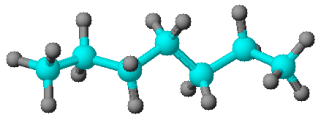
Representation of Organic Compounds

Three-dimensional structural formula

- Molecules are actual, three-dimensional entities.
- For example, the 7-carbon atom hydrocarbon molecule heptane exists as shown below:



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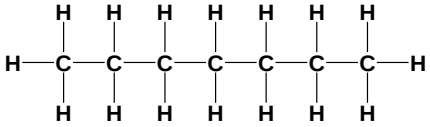
Two-dimensional structural formula

- For simplicity, the molecules are normally drawn in 2 dimensions
- Each carbon atom in a hydrocarbon forms a total of four bonds.



Heptane

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condensed structural formula

- A condensed structural formula includes all of the atoms but uses line bonds to emphasize the main structural characteristics of the molecule.

$CH_3–CH_2–CH_2–CH_2–CH_2–CH_2–CH_2–H$

Heptane

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condensed structural formula

- Taking out the lines representing the carbon—carbon bonds condenses this formula still more: $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$

Heptane

- Heptane has five repeating —CH_2— groups, called methylene groups. Because many organic molecules have such repetitive groups, an even more condensed notation shows these repeating units.

$CH_3(CH_2)_5CH_3$

Heptane

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bond-line structural formula

- Bond-line formulas are easy to draw and quickly convey the essential structure of a molecule. Both the ends and the angles of the structure represent the carbon atoms. C—H bonds are not shown, but you should assume that the appropriate number of hydrogen atoms is present to complete the four bonds required by carbon to have its octet of electrons.

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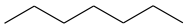
Examples of bond line structures

Bond-line formulas represent the carbon atoms as the intersection of lines and as line ends. You assume all the hydrogens needed to complete carbon's valences



Heptane

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Lewis Dot structures

- Dot Structures are diagrams that contain symbols of elements as well as dots.
- The symbols represent atoms in molecules and the dots represent valence electrons.
- These diagrams are used as a way to keep track of electrons so that it is possible to predict the number bonds between atoms in molecules, and the number electrons that are not part of these bonds.

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Lewis Dot structures

- The diagrams show bonding electrons between the element symbols and non-bonding electrons as dots that are located on the sides of the symbol.
- Often bonding electrons are replaced with lines. If there is 1 covalent bond between atoms and single line is shown, a double bond is 2 lines, and triple bond is 3 lines.

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Lewis Dot structures

In summary:

- Only the valence electrons appear in a Lewis structure.
- Bonds are made in order to fill the outer shell of the element.
- Bonds are indicated by electron pairs shown between the element symbols.
- There may be as many as three bonds between a pair of atoms.
- Stable molecules will only have paired electrons.

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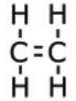
Examples of Lewis Dot structures

Water		
Ethylene		
Acetylene		

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Number of covalent bonds and lone pairs of some elements

Group 4A		Group 5A		Group 6A		Group 7A	
4 valence electrons 		5 valence electrons 		6 valence electrons 		7 valence electrons 	
4 bonds	No lone pairs	3 bonds	1 lone pair	2 bonds	2 lone pairs	1 bond	3 lone pairs
carbon – C 		nitrogen- N 		oxygen – O 		fluorine – F 	
		phosphorus – P 		sulfur – S 		chlorine – Cl 	
				selenium – Se 		bromine – Br 	
						iodine – I	

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covalent bonds and lone pairs of some elements

- These atoms (group 4 -7) acquire a maximum of 8 outermost electrons to be stable (the octet rule)
- Hydrogen on the other hand has one electron completes its shell with 2 electrons.
- It does this by receiving one electron from a donor atom to form a covalent bond.
- This means that a hydrogen atom has no lone pairs at all.

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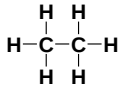
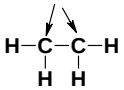
Simple structures

- Ethane, C_2H_6



  - Carbon forms four bonds, while hydrogen forms one bond.
- Consider the following molecule: C_2H_4

these carbons have 3 bonds i.e. 6 electrons



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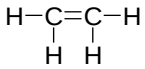

Complete structure

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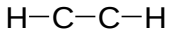
Simple structures

- What if we had a molecule with C_2H_2?



