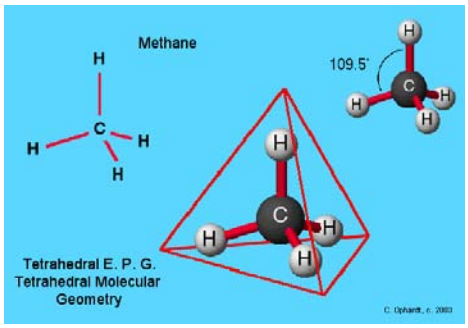
1.3 Geometry of C compounds:Valence Shell Electron Pair Repulsion Model(VSEPR Model)

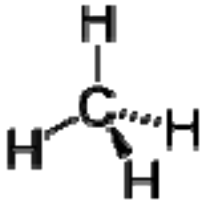
1.31 Geometry of C-C single bonds

Although we have drawn all the above molecules in 2 dimensions, they are in fact three dimensional molecules. The actual shape of methane (CH_4) is **tetrahedral** as shown in the model below.



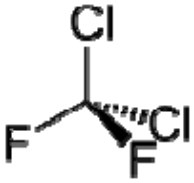
This shape can be justified on the basis that the 4 pairs of electrons in the C atom want to be as far apart as possible in 3 dimensional space because the negative charge of the outer valence electron pairs repel each other (hence the term valence shell electron pair repulsion model or VSEPR). This corresponds to a tetrahedral geometry with H-C-H bond angles of 109.5 ^{o}. Organic chemists frequently use a notation called wedge and dash notation to attempt to show the 3 dimensional tetrahedral shape in 2 dimensions.

Wedge and dash:

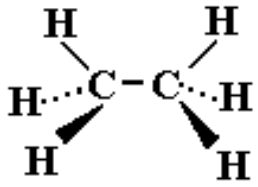


For methane one observes that two H atoms and one C atom can all be lined up in one plane. One remaining H atom sticks out towards the observer and its bond is represented with a wedge; the other H atom sticks out away from the observer and its direction is indicated with a series of dashes.

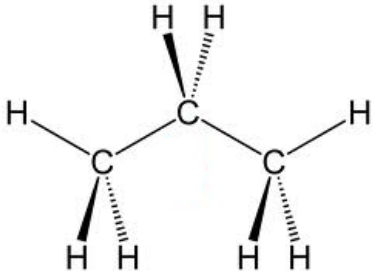
Exchanging H atoms for halogens, such as in Freon-12, $C_2Cl_2F_2$, still maintains the same basic tetrahedral geometry.



Similarly ethane has the following wedge and dash notation:

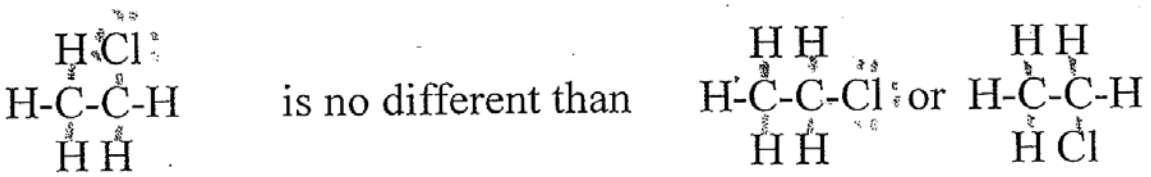


Likewise propane has the following wedge and dash notation:



Free rotation around C-C single bonds

C compounds are commonly drawn without using wedge and dash notation and the structures are drawn flat with bond angles that look like 90^o, but one should always keep in mind that they are really 3 dimensional molecules. Another important property is that there is free rotation around the C-C single bonds. Thus the structure:



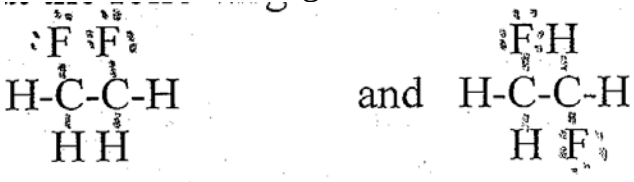
even though the structures may look different when drawn 2 dimensionally on paper.

Likewise the two structures:

are really the same because of free rotation found the second and third C atoms of the chain.

Whenever you are looking at chemical structures you always need to remember that these are really 3 dimensional molecules and that one can freely rotate around the single bonds.

Look at the following 2 structures. Are they the same molecule?



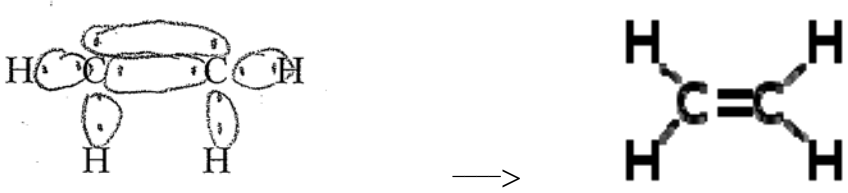
Are these 2 structures the same molecule?

