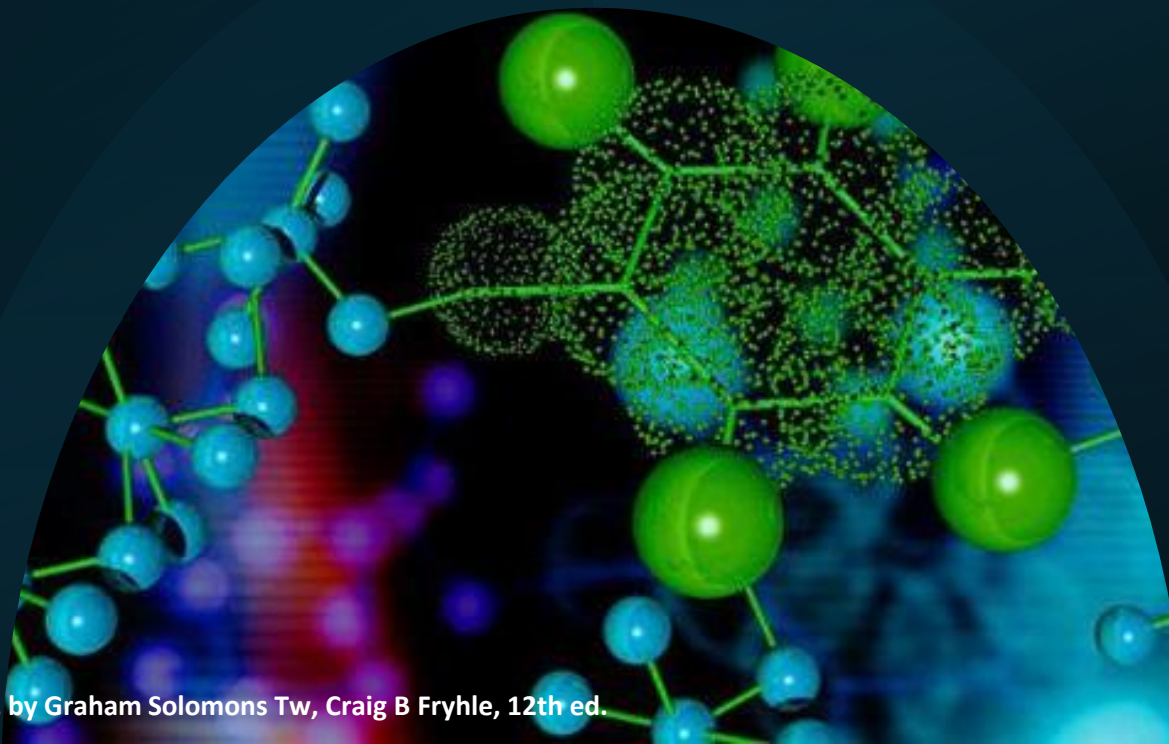




# Chapter 1

## Bonding and Molecular Structure

Carbon Compounds, Chemical Bonds and Hybridization



Slides are prepared by  
Dr. Heba Abbas Kashmery

Based on Organic Chemistry, by Graham Solomons Tw, Craig B Fryhle, 12th ed.

2026-01



## Why This Chapter?



Organic chemistry plays a role in all aspects of human lives including medicine, bioengineering etc.



**Biological Processes**



**By the end of this chapter, student will be able to:**

- Know the development of the science of organic chemistry.
- Understand the principles that determine how the atoms in organic molecules are bound together.
- Define the electronegativity and its effect on chemical bonding.
- Differentiate between ionic, polar and non-polar covalent bonds in a molecule.
- Identify the isomer
- Draw dash, condensed and bond-line, 3D structures of organic compounds.
- Identify the hybridization of carbon, nitrogen and oxygen atoms in a molecule.
- Determine the geometry, bond types and angles around atoms in a molecule.
- Compare bond lengths between C-C and C-H in alkanes, alkenes and alkynes.
- Recognize the effect of the type of hybridization on the acidity.

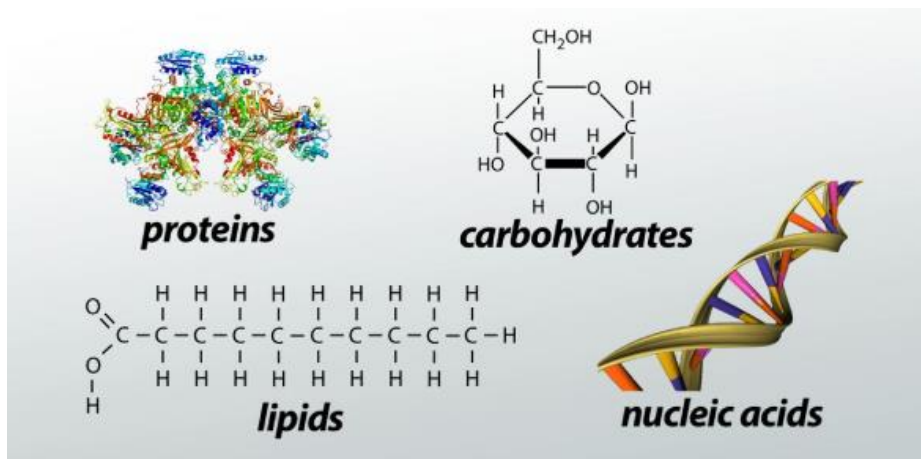


- **Introduction of Organic Chemistry**
- **Structural Theory**
- **Chemical Bonds, Electronegativity and the Octet Rule**
- **Isomers**
- **Representations of Structural Formulas**
- **Electron Configuration**
- **Hybridization**
- **The Structure of Methane and Ethane**
- **The Structure of Ethene**
- **The Structure of Ethyne**
- **Bond Lengths of Ethyne, Ethene and Ethane**
- **The Effect of Hybridization on Acidity**
- **Geometry of Ammonia, Water and Carbon dioxide**



## Organic Chemistry

- The chemistry of the compounds of **carbon**.
- The human body is largely composed of **organic compounds**.
- Carbon has the ability to form strong bonds to other carbon atoms and other elements such as hydrogen, nitrogen, oxygen, and sulfur.
- This property allows carbon to form the backbone of organic compounds, carbon-containing compounds, which are the basis of all known organic life.





## Organic and Inorganic Carbon

They are derived from **nonliving** components, and **natural inorganic processes**.

**Examples:** allotropes of carbon (graphite, diamond, etc.), carbon monoxide  $\text{CO}$ , carbon dioxide  $\text{CO}_2$ , and salts of inorganic anions such as carbonate  $\text{CO}_3^{2-}$ .

**Inorganic Compound**

They are derived from or produced by **living** organisms and have **carbon-hydrogen covalent bonds**.

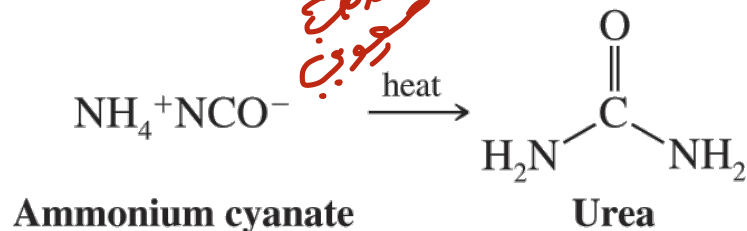
**Compounds of carbon with itself, hydrogen and other elements**

**Organic Compound**



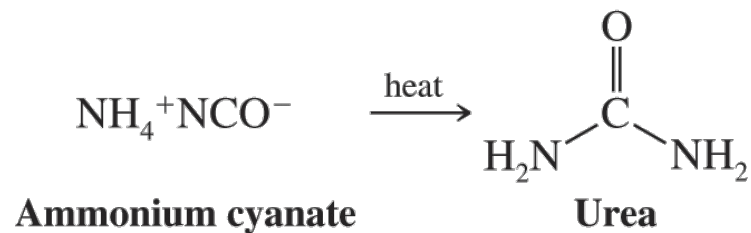
## Vitalism and Organic Chemistry

- It was originally thought organic compounds could be made only by living things by intervention of a “vital force” *قوة حيوية*
- Fredrich Wöhler disproved vitalism in 1828 by making the organic compound urea from the inorganic salt ammonium cyanate by evaporation *من مخرج مسجودين*

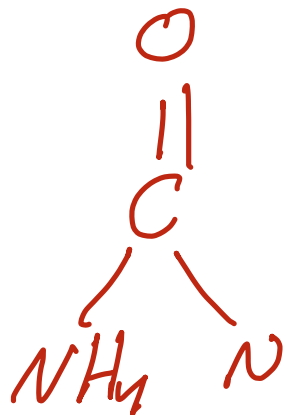


Despite the demise of vitalism in science, the word “organic” is still used today by some people to mean “coming from living organisms”





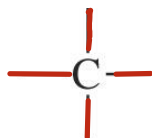
Write the structure of Ammonium cyanate?



## ♦ Structural Theory

### ● Central Premises → مبادئ

□ **Valency:** atoms in organic compounds form a fixed number of bonds  
عدد الروابط



Carbon atoms are **tetravalent**



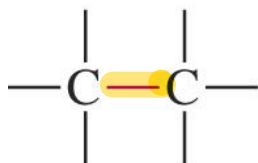
Oxygen atoms are **divalent**



Hydrogen and halogen atoms are **monovalent**

□ Carbon can form one or more bonds to other carbons

### Carbon-carbon bonds



Single bond



Double bond



Triple bond

## ◆ Chemical Bonds: The Octet Rule

### ● Octet Rule

- Atoms form bonds to produce the electron configuration of a noble gas (because the electronic configuration of noble gases is particularly stable)
- For most atoms of interest this means achieving a valence shell configuration of 8 electrons corresponding to that of the nearest noble gas
- Atoms close to helium achieve a valence shell configuration of 2 electrons
- Atoms can form either ionic or covalent bonds to satisfy the octet rule

# Periodic Table of the Elements

1  
IA  
**H**  
Hydrogen  
1.008  
1

2  
IIA  
**He**  
Helium  
4.0026  
2

3  
**Li**  
Lithium  
6.94  
3

4  
**Be**  
Beryllium  
9.0122  
4

11  
**Na**  
Sodium  
22.98976928  
11

12  
**Mg**  
Magnesium  
24.304  
12

19  
**K**  
Potassium  
39.0983  
19

20  
**Ca**  
Calcium  
40.078  
20

37  
**Rb**  
Rubidium  
85.4678  
37

38  
**Sr**  
Strontium  
87.62  
38

55  
**Cs**  
Cesium  
132.90545196  
55

56  
**Ba**  
Barium  
137.327  
56

87  
**Fr**  
Francium  
(223)  
223

88  
**Ra**  
Radium  
(226)  
226

Atomic Number →

← Symbol

Name →

← Atomic Weight

Electrons per shell →

13  
**Al**  
Aluminium  
26.982  
2-8-3

State of matter (color of name)  
GAS LIQUID SOLID UNKNOWN

Subcategory in the metal-metalloid-nonmetal trend (color of background)  
Alkali metals  
Alkaline earth metals  
Transition metals  
Lanthanides  
Actinides  
Post-transition metals  
Metalloids  
Reactive nonmetals  
Noble gases  
Unknown chemical properties

13  
IIIA  
**B**  
Boron  
10.81  
2-3

14  
IVA  
**C**  
Carbon  
12.011  
2-4

15  
VA  
**N**  
Nitrogen  
14.007  
2-5

16  
VIA  
**O**  
Oxygen  
15.999  
2-6

17  
VIIA  
**F**  
Fluorine  
18.998  
2-7

18  
VIIIA  
**Ne**  
Neon  
20.180  
2-8

31  
**Ga**  
Gallium  
69.723  
2-8-3

32  
**Ge**  
Germanium  
72.630  
2-8-4

33  
**As**  
Arsenic  
74.9216  
2-8-5

34  
**Se**  
Selenium  
78.9718  
2-8-6

35  
**Br**  
Bromine  
79.904  
2-8-7

36  
**Kr**  
Krypton  
83.798  
2-8-8

49  
**In**  
Indium  
114.818  
2-8-18-3

50  
**Sn**  
Tin  
118.710  
2-8-18-4

51  
**Sb**  
Antimony  
121.757  
2-8-18-5

52  
**Te**  
Tellurium  
127.603  
2-8-18-6

53  
**I**  
Iodine  
126.905  
2-8-18-7

54  
**Xe**  
Xenon  
131.29  
2-8-18-8

81  
**Tl**  
Thallium  
204.38  
2-8-18-32-3

82  
**Pb**  
Lead  
207.2  
2-8-18-32-4

83  
**Bi**  
Bismuth  
208.98  
2-8-18-32-5

84  
**Po**  
Polonium  
(209)  
2-8-18-32-6

85  
**At**  
Astatine  
(210)  
2-8-18-32-7

86  
**Rn**  
Radon  
(222)  
2-8-18-32-8

101  
**Ac**  
Actinium  
(227)  
2-8-18-32-10-2

90  
**Th**  
Thorium  
(232)  
2-8-18-32-10-2

91  
**Pa**  
Protactinium  
(231)  
2-8-18-32-10-2

92  
**U**  
Uranium  
(238)  
2-8-18-32-10-2

93  
**Np**  
Neptunium  
(237)  
2-8-18-32-10-2

94  
**Pu**  
Plutonium  
(244)  
2-8-18-32-10-2

95  
**Am**  
Americium  
(243)  
2-8-18-32-10-2

96  
**Cm**  
Curium  
(247)  
2-8-18-32-10-2

97  
**Bk**  
Berkelium  
(247)  
2-8-18-32-10-2

98  
**Cf**  
Californium  
(251)  
2-8-18-32-10-2

99  
**Es**  
Einsteinium  
(252)  
2-8-18-32-10-2

100  
**Fm**  
Fermium  
(257)  
2-8-18-32-10-2

101  
**Md**  
Mendelevium  
(258)  
2-8-18-32-10-2

102  
**No**  
Nobelium  
(259)  
2-8-18-32-10-2

103  
**Lr**  
Lawrencium  
(260)  
2-8-18-32-10-2

57  
**La**  
Lanthanum  
138.90547  
2-8-18-32-10-2

58  
**Ce**  
Cerium  
140.12  
2-8-18-32-10-2

59  
**Pr**  
Praseodymium  
140.90766  
2-8-18-32-10-2

60  
**Nd**  
Neodymium  
144.242  
2-8-18-32-10-2

61  
**Pm**  
Promethium  
(145)  
2-8-18-32-10-2

62  
**Sm**  
Samarium  
150.36  
2-8-18-32-10-2

63  
**Eu**  
Europium  
151.964  
2-8-18-32-10-2

64  
**Gd**  
Gadolinium  
157.25  
2-8-18-32-10-2

65  
**Tb**  
Terbium  
158.92534  
2-8-18-32-10-2

66  
**Dy**  
Dysprosium  
162.50  
2-8-18-32-10-2

67  
**Ho**  
Holmium  
164.93032  
2-8-18-32-10-2

68  
**Er**  
Erbium  
167.259  
2-8-18-32-10-2

69  
**Tm**  
Thulium  
168.93032  
2-8-18-32-10-2

70  
**Yb**  
Ytterbium  
173.05468  
2-8-18-32-10-2

71  
**Lu**  
Lutetium  
174.967  
2-8-18-32-10-2

السالبية  
الالكترونية

## Electronegativity

- Electronegativity is the ability of an atom to attract electrons
- It increases from **left to right** and from **bottom to top** in the periodic table (noble gases excluded)
  - Fluorine is the most electronegative atom and can stabilize excess electron density the best

