Chapter 1

1.1 Give the ground-state electron configuration for each of the following elements:

(a) Boron (b) Phosphorus (c) Oxygen (d) Chlorine

Solution: (a). B: $1s^22s^22p^1$

(b). P: [Ne] $3s^23p^3$

(c). O: [He] $2s^22p^4$

(d). Cl: [Ne] $3s^23p^5$

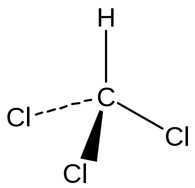
1.2 How many electrons does each of the following elements have in its outermost electron shell?

(a) Potassium (b) Aluminum (c) Krypton

Solution: (a) 1 (b) 3 (c) 8

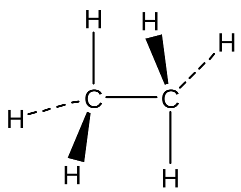
1.3 Draw a molecule of chloroform, $CHCl_3$, using solid, wedged, and dashed lines to show its tetrahedral geometry.

Solution:



1.4 Convert the following representation of ethane, C_2H_6, into a conventional drawing that uses solid, wedged, and dashed lines to indicate tetrahedral geometry around each carbon.

Solution:



1.5 What are likely formulas for the following substances?

(a) $GeCl_?$ (b)$AlH_?$ (c)$CH_?Cl_2$ (d)$SiF_?$ (e)$CH_3NH_?$

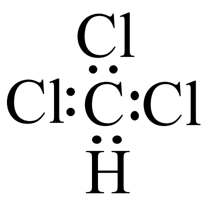
Solution:

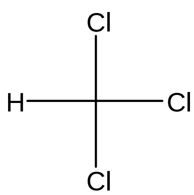
(a) $GeCl_4$ (b)AlH_3 (c)CH_2Cl_2 (d)SiF_4 (e)CH_3NH_2

1.6 Write both Lewis and line-bond structures for the following substances, showing all nonbonding electrons:

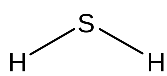
(a) $CHCl_3$, chloroform (b)H_2S, hydrogen sulfide (c)CH_3NH_2, methylamine (d)NaH, sodium hydride (e)CH_3Li, methyllithium

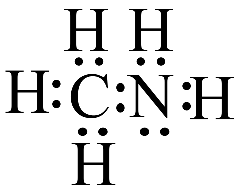
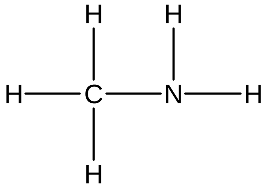
Solution:

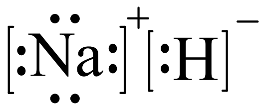
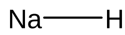
(a) 

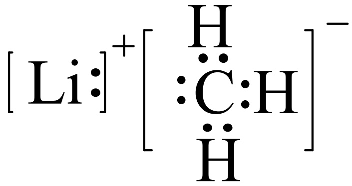
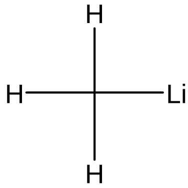


(b) 



(c)  

(d)  

(e)  

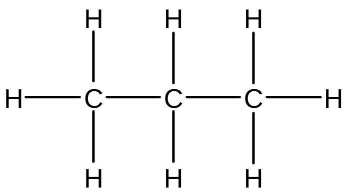
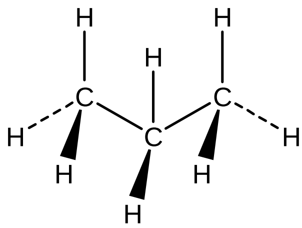
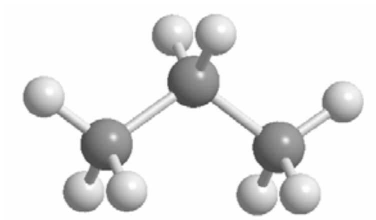
1.7 Why can't an organic molecular have the formula C_2H_7?

Solution

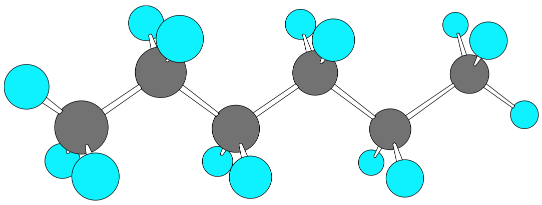
C_2H_7 has too many hydrogens for a compound with two carbons.

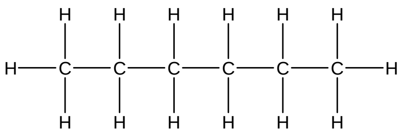
1.8 Draw a line-bond structure for propane, $CH_3CH_2CH_3$. Predict the value of each bond angle, and indicate the overall shape of the molecular

Solution

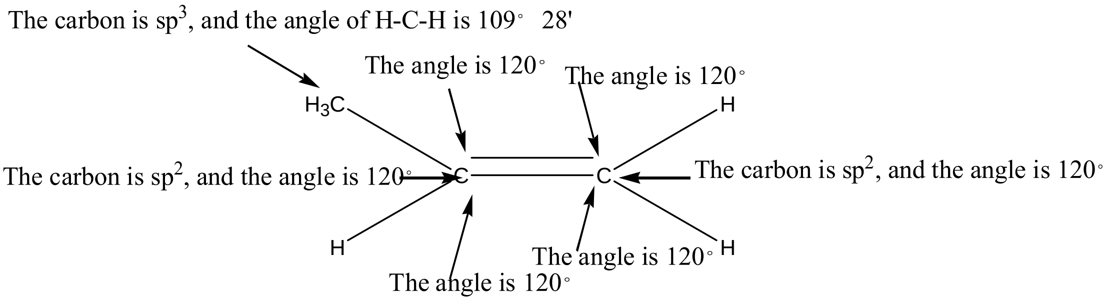
1.9 Convert the following molecular model of hexane, a component of gasoline, into a line-bond structure (gray = C, blue = H).