They are, because one can simply flip the molecule on the left over to produce the structure on the right.

Are these 2 structures the same molecule?

1.32 Geometry of C-C double bonds

C can also form double bonds with other atoms. For example: ethylene(ethene), C_2H_4, has the structure



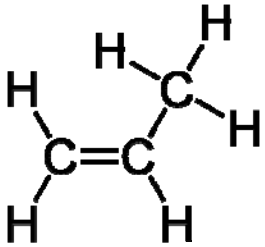
The actual geometry of the C=C in ethylene is **trigonal planar** (a flat planar structure with bond angles of 120^o) because the electrons in the C=C double bond and the two pairs of electrons in the C-H single bonds try to stay as far apart in space as possible. Unlike C-C single bonds there is **NO free rotation** around the C=C double bond. This will be important in future applications.

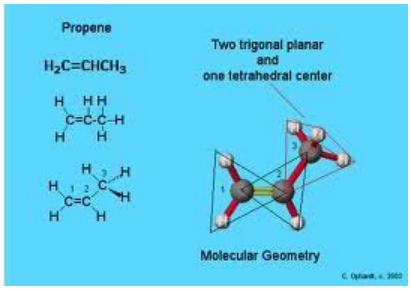
Ethylene is produced from crude oil and is the starting molecule for making the plastic material polyethylene. In rare instances vapors of ethylene from carbon deposits deep in the ground can rise to the surface along geological faults. Ethylene is a mild hallucinogen and it is thought that ethylene emanating into a cave at Delphi, Greece gave the oracles at Delphi their trances during which they made their predictions.

Wikimedia commons.This painting is by the Hon. John Collier and was painted in 1891. For more information on this artist, visit www.artmagick.com

delphic-oracle.info

One can have double bonds and single bonds in the same molecule, as in propene (propylene):



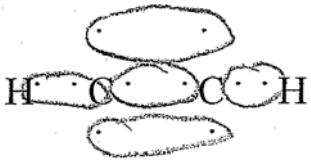


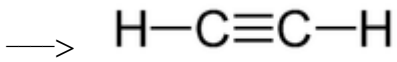
The geometry around the first two C atoms (from left to right) is **trigonal planar** with 120^o bond angle. The geometry of the H atoms around the third C atom is **tetrahedral** with 109.5^o bond angle.

1.33 Geometry around C-C triple bonds

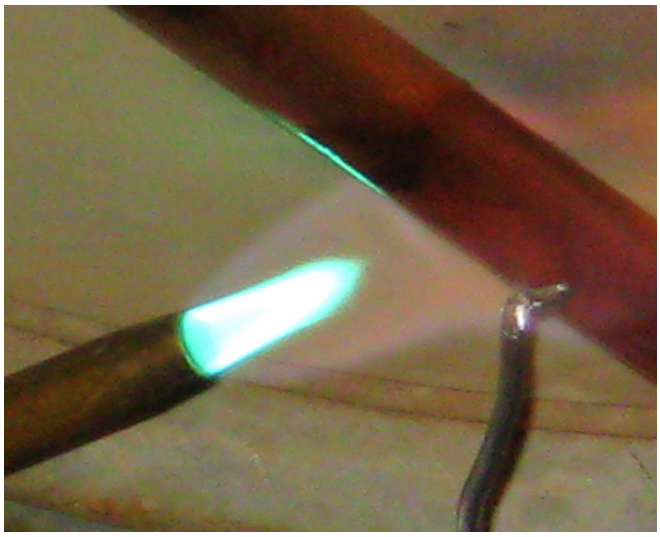
Carbon atoms can also form triple bonds with another atom

C_2H_2





Acetylene

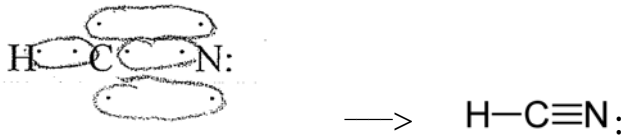


Wikimedia commons: Authors: Paul Anderson and Sheila

The geometry of acetylene (ethyne) is **linear** (bond angle 180^o) because the C-C triple bond stays as far away from the C-H single bond as it can, namely 180^o. Acetylene is the fuel used by welders in oxy-acetylene torches.

ronnormansculpture.com

HCN



Hydrogen cyanide

Hydrogen cyanide was one of the gases the Nazis used to kill people in the gas chambers and was also used in the 1950's in the US for executing prisoners given the death penalty.

Wikimedia commons: Bunker #16 in Poznan (Poland); author: Radomil