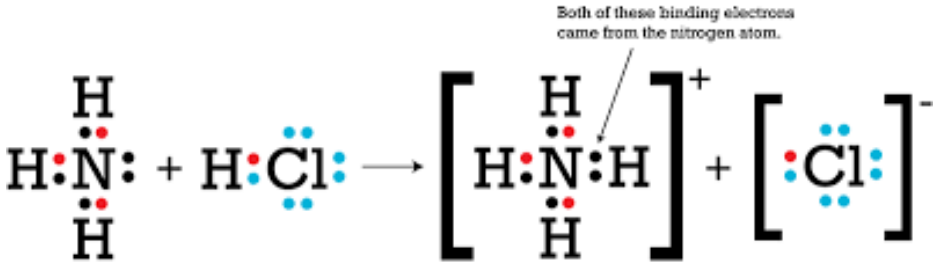
Electronic Structure and Bonding

Formal charge =
number of valence electrons -
number of lone pair electrons - 1/2 number of shared electrons)

Hydronium Ion, H_3O^+



ammonium chloride (NH_4Cl)



Electronic Structure and Bonding

Rules for Lewis Dot Structures:

1. All valence electrons are shown

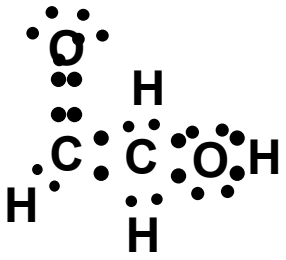
Total e^- = Sum of all valence electrons on all atoms involved

2. Determine connectivity. COH or OCH?
3. Add & subtract electrons for anionic and cationic charges, respectively.
4. Complete octet for each atom to fullest extent possible.

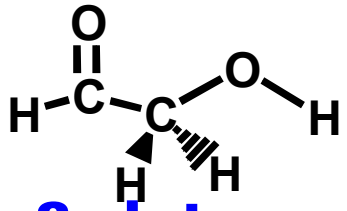
Electronic Structure and Bonding

Bonding Models

- **Lewis DOT structures – Uses DOTS to show covalent bonds & non-bonding valence electrons**



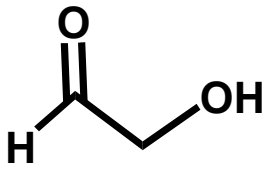
- **Kekulé line structures – Use of lines to show covalent bond(s)**