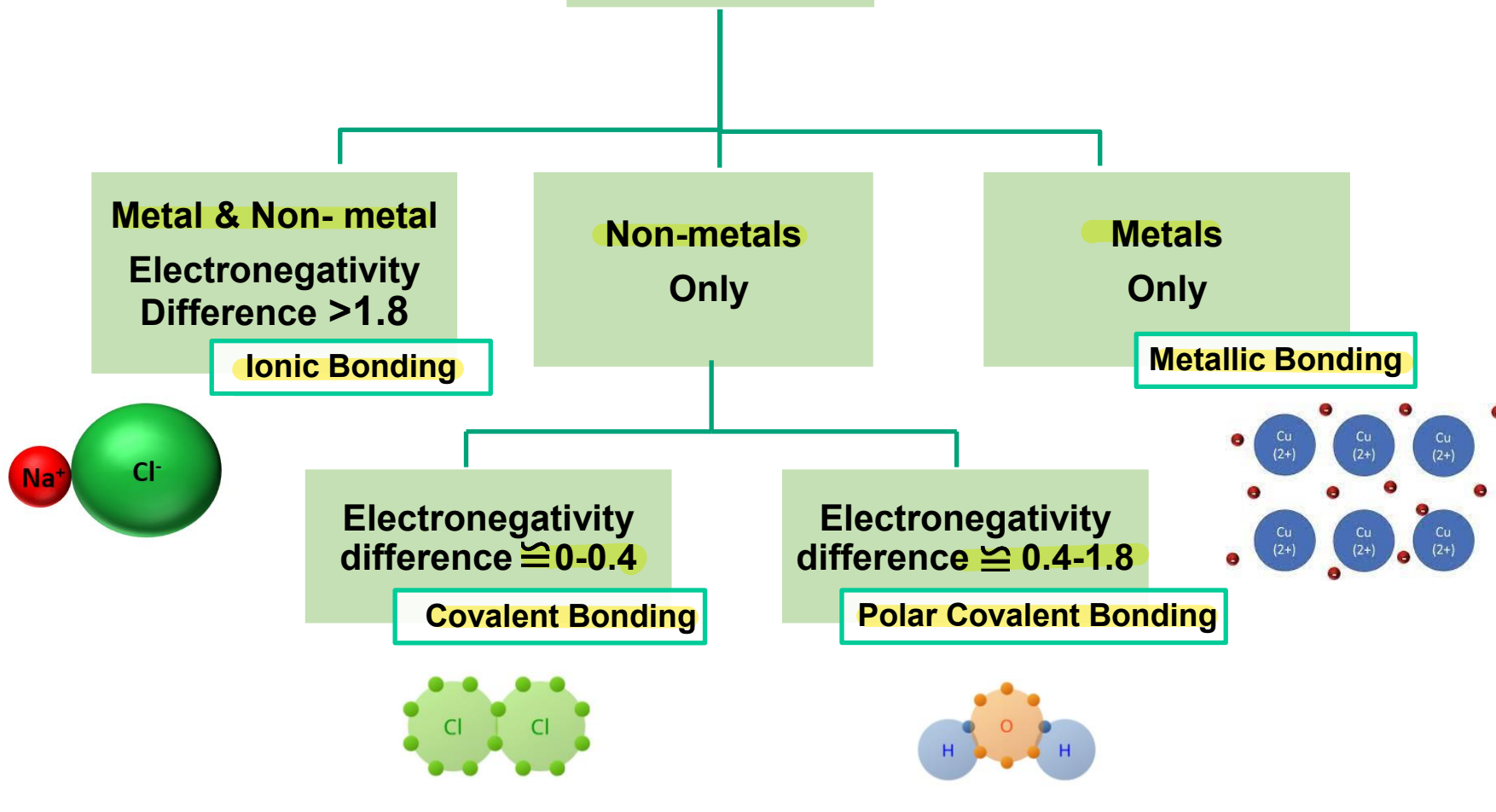
| Increasing electronegativity → |           |           |           |          |          |           | ↑<br>Increasing<br>electronegativity |
|--------------------------------|-----------|-----------|-----------|----------|----------|-----------|--------------------------------------|
|                                |           | H<br>2.1  |           |          |          |           |                                      |
| Li<br>1.0                      | Be<br>1.5 | B<br>2.0  | C<br>2.5  | N<br>3.0 | O<br>3.5 | F<br>4.0  |                                      |
| Na<br>0.9                      | Mg<br>1.2 | Al<br>1.5 | Si<br>1.8 | P<br>2.1 | S<br>2.5 | Cl<br>3.0 |                                      |
| K<br>0.8                       |           |           |           |          |          | Br<br>2.8 |                                      |



QUICK TIPS

Helpful to understand the properties and reactivity of organic molecules

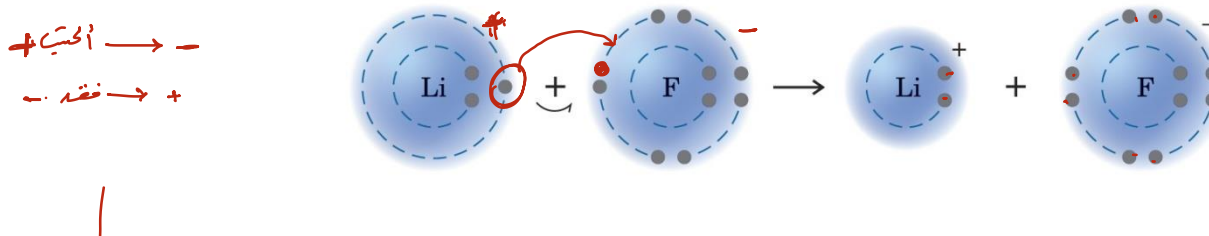
# Compound Components



مواصفات الجزيء

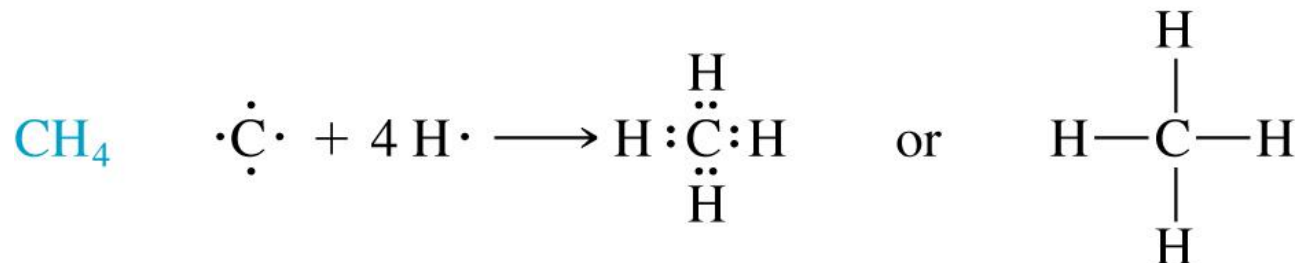
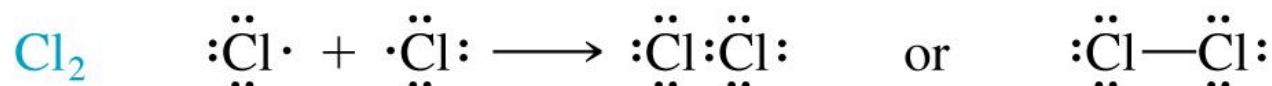
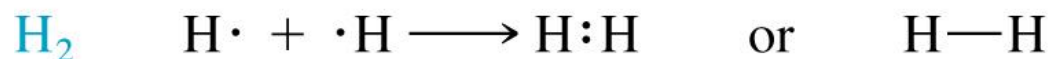
## ● Ionic Bonds

- When ionic bonds are formed atoms gain or lose electrons to achieve the electronic configuration of the nearest noble gas
  - In the process the atoms become ionic
- The resulting oppositely charged ions attract and form ionic bonds
- This generally happens between atoms of widely different electronegativities
- Example
  - Lithium loses an electron (to have the configuration of helium) and becomes positively charged
  - Fluoride gains an electron (to have the configuration of neon) and becomes negatively charged
  - The positively charged lithium and the negatively charged fluoride form a strong ionic bond (actually in a crystalline lattice)



## ● Covalent Bonds

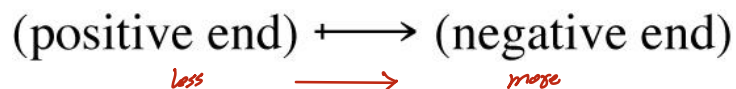
- Covalent bonds occur between atoms of similar electronegativity (close to each other in the periodic table)
- Atoms achieve octets by *sharing* of valence electrons
- Molecules result from this covalent bonding
- Valence electrons can be indicated by dots (electron-dot formula **or Lewis structures**) but this is time-consuming
- The usual way to indicate the two electrons in a bond is to use a line (one line = two electrons)



## ● Polar Covalent Bonds

### ● Polar covalent bonds occur when a covalent bond is formed between two atoms of differing electronegativities

- The more electronegative atom <sup>مقارب</sup> draws electron density closer to itself
- The more electronegative atom develops a partial negative charge ( $\delta^-$ ) and the less electronegative atom develops a partial positive charge ( $\delta^+$ )
- A bond which is polarized is a dipole and has a dipole moment
- The direction of the dipole can be indicated by a dipole arrow
  - The arrow head is the negative end of a dipole, the crossed end is the positive end



### ● Example: the molecule HCl

- The more electronegative chlorine draws electron density away from the hydrogen
  - Chlorine develops a partial negative charge



# Quick QUESTION

Periodic Table of the Elements

## ● PRACTICE PROBLEM 1.2

How many valence electrons does each of the following atoms have?

- (a) Na      (b) Cl      (c) Si      (d) B      (e) Ne      (f) N

## ● PRACTICE PROBLEM 1.3

Using the periodic table, which element in each pair is more electronegative?

- (a) Si, O      (b) N, C      (c) Cl, Br      (d) S, P

Consider the following compounds and decide whether the bond in them would be ionic or covalent.

- (a) KCl      (b) F<sub>2</sub>      (c) PH<sub>3</sub>      (d) CBr<sub>4</sub>

ion

cov

cov

cov

## ● PRACTICE PROBLEM 1.4

## ◆ Isomers

□ Isomers are different molecules with the same molecular formula

□ Many types of isomers exist

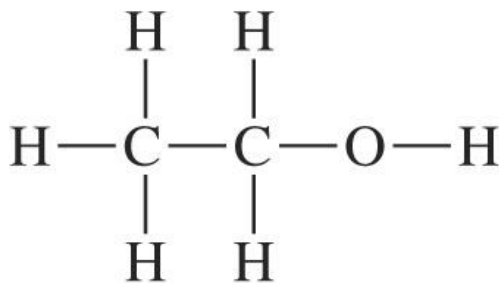
□ Example

C:2  
O:1  
H:6

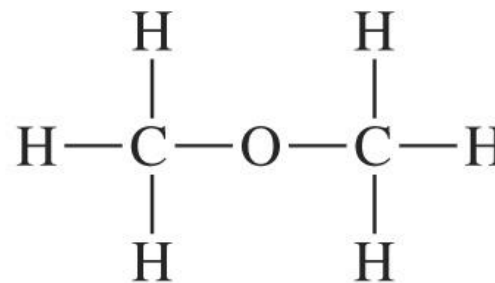
□ Consider two compounds with molecular formula  $C_2H_6O$

□ These compounds cannot be distinguished based on molecular formula; however they have different structures

□ The two compounds **differ in the connectivity of their atoms**



**Ethyl alcohol**



**Dimethyl ether**

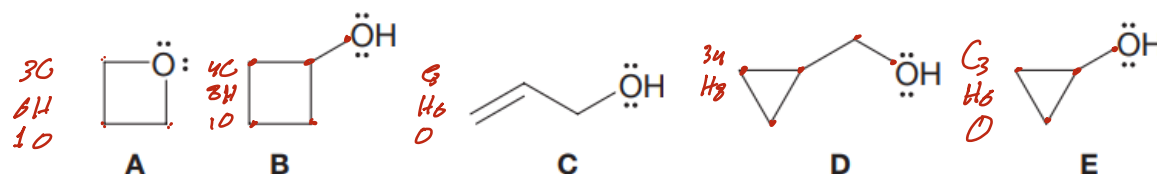
## ● Constitutional Isomers

- Constitutional isomers are one type of isomer
- They are different compounds that have the same molecular formula but different connectivity of atoms
- They often differ in physical properties (e.g. boiling point, melting point, density) and chemical properties

|                                      | Ethyl Alcohol<br>$\text{C}_2\text{H}_6\text{O}$ | Dimethyl Ether<br>$\text{C}_2\text{H}_6\text{O}$ |
|--------------------------------------|-------------------------------------------------|--------------------------------------------------|
| Boiling point ( $^{\circ}\text{C}$ ) | 78.5                                            | -24.9                                            |
| Melting point ( $^{\circ}\text{C}$ ) | -117.3                                          | -138                                             |

SOLVED PROBLEM 1.7

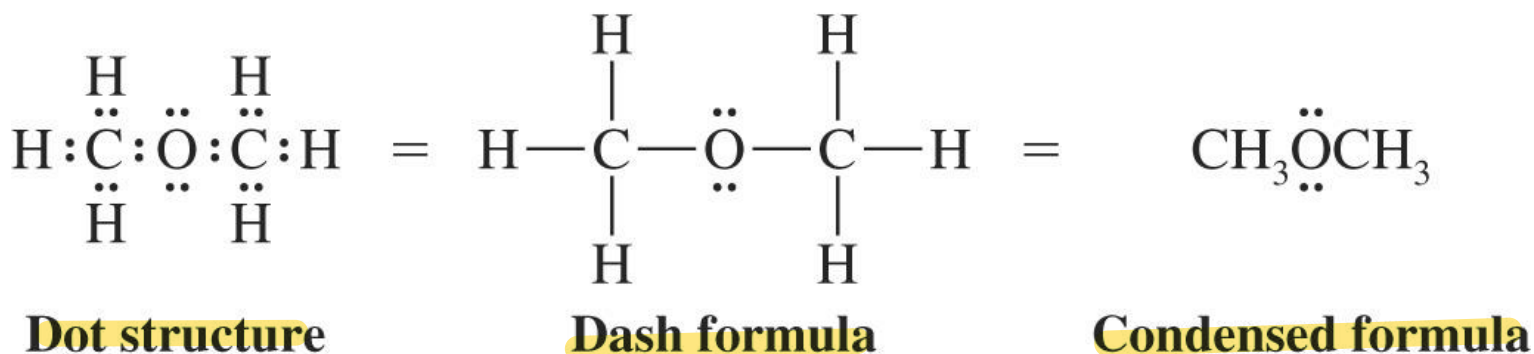
Which of the following compounds are constitutional isomers of one another?