Solution: 

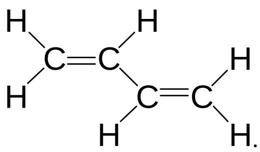
1.10 Draw a line-bond structure for propene, $H_3CHC{=}CH_2$, indicate the hybridization of each carbon, and predict the value of each bond angle.

Solution:



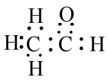
1.11 Draw a line-bond structure for 1,3-butadiene, $H_2C{=}CH{-}CH{=}CH_2$; indicate the hybridization of each carbon; and predict the value of each bond angle.

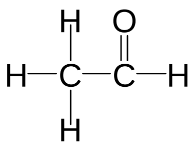
Solution:

The line-bond structure for 1,3-butadiene is . All of the four carbons are sp^2 hybridization. Each bond angle for two neighboring bonds is 120°.

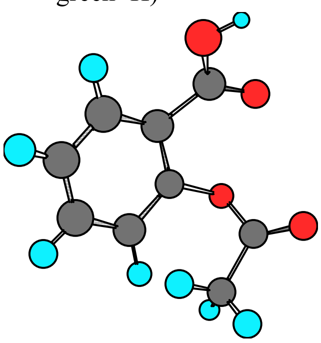
1.12 Draw both a Lewis structure and a line-bond structure for acetaldehyde, CH_3CHO

Solution:

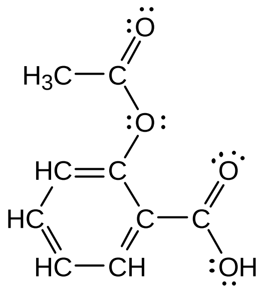
Lewis structure: 

Line-bond structure : 

1.13 Show below is a molecular of aspirin (acetylsalicylic acid). Identify the hybridization of each carbon atom in aspirin, and tell which atoms have lone pairs of electrons (gray=C, red=O, green=H)



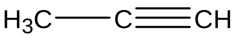
Solution:



All the carbons except CH_3 are sp^2 .CH_3 is sp^3. All the O atoms have lone pairs of electrons.

1.14 Draw a line-bond structure for propyne,CH3C≡CH, indicate the hybridization of each carbon, and predict a value for each bond angle.

Solution:



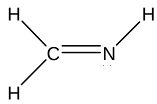
1 2 3

carbon 2, 3 are sp.

carbon 1 is sp^3.

The bond angle between carbon 1 and 2 is about 180 ° . So is the bond angle between carbon 2 and 3.

1.15 Draw Lewis and line-bond structures for CH_2NH.

Solution: structure 

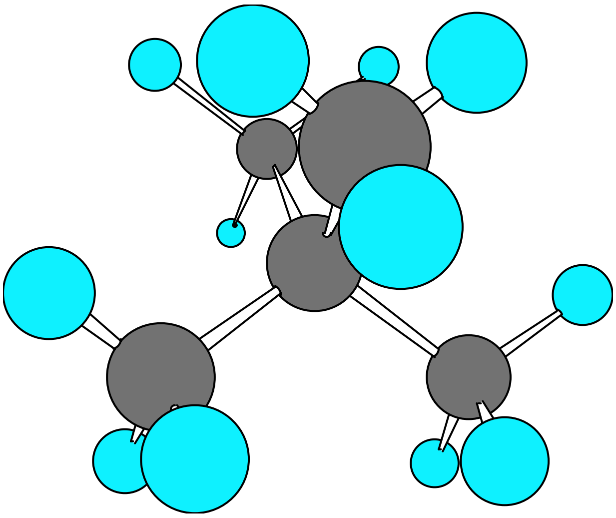
There are 4 electrons shared in the bond.

The N atom is sp2 hybridization.

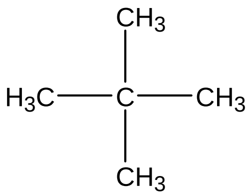
1.16 What geometry do you expect for each of the atoms?

Solution: The O atom in (a), N atom in (b) and P atom in (c) are sp3 hybridization. They all have roughly tetrahedral geometry.

1.17 Convert each of the following molecular models into a typical line-bond structure, and give the formula of each. Only the connections between atoms are shown; multiple bonds are not indicated (gray = C, red = O, blue = N, ivory = H).

