Name ______________________________

Lesson 1: Structure and bonding

Lesson one explores the fundamental concepts in chemistry related to the structure and bonding of atoms and molecules. Topics include the properties of atoms and valence electrons, hybridization and the formation of sigma and pi bonds, and the geometry and properties of molecules. Building models of organic molecules like methane, ethene, and ethyne, allow students to observe the relationship between hybridization and bond geometry. With the help of molecular modeling kits and online resources like Khan Academy, it is possible to visualize and understand the three-dimensional structures of molecules and their bonding patterns.

THINK! What are valence electrons and why are they important in chemical bonding?

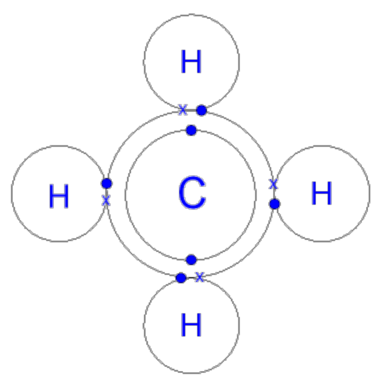
Valence electrons are the electrons in the outermost shell of an atom that are involved in chemical bonding. Atoms tend to form bonds with other atoms to achieve a more stable electron configuration, typically by gaining, losing, or sharing electrons. The valence electrons play a crucial role in this process because they are the electrons that are most available for bonding.

Go to https://www.khanacademy.org/science/organic-chemistry.
Watch the videos on Dot structures.

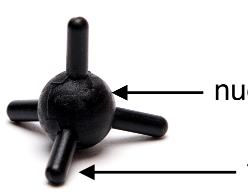
We will begin with a very simple molecule, methane, CH_4. Methane is in a group of molecules called the alkanes. Alkanes are hydrocarbons, compounds that contain only single bonds between the carbon and hydrogen atoms.

The carbon atom has six electrons represented by blue dots. Four electrons are valence electrons because they are in the second shell (or energy level) and are available to bond with the hydrogen atoms.

Lewis Structure of Methane, CH_4



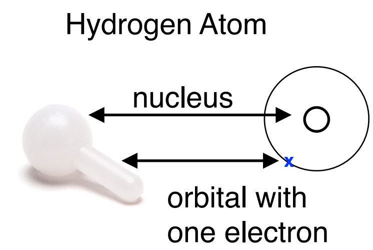
Carbon Atom



nucleus and two core electrons

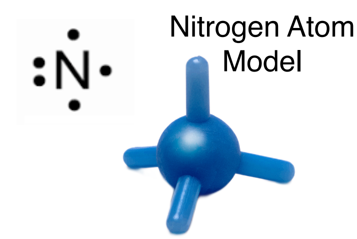
four orbitals with one valence electron in each orbital

Each hydrogen atom has one valence electron represented with a blue X in the Lewis structure. The hydrogen atom will be represented by a white model with a single orbital. Always use a 25 mm gray bond to join a hydrogen atom in a molecule.

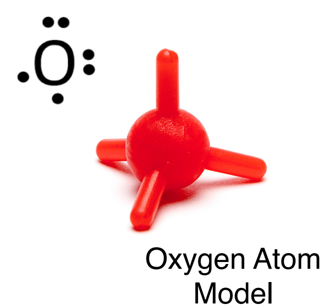


1. Build a model of methane, CH_4, the chief component of natural gas. How many electrons surround the carbon atom?

2. Nitrogen has five valence electrons located in four orbitals. Three of the orbitals have only one electron and will form covalent bonds with other atoms to achieve a more stable configuration. Build a model of methylamine, CH_3NH_2. Use a 40 mm gray or black bond between carbon and nitrogen atoms. When the structure is complete, how many unshared pairs of electrons are present on the nitrogen atom?



3. Oxygen has six valence electrons located in four orbitals. Build a model of methanol, CH_3OH. Use a 40 mm gray or black bond between carbon and oxygen atoms. Carbon and oxygen atoms follow the octet rule. How many unshared pairs of electrons are present on the oxygen atom?