**ANSWER:** First determine the molecular formula for each compound. You will then see that **B** and **D** have the same molecular formula ( $\text{C}_4\text{H}_8\text{O}$ ) but have different connectivities. They are, therefore, constitutional isomers of each other. **A**, **C**, and **E** also have the same molecular formula ( $\text{C}_3\text{H}_6\text{O}$ ) and are constitutional isomers of one another.

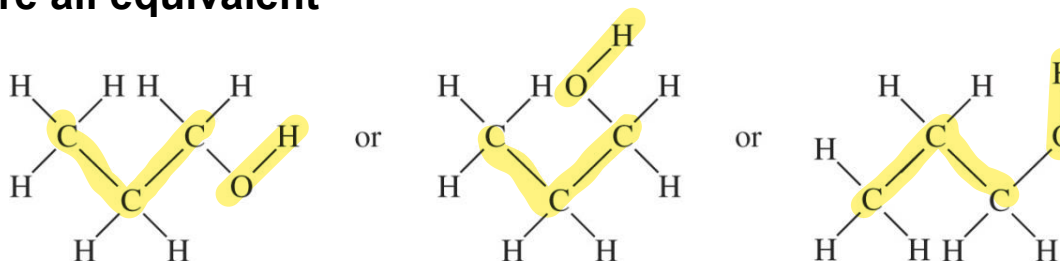
## ◆ Representations of Structural Formulas

- **Dot formulas** are more cumbersome to draw than dash formulas and condensed formulas
- Lone-pair electrons are often (but not always) drawn in, especially when they are crucial to the chemistry being discussed



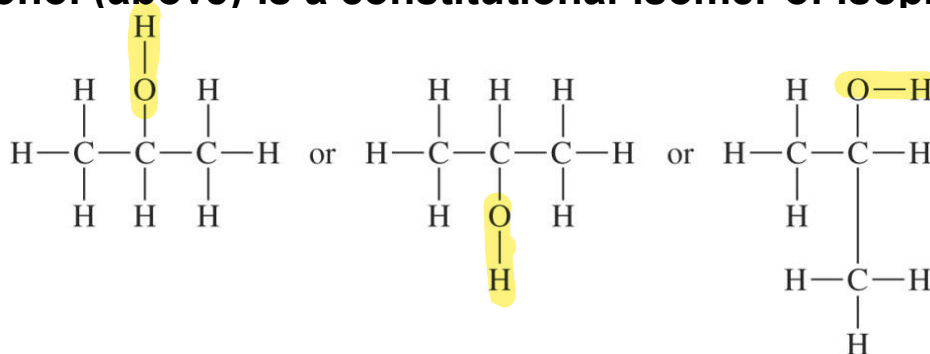
## ● Dash Formulas

- Each dash represents a pair of electrons
- This type of representation is meant to emphasize connectivity and does not represent the 3-dimensional nature of the molecule
  - The dash formulas of propyl alcohol appear to have  $90^\circ$  angles for carbons which actually have tetrahedral bond angles ( $109.5^\circ$ )
- There is relatively free rotation around single bonds so the dash structures below are all equivalent



Equivalent dash formulas for **propyl alcohol**

- Propyl alcohol (above) is a constitutional isomer of isopropyl alcohol (below)

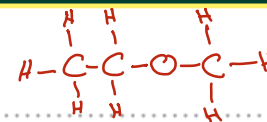


Equivalent dash formulas for **isopropyl alcohol**

# Quick QUESTION

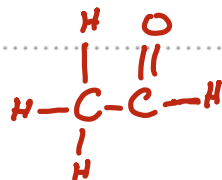
There are actually three constitutional isomers with the molecular formula  $C_3H_8O$ . We have seen two of them in propyl alcohol and isopropyl alcohol. Write a dash formula for the third isomer.

## • PRACTICE PROBLEM 1.12



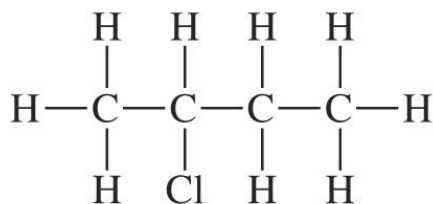
## • PRACTICE PROBLEM 1.7

Write a dash structural formula showing all valence electrons for  $\text{CH}_3\text{CHO}$  (acetaldehyde).

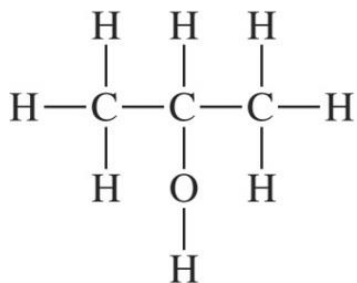


## ● Condensed Structural Formulas

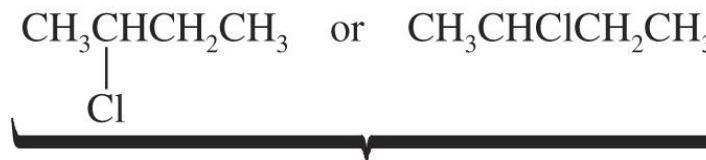
- In these representations, some or all of the dash lines are omitted
- In partially condensed structures all hydrogens attached to an atom are simply written after it but some or all of the other bonds are explicitly shown
- In fully condensed structure all bonds are omitted and atoms attached to carbon are written immediately after it
- For emphasis, branching groups are often written using vertical lines to connect them to the main chain



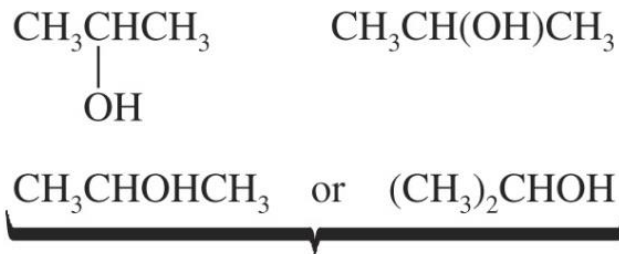
Dash formula



Dash formula

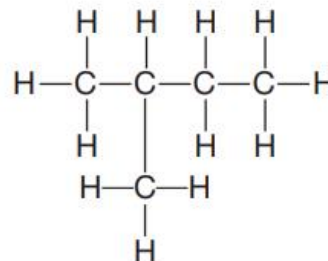
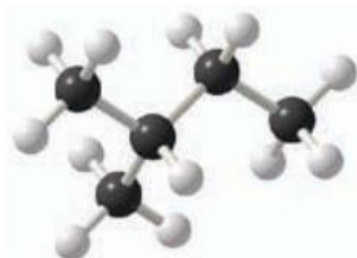


Condensed formulas

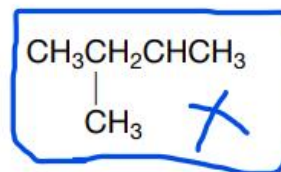
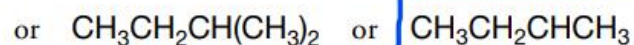
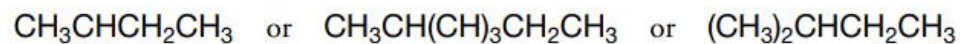


Condensed formulas

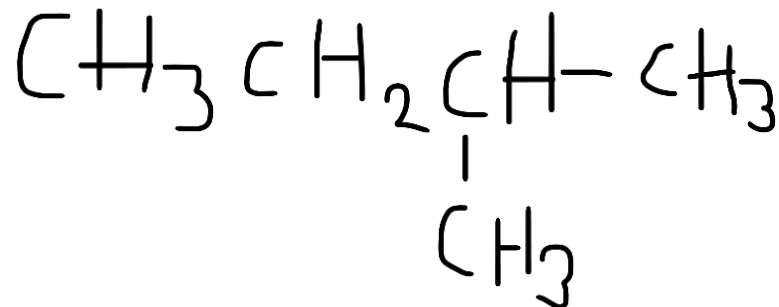
Write a condensed structural formula for the compound that follows:



ANSWER:

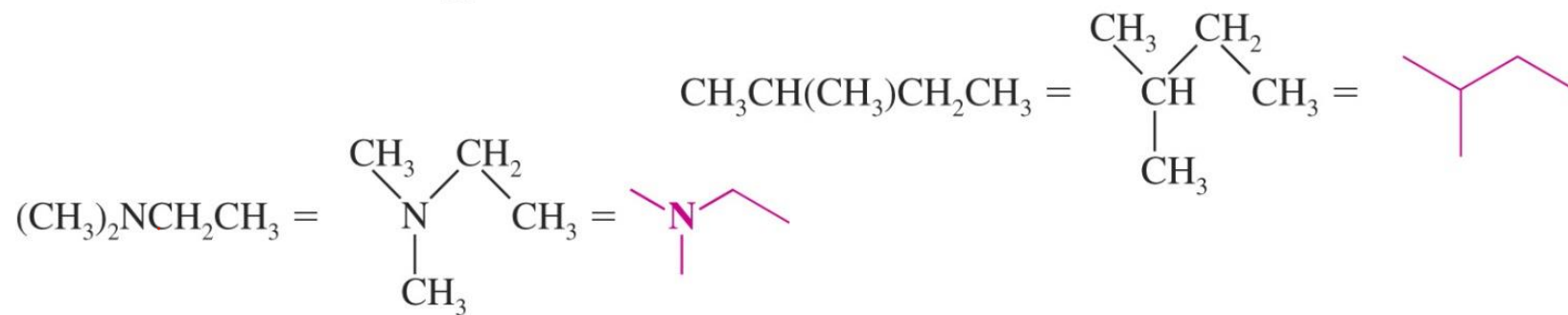
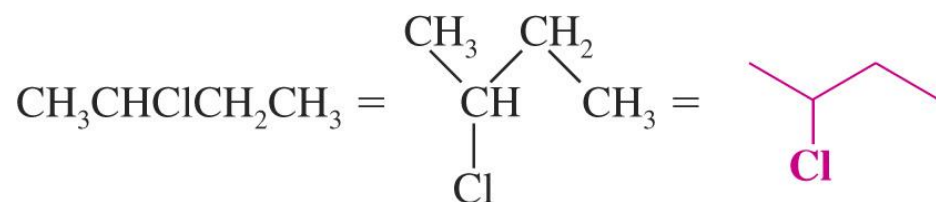


Correct this please



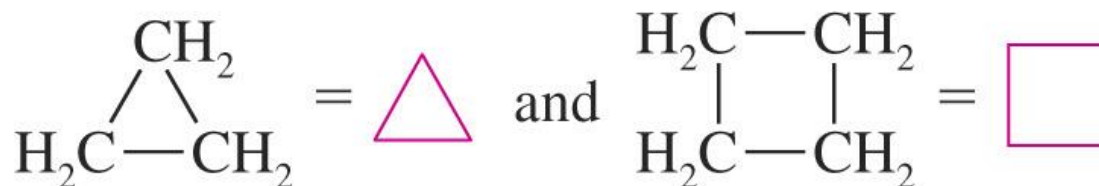
## ● Bond-Line Formulas

- A further simplification of drawing organic molecules is to completely omit all carbons and hydrogens and only show heteroatoms (e.g. O, Cl, N) explicitly
- Each intersection or end of line in a zig-zag represents a carbon with the appropriate amount of hydrogens
  - Heteroatoms with attached hydrogens must be drawn in explicitly

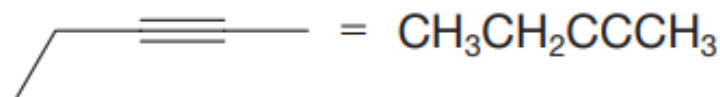
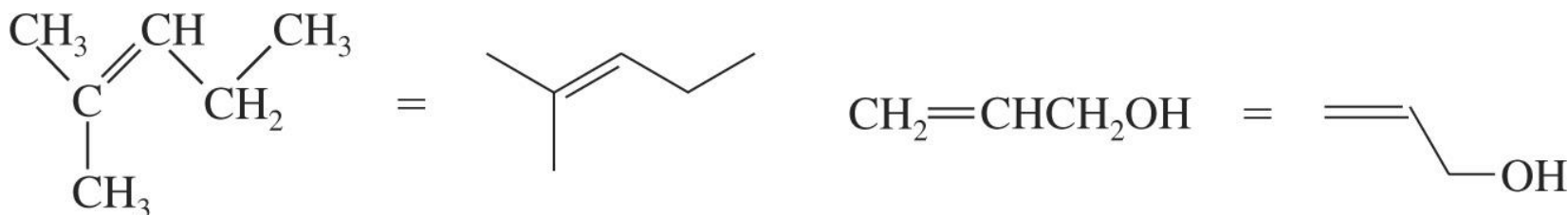


Bond-line  
formulas

- Cyclic compounds are condensed using a drawing of the corresponding polygon



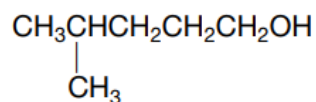
- Multiple bonds are indicated by using the appropriate number of lines connecting the atoms