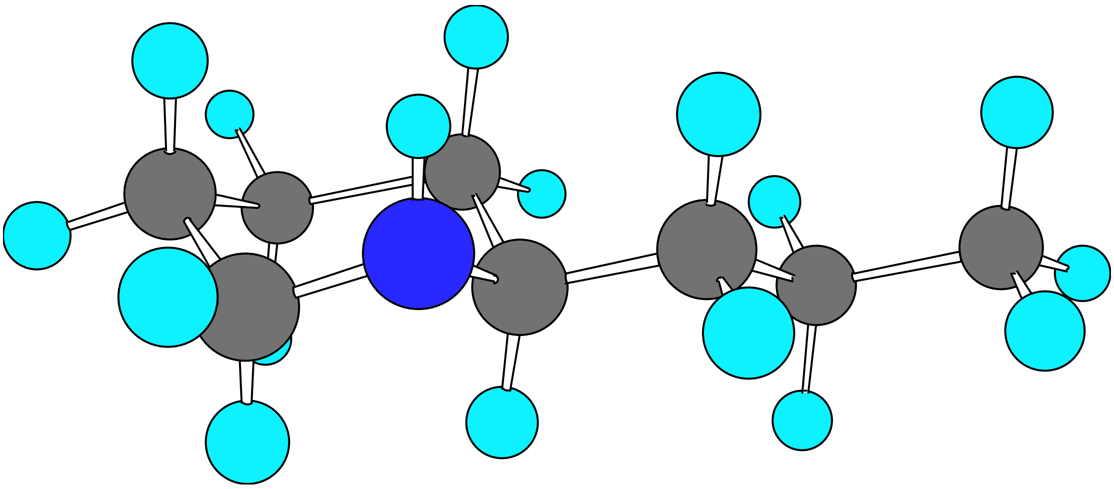


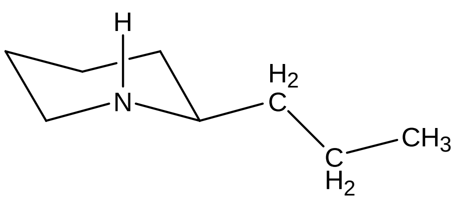
(a)

Solution: 

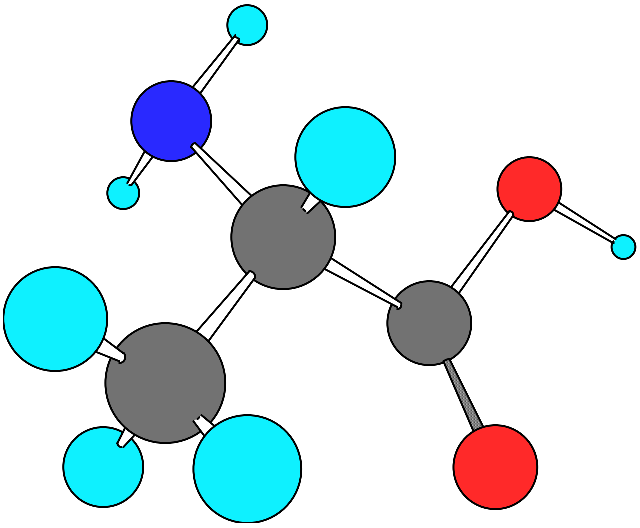
Its formula is C_5H_{12}.

(b)

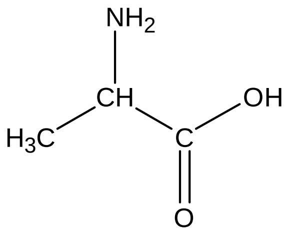


Solution: 

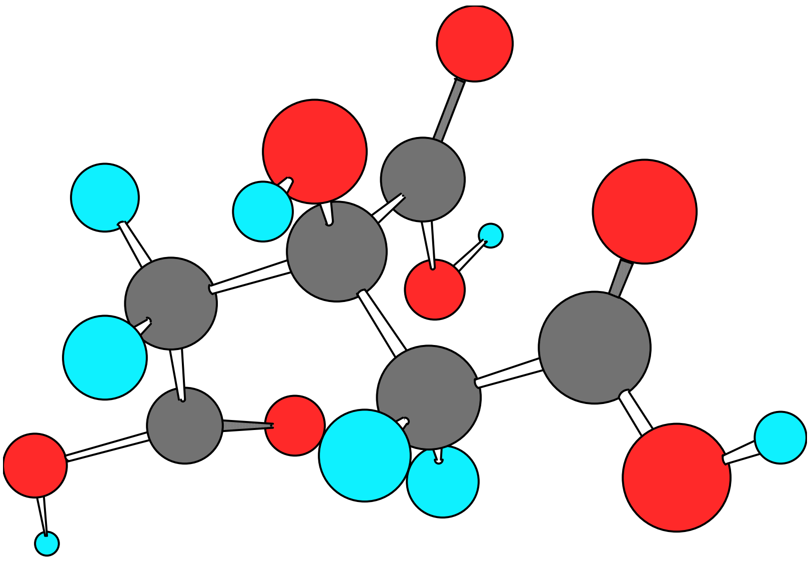
Its formula is $C_8H_{17}N$.