- **Condensed structures – eliminates all lines & dots**

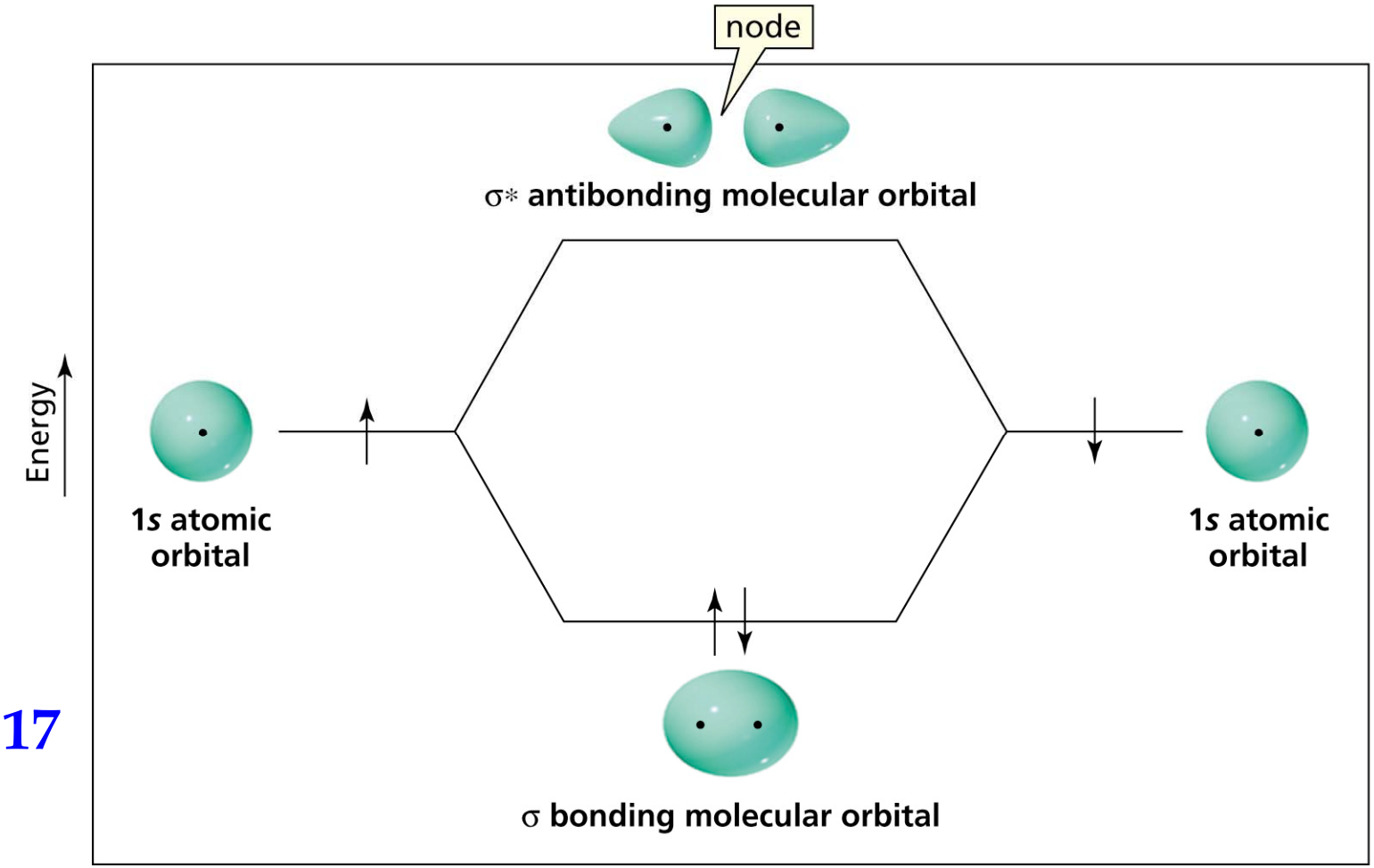
- **Organic structures – use of corners to show carbons, fill in other elements**