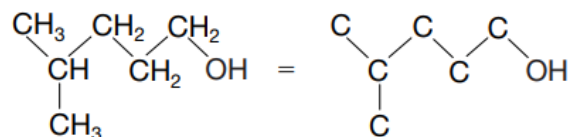
**Revise from the book the rules to understand How To Draw Bond-Line Formulas**

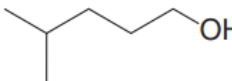
SOLVED PROBLEM 1.9

Write the bond-line formula for

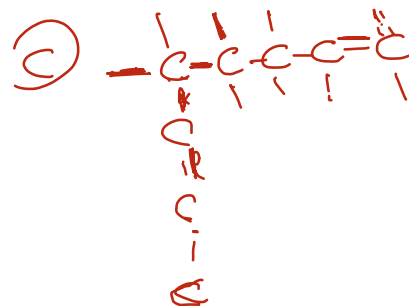
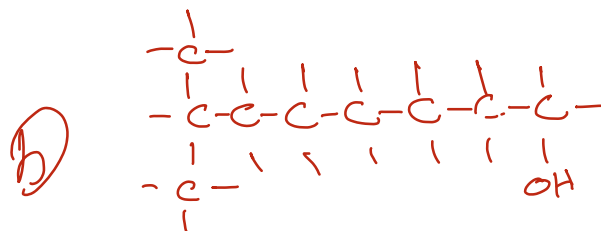
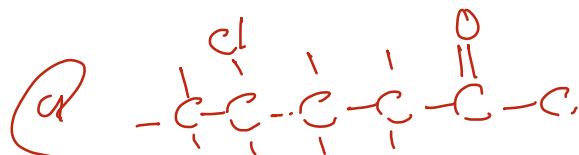
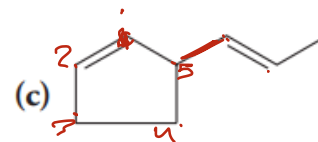
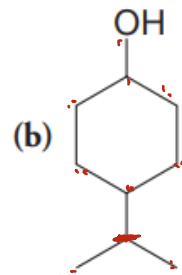
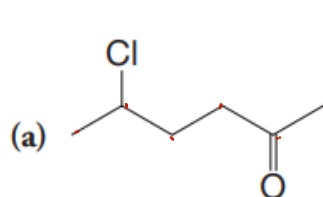


**STRATEGY AND ANSWER:** First, for the sake of practice, we outline the carbon skeleton, including the OH group, as follows:



Then we write the bond-line formula as . As you gain experience you will likely skip the intermediate steps shown above and proceed directly to writing bond-line formulas.

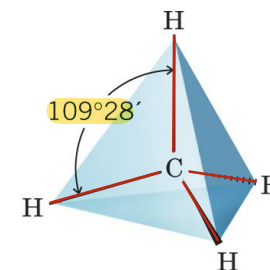
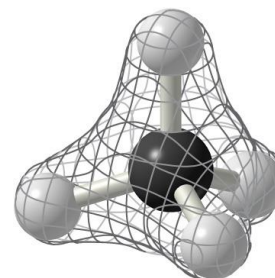
● PRACTICE PROBLEM 1.16 Write a dash formula for each of the following bond-line formulas:

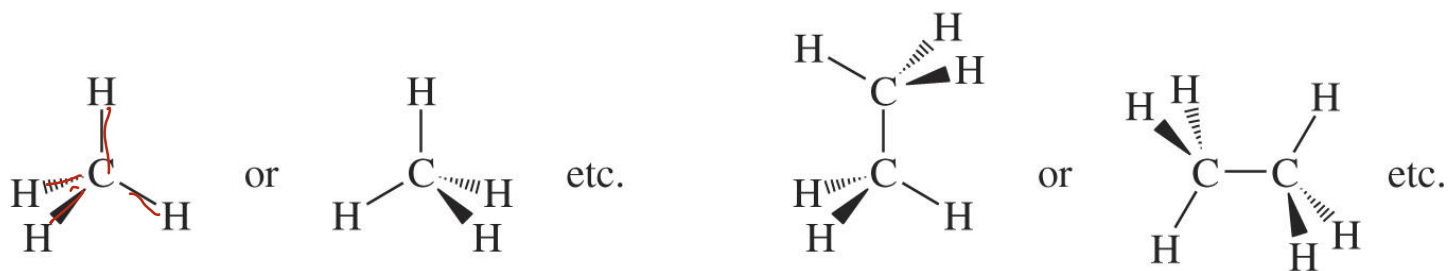
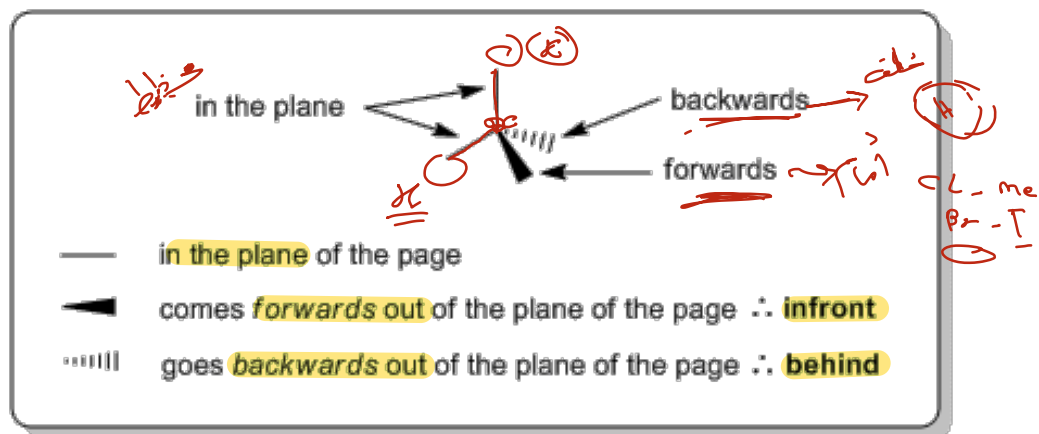


## ● Three-Dimensional Formulas

- ❑ Virtually all molecules possess a 3-dimensional shape which is often not accurately represented by drawings
- ❑ It is often important to be able to convey their shape.
- ❑ The conventions for this are:
  - ❑ Bonds that lie in the plane of the paper are indicated by a simple line
  - ❑ Bonds that come forward out of the plane of the paper are indicated by a solid wedge
  - ❑ Bonds that go back out of the plane of the paper are indicated by a dashed wedge
- ❑ Generally to represent a **tetrahedral atom**:
  - ❑ **Two** of the **bonds** are drawn in the plane of the paper about **109°** apart
  - ❑ The other two bonds are drawn in the opposite direction to the in- plane bonds but right next to each other

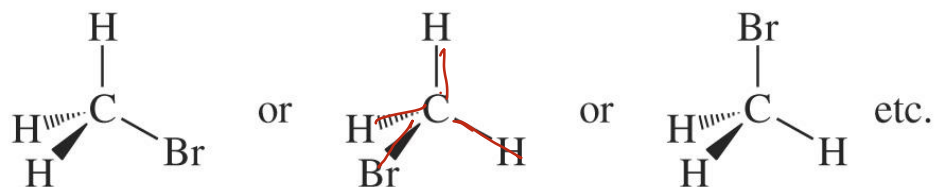
It was proposed in 1874 by van't Hoff and le Bel that the four bonds around carbon where not all in a plane but rather in a tetrahedral arrangement i.e. the four C-H bonds point towards the corners of a regular tetrahedron





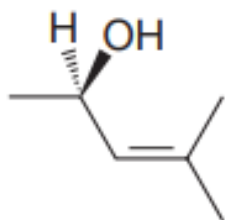
**Methane**

**Ethane**



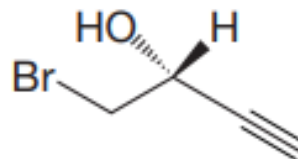
**Bromomethane**

- **Trigonal planar** arrangements of atoms can be drawn in 3-dimensions in the plane of the paper
  - Bond angles should be approximately **120°**
  - These can also be drawn **side-on** with the central bond in the plane of the paper, **one bond forward and one bond back**
- Linear arrangements of atoms are always best drawn in the plane of the paper



An example involving **trigonal planar geometry**

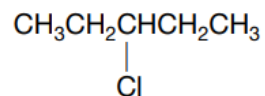
Bonds to the **carbon with the double bond** are in the plane of the paper and separated by **120°**.



An example involving **linear geometry**

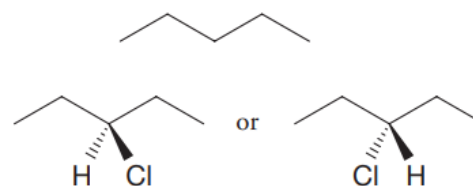
Bonds to the **carbon with the triple bond** are in the plane of the paper and separated by **180°**.

Write a bond-line formula for the following compound showing three dimensions at the carbon bearing the chlorine atom.



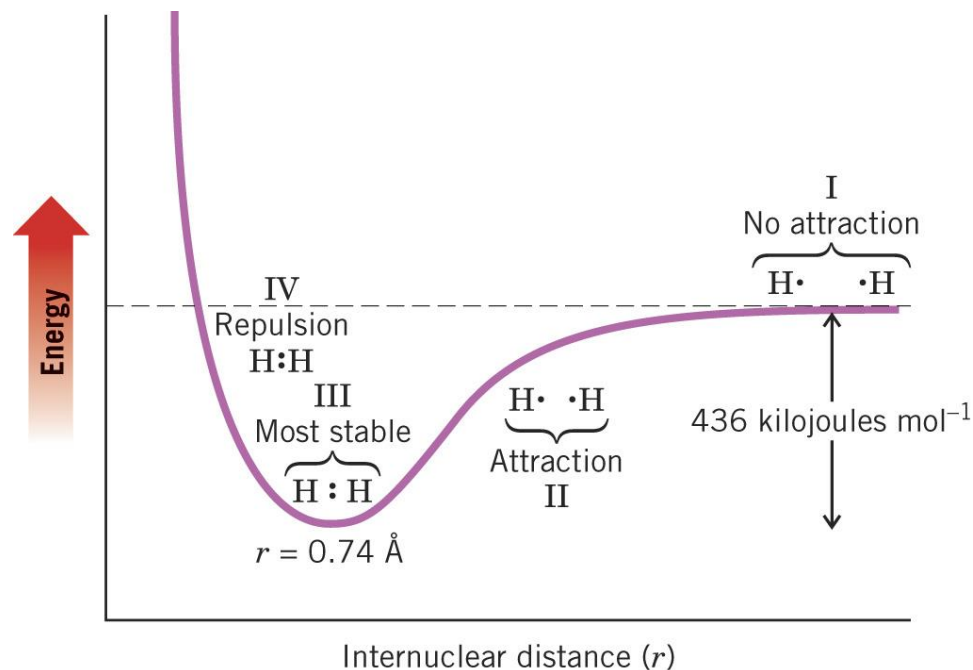
**STRATEGY AND ANSWER:** First draw the carbon skeleton, placing as many carbon atoms in the plane of the paper as possible (which is all of them, in this case).

Then add the chlorine atom at the appropriate carbon using a three-dimensional representation.



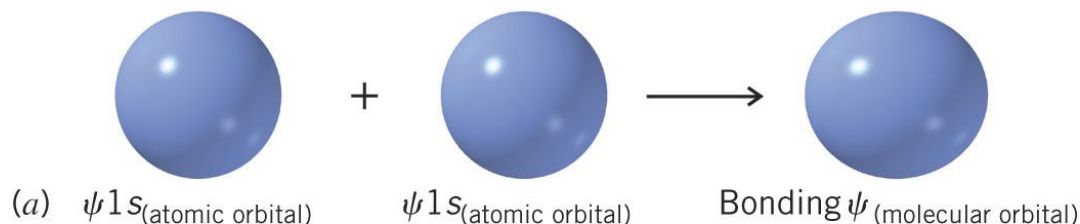
## ◆ Molecular Orbitals (MOs)

- A simple model of bonding is illustrated by forming molecular H<sub>2</sub> from H atoms and varying distance:
- Region I: The total energy of two isolated atoms
  - Region II: The nucleus of one atom starts attracting the electrons of the other; the energy of the system is lowered
  - Region III: at 0.74 Å the attraction of electrons and nuclei exactly balances repulsion of the two nuclei; this is the bond length of H<sub>2</sub>
  - Region IV: energy of system rises as the repulsion of the two nuclei predominates



## ● Bonding Molecular Orbitals ( $\Psi_{\text{molec}}$ )

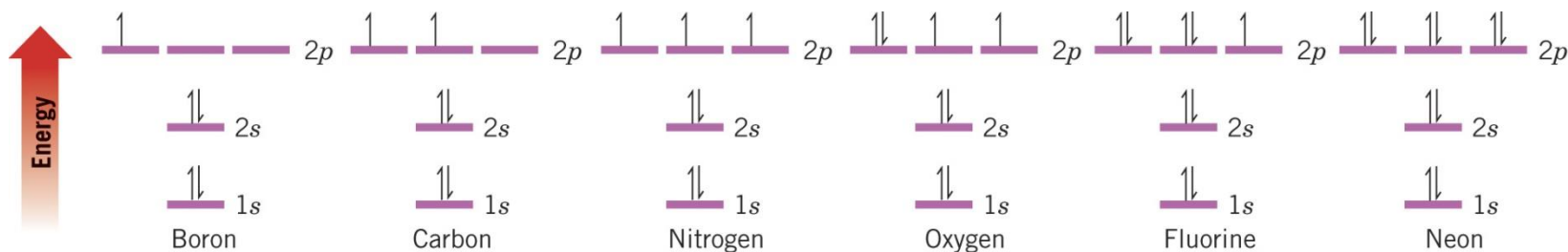
- AOs combine by addition (the AOs of the same phase sign overlap)
- The wave functions reinforce
- The value of  $\Psi$  increases between the two nuclei
- The value of  $\Psi^2$  (electron probability density) in the region between the two nuclei increases
- The two electrons between the nuclei serve to attract the nuclei towards each other
- This is the ground state (lowest energy state) of the MO



## ◆ Electron Configurations

- Atoms can be assigned <sup>تعیین</sup> electronic configuration using the following rules:

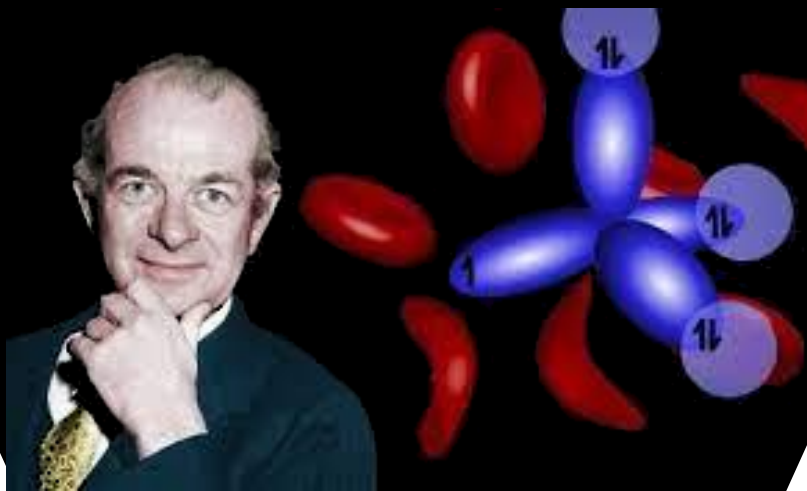
- <sup>اُچھے باؤ</sup> □ Aufbau Principle: The lowest energy orbitals are filled first
- <sup>استبعاد باؤی</sup> □ Pauli Exclusion Principle: A maximum of two spin paired electrons may be placed in each orbital
- <sup>ہارونڈ</sup> □ Hund's Rule: One electron is added to each degenerate (equal energy orbital) before a second electron is added
- Electronic Configurations of Some Second Row Elements



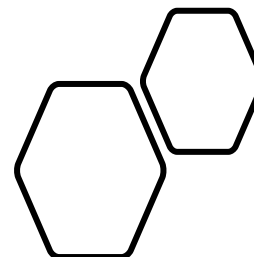
**Linus Carl Pauling**  
(February 28, 1901-August 19, 1994)

**Chemist Linus Carl Pauling first developed the hybridization theory in 1931 in order to explain the structure of simple molecules such as methane ( $\text{CH}_4$ ) using atomic orbitals.**

**Linus Carl Pauling was awarded the nobel prize in chemistry in 1954**



## ◆ Hybridization



# What is Hybridization?

It is the process of mixing and recasting atomic orbitals of the same atom with slightly different energies to form an equal number of new orbitals with equivalent energy, maximum symmetry and definite orientation in space.

إعدادة المدارات

وتماثلها

## Purposes of Hybridization:

To see the types of bonds that the atoms share with each other "Sigma or pi bonds"

$\sigma$

$\pi$

The difference types of bonds allow different properties.

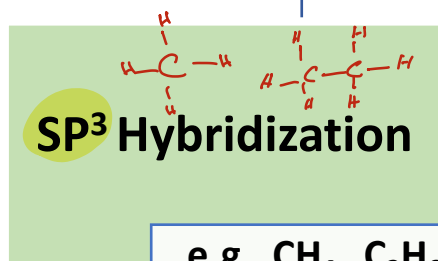
"How pi bonds do not allow rotation whereas sigma bonds are rotational"

بسم الله الرحمن الرحيم  
عنه ما يخلط

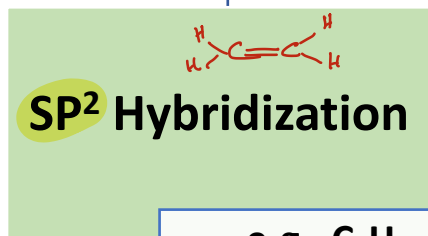
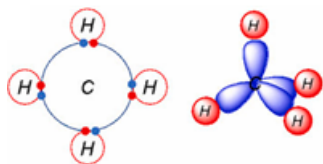
## Steps of Hybridization

- ✓ **Formation Of An Excited State :** No. Of unpaired electron in ground state of an atom is less than the observed valency of atom in its stable compd. Then one or more electron are uncoupled and promoted to the vacant orbitals of higher energy level.
- ✓ **Mixing And Recasting Of Atomic Orbital :** Mixing & redistribution of atomic orbital of the atom having same energy to form new orbital of equal energy.
- ✓ **Orientation Of Hybrid Orbitals :** Hybrid orbital orients themselves in a space in such a way that they minimize the inter electronic repulsion to acquire max. Stability.
- ✓ **Energy Of Orbitals :** Hybrid Orbitals Have Equivalent Energy And Differ Only In Orientation.

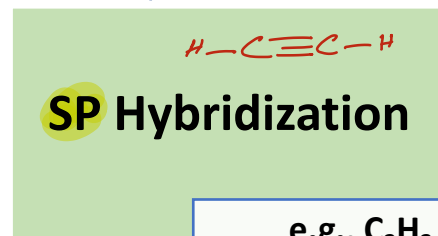
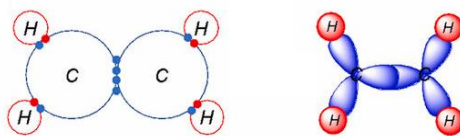
# Types of Hybridization



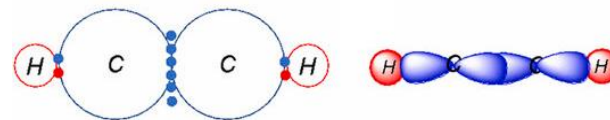
e.g., CH<sub>4</sub>, C<sub>2</sub>H<sub>6</sub>



e.g., C<sub>2</sub>H<sub>4</sub>

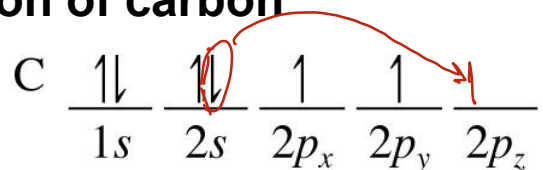


e.g., C<sub>2</sub>H<sub>2</sub>



## ◆ The Structure of Methane (CH<sub>4</sub>): sp<sup>3</sup> Hybridization

- The structure of methane with its four identical **tetrahedral** bonds cannot be adequately explained using the electronic configuration of carbon

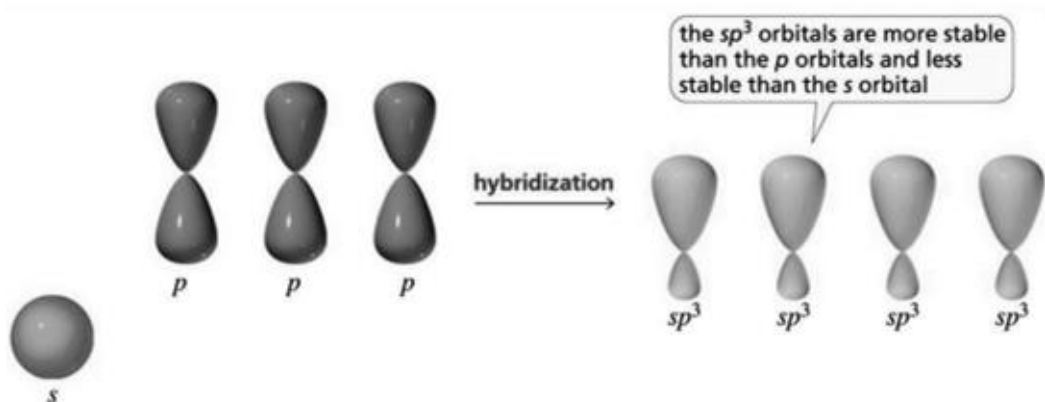


Ground state of a carbon atom

- Hybridization of the valence orbitals (2s and 2p) provides four new identical orbitals which can be used for the bonding in methane
- *Orbital hybridization* is a mathematical combination of the 2s and 2p wave functions to obtain wave functions for the new orbitals

- When one 2s orbital and three 2p orbitals are hybridized four new and identical  $sp^3$  orbitals are obtained
  - When four orbitals are hybridized, four orbitals must result
  - Each new orbital has one part s character and 3 parts p character
  - The four identical orbitals are oriented in a tetrahedral arrangements
- The four  $sp^3$  orbitals are then combined with the 1s orbitals of four hydrogens to give the molecular orbitals of methane
- Each new molecular orbital can accommodate 2 electrons

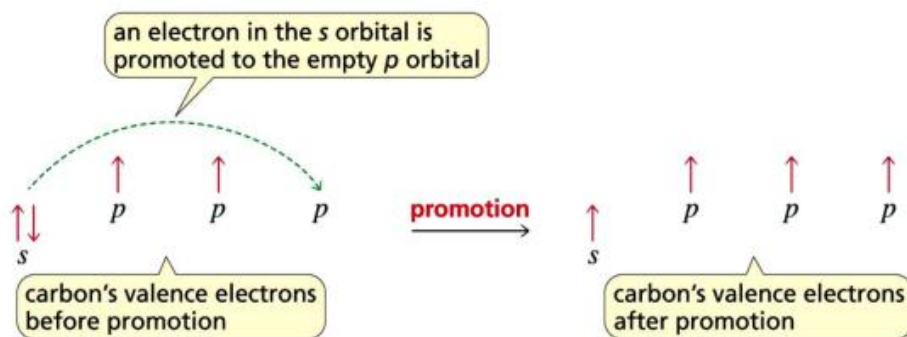
## The Carbon in Methane is $sp^3$



# The Structure of Methane (CH<sub>4</sub>): sp<sup>3</sup> Hybridization

The observed valency of carbon in methane is four and it has a bond angle of 109° with a tetrahedron geometry which can be explained on the basis of hybridization

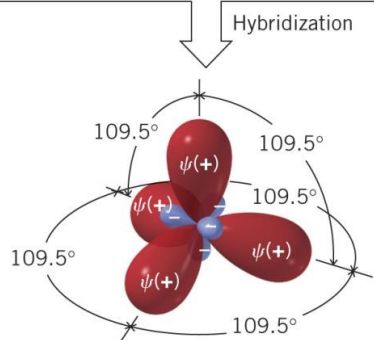
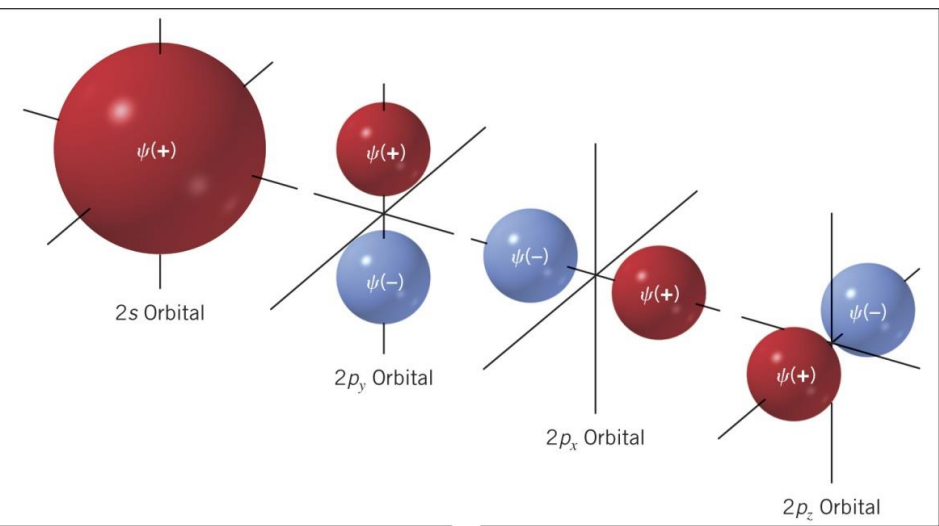
**In order to Form Four Bonds, Carbon Must Promote an Electron**



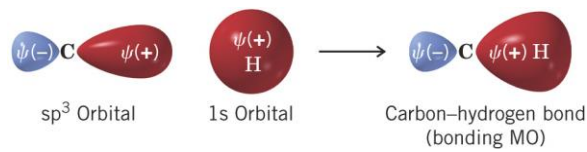
**Four Orbitals are Mixed to Form Four Hybrid Orbitals**



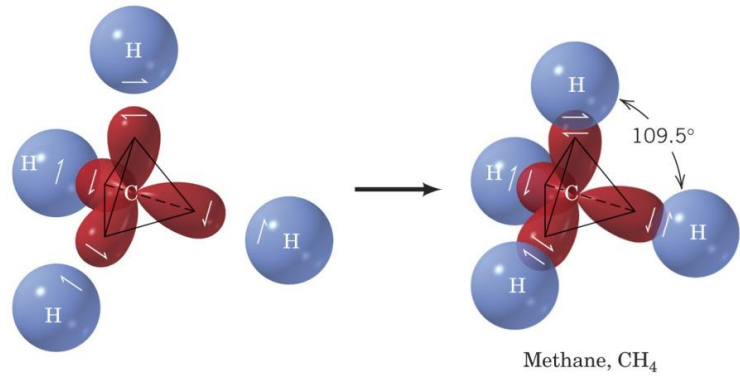
$$1s + 3p = 4 sp^3 \text{ orbitals}$$



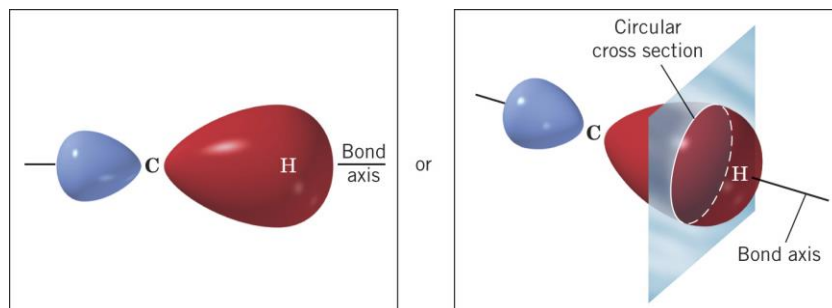
- An  $sp^3$  orbital looks like a p orbital with one lobe greatly extended
- Often the small lobe is not drawn
- The extended  $sp^3$  lobe can then overlap well with the hydrogen 1s to form a strong bond



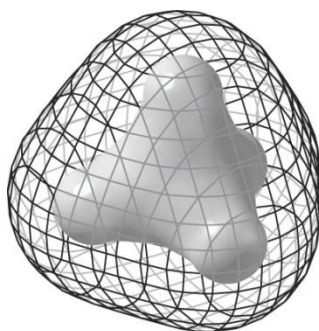
**Orbital Overlap:** each half filled hybrid orbital of carbon atom overlap axially with half filled 1s orbital of hydrogen atom containing electron with opposite spin thus the  $CH_4$  molecule is formed.