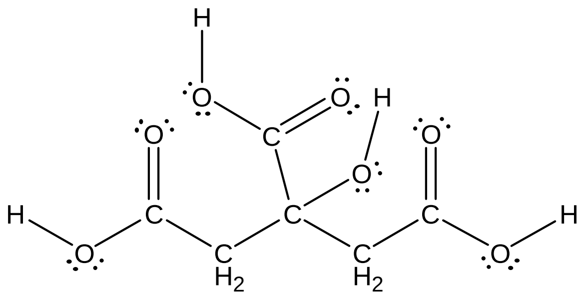


(c)

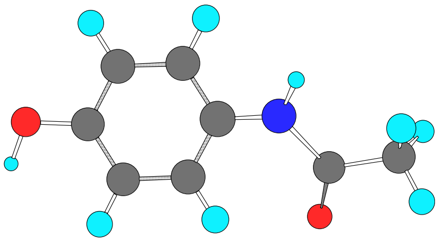
Solution:  Its formula is $C_3H_7NO_2$.

1.18 Shown below is a model of citric acid, the key substance in the so-called citric acid cycle by which food molecules are metabolized in the body. Only the connections between atoms are shown; multiple bonds are not indicated. Complete the structure by indicating the positions of multiple bonds and lone-pair electrons(gray = C, red = O, ivory = H).



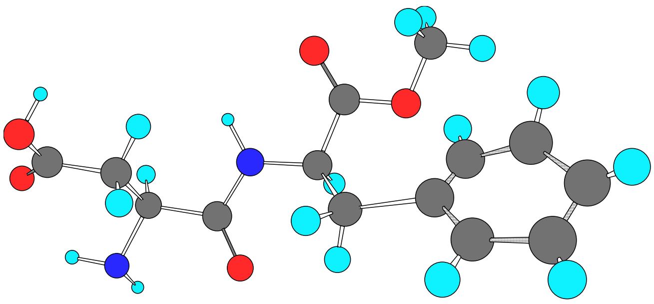
Solution: 

1.19 Shown below is a model of acetaminophen, a pain-reliever sold in drugstores as Tylenol. Identify the hybridization of each carbon atom in acetaminophen, and tell which atoms have lone pairs of electrons (gray=C, red=O, blue=N, light-blue=H).

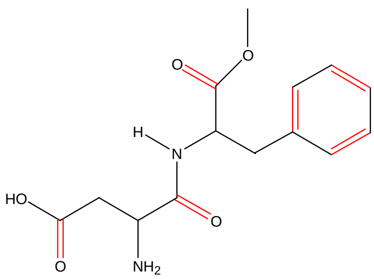


Solution: Except the carbon of the methyl is sp^3 hybridized, the other carbons are all sp^2 hybridized. And all of the two O and one N atoms have lone pairs of electrons.

1.20 Shown below is a model of aspartame, C14H18N2O5, known commercially as NutraSweet. Only the connections between atoms are shown; multiple bonds are not indicated. Complete the structure by indicating the positions of multiple bonds (gray=C, red=O, blue=N, light-blue=H).



Solution:



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

(a) Calcium (b) Chlorine (c) Germanium (d) Strontium

Solution: (a) Calcium has 2 valence electrons

(b) Chlorine has 7 valence electrons

(c) Germanium has 4 valence electrons

(d) Strontium has 2 valence electrons

1.22 Give the ground-state electron configuration for each of the following elements:

(a) Potassium (b) Sulfur (c) Aluminum (d) Bromine

Solution: (a) Potassium: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^1$

(b) Sulfur: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^4$

(c) Aluminum: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^1$

(d) Bromine: $1s^2\ 2s^2\ 2p^6\ 3s^2\ 3p^6\ 4s^2\ 3d^{10}\ 4p^5$

1.23 What are likely formulas for the following molecules?

(a)$CH_?OH$ (b)$AlCl_?$ (c)$CF_2Cl_?$ (d)$NI_?$

Solution: (a)CH_3OH

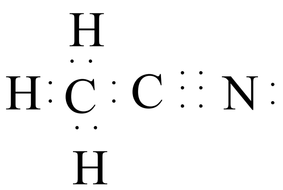
(b)$AlCl_3$

(c)CF_2Cl_2

(d)NI_3

1.24 Write a Lewis (electron-dot) structure for acetonitrile, C2H3N, which contains a carbon-nitrogen triple bond. How many electrons does the nitrogen atom have in its outer shell? How many are bonding, and how many are nonbonding?

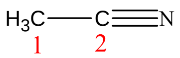
Solution:



The nitrogen has 5 electrons in its outer shell, while 3 of them are bonding, and 2 of them are nonbonding.

1.25 What is the hybridization of each carbon atom in acetonitrile (Problem 1.24)?

Solution:

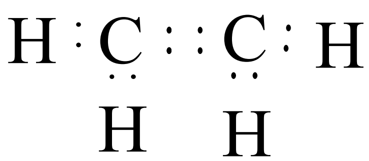


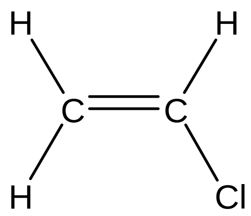
C1 is sp^3-hybridized, and C2 is sp-hybridized.

1.26 Draw both a Lewis structure and a line-bond structure for vinyl chloride, C_2H_3Cl, the starting material from which PVC [poly (vinyl chloride)] plastic is made.