$C_2O_2H_4$ $HCOCH_2OH$



Molecular Orbital Theory

In-phase overlap forms a bonding MO
Out-of-phase overlap forms an antibonding MO



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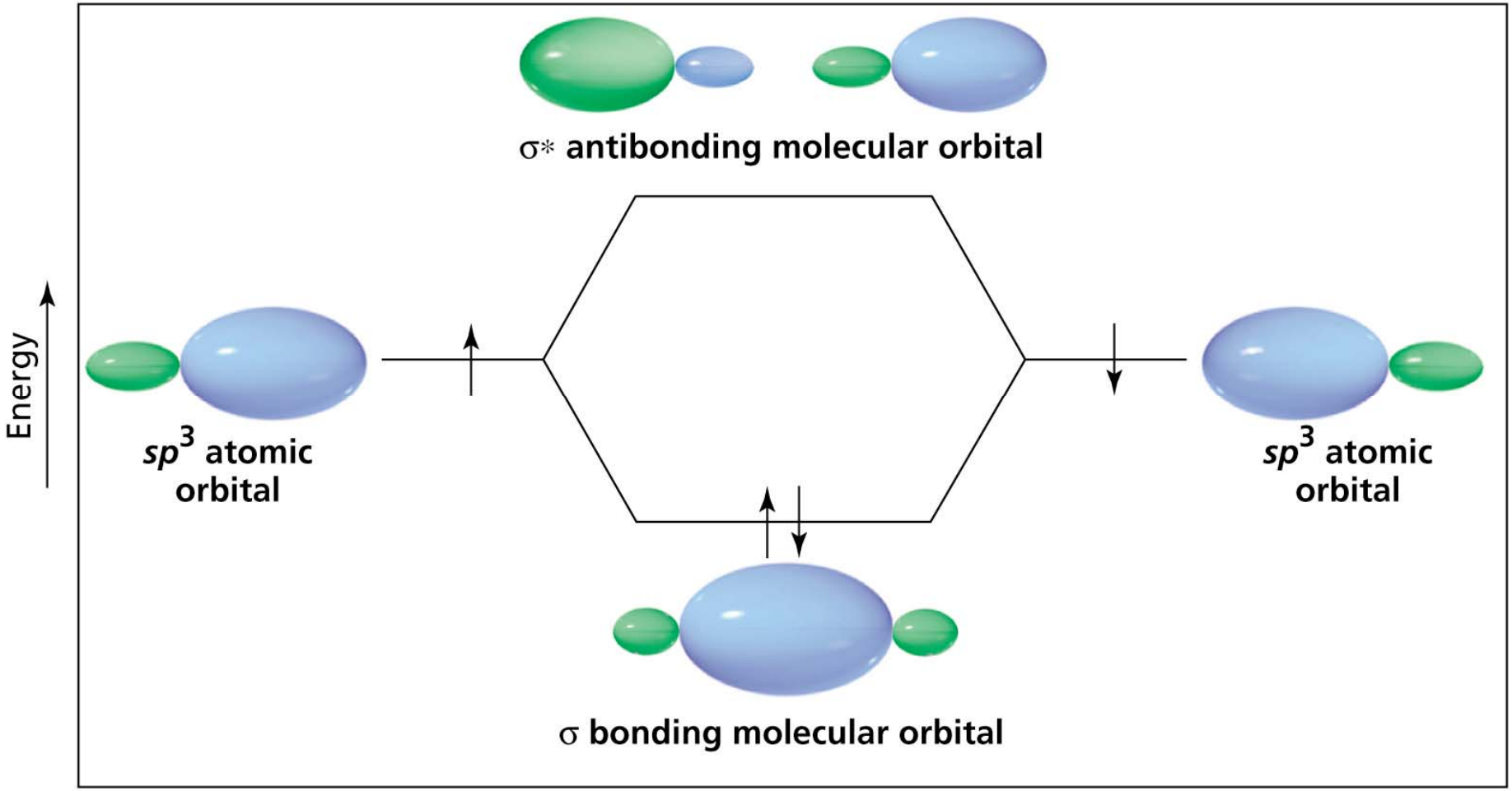
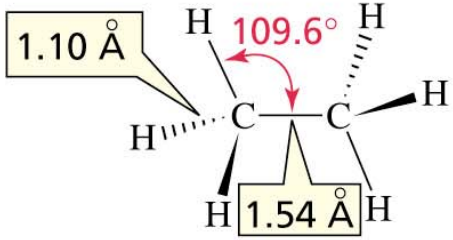
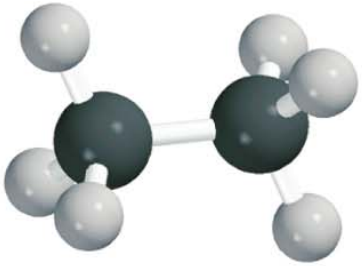
Hybrid Orbitals of Ethane, C_2H_6