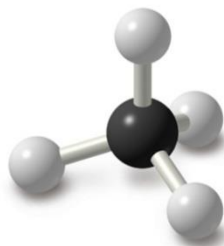
- The bond formed is called a **sigma ( $\sigma$ )** bond because it is circularly symmetrical in cross section when view along the bond axis



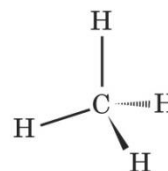
- A variety of representations of methane show its tetrahedral nature and electron distribution
  - a. calculated electron density surface b. ball-and-stick model
  - c. a typical 3-dimensional drawing



(a)



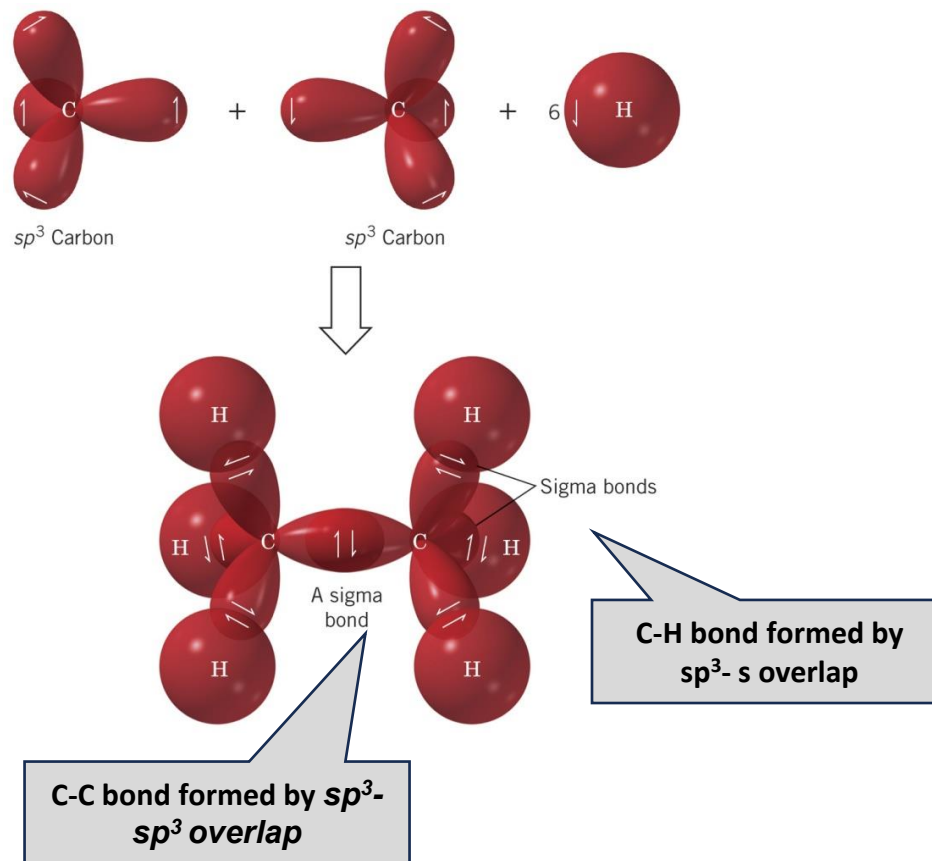
(b)



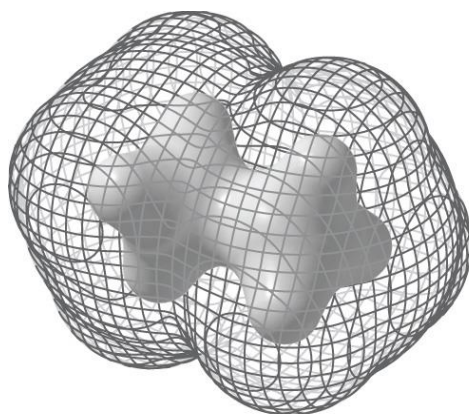
(c)

## ◆ The Structure of Ethane ( $\text{C}_2\text{H}_6$ ): $sp^3$ Hybridization

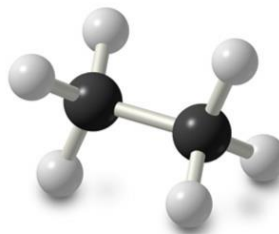
- The carbon-carbon bond is made from overlap of two  $sp^3$  orbitals to form a  $\sigma$  bond
- The molecule is approximately tetrahedral around each carbon



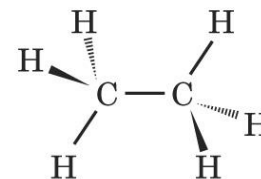
- The representations of ethane show the tetrahedral arrangement around each carbon
  - a. calculated electron density surface    b. ball-and-stick model
  - c. typical 3-dimensional drawing



(a)



(b)

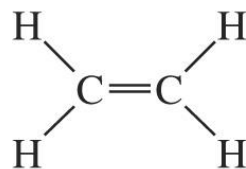


(c)

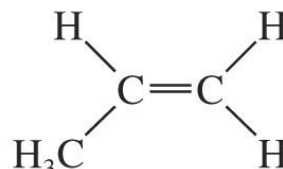
- Generally there is relatively free rotation about  $\sigma$  bonds
  - Very little energy (13-26 kcal/mol) is required to rotate around the carbon-carbon bond of ethane

## ◆ The Structure of Ethene (Ethylene) : $sp^2$ Hybridization

- Ethene ( $C_2H_4$ ) contains a carbon-carbon double bond and is in the class of organic compounds called *alkenes*
  - Another example of the alkenes is propene

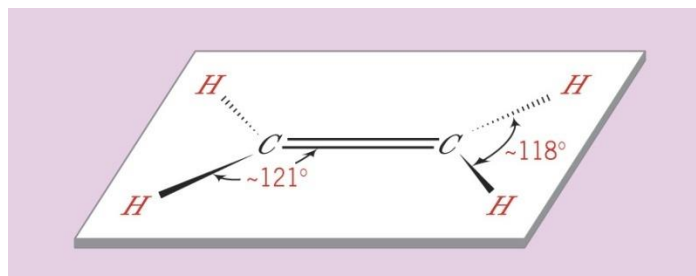


Ethene



Propene

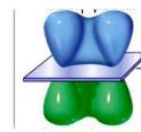
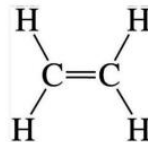
- The geometry around each carbon is called *trigonal planar*
  - All atoms directly connected to each carbon are in a plane
  - The bonds point **towards** the corners of a **regular triangle**
  - The bond angle are approximately  $120^\circ$



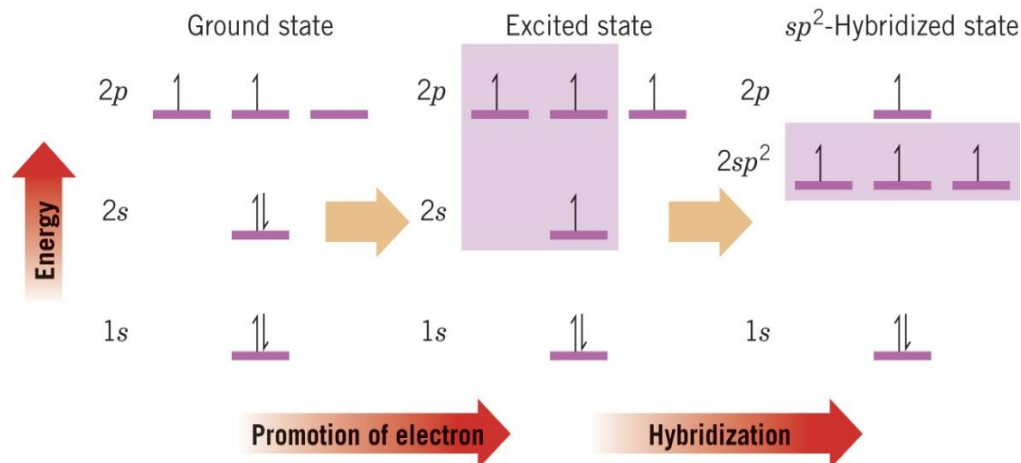
The observed valency of carbon in ethene is four and it has a bond angle of  $120^\circ$  with a trigonal geometry which can be explained on the basis of hybridization

Ethene (Ethylene): double bond

double bond =  $\sigma$  bond +  $\pi$  bond



need a  $p$  orbital!



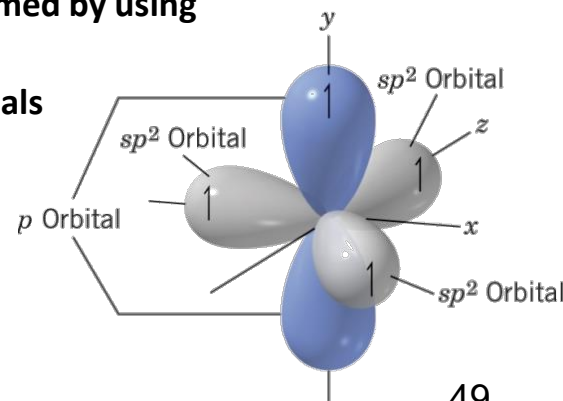
An unhybridized  $P$  orbital  
3 hybrid orbitals are formed



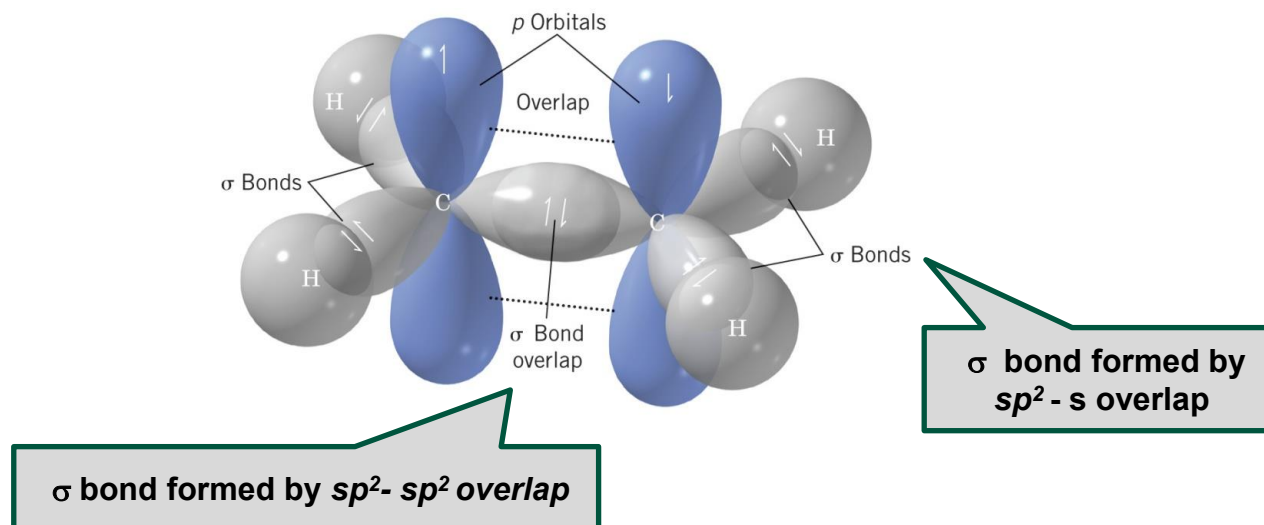
three orbitals are hybridized  
(one  $2s$  + two  $2p$  = three  $sp^2$  orbitals)

Carbon bonds to 3 atoms, so it needs to hybridize 3 atomic orbitals.

- There are **three  $\sigma$  bonds** around each carbon of ethene and these are formed by using  $sp^2$  hybridized orbitals
- The three  $sp^2$  hybridized orbitals come from mixing one  $s$  and two  $p$  orbitals
  - One  $p$  orbital is left unhybridized
- The  $sp^2$  orbitals are arranged in a **trigonal planar** arrangement
  - The  $p$  orbital is perpendicular (orthogonal) to the plane

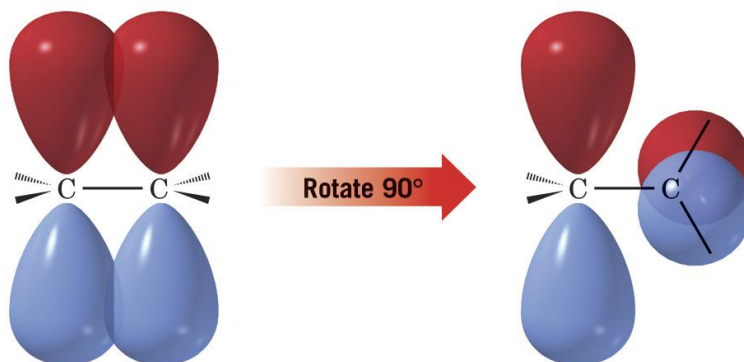


- **Overlap of  $sp^2$  orbitals in ethylene results in formation of a  $\sigma$  framework**
  - **One  $sp^2$  orbital on each carbon overlaps to form a carbon-carbon  $\sigma$  bond; the remaining  $sp^2$  orbitals form bonds to hydrogen**
- **The leftover  $p$  orbitals on each carbon overlap to form a bonding  $\pi$  bond between the two carbons**
- **A  $\pi$  bond results from overlap of  $p$  orbitals above and below the plane of the  $\sigma$  bond**
  - **It has a nodal plane passing through the two bonded nuclei and between the two lobes of the  $\pi$  molecular orbital**



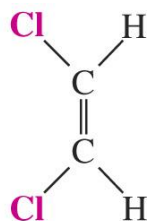
## ● Restricted Rotation and the Double Bond

- There is a large energy barrier to rotation (about 264 kJ/mol) around the double bond
  - This corresponds to the strength of a  $\pi$  bond
  - The rotational barrier of a carbon-carbon single bond is 13-26 kJ/mol
- This rotational barrier results because the  $p$  orbitals must be well aligned for maximum overlap and formation of the  $\pi$  bond
- Rotation of the  $p$  orbitals  $90^\circ$  totally breaks the  $\pi$  bond

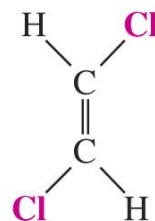


## ● Cis-trans isomers

- Cis-trans isomers are the result of restricted rotation about **double bonds**
- These isomers have the same connectivity of atoms and differ only in the arrangement of atoms in space
  - This puts them in the broader class of stereoisomers
- The molecules below do not *superpose* on each other
- One molecule is designated *cis* (groups on same side) and the other is *trans* (groups on opposite side)