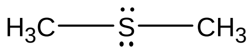
Solution:

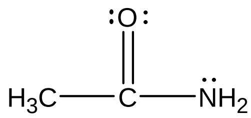
Lewis structure:

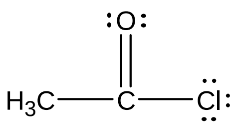


Line-bond structure: 

1.27 Fill in any nonbonding valence electrons that are missing from the following line-bong structure:

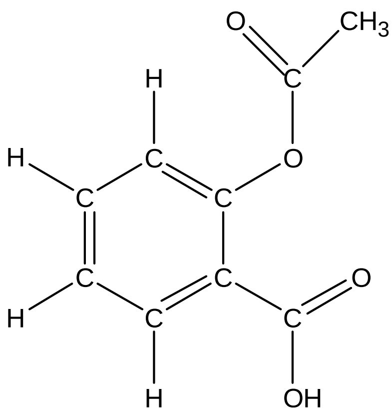
(a) 

(b) 

(c) 

1.28 Convert the following line-bond structures into molecular formulas:

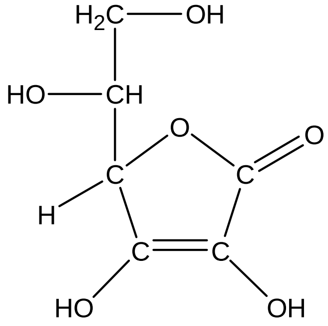
(a)



Aspirin

Solution: $C_9H_8O_4$

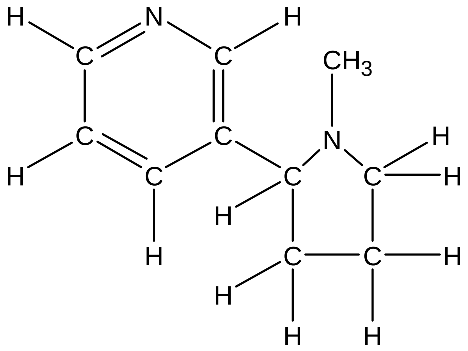
(b)



Vitamin C

Solution: $C_6H_8O_6$

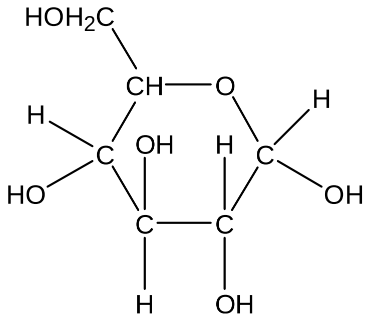
(c)



Nicotine

Solution: $C_{10}H_{14}N_2$

(d)



Glucose

Solution: $C_6H_{12}O_6$

1.29 Convert the following molecular formulas into line-bond structure that are consistent with valence rules:

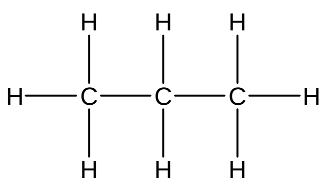
(a).C_3H_8 (b).CH_5N

(c).C_2H_6O (2 possibilities) (d).C_3H_7Br (2 possibilities)

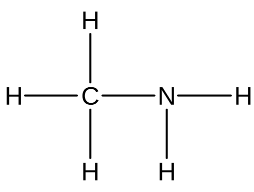
(e).C_2H_4O (3 possibilities) (f).C_3H_9N (4 possibilities)

Solution:

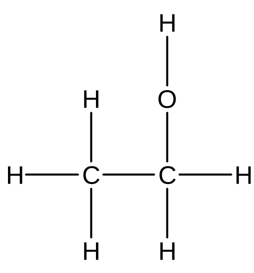
(a)

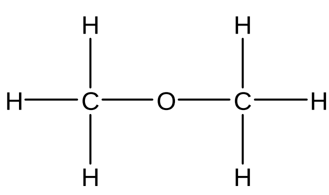


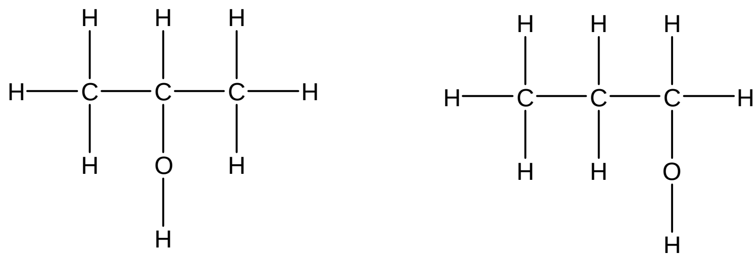
(b)



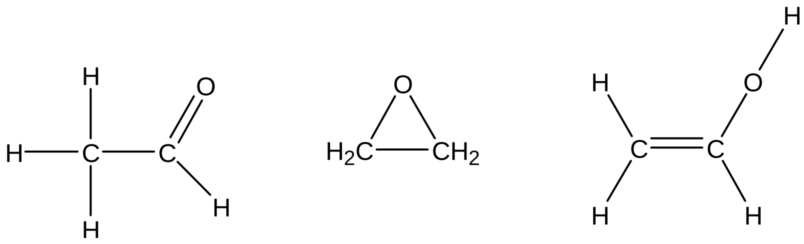
(c)