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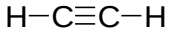
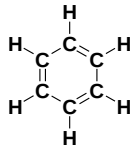


Complete structure

- A carbon molecule can also exist in a ring e.g. C_6H_6



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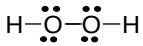
Simple structures

- As we saw in the table earlier, when we have oxygen, sulphur, phosphorus, and the halogens e.g. chlorine, then we need to include lone pairs of electrons for the structure to be complete, e.g. as in Hydrogen peroxide, H_2O_2
  - Hydrogen atoms always have one covalent bond and no lone pairs, and oxygen atoms usually have two covalent bonds and two lone pairs.



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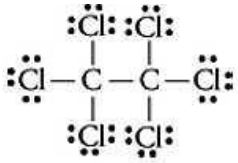
Simple structures

- Consider the following structure, C_2Cl_6
  - Carbon atoms usually have four covalent bonds and no lone pairs, and chlorine atoms usually have one covalent bond and three lone pairs.



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Simple structures

- Note that Lewis structures are useful for showing how the atoms in a molecule are connected by covalent bonds, but they do not always give a clear description of how the atoms are arranged in space since molecules are actually three dimensional in nature.
- Remember we learnt about tetrahedral, trignal structures etc, and bond angles between the atoms. For example, for tetrahedral structures, the bond angle between atoms (without lone pairs) is 109.5°

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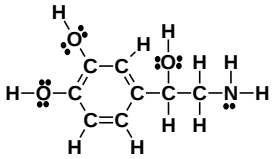
Complex structures

- In this Lewis structure, all the bonds and lone pairs are shown on the structure.



- It can be cumbersome in drawing big structures.

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Simplifying complex structures

- There are some types of structures used to simplify the way organic molecules are represent ed.
- These are:
  - Kekule structures
  - Condensed structures

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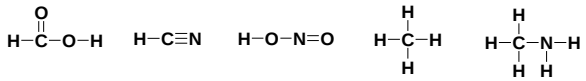
Simplifying complex structures: Kekulé Structures

- In **Kekulé structures**, the bonding electrons are drawn as lines and the lone-pair electrons are usually left out entirely, unless they are needed to draw attention to some chemical property of the molecule. (Although lone-pair electrons may not be shown, you should remember that neutral nitrogen, oxygen, and halogen atoms always have them: one pair in the case of nitrogen, two pairs in the case of oxygen, and three pairs in the case of a halogen



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Simplifying complex structures: Condensed Structures

- Frequently, structures are simplified by omitting some (or all) of the covalent bonds and listing atoms bonded to a particular carbon (or nitrogen or oxygen) next to it with a subscript to indicate the number of such atoms.
- These kinds of structures are called **condensed structures**. Compare the preceding structures with the following ones

HCO_2H HCN HNO_2 CH_4 CH_3NH_2

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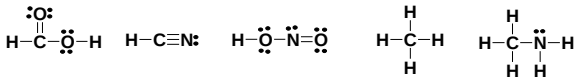
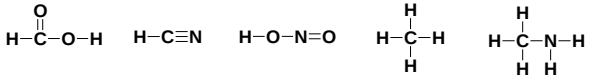
Comparison between Lewis, Kekulé and Condensed Structures

- Lewis Structures



- **Kekulé Structures**



- **Condensed Structures**

HCO_2H **HCN** **HNO_2** **CH_4** **CH_3NH_2**

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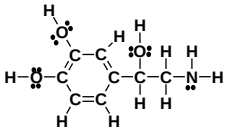
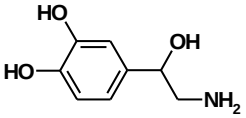
Bond line structures of complex molecules

- It is easier to draw complex molecules using bond line structures.



Lewis Dot structure

- Carbon and hydrogen atoms and lone pairs are not shown (except in mechanisms).



Bond line Structure

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