1.S: STRUCTURE AND BONDING (SUMMARY)

CONCEPTS & VOCABULARY

1.0: Prelude to Structure and Bonding

- Organic compounds contain carbon atoms bonded hydrogen and other carbon atoms.
- Organic chemistry studies the properties and reactions of organic compounds.

1.1: Atomic Structure: The Nucleus

- Atoms are comprised of **protons**, **neutrons** and **electrons**. Protons and neutrons are found in the nucleus of the atom, while electrons are found in the electron cloud around the nucleus. The relative electrical charge of a proton is +1, a neutron has no charge, and an electron's relative charge is -1.
- The number of protons in an atom's nucleus is called the **atomic number, *Z***.
- The **mass number, *A***, is the sum of the number of protons and the number of neutrons in a nucleus.
- The type of element an atom represents is defined by the atomic number, *Z* in the atom. All atoms of one specific element have the same number of protons (Z).
- Atoms that have the same atomic number (Z), but different mass numbers (A) are called **isotopes**.

1.2: Atomic Structure: Orbitals

- An **atomic orbital** is the probability description of where an electron can be found. The four basic types of orbitals are designated as ***s***, ***p***, ***d***, and ***f***.

1.3: Atomic Structure: Electron Configurations

- The order in which electrons are placed in atomic orbitals is called the **electron configuration** and is governed by the ***aufbau* principle**.
- Electrons in the outermost shell of an atom are called **valence electrons**. The number of valence electrons in any atom is related to its position in the periodic table. Elements in the same periodic group have the same number of valence electrons.

1.4: Development of Chemical Bonding Theory

- **Lewis Dot Symbols** are a way of indicating the number of valence electrons in an atom. They are useful for predicting the number and types of covalent bonds within organic molecules.
- The **molecular shape** of molecules is predicted by Valence Shell Electron Pair Repulsion (VSEPR) theory. The shapes of common organic molecules are based on **tetrahedral**, **trigonal planar** or **linear** arrangements of electron groups.

1.5: The Nature of Chemical Bonds: Valence Bond Theory

- **Covalent bonds** form as valence electrons are shared between two atoms.
- **Lewis Structures** and **structural formulas** are common ways of showing the covalent bonding in organic molecules.
- **Formal charge** describes the changes in the number of valence electrons as an atom becomes bonded into a molecule. If the atom has a net loss of valence electrons it will have a positive formal charge. If the atom has a net gain of valence electrons it will have a negative formal charge.
- Atomic orbitals often change as they overlap to form molecular orbitals. This process is known as **orbital hybridization**. The common types of hybrid orbitals in organic molecules are ***sp*^{3}**, ***sp*^{2}**, and ***sp***.

1.6: sp^3 Hybrid Orbitals and the Structure of Methane

- The four identical C-H single bonds in CH_4 form as the result of sigma bond overlap between the sp^3 hybrid orbitals of carbon and the *s* orbital of each hydrogen.

1.7: sp^3 Hybrid Orbitals and the Structure of Ethane

- The C-C bond in C_2H_6 forms as the result of sigma bond overlap between a sp^3 hybrid orbital on each carbon. and the *s* orbital of each hydrogen. The six identical C-H single bonds in form as the result of sigma bond overlap between the sp^3 hybrid orbitals of carbon and the *s* orbital of each hydrogen.

1.8: sp^2 Hybrid Orbitals and the Structure of Ethylene

- The C=C bond in C_2H_4 forms as the result of both a sigma bond overlap between a sp^2 hybrid orbital on each carbon and a pi bond overlap of a *p* orbital on each carbon

1.9 *sp* Hybrid Orbitals and the Structure of Acetylene

- The carbon-carbon triple bond in C_2H_4 forms as the result of one sigma bond overlap between a *sp* hybrid orbital on each carbon and two pi bond overlaps of *p* orbitals on each carbon.

1.10: Hybridization of Nitrogen, Oxygen, Phosphorus and Sulfur

- The atomic orbitals of nitrogen, oxygen, phosphorus and sulfur can hybridize in the same way as those of carbon.

1.11: The Nature of Chemical Bonds: Molecular Orbital Theory

- **Molecular Orbital theory (MO)** is a more advanced bonding model than Valence Bond Theory, in which two atomic orbitals overlap to form *two* molecular orbitals – a bonding MO and an anti-bonding MO.

1.12: Drawing Chemical Structures

- **Kekulé Formulas** or **structural formulas** display the atoms of the molecule in the order they are bonded.
- **Condensed structural formulas** show the order of atoms like a structural formula but are written in a single line to save space.
- **Skeleton formulas** or **Shorthand formulas** or **line-angle formulas** are used to write carbon and hydrogen atoms more efficiently by replacing the letters with lines.
- **Isomers** have the same molecular formula, but different structural formulas

SUMMARY PROBLEMS

EXERCISE 1.S.1

The following molecule is highly reactive and contains a functional group called a ketene. For each numbered atom, list the geometry, bond angle, hybridization, orbitals present, and orbital function. Notes: Ignore the geometry and bond angle for atom #1. For orbitals present, list all of the orbitals at that atom. For orbital function, describe what each orbital is doing (e.g., participating in a sigma bond, containing lone pair electrons, etc.).