THINK! What is hybridization and why is it important in chemical bonding?

Hybridization is defined as the concept of mixing two atomic orbitals to give rise to new types of orbitals called hybrid orbitals. This intermixing usually results in the formation of hybrid orbitals having entirely different energy and shapes. Hybridized orbitals lead to greater overlap when forming bonds. Hybridization results in stronger bonds and more stable compounds.

Go to https://www.khanacademy.org/science/organic-chemistry.
Watch the videos on Hybridization.

Hybridization occurs only during the bond formation and not in an isolated gaseous atom. Not all half-filled orbitals in an atom must participate in hybridization. Some half-filled orbitals may remain unhybridized. Finally, the number of hybrid orbitals formed always equals the number of atomic orbitals mixed.

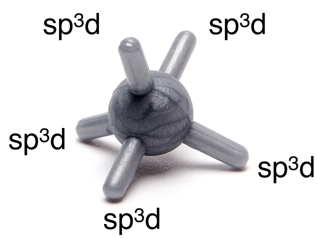
The Geometries of Hybrid Atomic Orbitals

Two hybrid sp orbitals are oriented in a linear geometry with a bond angle of 180^{o}.

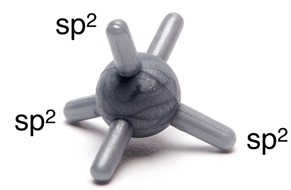
Three hybrid sp^2 orbitals are oriented in a planar triangular shape with bond angles of 120^{o}.

Four hybrid sp^3 orbitals are oriented in a tetrahedral arrangement with bond angles of 109.5^{o}.

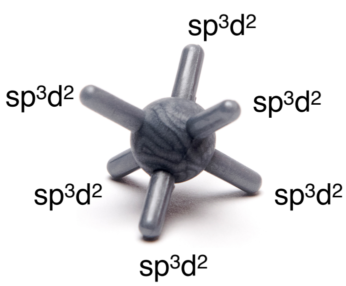
Five sp^3d hybrid orbitals are oriented in a trigonal bipyramidal geometry with bond angles of 90^{o} and 120^{o}.



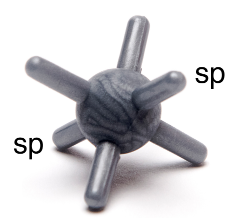
The hybridization used in forming a double bond is three sp^2 hybrid orbitals and one unhybridized p orbital.



Six sp^3d^2 hybrid orbitals are oriented in an octahedral shape with bond angles of 90^{o}.



The hybridization used in forming a triple bond (or two double bonds) is two sp hybrid orbitals and two unhybridized p orbitals.



4. What hybrid orbitals are used by the oxygen atom in methanol, CH_3OH?

5. What hybrid orbitals are used by the carbon atoms in acetylene, $HC{\equiv}CH$?

6. What hybrid orbitals are used by the carbon atoms in ethene, $H_2C{=}CH_2$?

THINK! What is the difference between a sigma bond and a pi bond?

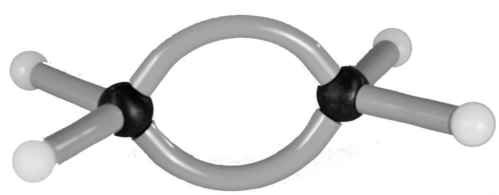
A sigma bond is a bond formed by the overlap of orbitals in an end-to-end fashion, with the electron density concentrated between the nuclei of the bonding atoms. Sigma bonds are the strongest type of chemical covalent bond. A pi bond is a bond formed by the overlap of orbitals in a side-by-side fashion with the electron density concentrated above and below the plane of the nuclei of the bonding atoms.

7. Build a model of ethane, C_2H_6. Use a 40 mm black bond between carbon atoms. All of the bonds in ethane are sigma bonds. Observe the rotation around the single bond between carbon atoms. How many sigma bonds are in ethane?

