Organic Compounds
1 - Writing Organic Structures

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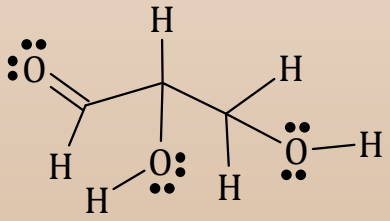
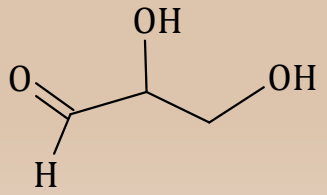
Chemical Formulas

Chemical structures are written in various ways. The most common are empirical and molecular. In organic chemistry there are also the condensed formulas, expanded structures and line structures.

- Empirical formula: Smallest ratio of elements. CH_2O
- Molecular formula: Actual ratio of elements in a compound. Here I have multiplied the above formula by 3. $C_3H_6O_3$
- Condensed formula: A structure that shows the structure with functional groups and carbon chains. No bonds are shown. $CH_2OHCHOHCHO$
- Expanded structure: Shows the Lewis structure with all bonds. (Lone pairs of electrons don't have to be shown).



- Line formula: Carbons, as each point, are connected by lines; no hydrogens are shown but all heteroatoms are shown and any atoms on heteroatoms are drawn.



Chemical Formulas

Which formula is used when? It depends on what is being studied.

In general chemistry, chemical formulas are usually empirical formulas as the ionic compounds are the lowest ratios of atoms. They are used in reactions and usually written to avoid writing names all the time.

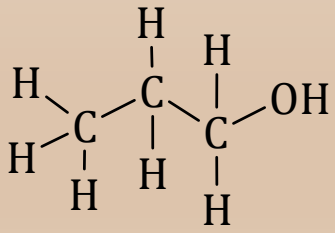
In organic chemistry empirical formulas are used only in certain cases for e.g. in constitutional isomer problems or when determining structure in spectroscopy. Expanded structures are used to understand bonding and sometimes reactions. Condensed structures are commonly used for small molecules. They don't show any bonds, so it is important to have a good understanding of structure and bonding before writing them.

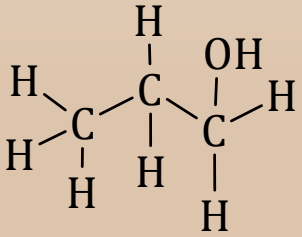
The most common structures used in organic chemistry are line structures as one does not have to draw out all the atoms. They are easy and fast to write. They are used routinely to write reactions. The key to avoid making mistakes in line structures is how many atoms are attached to each carbon.

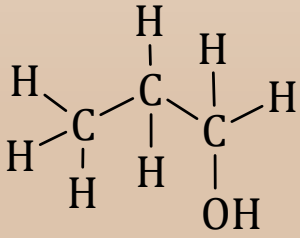
Expanded (Dash) formulas

This representation emphasizes connectivity and does not represent the 3-dimensional nature of the molecule. It is the Lewis structure of the compound where each line represents a pair of electrons. We can skip the lone pair of electrons unless we are writing out a reaction where it might be necessary to show the electrons.

There is free rotation around single bonds, so all the structures below are equivalent. No matter where the OH is written, up or down, so long it is on the same carbon, the structure is the same. Note that in the structures below, I did not show the bond drawn out between O and H. We will learn later in the chapter where we should show the bond and where we can skip it.



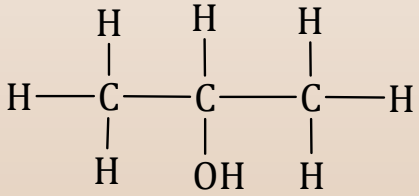




Condensed Structural Formulas

In fully condensed structure all bond lines are omitted, and atoms attached to carbon are written immediately after it.

Expanded Structure



Condensed Structures

$CH_3CHOHCH_3$

OR $CH_3CH(OH)CH_3$

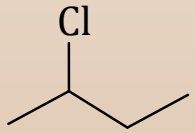
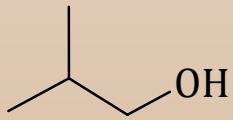
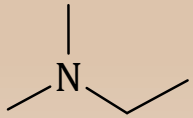
OR $(CH_3)_2CHOH$

In the condensed structures we can use parenthesis to help separate the groups attached on carbons. This is an option, not requirement. Parenthesis help when we need to show two of the same groups as shown in the third structure. Hydrogens are never placed in parenthesis.