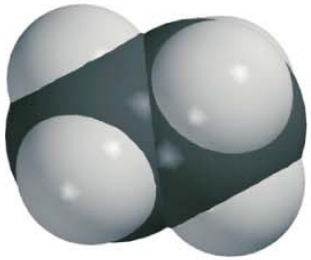


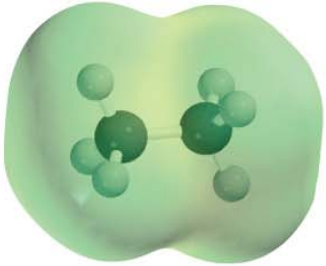
Hybrid Orbitals of Ethane, C_2H_6



perspective formula of ethane


ball-and-stick model of ethane


space-filling model of ethane


electrostatic potential map for ethane

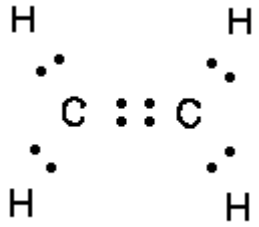
- Ethane has both carbons sp^3 hybridized and tetrahedral.
- The sp^3 orbitals which overlap to form the C-C bond are shaped such that rotation about the bond axis does not interfere with their overlap.
- Structures that differ only in rotation about a single bond are called different Conformations.

Molecular Orbital Theory

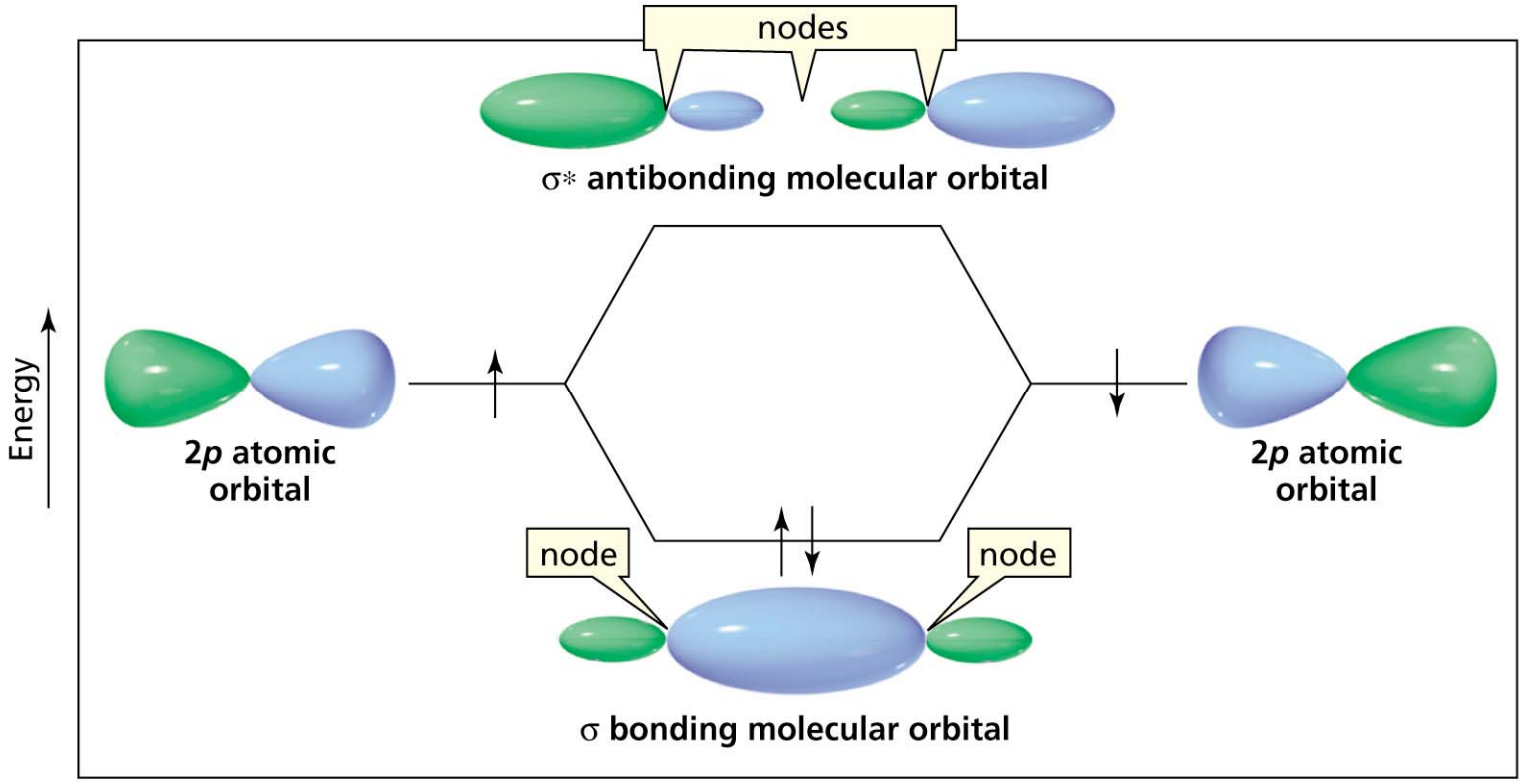
So let's look at Ethene (Ethylene) . . .