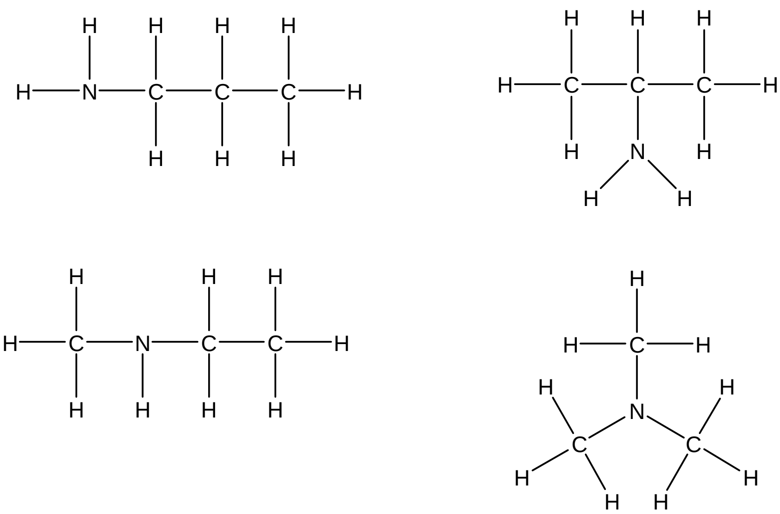




(d)

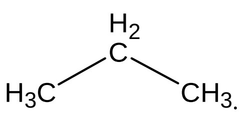
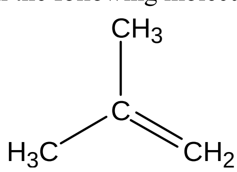


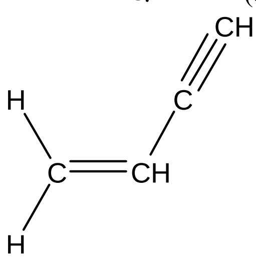
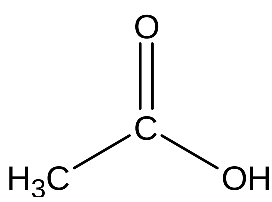
(e)



(f)

1.30 What kinds of hybridization do you except for each carbon atom in the following molecules?

(a).Propane,  (b).2-Methylpropene, 

(c).1-buten-3-yne,  (d).Acetic acid, 

Solution:

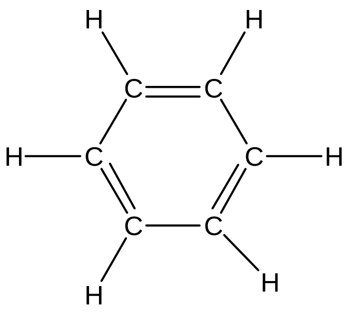
(a). All the three carbon is sp^3 hybridized

(b).The two carbon linked with double bond are sp^2 hybridized, others are sp^3 hybridized.

(c). The two carbon linked with double bond are sp^2 hybridized, others are sp hybridized

(d). The carbon linked with double bond is sp^2 hybridized, the other one is sp^3 hybridized

1.31 What is the shape of benzene, and what hybridization do you expect for each carbon?



Benzene

All the carbons and hydrogens of benzene lie in the same plane. So the shape of benzene is a plane. All the carbons form sp^2 hybridization.

1.32 What bond angles do you expect for each of the following, and what kind of hybridization do you expect for the central atom in each?

(a) The C-O-C angle in CH_3-O-CH_3

bond angle >104.5^0, sp^3

(b) The C-N-C angle in CH_3-NH-CH_3

bond angle >107.3^0, sp^3

(c) The C-N-H angle in CH_3-NH-CH_3

bond angle <107.3^0, sp^3

(d) The O-C-O angle in acetic acid (See Problem 1.30d.)

bond angle 120^0,sp^2

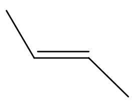
1.33 Propose structures for molecules that meet the following descriptions:

(a) Contains two sp^2-hybridized carbons and two sp^3-habridized carbons.

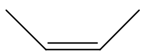
(b) Contain only four carbons, all of which are sp^2-hybridized.

(c) Contains two sp-hybridized carbons and two sp^2-hybridized carbons.

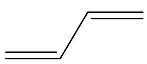
Solution: (a)



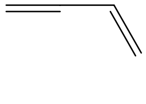
or



(b)



(c)



1.34 Why can't molecules with the following formulas exist?

(a) CH_5 (b) C_2H_6N (c) $C_3H_5Br_2$

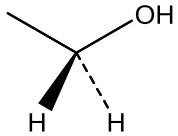
Solution: (a) The center carbon has only 4 sp^3 orbitals, it can only form 4 carbon-hydrogen bonds.

(b) NH_2 equals to H, So the formula equals to C_2H_5, it could not exist.

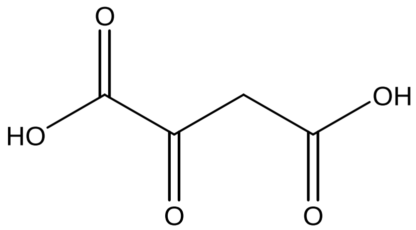
(c) As same as (b), the formula equals to C_3H_7, it could not exist.

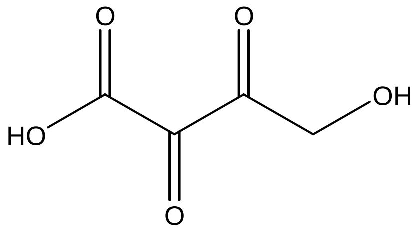
1.35 Draw a three-dimensional representation of the oxygen-bearing carbon atom in ethanol, CH_3-

-CH_2-OH, using the standard convention of solid, wedged and dashed lines.



