Objective 1: Represent organic molecules with chemical formulas, expanded formulas, Lewis structures, skeletal structures. Determine shape (VSEPR), bond polarity, and molecule polarity. Identify functional groups.

Quiz Practice problems

Key ideas:

There are different ways to represent an organic compound: chemical formula, expanded formula, Lewis structure, skeletal structure.

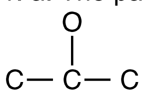
Structure determines shape which determines polarity which determines properties.

Skills:

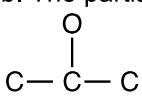
Convert Lewis structure to skeletal structure and vice versa.
Convert structure to expanded formula and and vice versa.
Use electronegativity to determine bond polarity.
Determine shape using VSEPR theory.
Determine polarity of molecule.
Identify functional groups.

For neutral molecule: C = 4 bonds, N = 3 bonds and 1 l.p., O = 2 bonds and 2 l.p., H = 1 bond and 0 l.p.

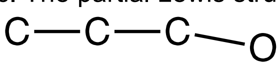
1. a. The partial Lewis structure of C_3H_8O is shown below. Draw in H's and lone pairs. Identify the functional group.



b. The partial Lewis structure of C_3H_6O is shown below. Draw in H's and lone pairs. Identify the functional group.

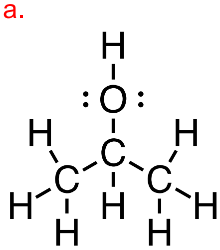


c. The partial Lewis structure of C_3H_6O is shown below. Draw in H's and lone pairs. Identify the functional group.



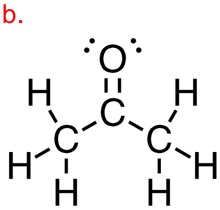
Answers:

a.



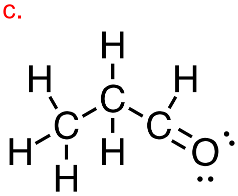
This compound is isopropanol (rubbing alcohol).
alcohol functional group

b.



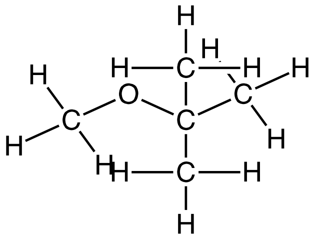
This compound is acetone (propanone).
ketone functional group

c.

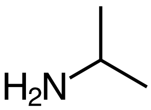


This compound (Propionaldehyde or propanal) is an isomer of acetone (same chemical formula, different bonding).
aldehyde functional group

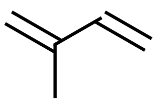
2. a. Methyl-t-butyl ether (MTBE) is a common organic solvent and used to be a gasoline additive. Draw the skeletal structure.



b. The expanded formula for acetone is CH_3COCH_3. Draw the skeletal structure.
c. This chemical might smell like dirty socks. Draw in H's and lone pairs. Write the chemical formula and the expanded formula.

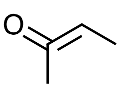


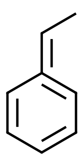
d. Isoprene is a building block for many essential oils. Draw in H's and lone pairs. Write the chemical formula and expanded formula.

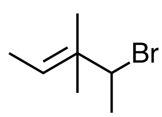


e. The CHF_2CHCl_2 is a CFC. (What is a CFC?) Draw the skeletal structure.

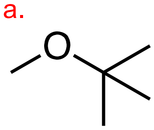
f. What is wrong with these structures? Draw a correct structure.



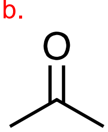




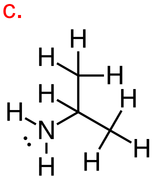
Answers:
a.



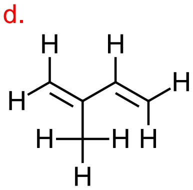
b.



c.

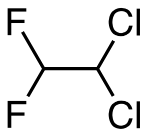


Chemical formula: C_3H_9N
Expanded formula: $CH_3CHNH_2CH_3$
d.