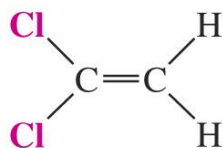


*cis*-1,2-Dichloroethene

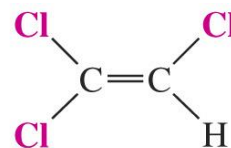


*trans*-1,2-Dichloroethene

- **Cis-trans isomerism is not possible if one carbon of the double bond has two identical groups**

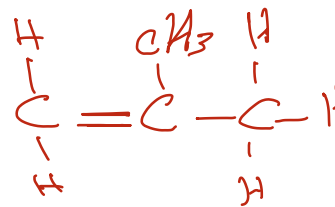
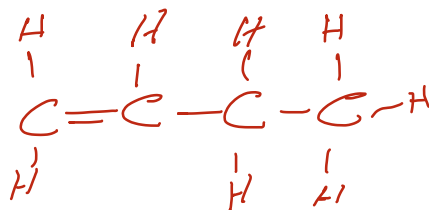


1,1-Dichloroethene  
(no *cis-trans* isomerism)



1,1,2-Trichloroethene  
(no *cis-trans* isomerism)

# Quick QUESTION



## PRACTICE PROBLEM 1.22

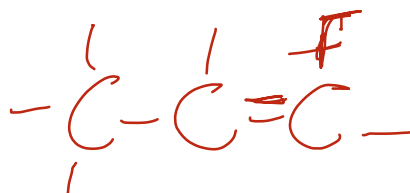
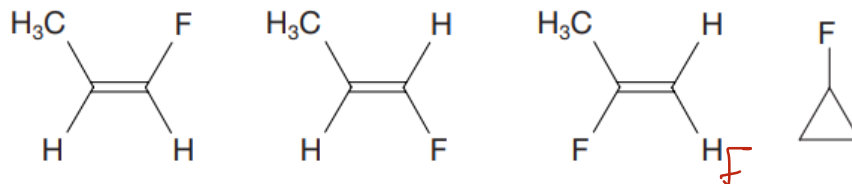
Which of the following alkenes can exist as **cis-trans isomers**? Write their structures. Build hand-held models to prove that one isomer is not superposable on the other.

- (a)  $\text{CH}_2=\text{CHCH}_2\text{CH}_3$     (c)  $\text{CH}_2=\text{C}(\text{CH}_3)_2$   
 (b)  $\text{CH}_3\text{CH}=\text{CHCH}_3$     (d)  $\text{CH}_3\text{CH}_2\text{CH}=\text{CHCl}$

## SOLVED PROBLEM 1.12

Write structures of all the isomers of  $\text{C}_3\text{H}_5\text{F}$ .

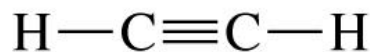
**ANSWER:** Taking into account cis-trans isomerism and the possibility of a ring we have the following four possibilities.



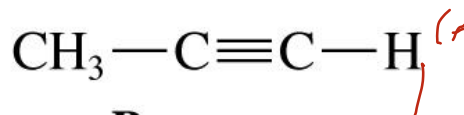


## ◆ The Structure of Ethyne (Acetylene): sp Hybridization

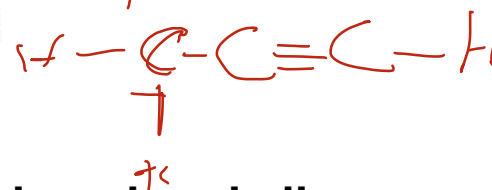
- Ethyne (acetylene) is a member of a group of compounds called alkynes which all have carbon-carbon triple bonds
  - Propyne is another typical alkyne



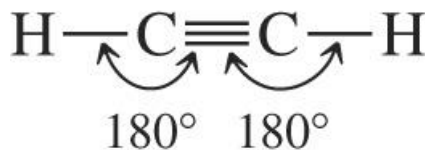
Ethyne  
(acetylene)  
(C<sub>2</sub>H<sub>2</sub>)



Propyne  
(C<sub>3</sub>H<sub>4</sub>)



- The arrangement of atoms around each carbon is linear with bond angles 180°

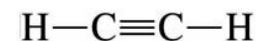


The observed valency of carbon in ethyne is four and it has a bond angle of  $180^\circ$  with a linear geometry which can be explained on the basis of hybridization

## Ethyne (Acetylene)

triple bond =  $\sigma$  bond +  $2\pi$

bond



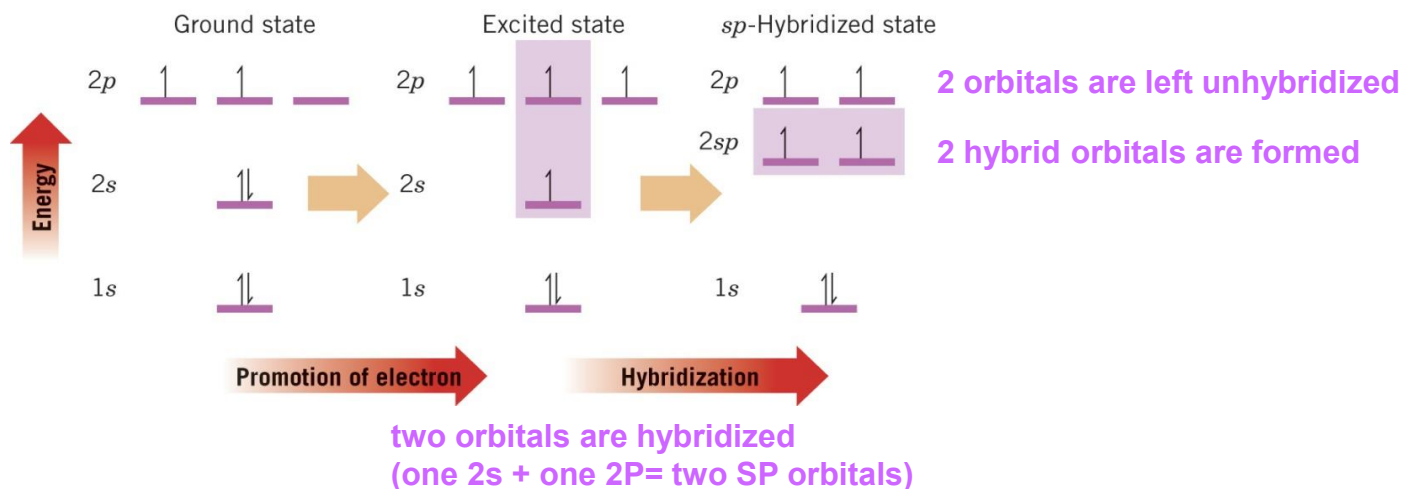
need 2 *p* orbitals!

□ The carbon in ethyne is *sp* hybridized

□ One *s* and one *p* orbital are mixed to form two *sp* orbitals

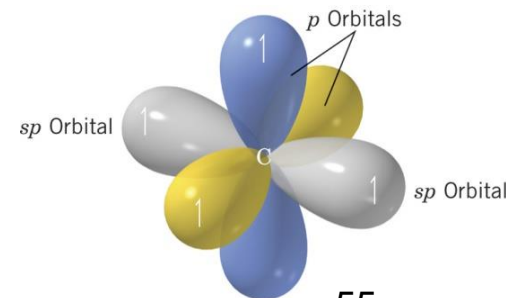
□ Two *p* orbitals are left unhybridized

Carbon bonds to 2 atoms, so it needs to hybridize 2 atomic orbitals.

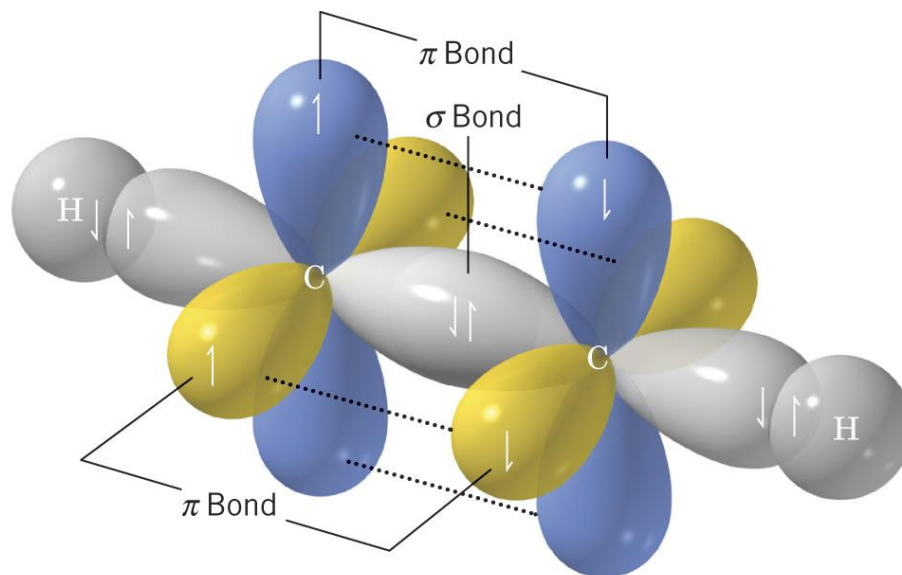


□ The two *sp* orbitals are oriented  $180^\circ$  relative to each other around the carbon nucleus

□ The two *p* orbitals are perpendicular to the axis that passes through the center of the *sp* orbitals



- In ethyne the  $sp$  orbitals on the two carbons overlap to form a  $\sigma$  bond
  - The remaining  $sp$  orbitals overlap with hydrogen  $1s$  orbitals
- The  $p$  orbitals on each carbon overlap to form two  $\pi$  bonds
- The triple bond consists of one  $\sigma$  and two  $\pi$  bonds

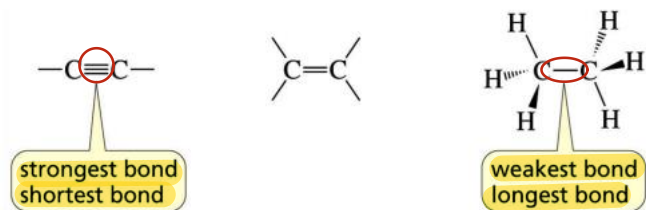


## ◆ Bond Lengths of Ethyne, Ethene and Ethane

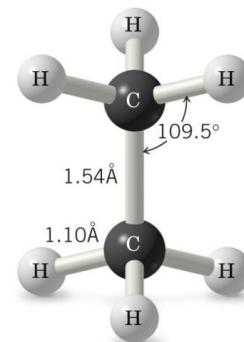
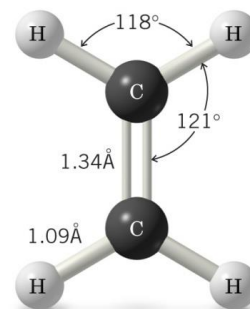
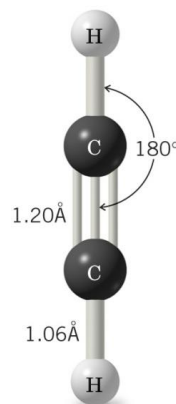
- The carbon-carbon bond length is shorter as more bonds hold the carbons together
  - With more electron density between the carbons, there is more “glue” to hold the nuclei of the carbons together
- The carbon-hydrogen bond lengths also get shorter with more s character of the bond
  - 2s orbitals are held more closely to the nucleus than 2p orbitals
  - A hybridized orbital with more percent s character is held more closely to the nucleus than an orbital with less s character
  - The  $sp$  orbital of ethyne has 50% s character and its C-H bond is shorter
  - The  $sp^3$  orbital of ethane has only 25% s character and its C-H bond is longer

## Bond Strength and Bond Length

The **more bonds** holding 2 atoms together, the **stronger** and **shorter** it is.



**Bond strength decreases as bond length increases**

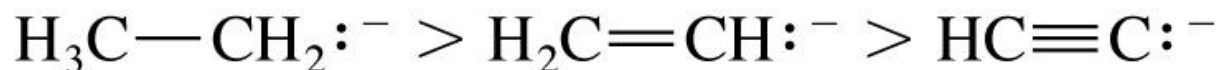
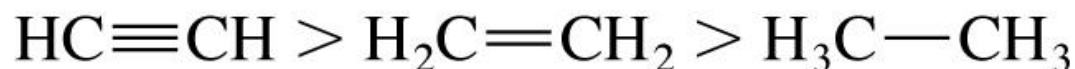


## ◆ The Effect of Hybridization on Acidity

- Hydrogens connected to orbitals with more *s* character will be more acidic

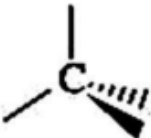
□ *s* orbitals are smaller and closer to the nucleus than *p* orbitals

□ ← انيون Anions in hybrid orbitals with more *s* character will be held more closely to the nucleus and be more stabilized



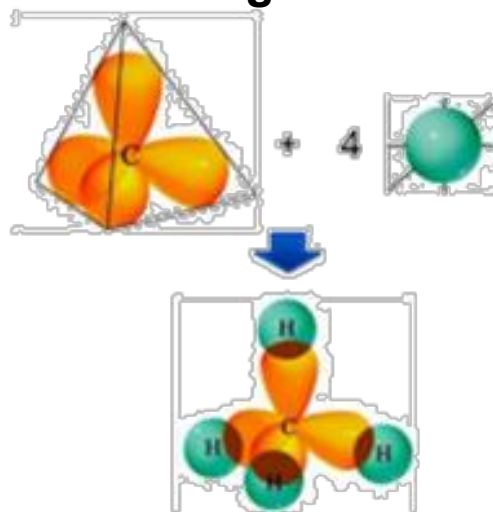
# Summary of Hybridization

- The number of molecular orbitals formed equals the number of the atomic orbitals used
- Hybridized orbitals are obtained by mixing the wave functions of different types of orbitals
  - **Four  $sp^3$**  orbitals are obtained from mixing **one s and three p orbitals**
    - The geometry of the four orbitals is **tetrahedral**
    - This is the hybridization used in the carbon of methane
  - **Three  $sp^2$**  orbitals are obtained from mixing **one s and two p orbitals**
    - The geometry of the three orbitals is **trigonal planar**
    - The left over *p* orbital is used to make a  $\pi$  bond
    - This is the hybridization used in the carbons of ethene
  - **Two  $sp$**  orbitals are obtained from mixing **one s and one p orbital**
    - The geometry of the two orbitals is **linear**
    - The two leftover *p* orbitals are used to make two  $\pi$  bonds
    - This is the hybridization used in the carbons of ethyne
  - **Sigma ( $\sigma$ )** bonds have circular symmetry when viewed along the bond axis
  - **Pi ( $\pi$ )** bonds result from sideways overlap of two *p* orbitals