Line Structures

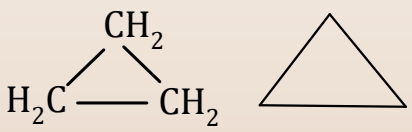
In line formulas organic molecules are drawn to completely omit all carbons and hydrogens and only show heteroatoms (*e.g*. O, Cl, N etc.) explicitly.

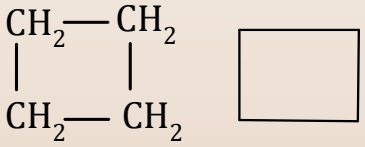
- Each intersection or end of line in a zig-zag represents a carbon with the appropriate number of hydrogens. The zig-zag is a 109°/120° angle as part of the sp^3 and sp^2 hybridization.
- Heteroatoms with attached hydrogens must be drawn in explicitly (as shown below with OH).

Condensed structure	**Line structure**
$CH_3CHClCH_2CH_3$	
$(CH_3)_2CHCH_2OH$	
$(CH_3)_2NCH_2CH_3$	

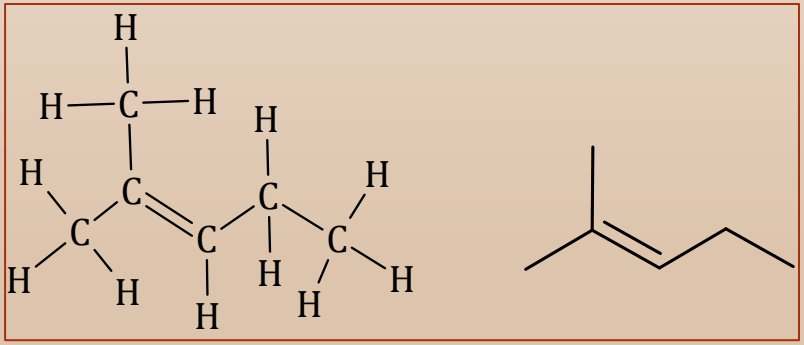
Line Structures - 2

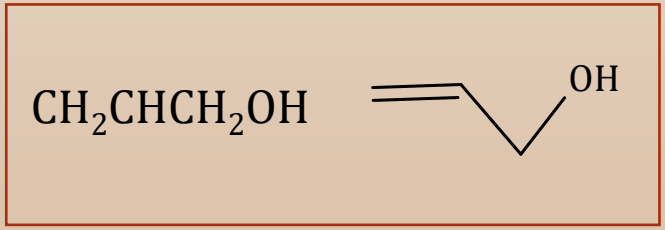
- Cyclic compounds are condensed using a drawing of the corresponding polygon.





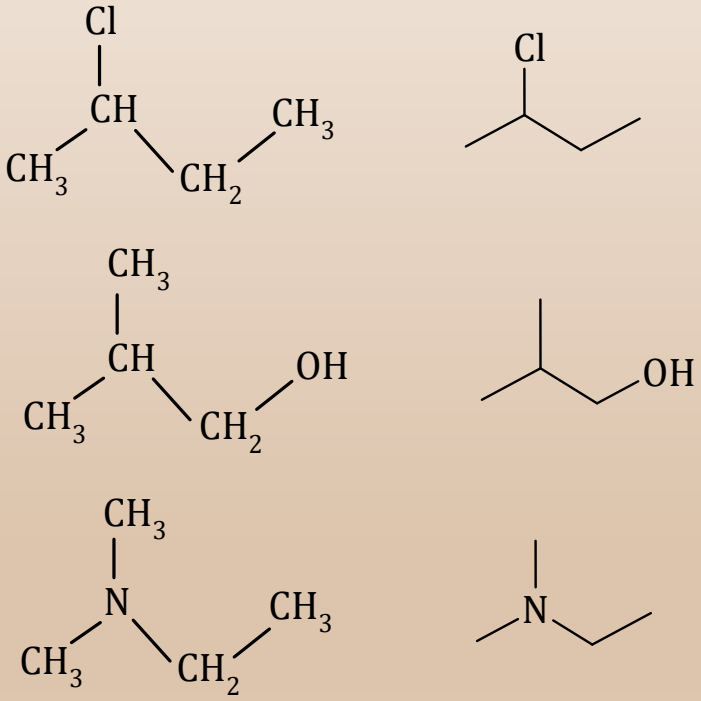
- Multiple bonds are indicated by using the appropriate number of lines connecting the atoms. Note 1) that H connected to heteroatom is written and 2) multiple bond (double bond) is not written in the condensed structure.