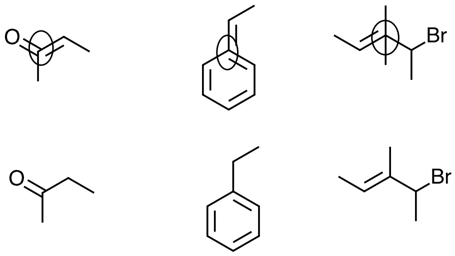


Chemical formula: C_5H_8
Expanded formula: $CH_2CCH_3CHCH_2$

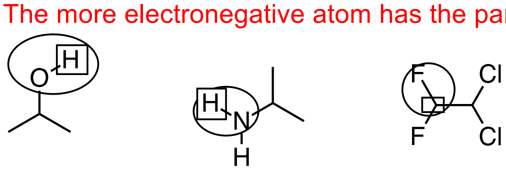
e. CFC is a chlorofluorocarbon



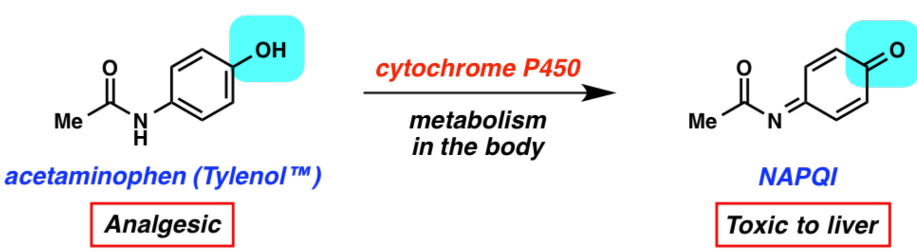
f. Circled C has too many bonds (violates octet rule).



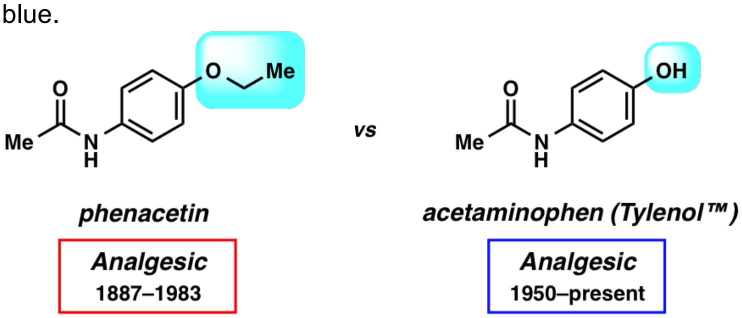
3. See an electronegativity table. Compare C, H, O, and N. Rank these elements from the most electronegative to least electronegative.
In the structures in Questions 1a and 2c and 2e, circle the most polar bond. Box the atom with the partial positive charge.
Answers:
O (3.5) > N (3.0) > C (2.5) > H (2.1)
F is the most electronegative element = 4.0, Cl has the same electronegativity as N = 3.0
The most polar bond has the largest electronegativity difference.
For isopropanol, O-H bond has an electronegativity difference = 3.5 – 2.1 = 1.4
And C-O bond has an electronegativity difference = 3.5 – 2.5 = 1.0
So O-H bond is the most polar bond.
The less electronegative atom has the partial positive charge.
The more electronegative atom has the partial negative charge.



4. 40,000 tons of acetaminophen are consumed per year. Misuse causes liver damage. Identify the functional groups in blue. (Me = methyl group = CH_3-)



Phenacetin is a carcinogen and damages kidneys; it was replaced by acetaminophen. Identify the functional groups in blue.



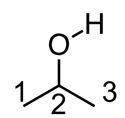
Answers:

Acetaminophen: alcohol
NAPQI: ketone
Phenacetin: ether

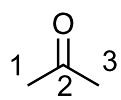
5. Valence Shell Electron Pair Repulsion (VSEPR) theory – the shape at a central atom is based on the number of bonding pairs and lone pairs surrounding a central atom.
Tetrahedral = 4 bonds and 0 l.p.
Trigonal pyramid = 3 bonds and 1 l.p.
Bent = 2 bonds and 2 l.p.
Trigonal planar = 3 bonds and 0 l.p.
a. For each compound in Question 1, determine the shape at each central atom using VSEPR theory.

b. Structure determines shape, shape determines polarity.
For each compound in Question 1, determine whether the compound is polar or non-polar.

