Objectives

After completing this section, you should be able to

1. propose one or more acceptable Kekulé structures (structural formulas) for any given molecular formula
2. write the molecular formula of a compound, given its Kekulé structure.
3. draw the shorthand structure of a compound, given its Kekulé structure.
4. interpret shorthand structures and convert them to Kekulé structures.
5. write the molecular formula of a compound, given its shorthand structure.

Study Notes

When drawing the structure of a neutral organic compound, you will find it helpful to remember that

• each carbon atom has four bonds.
• each nitrogen atom has three bonds.
• each oxygen atom has two bonds.
• each hydrogen atom has one bond.

It is necessary to draw structural formulas for organic compounds because in most cases a molecular formula does not uniquely represent a single compound. Different compounds having the same molecular formula are called isomers, and the prevalence of organic isomers reflects the extraordinary versatility of carbon in forming strong bonds to itself and to other elements. When the group of atoms that make up the molecules of different isomers are bonded together in fundamentally different ways, we refer to such compounds as constitutional isomers. There are seven constitutional isomers of \( \text{C}_4\text{H}_{10}\text{O} \), and structural formulas for these are drawn in the following table. These formulas represent all known and possible \( \text{C}_4\text{H}_{10}\text{O} \) compounds, and display a common structural feature. There are no double or triple bonds and no rings in any of these structures.
Simplification of structural formulas may be achieved without any loss of the information they convey. In condensed structural formulas the bonds to each carbon are omitted, but each distinct structural unit (group) is written with subscript numbers designating multiple substituents, including the hydrogens. Shorthand (line) formulas omit the symbols for carbon and hydrogen entirely (unless the hydrogen is bonded to an atom other than carbon). Each straight line segment represents a bond, the ends and intersections of the lines are carbon atoms, and the correct number of hydrogens is calculated from the tetravalency of carbon. Non-bonding valence shell electrons are omitted in these formulas.

Developing the ability to visualize a three-dimensional structure from two-dimensional formulas requires practice, and in most cases the aid of molecular models. As noted earlier, many kinds of model kits are available to students and professional chemists, and the beginning student is encouraged to obtain one.

Kekulé Formula

A Kekulé Formula or structural formula displays the atoms of the molecule in the order they are bonded. It also depicts how the atoms are bonded to one another, for example single, double, and triple covalent bond. Covalent bonds are...
shown using lines. The number of dashes indicate whether the bond is a single, double, or triple covalent bond. Structural formulas are helpful because they explain the properties and structure of the compound which empirical and molecular formulas cannot always represent.

\[ \text{H} \quad \text{H} \]
\[ \text{H} \quad \text{C} \quad \text{C} \quad \text{O} \quad \text{H} \]
\[ \text{H} \quad \text{H} \]

**Figure 1:** Kekulé Formula for Ethanol

### Condensed Formula

Condensed structural formulas show the order of atoms like a structural formula but are written in a single line to save space and make it more convenient and faster to write out. Condensed structural formulas are also helpful when showing that a group of atoms is connected to a single atom in a compound. When this happens, parenthesis are used around the group of atoms to show they are together.

Ex. Condensed Structural Formula for Ethanol: CH\(_3\)CH\(_2\)OH (Molecular Formula for Ethanol C\(_2\)H\(_6\)O).

### Shorthand Formula

Because organic compounds can be complex at times, line-angle formulas are used to write carbon and hydrogen atoms more efficiently by replacing the letters with lines. A carbon atom is present wherever a line intersects another line. Hydrogen atoms are then assumed to complete each of carbon's four bonds. All other atoms that are connected to carbon atoms are written out. Line angle formulas help show structure and order of the atoms in a compound making the advantages and disadvantages similar to structural formulas.

\[ \text{OH} \]

**Figure 2:** Shorthand Formula for Ethanol

### Exercises

Write down the molecular formula for each of the compounds shown here.

compounds A through D for naming

**Answers:**

A. C\(_7\)H\(_7\)N
B. C\(_5\)H\(_{10}\)
C. $C_5H_4O$
D. $C_5H_6Br_2$

Questions
Q1.12.1

Below is the molecule for caffeine. Give the molecular formula for it.

![Caffeine Molecule]

Solutions
S1.12.1

$C_8H_{10}O_2N_4$

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