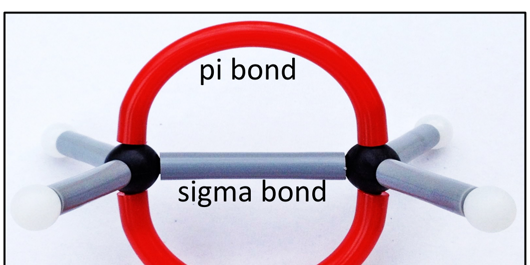
Alkenes are hydrocarbons that have at least one C=C double bond in their structure. A double bond has one sigma bond and one pi bond. The double bond in ethene (also called ethylene), C_2H_4, can be constructed in two ways.

Method 1: Two carbon models with four sp^3 orbitals are connected using two 51 mm gray links as shown to the right. The ethene molecule has one double bond and four single bonds. This method illustrates the planarity of the molecule and prevents rotation around the double bond.

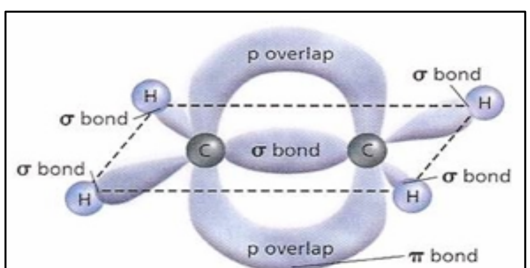
Ethene



Method 2: Select carbon atoms with three sp^2 orbitals and one unhybridized p orbital when forming a double bond. Use a 40 mm gray bond to represent the sigma bond between the nuclei of the carbon atoms. As shown below, the pi bond is constructed using two long (83 mm) red bonds to connect the adjacent unhybridized p orbitals. This method clearly distinguishes between sigma and pi bonds and shows the correct hybridization around the carbon atom.



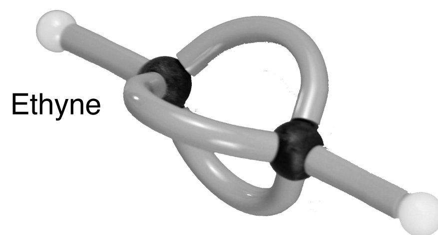
Ethene



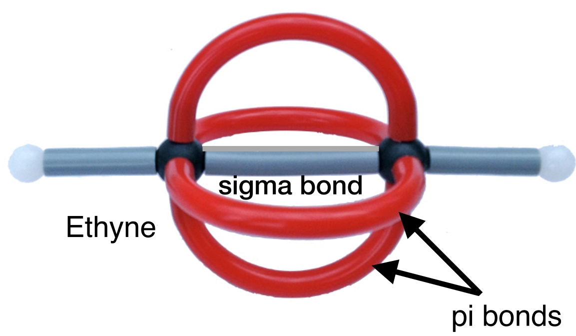
Ethene

Alkynes are hydrocarbons that have at least one triple bond. Triple bonds (one sigma and two pi bonds) can also be constructed in two different ways.

Method 1: Build ethyne (also called acetylene), C_2H_2. Two carbon models with four sp^3 orbitals are connected using three 51 mm gray bonds. This method illustrates the planarity of the molecule.



Method 2: Carbon will hybridize to form two sp orbitals and two unhybridized p orbitals when forming a triple bond. The molecule of acetylene has three sigma bonds and two pi bonds. This method clearly distinguishes between sigma and pi bonds and shows the correct hybridization around the carbon atom.



Identify the type of hybridization for the carbon atom in each molecule. Write the geometry and the bond angle around the carbon atom.

Molecule	Hybridization	Geometry	Bond Angle
8. methane			
9. acetylene			
10. ethene			
11. methanol			
12. methylamine			

Keep the methane model. Disassemble the other molecules!

THINK! What are bond-line structures?

> Bond-line notation is a convention used by organic chemists to represent molecular structures. A bond between two atoms is depicted as a line. Only non-carbon and non-hydrogen atoms are specifically depicted.