CH_2CH_2

Draw a Lewis Dot Structure for Ethene

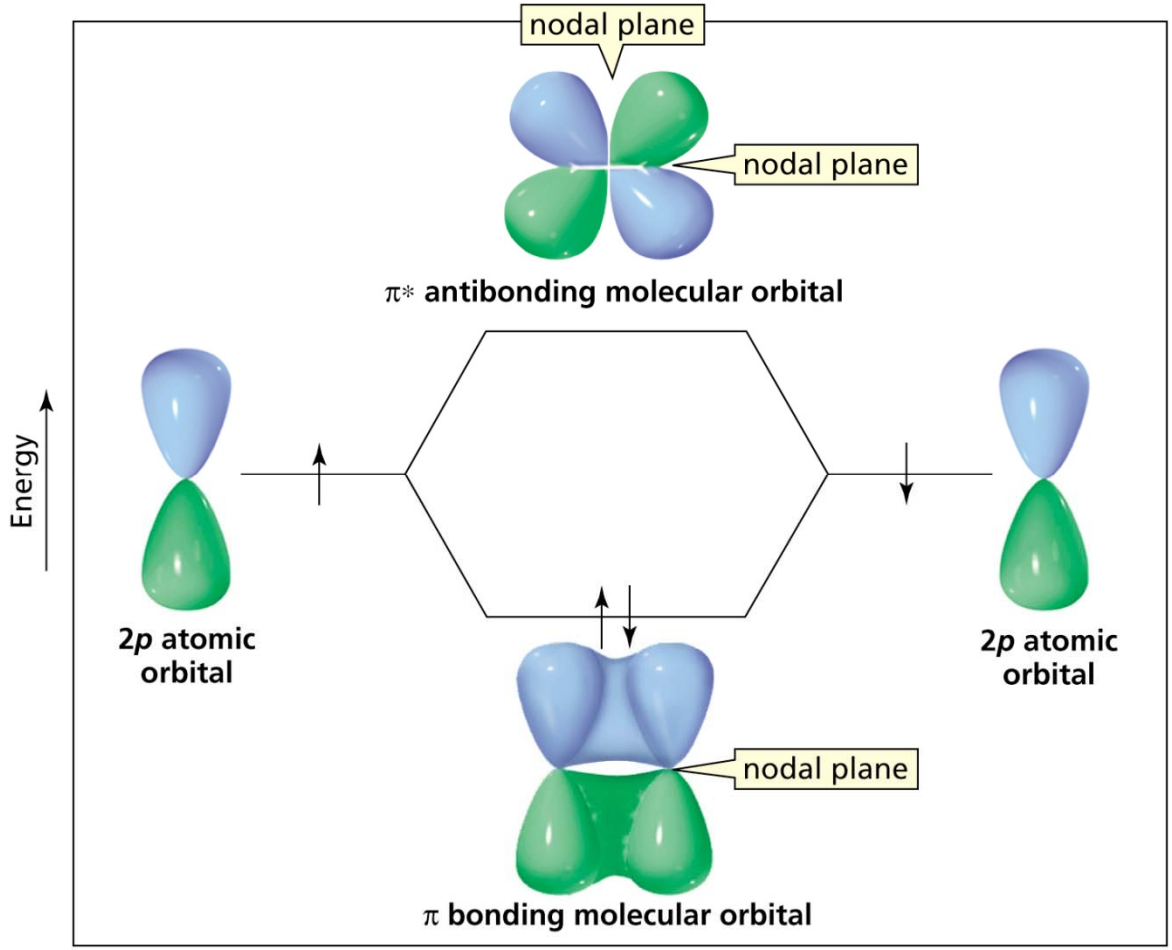


Hybrid Orbitals of Ethene, C_2H_4



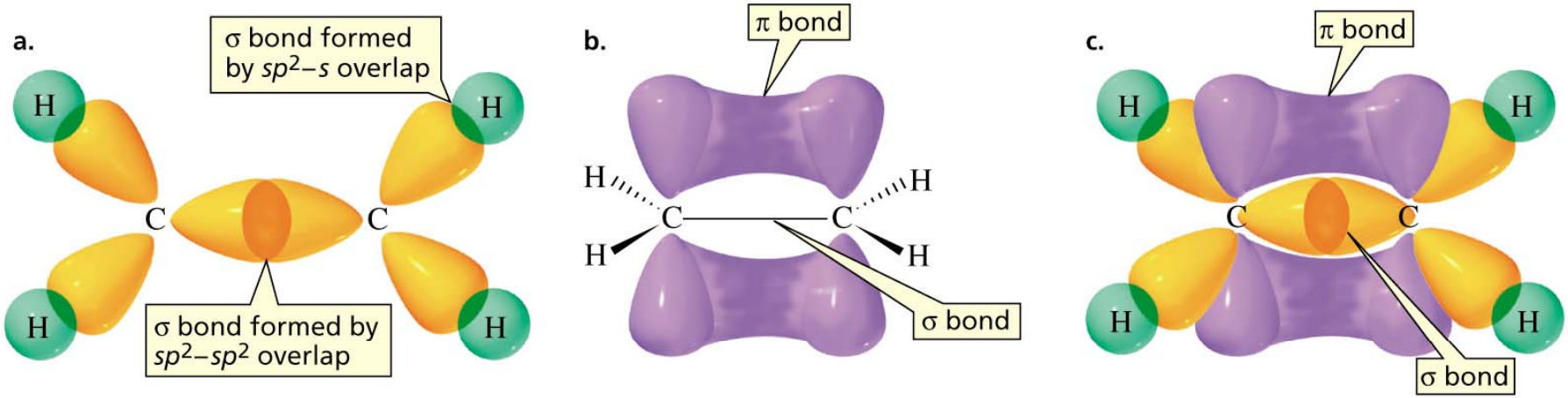
Sigma bond (s) is formed by end-on overlap of t
***p* orbitals.**

Hybrid Orbitals of Ethene, C_2H_4



Pi bond (π) is formed by sideways overlap of two parallel *p* orbitals

Hybrid Orbitals of Ethene, C_2H_4



Bonding in Ethene (Ethylene): A Double Bond

- The sigma bond is unaffected by rotation of one of the CH_2 groups.
- The overlap of the p orbitals is disrupted by rotation of one of the CH_2 groups.
- This would cause the double bond to break.

For Next Time….

- Monday Chapter 2 Sections 2.1-2.7

- Homework Practice Problems Chapter 1

  #8,12,15,37,39,43,45,48,49,53,56

- Homework Practice Problems Chapter 2

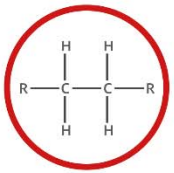
  #1,5,12,16,25,34,40,47,48,54,55,64, 66

  *know the functional groups in table 2.1

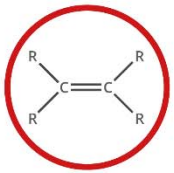
FUNCTIONAL GROUPS IN ORGANIC CHEMISTRY

FUNCTIONAL GROUPS ARE GROUPS OF ATOMS IN ORGANIC MOLECULES THAT ARE RESPONSIBLE FOR THE CHARACTERISTIC CHEMICAL REACTIONS OF THOSE MOLECULES. IN THE GENERAL FORMULAE BELOW, 'R' REPRESENTS A HYDROCARBON GROUP OR HYDROGEN, AND 'X' REPRESENTS ANY HALOGEN ATOM.

