Objective 2: Compare 2 or more compounds and determine whether the compounds are structural isomers, the same compound, or different compounds. Calculate formal charge and determine most likely structure. **Quiz Practice problems**

Key ideas:

General bonding rules for a 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.

As organic compounds get bigger, there are more ways to connect the atoms. Experiments can determine the actual structure but looking at formal charges allows you to predict the most likely structure.

Formal charge on an atom = # of valence electrons - # of bonds - # of electrons in lone pairs

Formal charge rules: structure in which every atom has a formal charge = 0 is the most likely structure.

A structure in which C, N, O fit the octet rule is more stable than a structure in which atoms lack an octet.

Negative formal charge on the more electronegative atom is preferred.

Skills:

Draw isomers of a compound.

Given two or more structures, determine whether compounds are the same compound, isomers, or different compounds. Calculate formal charge on an atom in a compound.

Determine most likely structure based on formal charge rules.

1. Glycine is the simplest amino acid.

glycine at low pH glycine at intermediate pH

a. Draw in H's and lone pairs.

b. Confirm that when C has 4 bonds and O has 2 bonds and 2 l.p., the formal charge is 0.

c. Confirm that when N has 4 bonds and 0 l.p., the formal charge is 1.

d. Confirm that when O has 1 bond and 3 l.p., the formal charge is -1.

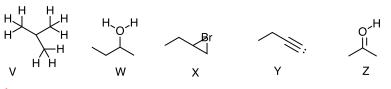
Answers:

b. Formal charge on C bonded to two O's = 4 - 4 - 0 = 0Formal charge on C bonded to N = 4 - 4 - 0 = 0c. Formal charge on N = 5 - 4 - 0 = 1d. Formal charge on O bonded to H = 6 - 2 - 4 = 0Formal charge on O with -1 charge = 6 - 1 - 6 = -1

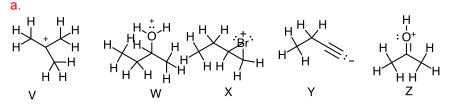
2. We will see some of these compounds in Chem 12. Compound V has a charge of +1, W = +1, X = +1, Y = -1, and Z = +1.

a. Draw in H's and lone pairs.

b. Use formal charge to determine which atom is charged in each compound.

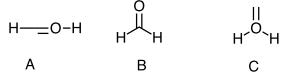


Answers:



b. Compound V: Formal charge on carbon with 3 bonds = 4 - 3 - 0 = 1Compound W: Formal charge on O = 6 - 3 - 2 = 1 Compound X: Formal charge on Br = 7 - 2 - 4 = 1Compound Y: Formal charge on C with lone pair = 4 - 3 - 2 = -1Compound Z: Formal charge on O = 6 - 3 - 2 = 1

3. Formaldehyde (CH₂O) is a common organic solvent. Three structures of formaldehyde are shown below.



a. Determine the number of valence electrons in formaldehyde.

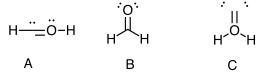
b. Draw in the lone pairs in each structure.

c. For each strucure, calculate the formal charge on each atom.

- d. Apply formal charge rules to determine more plausible structure.
- e. Which structure has the aldehyde functional group?

Answers:

a. CH_2O has 10 valence electrons (C = 4 valence electrons, 2 H = 2(1 valence electron) = 2, O = 6 valence electrons) b. The C's and O in each structure should fit the octet rule.



c. A: FC on C = 4 - 3 - 2 = -1, FC on O = 6 - 3 - 2 = 1, FC on each H = 1 - 1 - 0 = 0B: FC on C = 4 - 4 - 0 = 0, FC on O = 6 - 2 - 4 = 0, FC on each H = 1 - 1 - 0 = 0C: FC on C = 4 - 2 - 4 = -2, FC on O = 6 - 4 - 0 = 2, FC on each H = 1 - 1 - 0 = 0d. The most plausible structure is B ==> no formal charge on each atom. e. B has the aldehyde functional group.

4. a. Draw the Lewis structure of C₃H₈. Does this compound have any isomers?

b. C_4H_8 has at least 2 isomers. Draw the Lewis and skeletal structures of the isomers of C_4H_8 .

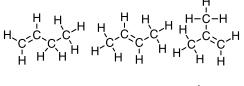
c. C₃H₅Br has at least 2 isomers. Draw the Lewis and skeletal structures of the isomers of C₃H₅Br.

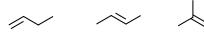
d. C₂H₆O has at least 2 isomers. Draw the Lewis and skeletal structures of the isomers of C₂H₆O.

e. C_3H_6O has at least three isomers. Draw the Lewis structure and skeletal structure each isomer. Answers:

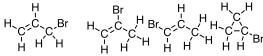
a. C₃H₈ does not have any isomers.

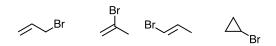
b. C₄H₈ has 3 isomers



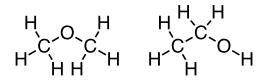


c. C₃H₅Br has 4 isomers.



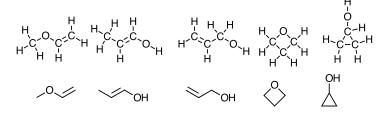








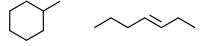
e. C_3H_6O has several isomers.



5. a. Are D and E the same compound, different compounds, or isomers?



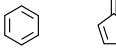
b. Are the two compounds the same, different, or isomers? Hint: count the number of carbons in each compound. Determine the chemical formula of each compound.



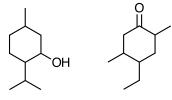
c. Are the two compounds the same, different, or isomers?



d. Are the two compounds the same, different, or isomers?



e. The compound on the left is menthol, which is responsible for cool sensations in your mouth. Is the compound on the right the same compound, different, or an isomer of menthol?



Answers:

- a. isomers same chemical formula (C₁₂H₂₆), different bonding
- b. isomers same chemical formula (C7H14), different bonding
- c. different different chemical formula (left compound = C_7H_{12} , right compound = C_7H_{14})
- d. isomers same chemical formula (C₆H₆), different bonding
- e. different different chemical formula (left compound = $C_{10}H_{20}O$, right compound = $C_{10}H_{18}O$)