Answer

#1 - sp^2 hybridization; 3 sp^2 orbitals and 1 p orbital present; p orbital participates in a pi bond, 1 sp^2 orbital participates in a sigma bond, 2 sp^2 orbitals contain lone pair electrons

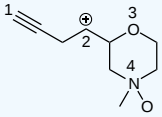
#2 - linear; 180 degrees; sp hybridization; 2 sp orbitals and 2 p orbitals present; p orbitals participate in two pi bonds, s sp^2 orbitals participate in two sigma bonds

#3 - trigonal planar; 120 degrees; sp^2 hybridization; 3 sp^2 orbitals and 1 p orbital present; p orbital participates in a pi bond, 3 sp^2 orbitals participate in three sigma bonds

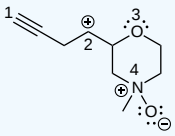
#4 - tetrahedral; 109.5 degrees; sp^3 hybridization; 4 sp^3 orbitals present; 4 sp^3 orbitals participate in four sigma bonds

EXERCISE 1.S.2

First, add lone pair electrons and formal charges to the molecule shown below; its net charge is plus one. (The only formal charge on a carbon atom has already been added for you.) Second, for each numbered atom, list the geometry, bond angle, hybridization, orbitals present, and orbital function. Notes: For orbitals present, list all of the orbitals at that atom. For orbital function, describe what each orbital is doing (e.g., participating in a sigma bond, containing lone pair electrons, etc.).



Answer



#1 - linear; 180 degrees; sp hybridization; 2 sp orbitals and 2 p orbitals present; p orbitals participate in two pi bonds, s sp^2 orbitals participate in two sigma bonds

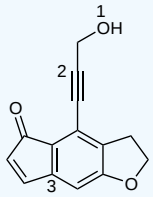
#2 - trigonal planar; 120 degrees; sp^2 hybridization; 3 sp^2 orbitals and 1 p orbital present; p orbital is empty, 3 sp^2 orbitals participate in three sigma bonds

#3 - bent; <109.5 degrees; sp^3 hybridization; 4 sp^3 orbitals present; 2 sp^3 orbitals participate in two sigma bonds, 2 sp^3 orbitals contain two lone pairs

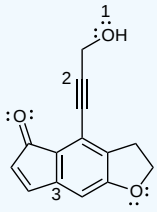
#4 - tetrahedral; 109.5 degrees; sp^3 hybridization; 4 sp^3 orbitals present; 4 sp^3 orbitals participate in four sigma bonds

EXERCISE 1.S.3

First, add lone pair electrons and formal charges to the molecule shown below. Second, for each numbered atom, list the geometry, bond angle, hybridization, orbitals present, and orbital function. Third, clearly identify on the structure below sigma bonds formed by overlap of the following orbitals: sp-sp^2 (label as "a"), sp-sp^3 (label as "b"), sp^2-sp^2 (label as "c"), sp^2-sp^3 (label as "d"), and sp^3-sp^3 (label as "e"). Notes: For orbitals present, list all of the orbitals at that atom. For orbital function, describe what each orbital is doing (e.g., participating in a sigma bond, containing lone pair electrons, etc.). When identifying particular types of sigma bonds, there will be more than one correct answer for some options.



Answer

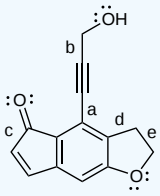


All atoms are neutral in this molecule.

#1 - bent; <109.5 degrees; sp^3 hybridization; 4 sp^3 orbitals present; 2 sp^3 orbitals participate in two sigma bonds, 2 sp^3 orbitals contain two lone pairs

#2 - linear; 180 degrees; sp hybridization; 2 sp orbitals and 2 p orbitals present; p orbitals participate in two pi bonds, s sp^2 orbitals participate in two sigma bonds

#3 - trigonal planar; 120 degrees; sp^2 hybridization; 3 sp^2 orbitals and 1 p orbital present; p orbital participates in a pi bond, 3 sp^2 orbitals participate in three sigma bonds



For a and b, these are the only bonds that are correct. For c, there are several correct options. For d, there is one other option (from the benzene ring to the O in the five-membered ring. For e, there are several correct options.

SKILLS TO MASTER

Skill 1.1 Determine the number of protons, neutrons, and electrons in a nuclide.

Skill 1.2 Write the electron configuration and orbital diagram for an atom.

Skill 1.3 Determine the number of valence electrons in an atom.

Skill 1.4 Draw the molecular formula, Lewis Dot Structure, structural formula, condensed structural formula, shorthand formula and wedge-dash structure of simple organic molecules.

Skill 1.5 Use Lewis Dot structures to predict molecular shape, bond angle, hybridization.

Skill 1.6 Calculate formal charge on an atom in a molecule.

Skill 1.7 Determine the number of sigma and pi bonds in organic molecules.

Skill 1.8 Determine relative bond energy and bond length based on atoms involved in the bond and bond type.

Skill 1.9 Describe and draw the orbital overlap and types of bonding in simple organic molecules like methane, ethane, ethylene and acetylene.

Skill 1.10 Describe the bonding in organic molecules using both the Valence Bond Theory and Molecular Orbital Theory.

MEMORIZATION TASKS (MT)

MT 1.1 Memorize the number of valence electrons in the atoms - C, H, N, O, and the halides.

MT 1.2 Memorize the number of bonds and lone pairs to atoms of carbon, hydrogen, oxygen and nitrogen that result in formal charges of zero.