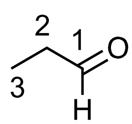
c. A carbocation is a carbon that is bonded to three atoms and has a +1 charge. Carbocations are formed as intermediates in some types of substitution, elimination, and addition reactions (which we will look at later in Chem 12A).
(i) CH_3^+ is a carbocation. Draw the structure of this carbocation. Identify the shape at the carbon using VSEPR theory.
(ii) Draw the structure of the $CH_3CH^+CH_3$ carbocation. Identify the shape at each carbon using VSEPR theory.
Answers:
a and b.



isopropanol



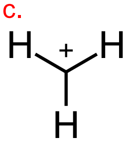
acetone



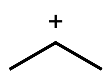
propanal

Each C is labeled according to naming rules (we'll cover naming organic compounds later).
isopropanol: each C = tetrahedral, O = bent ==> isopropanol is polar
acetone: C1 and C3 = tetrahedral, C2 = trigonal planar ==> acetone is polar
propanal: C1 = trigonal planar, C2 and C3 = tetrahedral ==> propanal is polar

c.



trigonal planar



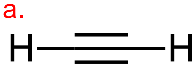
C1 and C3 = tetrahedral, C3 = trigonal planar

6. Valence bond (VB) theory – the shape of a molecule is explained with VB theory.
Electrons in carbon occupy s and p atomic orbitals. These orbitals have a certain shape and are oriented in specific directions. In VB theory, s and p atomic orbitals combine together to form hybrid orbitals. See Objective 1 Lecture Slides 48-52.
Table. Shape and hybrid orbitals relationship.

# of bonds to carbon	Shape at C	VB Hybrid orbitals
4 single bonds	Tetrahedral	four sp^3 hybrid orbitals
1 double bond and 2 single bonds	Trigonal planar	three sp^2 hybrid orbitals (and one p orbital left over)
1 triple bond and 1 single bond	Linear	two sp hybrid orbitals (and two p orbitals left over)

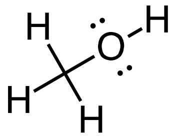
a. Draw the structure of C_2H_2. Determine the shape at each carbon. Identify the VB hybrid orbitals in each carbon. Describe the bonding in C_2H_2. In other words,
C1-C2 σ bond forms between ________ orbital on C1 and________ orbital on C2.
C1-C2 π bond forms between ________ orbital on C1 and________ orbital on C2.
H-C1 σ bond forms between ________ orbital on H and________ orbital on C1.

b. Draw the structure of CH_3OH. Determine the shape at each central atom. Identify the VB hybrid orbitals in each central atom. Describe the bonding in CH_3OH.
c. You looked at the structure and shape of the CH_3^+ carbocation in Question 5. Identify the VB hybrid orbitals in the carbon. Describe the bonding in CH_3^+.
Answers:
a.



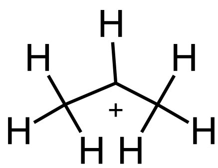
Hybrid orbitals: sp at each C.
C1-C2 σ bond forms between sp orbital on C1 and sp orbital on C2.
C1-C2 π bond forms between p orbital on C1 and p orbital on C2.
2nd C1-C2 π bond forms between p orbital on C1 and p orbital on C2.
H-C1 σ bond forms between s orbital on H and sp orbital on C1.

b.



Hybrid orbitals: sp^3 at C and O.
C-O σ bond forms between sp^3 orbital on C and sp^3 orbital on O.
H-O σ bond forms between s orbital on H and sp^3 orbital on O.
H-C σ bond forms between s orbital on H and sp^3 orbital on C1.

c.



Hybrid orbitals: sp^3 at C1 and C3, sp^2 at C2 (middle C).
C1-C2 σ bond forms between sp^3 orbital on C1 and sp^2 orbital on C2.
C3-C2 σ bond forms between sp^3 orbital on C3 and sp^2 orbital on C2.
On C1 and C3, H-C σ bond forms between s orbital on H and sp^3 orbital on C1 or C3.
On C2, H-C σ bond forms between s orbital on H and sp^2 orbital on C2.