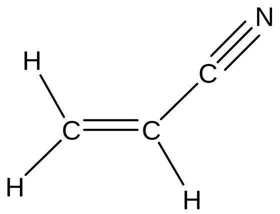
1.36 Oxaloacetic acid, an important intermediate in food metabolism, has the formula $C_4H_4O_5$ and contains three C=O bonds and two O-H bonds. Propose two possible line-bond structures for the molecule.



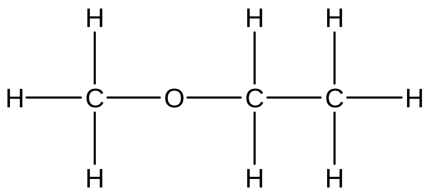


1.37 Draw line-bond structures for the following molecules:

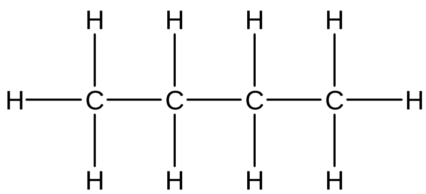
(a) Acrylonitrile, C_3H_3N, which contains a carbon-carbon double bond and a carbon-nitrogen triple bond.

Solution: 

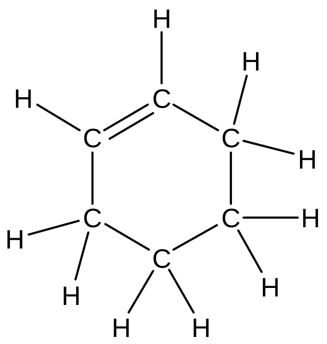
(b) Ethyl methyl ether, C_3H_8O, which contains an oxygen atom bonded to twocarbons

Solution: 

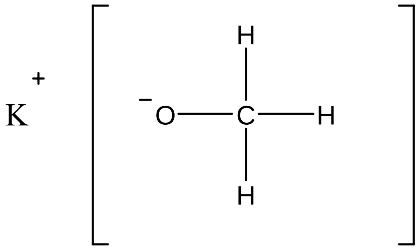
(c) Butane, C_4H_{10}, which contains a chain of four carbons atoms

Solution: 

(d) Cyclohexene, C_6H_{10}, which contains a ring of six carbon atoms and one carbon-carbon double bond

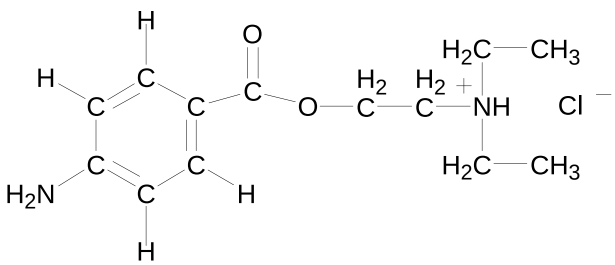
Solution: 

1.38 Potassium methoxide, $KOCH_3$, contains both covalent and ionic bonds. Which do you think is which?

Solution: 

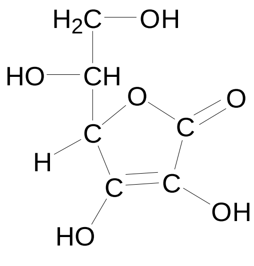
1.39 What kind of hybridization do you expect for each carbon atom in the following molecules?

(a)



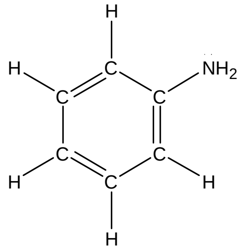
The molecular will carry out syn-addition with H_2 to the C=C bond by catalyst

(b)

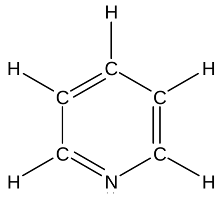


The molecular will carry out syn-addition with H_2 to the C=C bond by catalyst.

1.40 What bond angles do you expect for the following?



(a) The C-N-H angle in aniline.



(b) The C-N-C angle in pyridine.

(c) The C-P-C angle in trimethylphosphine, $P(CH_3)_3$.

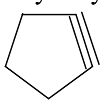
Solution:

(a)107.3° (around 109.5°)

(b)120°

(c)Around 109.5°

1.41 Why do you suppose no one has ever been able to make cyclopentyne as a stable molecule?



cyclopentyne

Solution:

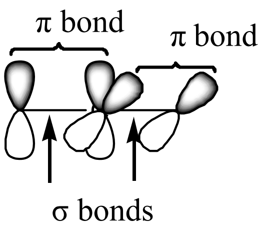
Two of the five C are sp hybridized, so the carbon carbon single bond on each of the two carbons should be 180 degree. But in cyclopentyne, it should be nearly 360/5=72 degree. So it is not able to be stable.

1.42 What is wrong with the following sentence? "The π bonding molecular orbital in ethylene results from sideways overlap of two p atomic orbitals."

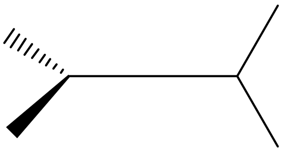
solution: The π bonding molecular orbital in ethylene results from sideways overlap of two p atomic orbitals with the same algebraic sign.