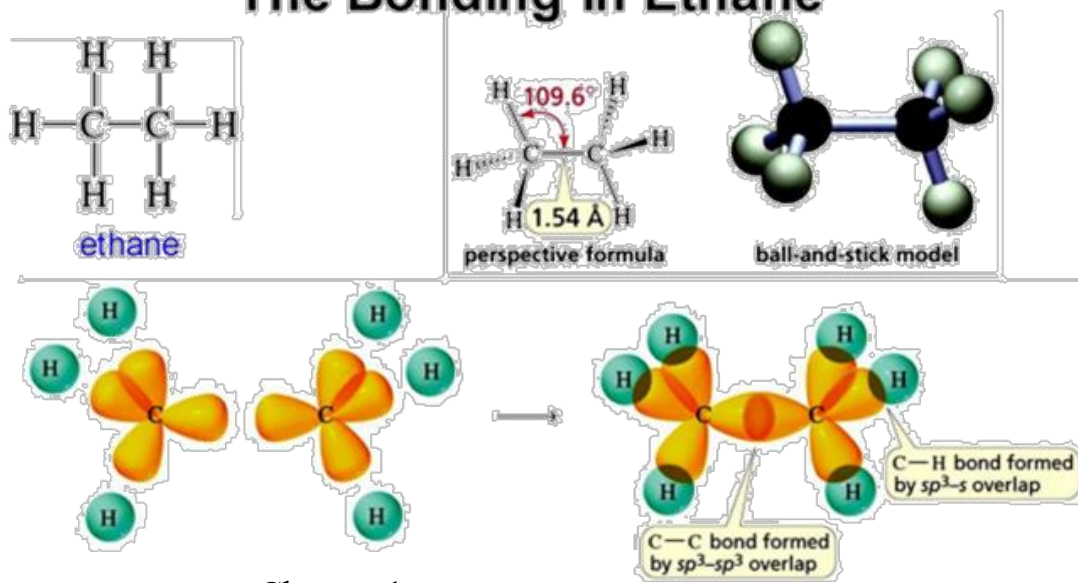
| Type of hybrid                   | sp <sup>3</sup> hybridization                                                      | sp <sup>2</sup> hybridization                                                       | sp hybridization                                                                    |
|----------------------------------|------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|-------------------------------------------------------------------------------------|
| Diagram                          |  |  |  |
| Atomic orbitals used             | s, p, p, p                                                                         | s, p, p                                                                             | s, p                                                                                |
| Orbitals Combined                | s-orbital + 3 p-orbitals                                                           | s-orbital + 2 p-orbitals                                                            | s-orbital + 1 p-orbital                                                             |
| Resulting Orbitals               | 4 sp <sup>3</sup> orbitals (no p-orbitals)                                         | 3 sp <sup>2</sup> orbitals + 1 p-orbital                                            | 2 sp orbitals + 2 p-orbitals                                                        |
| Number of hybrid orbitals formed | 4                                                                                  | 3                                                                                   | 2                                                                                   |
| Number of atoms bonded to the C  | 4                                                                                  | 3                                                                                   | 2                                                                                   |
| Geometry                         | tetrahedral                                                                        | triangular planer                                                                   | Linear                                                                              |
| angle                            | 109.5°                                                                             | 120°                                                                                | 180°                                                                                |
| Bonds                            | single bonds                                                                       | double bonds                                                                        | triple bonds                                                                        |

# Summary

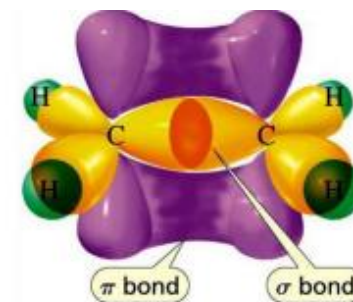
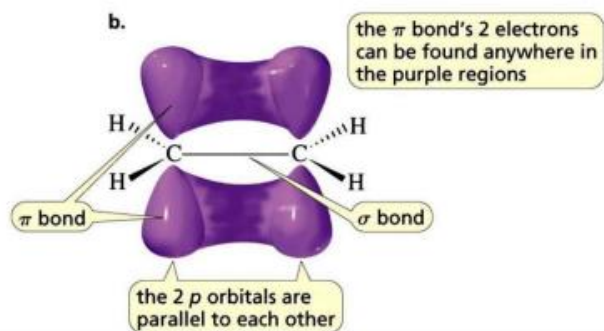
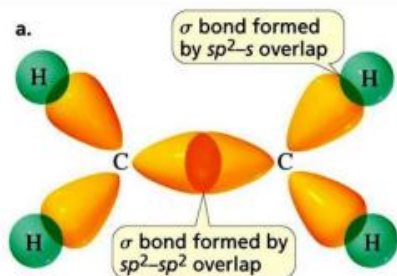
## The Bonding in Methane



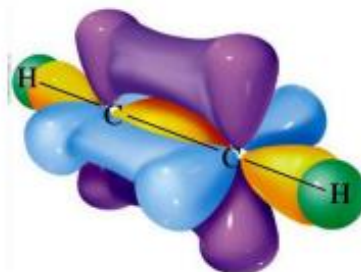
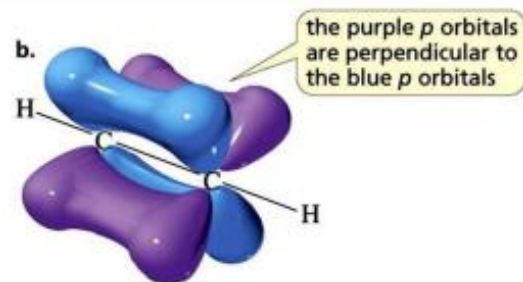
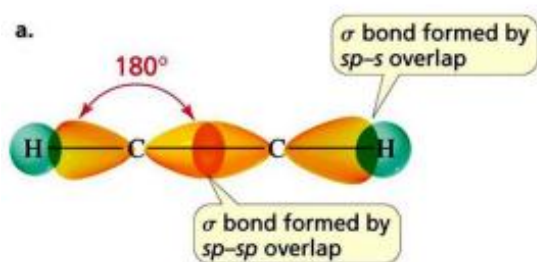
## The Bonding in Ethane



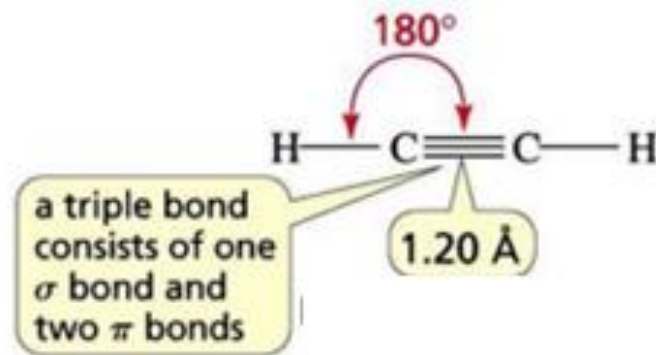
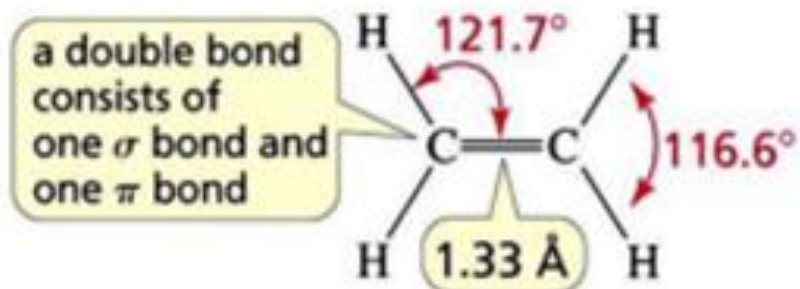
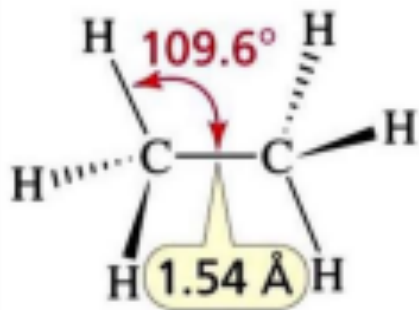
## The Bonding in Ethene



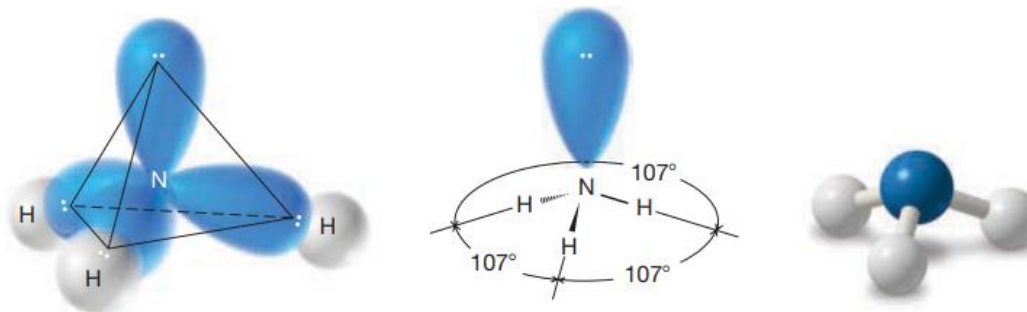
## The Bonding in Ethyne



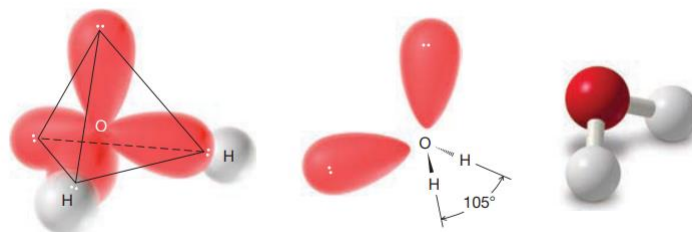
# Summary



## ◆ Geometry of Ammonia $\text{NH}_3$ , Water $\text{H}_2\text{O}$ and Carbon Dioxide $\text{CO}_2$



**Trigonal pyramid**



**Angular or bent shape**

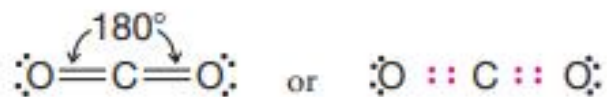
What do the bond angles of ammonia suggest about the hybridization state of the nitrogen atom of ammonia?

● **PRACTICE PROBLEM 1.23**

What do the bond angles of water suggest about the hybridization state of the oxygen atom of water?

● **PRACTICE PROBLEM 1.24**

## Carbon dioxide

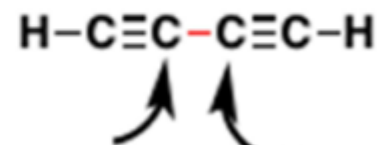
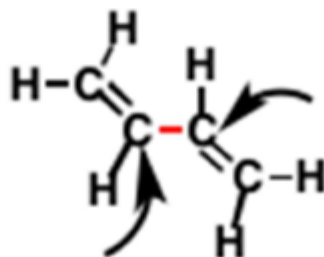
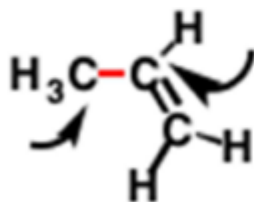
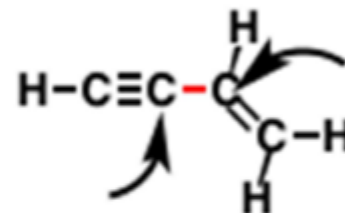
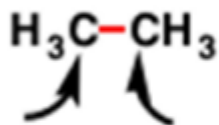


The four electrons of each double bond act as a single unit and are maximally separated from each other.



## Practice

### Some examples



# Group Activity In BB (8 threads)

Chapter 1

Tasks

Student Mark 12



Condensed structure and molecular formula

2

Q 1.33 a-d



Q 1.34 a-d



3D structure

1

Q 1.17 a-d



Bond-line structure

1

Q 1.36 a-f



Bond-line and constitutional isomer

2

Q 1.14 a-h



Q 1.15 a-h



\*Bond-line, condensed structures and constitutional isomer

2

Q 1.49 a-d



Each student choose 2 points one line bond and one condensed structures

constitutional isomer

1

Q 1.35 a-p



Resonance and constitutional isomer

1

Q 1.50 a-f



Resonance

2

Q 1.20 a-f



Q 1.41 a-i



Total

/76

/8

/4

/6

/11

/8

/16

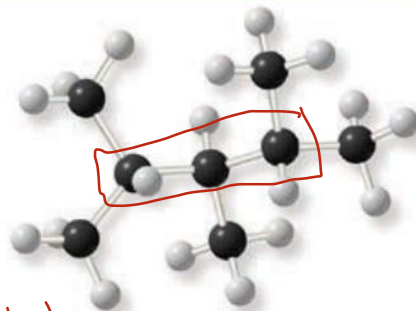
/6

/17

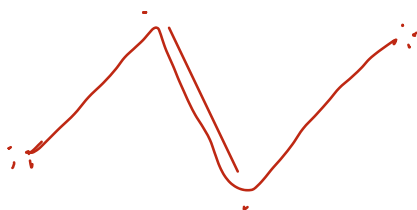
# Practice

● PRACTICE PROBLEM 1.13

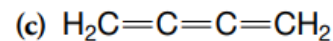
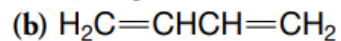
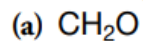
Write a condensed structural formula for the following compound.



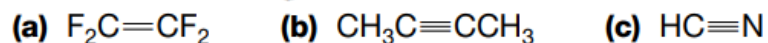
**1.37** Write bond-line formulas for all of the constitutional isomers with the molecular formula  $C_4H_8$ .



**1.46** Draw a three-dimensional orbital representation for each of the following molecules, indicate whether each bond in it is a  $\sigma$  or  $\pi$  bond, and provide the hybridization for each non-hydrogen atom.



Predict the bond angles of



● PRACTICE PROBLEM 1.28