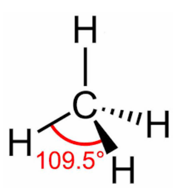
Go to https://www.khanacademy.org/science/organic-chemistry
Watch the videos on Bond-line structures.

13. Build and draw the bond-line structure for 2-propanol, CH_3CHCH_3 (with OH on the central carbon)

$$\begin{array}{c} CH_3\underset{\displaystyle |}{C}HCH_3 \\ \quad OH \end{array}$$

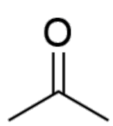
14. Look at the models of methane and 2-propanol. Both molecules are three-dimensional. To draw the 3-D structure of an organic compound, you can use wedge-dash representation. A bond that protrudes out of the plane of paper towards the viewer is denoted by a solid wedge. A bond that projects away from the viewer or into the plane of the paper is denoted by a dashed wedge and the bond in the plane of the paper is represented by a line. The 3-D bond-line structure for methane is shown below. Draw the 3-D bond-line structure for 2-propanol.

3-D Bond-line Structure
for Methane



15. Build a model of acetone. Are the carbon atoms in this structure in the same plane? Draw the thee-dimensional bond-line structure for acetone. Identify the hybridization of each carbon atom in the structure.

Bond-line Structure
for Acetone



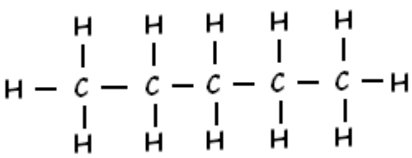
Disassemble the molecules!

THINK! How can the structure of a molecule affect its physical and chemical properties?

One of the interesting aspects of organic chemistry is that molecules have a definite three-dimensional geometry. The types of atoms and bonds present in the molecule and the size of the molecule determine its reactivity, stability, and other chemical properties. The distribution of electrons within a molecule effects the strength and type of intermolecular forces which effects its polarity and determines the boiling and melting points, solubility, and other physical properties of a molecule.

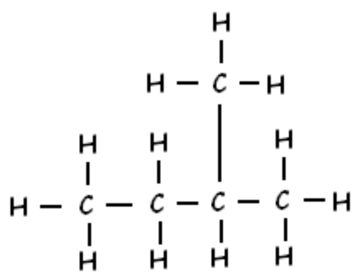
Go to https://www.khanacademy.org/science/organic-chemistry
Watch the videos on Electronegativity.

16. Structural isomers are molecules that have the same molecular formula, but have a different arrangement of the atoms in space. All of the isomers of pentane, C_5H_{12} are non-polar molecules. London dispersion forces exist between the molecules. Look at the bond-line structures of pentane and determine the effect of branching on the boiling point of the molecules?



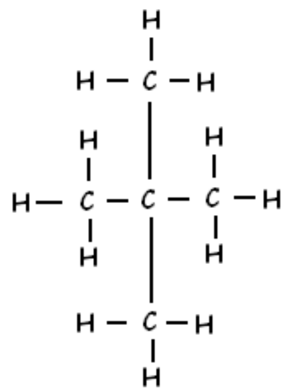
n-pentane

BP = 36 °C



Iso-pentane

BP = 28 °C

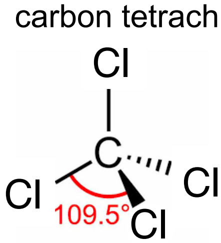


Neo-pentane

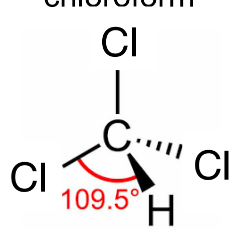
BP = 10 °C

17. Electronegativity is the power of an atom in a molecule to attract electrons to itself. Build models of the molecules, carbon tetrachloride, chloroform, and water. Use the electronegativity table to determine the bond polarity and the molecular polarity of each molecule. Order the molecules from least to greatest molecular polarity. Explain your rankings.