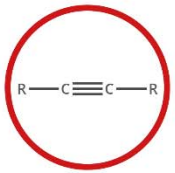
HYDROCARBONS · SIMPLE OXYGEN HETEROATOMICS · HALOGEN HETEROATOMICS · CARBONYL COMPOUNDS · NITROGEN BASED · SULFUR BASED · AROMATIC



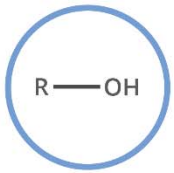
ALKANE
Naming: -ane
e.g. ethane



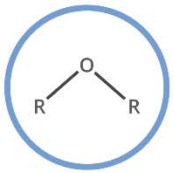
ALKENE
Naming: -ene
e.g. ethene



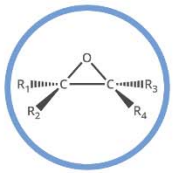
ALKYNE
Naming: -yne
e.g. ethyne



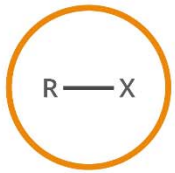
ALCOHOL
Naming: -ol
e.g. ethanol



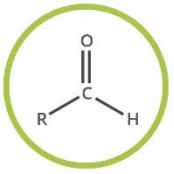
ETHER
Naming: -oxy -ane
e.g. methoxyethane



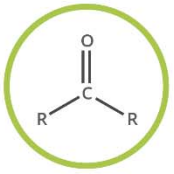
EPOXIDE
Naming: -ene oxide
e.g. ethene oxide



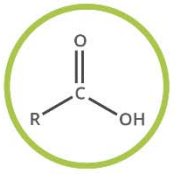
HALOALKANE
Naming: halo-
e.g. chloroethane



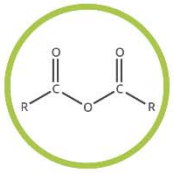
ALDEHYDE
Naming: -al
e.g. ethanal



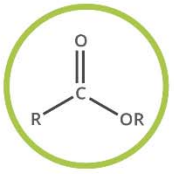
KETONE
Naming: -one
e.g. propanone



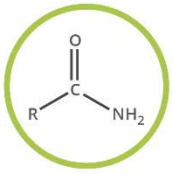
CARBOXYLIC ACID
Naming: -oic acid
e.g. ethanoic acid



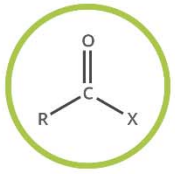
ACID ANHYDRIDE
Naming: -oic anhydride
e.g. ethanoic anhydride



ESTER
Naming: -yl -oate
e.g. ethyl ethanoate



AMIDE
Naming: -amide
e.g. ethanamide

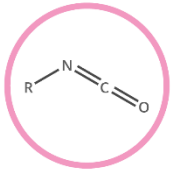


ACYL HALIDE
Naming: -oyl halide
e.g. ethanoyl chloride

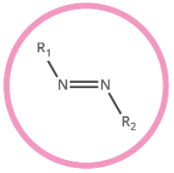
AMINE
Naming: -amine
e.g. ethanamine

NITRILE
Naming: -nitrile
e.g. ethanenitrile

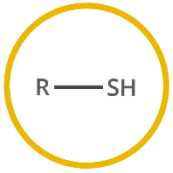
IMINE
Naming: -imine
e.g. ethanimine



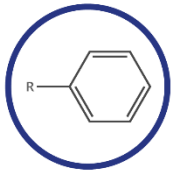
ISOCYANATE
Naming: -yl isocyanate
e.g. ethyl isocyanate



AZO COMPOUND
Naming: azo-
e.g. azoethane



THIOL
Naming: -thiol
e.g. methanethiol



ARENE
Naming: -yl benzene
e.g. ethyl benzene