Lesson 9: Valence Shell Electron Pair Repulsion (VSEPR) Theory II

*Read through the lesson notes. You can write them out, print them or save them.

*Once you have tried to understand the lesson answer the questions that follow at the end.

*The answers to the question sheet(s) will be posted later and this will allow you to self-evaluate your learning.

Learning Intentions

-Learn about the effect of lone pairs on the bond angles of basic molecules.

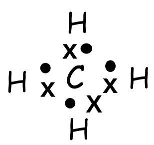
-Learn about the shapes of polyatomic ions.

Background

This lesson builds on lesson 8, VSEPR Theory I, and looks specifically at the effect that lone pairs have on bond angles.

The following three examples, methane, ammonia and water are useful to illustrate how bonded pairs of electrons interact with lone pairs of electrons to alter the shape of molecules.

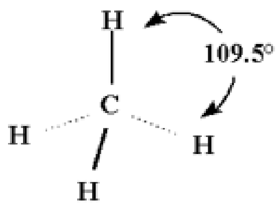
Methane (CH_4)



4 electron pairs (all bonded)

Shape of molecule: tetrahedral

Bond angle: 109.5°



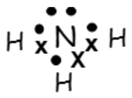
* Electron pairs = $\frac{4 \text{ (carbon has 4 outer electrons)} + 4 \text{ (number of hydrogen atoms)}}{2}$

Electron pairs = 8/2 → 4 electron pairs

→4 bonded pairs and 0 non-bon-bonded pairs (lone pair)

There are only bonding pairs. There is an even degree of repulsion between the bonded pairs of electrons which creates a bond angle of 109.5°.

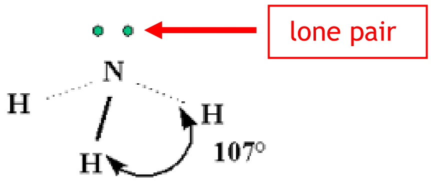
Ammonia (NH_3)



4 electron pairs (3 bonded and 1 lone)

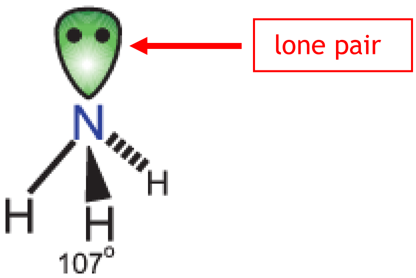
Shape of molecule: trigonal pyramidal

Bond angle: 107°



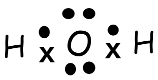
There is one non-bonding pair of electrons so there will be slightly more repulsion between this non-bonded pair and the bonded pairs of electrons. This causes the bonds to push together slightly more and therefore creates a bond angle of 107°.

It is also convenient to represent ammonia in the following way:



*It is important to understand, that the shape of the molecule is trigonal pyramidal BUT the shape of ALL electron pairs (both bonded and non-bonded) is tetrahedral.

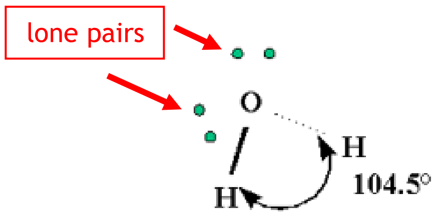
Water (H_2O)



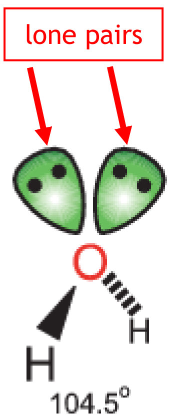
4 electron pairs (2 bonded and 2 lone)

Shape of molecule: angular or bent

Bond angle: 104.5°



The two non-bonding pairs of electrons cause a lot of repulsion. This causes the bonds to push together to a greater extent and therefore reduces the bond angle to 104.5°.



*It is important to note, that the shape of the molecule is angular BUT the shape of ALL electron pairs (both bonded and non-bonded) is tetrahedral.