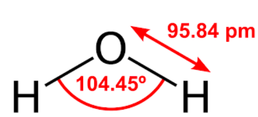
carbon tetrachloride



chloroform

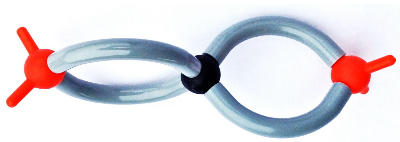


water

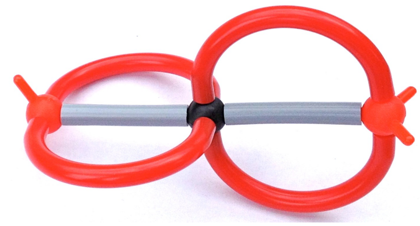


18. Build a model of carbon dioxide, CO_2. Use the electronegativity table to determine the bond polarity and the molecular polarity. Explain how a molecule with polar covalent bonds can be a non-polar molecule.

Method 1
CO_2.



Method 2
CO_2



Electronegativity values of the elements

H 2.1																	He
Li 1.0	Be 1.5											B 2.0	C 2.5	N 3.0	O 3.5	F 4.0	Ne
Na 0.9	Mg 1.2											Al 1.5	Si 1.8	P 2.1	S 2.5	Cl 3.0	Ar
K 0.8	Ca 1.0	Sc 1.3	Ti 1.5	V 1.6	Cr 1.6	Mn 1.5	Fe 1.8	Co 1.8	Ni 1.8	Cu 1.9	Zn 1.6	Ga 1.6	Ge 1.8	As 2.0	Se 2.4	Br 2.8	Kr 3.0
Rb 0.8	Sr 1.0	Y 1.2	Zr 1.4	Nb 1.6	Mo 1.8	Tc 1.9	Ru 2.2	Rh 2.2	Pd 2.2	Ag 1.9	Cd 1.7	In 1.7	Sn 1.8	Sb 1.9	Te 2.1	I 2.5	Xe 2.6
Cs 0.7	Ba 0.9	La 1.1	Hf 1.3	Ta 1.5	W 1.7	Re 1.9	Os 2.2	Ir 2.2	Pt 2.2	Au 2.4	Hg 1.9	Ti 1.8	Pb 1.8	Bi 1.9	Po 2.0	At 2.2	Rn 2.4
Fr 0.7	Ra 0.7	Ac 1.1															

Ce 1.1	Pr 1.1	Nd 1.1	Pm 1.1	Sm 1.1	Eu 1.1	Gd 1.1	Tb 1.1	Dy 1.1	Ho 1.1	Er 1.1	Tm 1.1	Yb 1.1	Lu 1.2
Th 1.3	Pa 1.5	U 1.7	Np 1.3	Pu 1.3	Am 1.3	Cm 1.3	Bk 1.3	Cf 1.3	Es 1.3	Fm 1.3	Md 1.3	No 1.3	Lr

19. Alcohols are organic compounds containing an -OH group attached to a carbon atom. Draw the Lewis structure of ethanol (also called ethyl alcohol), C_2H_5OH. Build two models of ethanol. An attractive force between two molecules is called an intermolecular force or van der Waals force. The van der Waals forces are classified from weakest to strongest into three types of forces: London dispersion forces, dipole-dipole forces, and hydrogen bonding. Examine the models and determine the strongest intermolecular force?

20. As a result of the intermolecular force, ethanol is miscible with water. As the number of carbon atoms in an alcohol increases, the solubility of the alcohol in water decreases. Thus, octanol (or octyl alcohol), $C_8H_{17}OH$, is practically insoluble in water. What characteristics of the C_8H_{17}- cause octanol to be insoluble in water?

In conclusion, this lesson about the structure and bonding of atoms and molecules has covered fundamental concepts in chemistry. The importance of valence electrons and hybridization in chemical bonding was highlighted, along with the use of Lewis and bond-line structures to represent molecules. With the help of Mega Molecules modeling kits and online resources like Khan Academy, this lesson provided a solid foundation for understanding the structure and bonding of atoms and molecules.