Carbon Chain Structures

Carbon chain structures is another convenient way of writing structures. It is not a formal method, but it used in organic chemistry to quickly see the bonding and number of hydrogens on each atom without drawing the expanded structure. The structures shown in the left column is carbon chain structures.



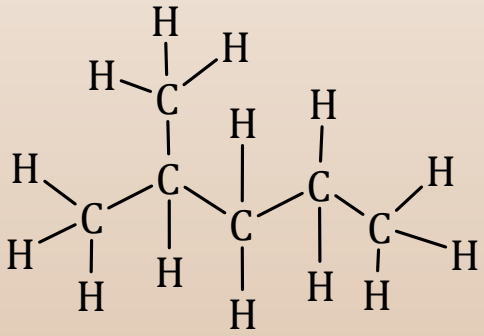
Solved Example: Writing all structure types

Write all the structures for the condensed structure given below.

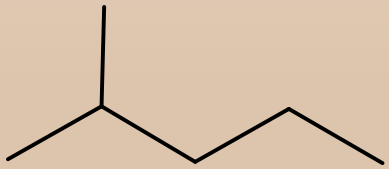
$CH_3CH\,(CH_3)CH_2CH_2CH_3$

ANSWER

- Molecular Formula – C_6H_{14}
- Expanded structure –

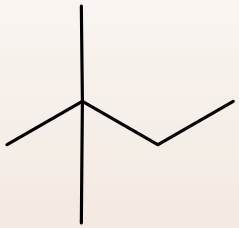


- Line structure –



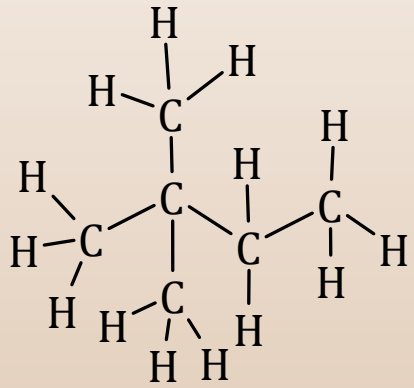
Solved Example: Writing all structure types

Write all the structures for the line structure given.



ANSWER

- Expanded structure –

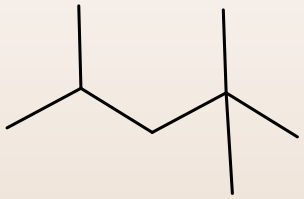


- Molecular Formula – C_6H_{14}

- Condensed Structure – $(CH_3)_3CCH_2CH_3$ or $CH_3C(CH_3)_2CH_2CH_3$

Solved Example: Determine the number of hydrogens

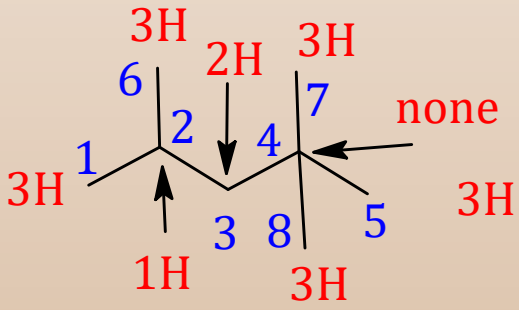
Write the number of hydrogens on each carbon for the structure below.



ANSWER

For each structure, note how many bonds are coming out of each line.

- **Carbon 1**, there is only one line going to carbon 2 so the other 3 bonds must be H.
- **Carbon 2** has two lines going to 3 carbons 1, 6 and 3, so the remaining one bond must be one H,
- **Carbon 3** is attached to carbons 2 and 4, two bonds remaining must be 2H.
- **Carbon 4** has no H since it is attached to carbons 5, 7 and 8.
- **Carbons 1,6, 7, 8 and 5** are terminal carbons (they have only one bond) and they have 3 Hs as the other bonds.



Key Words/Concepts

- Writing Organic Compounds
  - Molecular formula
  - Structural formula
  - Line structure
  - Expanded structure