In the three examples above, (water, ammonia and methane) each molecule has 4 bonding pairs of electrons. However, the important point to note is that each molecule has a different number of non-bonding (lone) pairs.

According to VSEPR theory, the interactions between bonding pair electrons and non-bonding (lone) pair electrons causes a degree of repulsion and therefore alters the shape and bond angle of the molecule.

VSEPR theory tells us that the pairs of electrons that surround the central atom of a molecule or ion are arranged as far apart as possible to minimise electron-electron repulsion. In the case of non-bonding (lone) pairs there is a greater degree of repulsion and this ultimately alters the bond angle in a molecule.

In summary

non-bonded pair:non-bonded pair

non-bonded pair:bonded pair

bonded pair: bonded pair

Increase repulsion.

Polyatomic ions

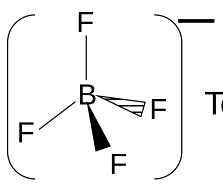
Polyatomic ions are those which contain more than one type of atom. It is also possible to predict the number of electron pairs of polyatomic ions.

When calculating the number of electron pairs of a polyatomic ion:

-add an electron for each negative charge

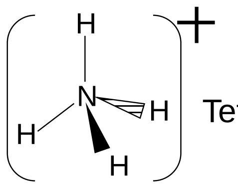
-subtract an electron for each positive charge

BF_4^- Electron pairs= $\frac{3 + 4 + 1}{2}$ 4 electron pairs and all bonding



Tetrahedral

NH_4^+ Electron pairs= $\frac{5 + 4 - 1}{2}$ 4 electron pairs and all bonding



Tetrahedral

Additional Resources

-The University of Bristol has a good set of animations which help to view the molecules in 3D. For this lesson use the tab "Lone pairs" and "Charged species"

VSEPR Theory (University of Bristol)

https://www.youtube.com/watch?v=e99iaUKsucc

-Read Scholar Sections 2.10, 2.11 and 2.12

-Read BrightRed textbook pages 18 and 19

-Answer the Question from Sheet 1.12 and check the answers when you have completed them.

-If there are any questions regarding this lesson or the questions from sheet 1.12 then please leave a post on Microsoft Teams.

1.12 Valency Shell Electron Pair Repulsion Theory II

1. Fluorine is the most reactive non-metal. It forms compounds with most other elements. Five of the compounds of fluorine are: BF_3, NF_3, CF_4, PF_5 and SF_6.

   For each compound:
   (a) Calculate the number of bonding and non-bonding electron pairs.
   (b) Name and draw the shape of the molecules.
   (c) In CF_4 the bond angle θ is 109·5°, whereas in NF_3 the bond angle is 107°. Explain this.
   (d) There are two different bond angles in PF_5. Draw a molecule of PF_5 with the angles labelled and the size of each angle shown.

2. The table below gives information about three compounds containing fluorine.

Fluorine compound	Shape	Bond angle
$BF_3(g)$		120°
$CF_4(g)$	Tetrahedral	109.5°
$NF_3(g)$	Pyramidal	107°

   (a) What is the shape of the BF_3 molecule?
   (b) In terms of electron-pair repulsions, account for the difference in bond angle between BF_3 and NF_3.

3. (a) Sketch the shapes of NH_3 and H_2S molecules, showing clearly all the bond angles and their values.
   (b) Explain why the bond angles in both molecules are different.

4. For the following substances:
   i) Calculate the number of bonding and non-bonding electron pairs around the central atom.
   ii) Name the shape adopted by ALL electron pairs.

   (a) SiF_4 (b) PCl_3 (c) Cl_2O (d) ClF_3 (e) IF_4^-

5. The following reaction involves the conversion of water into the hydronium ion.

   $H_2O + H^+ \rightarrow H_3O^+$

   a) What shape do **all the electron pairs** adopt in the water molecule?
   b) i) What shape does the water molecule adopt?
   ii) Account for this shape by including the bond angles involved.
   c) How many bonding pairs and lone pairs of electrons does the hydronium ion contain?