1.43 Allene, $H_2C=C=CH_2$, is somewhat unusual in that it has two adjacent double bonds. Draw a picture showing the orbitals involved in the σ and π bonds of allene. Is the central carbon atom sp^2- or sp-hybridized? What about the hybridization of the terminal carbons? What shape do you predict for allene?

Solution:



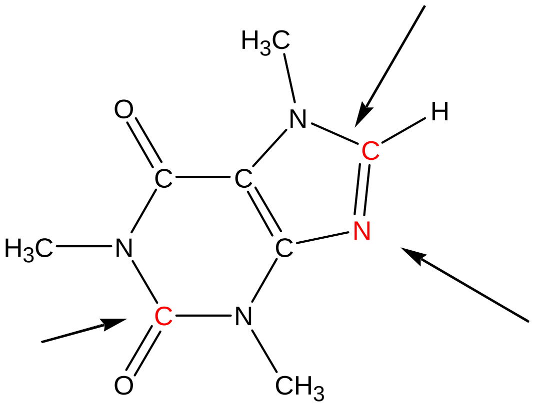
The central carbon atom is sp-hybridized, and the terminal carbons are sp^2-hybridized.

The shape is like this  .

1.44 Allene (see Problem 1.43) is related structurally to carbon dioxide, CO_2. Draw a picture showing the orbitals involved in the σ and π bonds of CO_2, and identify the hybridization of carbon.

Solution: The carbon is sp hybridized. One of its hybridized sp orbital overlap a p orbital of one oxygen to form a σ bond. And one p orbital overlap another p orbital of the oxygen to form a π bond. So as with another oxygen.

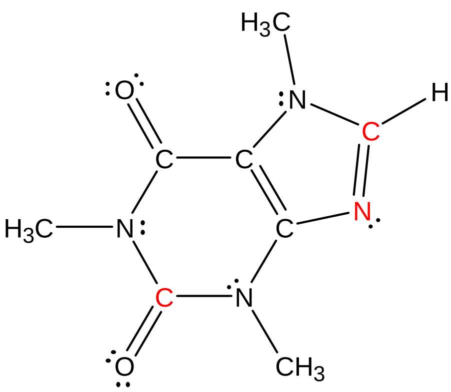
1.45 Complete the Lewis (electron-dot) structure of caffeine, show all lone-pair electrons, and identify the hybridization of the indicated atoms.



caffeine

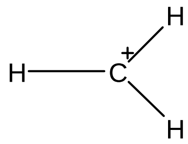
Solution:

The Lewis (electron-dot) structure of caffeine as follow:



and all the atoms indicated is sp^2 hybrids.

1.46 Although almost all stable organic species have tetravalent carbon atoms, species with trivalent carbon atoms also exist. Carbocations are one such class of compounds.



(a) How many valence electrons does the positively charged carbon atom have?

(b) What hybridization do you expect this carbon atom to have?

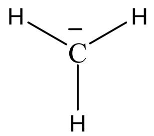
(c) What geometry is the carbocation likely to have?

Solution: (a) 6

(b) sp^2

(c) planar

1.47 carbanion is a species that contains a negatively charged, trivalent carbon.



(a) What is the relationship between a carbanion and a trivalent nitrogen compound such as NH3

(b) How many valence electrons does the negatively charged carbon atom have?

(c) What hybridization do you expect this carbon atom to have?

(d) What geometry is the carbonion likely to have?

Solution:

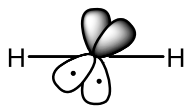
(a) They are all octet, and the number of electrons is the same.

(b) 8

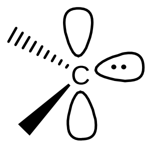
(c) sp3

(d) tetrahedral

1.48 Divalent carbon species called carbenes are capable of fleeting existence. For example, methylene, $:CH_2$, is the simplest carbene. The two unshared electrons in methylene can be either spin-paired in a single orbital or unpaired in different orbitals. Predict the type of hybridization you expect carbon to adopt in singlet (spin-paired) methylene and triplet (spin-unpaired) methylene. Draw a picture of each, and identify the types of carbon orbitals present.



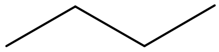
triplet methylene



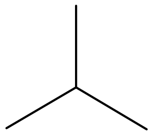
singlet methylene

1.49 There are two different substances with the formula C_4H_{10}. Draw both, and tell how they differ.

Solution:



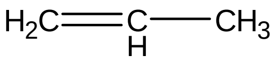
and

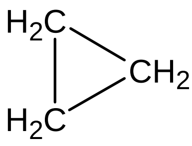


They have the same numbers and kinds of atoms but differ in the way the atoms are arranged. The atoms of them are connected differently.

1.50 There are two different substances with the formula C3H6. Draw both, and tell how they differ. (See Section 3.2.)

Solution:

(a) 

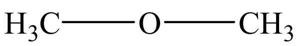
(b) 

(a) has a carbon-carbon single bond and a carbon-carbon double bond

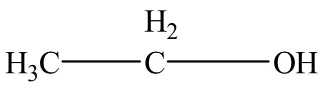
(b) has three carbon-carbon single bonds.

1.51 There are two different substance with the formula C_2H_6O . Draw both , and tell how they differ.

Solution:



and



They are ether and Alcohol.

1.52 There are three different substances that contain a carbon-carbon double bond and have the formula C_4H_8. Draw them, and tell how they differ. (See section 6.5)

Solution: