Chem Factsheet

September 2000 Number 04

# Shapes of Molecules and Ions

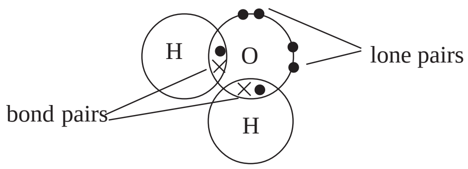
**To succeed with this topic you need to:**
- be able to find an atom/element in the Periodic Table and decide which group it is in
- know that the number of the group an element is in tells you how many electrons it has in its outer shell
- understand how to draw dot-and-cross diagrams to show covalent bonding
- understand that positive ions have lost electrons, and negative ions have gained them, and that the size of the charge on the ion tells you how many electrons are involved

**After working through this Factsheet you will:**
- have met the commonest examples of the shapes used in 'AS' level examination questions
- be able to work out the shape of any molecule from its dot-and-cross diagram

## Examination guide
Success in this topic relies on you understanding how shapes of molecules are determined and learning the names of, and diagrams for, the basic shapes. It is very important to name the shapes correctly and present the shapes clearly as 3D structures.

## What determines the shape of a molecule?
In a molecule there are covalent bonds that hold the group of atoms together. A single covalent bond is **a shared pair of electrons** (called a **bond pair**) between two nuclei (the central parts of the two atoms involved). It is **negative in charge** because the electrons have a negative charge themselves.

Not all electrons around an atom are in a bond. We can see this by looking at a dot and cross diagram, like the one below for water ($H_2O$). A pair of electrons not in a bond is called a **lone pair**.




If you have several electron pairs (bond pairs or lone pairs) around an atom then they will **repel** one another (two negatives repel -electrostatic repulsion) and because of this the electron pairs become as **far apart as possible**. This is the basic principle on which this topic is based. This theory is called **'valence shell electron pair repulsion (vsepr)'** and you may be asked to explain it.

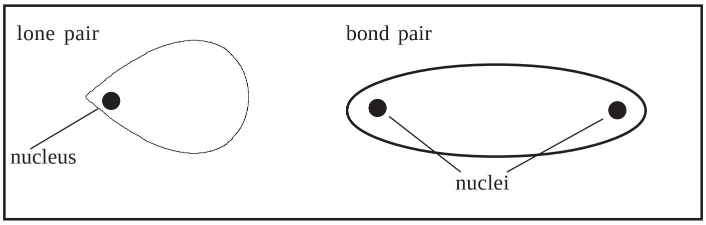
> *VSEPR theory states that each electron pair tries to separate itself as much as possible from other electron pairs (due to electrostatic repulsion.)*
>
> *The shapes of molecules and ions are thus determined by the number of electron pairs* ***not*** *by the atoms.*

**Electron clouds and orbitals**
Although at GCSE we always thought of electrons as simple particles, and we show them like that in dot and cross diagrams, it's not really as simple as that! We never know exactly where an electron is in an atom - just that it's somewhere in a region of space called an **orbital** (see Factsheet 1 - Atomic Structure). Each pair of electrons has its own orbital. Because we can't know where in the orbital the electrons are, the most helpful way of thinking about an electron pair is as a kind of cloud of negative charge - the shape of the orbital tells you the shape of the cloud. Electron clouds are three dimensional - it can help to think of them as like balloons!

**Bond pairs, lone pairs and electron clouds**
The electrons in a bond pair are shared between two atoms. The positive nuclei of both atoms are attracting the negative electrons, so the electron cloud for a bond pair is pulled between the nuclei.

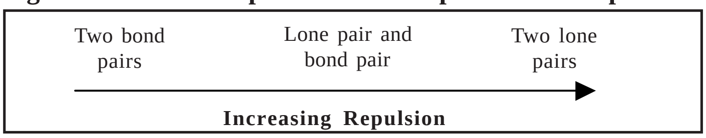
In a lone pair, only one nucleus is attracting the electrons, so the electron cloud is close to that nucleus. This means that the electron cloud for a lone pair looks "short and fat", and for a bond pair "long and thin" (Fig 1.)

**Fig 1. Lone pair and bond pair electron clouds**




**Repulsion, bond pairs and lone pairs**
The shape of the electron cloud for bond pairs and lone pairs matters because it affects the amount of repulsion between them. Both types of electron cloud have the same total charge (-2 from the two electrons), but with the lone pair, the charge is concentrated close to the nucleus. This means the lone pair has a higher **charge density** - so it repels more strongly than a bond pair does. (You can imagine this with balloons as well - each lone pair is a short fat balloon, and each bond pair a long thin balloon. To model the water molecule shown in the first column, (which has two LP and two BP around the oxygen atom) we'd tie two short fat balloons and two long thin balloons to one point. The short fat balloons will push the other balloons away more effectively!) Fig 2 shows how repulsion varies for lone pairs and bond pairs.

**Fig 2. Differences in repulsion with lone pairs and bond pairs**

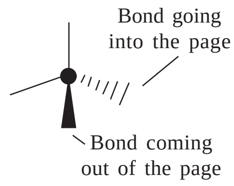



**N.B.** The difference between lone and bond pairs does **not** alter the basic shape of a molecule **BUT** it does distort it and so alter **bond angles** (i.e. the angle between two adjacent bond pairs).

**Finding the shape**
To find the shape of any molecule, go through the following procedure:
1. Draw a dot and cross diagram
2. Count the number of electron pairs (both types) around the central atom.
3 Decide the shape adopted by the electron pairs (see table below)
4 Look at the number of lone pairs, and decide the shape adopted by the atoms (see table on page 3)
5. Draw the shape, including bond angles

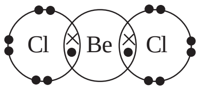
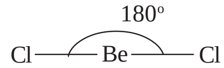
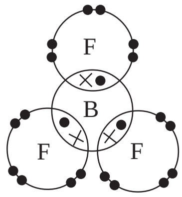
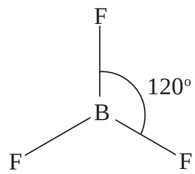
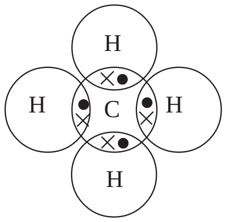
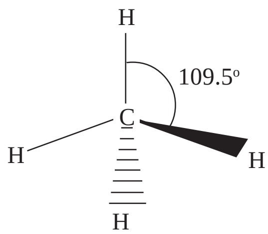
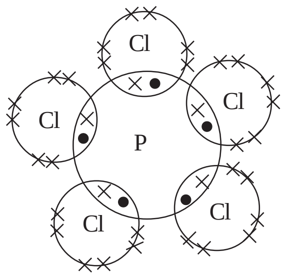
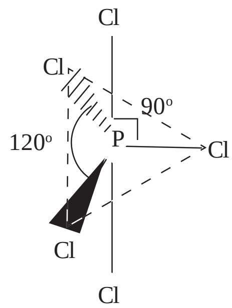
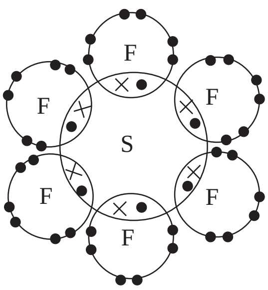
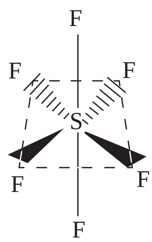
> ***Exam Hint: -*** *Although you have to work out the shape adopted by the electron pairs first, your* ***answer*** *must always be the shape adopted by the* ***atoms***

**Drawing 3D shapes**
No one finds drawing 3D shapes very easy! One way of showing things more clearly is to use different sorts of line to show bonds coming out of the page towards you and bonds going into the page away from you. Other bonds - shown with a normal line - are in the plane of the page, going along it. You can also add dotted lines to diagrams to make the shape clearer.




> ***Exam Hint: -*** *Learn the names, examples and diagrams (with angles!) in tables 1 and 2 - they cover all the common cases you can be asked in the exam.*

**Table 1. Shapes of molecules and ions**

| electron pairs around central atom | Example molecule | dot - cross diagram | Name of shape | Bond angles |
|---|---|---|---|---|
| 2 | $BeCl_2$ |  | linear |  |
| 3<br>Note that in these first two, the central atom does not have 8 electrons - they are *electron deficient*. You'll learn more about this later! | $BF_3$ |  | trigonal planar |  |
| 4 | $CH_4$ |  | tetrahedral |  |
| 5 | $PCl_5$ |  | trigonal bipyramidal |  |
| 6<br>Note in these last two, the central atom has more than 8 electrons. That's because it's using its d-orbitals, so there's extra space. | $SF_6$ |  | octahedral |  all angles 90° |

### Effect of lone pairs on shape

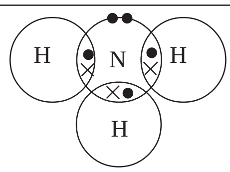
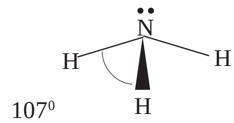
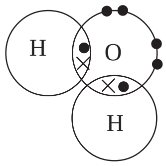
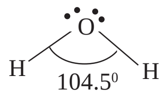
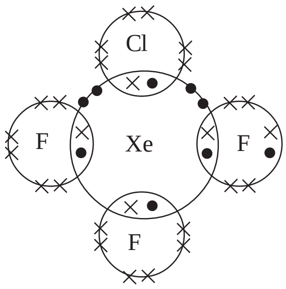
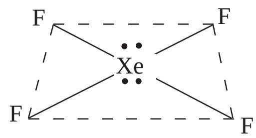
Although the overall shape is determined by the **total** number of electron pairs, lone pairs are important because they affect the shape in two ways:

- **The bond angles are reduced**
  Because lone pairs have a greater repulsive effect, they push the bond pairs closer together. **Learn** the **angles** in table 2.
- **The name of the shape is different**
  Because we can't actually "see" lone pairs, the name of the shape depends on the bond pairs. **Learn** the **shape names** in table 2.

The best examples to look at are $CH_4$, $NH_3$ and $H_2O$. Each of these have four pairs of electrons.

- $CH_4$ is a perfect tetrahedral (4 bond pairs).
- $NH_3$ is based on a tetrahedral shape as it has 4 electron pairs, but because it has 3 bond pairs and 1 lone pair, the bond angle is less due to the increased repulsion from the lone pair. The shape is trigonal pyramidal.
- $H_2O$, similarly, is based on a tetrahedral, but as it has 2 bond pairs and 2 lone pairs, the bond angle is even less due to the repulsion from the two lone pairs.The shape is bent.

**Table 2. Distortion of the basic shapes due to lone pairs**

| molecule | electron pairs around orbital atom | dot - cross diagram | Name of shape | Bond angles |
|---|---|---|---|---|
| $NH_3$ | 4<br>3 BP + 1 LP |  | trigonal pyramidal |  |
| $H_2O$ | 4<br>2 BP. + 2 LP |  | bent |  |
| $XeF_4$ | 6<br>4 BP + 2 LP |  | square planar | <br>*the lone pairs get as far as possible from each other* |

### Multiple bonds and shapes

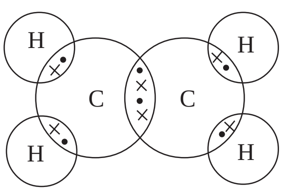
Some molecules - most commonly ethene ($C_2H_4$), ethyne ($C_2H_2$), CO, $CO_2$ and $SO_2$ - contain double or even triple bonds. This is the rule:

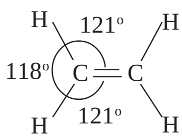
When working out the shape of a molecule a double or triple bond counts as **1 bond pair. But it has greater repulsive power!**

***Exam Hint:-*** *Some molecules and ions (like CO on this page) contain* ***dative bonds*** *(shown as →), where both electrons come from one atom. These behave just like normal single bonds - once the bond is formed, it doesn't matter where the electrons came from in the first place!*

**Fig 3. Shapes of molecules with multiple bonds**

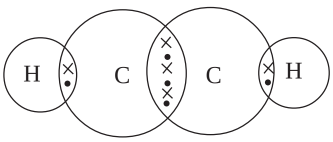
$C_2H_4$

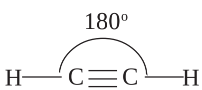





trigonal planar

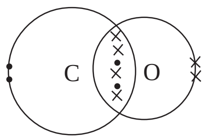
$C_2H_2$





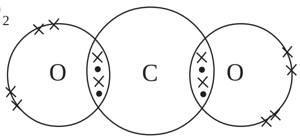

linear

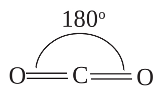
CO




linear

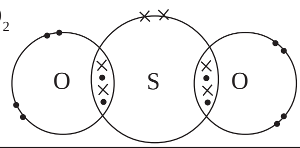
$CO_2$

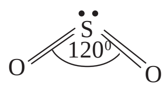





linear

$SO_2$






bent

## Shapes of ions

Working out shapes of ions is very similar to molecules. You draw a dot and cross diagram as before, but you must remember:

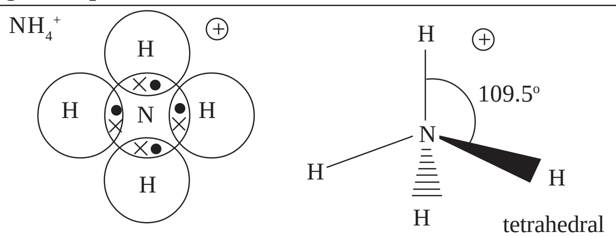
- If it's a **positive** ion (cation), **remove** the same number of electrons as the charge on the ion.
- If it's a **negative** ion (anion), **add** the same number of electrons as the charge on the ion

This will give the central atom a full outer shell.

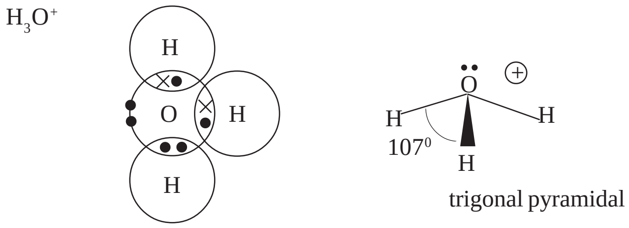
**1. Cations**

You only need to know two of these - $NH_4^+$ and $H_3O^+$

**Fig 4. Shapes of cations**




(4 bond pairs, so the same shape as $CH_4$)




(3 bond pairs + 1 lone pair, so the same shape as $NH_3$)

**2. Anions**

You need to know $NO_3^-$, $SO_4^{2-}$ and $CO_3^{2-}$

All of these ions, from the dot and cross diagrams, appear to contain a mixture of normal single bonds, dative single bonds and double bonds. Although the dative bonds wouldn't affect the shape, the double bonds normally would. But they don't in these anions! **All the bond angles are the same!**

This is because of something called **delocalisation**, which you will study properly in organic chemistry. What it basically means is that in, for example, the nitrate ion, instead of having one normal single bond, one dative bond and one double bond, the "spare" electrons in the double bond are "shared" between all three bonds, so that all the bonds are the same. You don't have to worry about the details of this yet!

*Exam Hint:- Learn the dot and cross diagrams for the ions - they may not be that easy to work out in an exam!*

**Useful Websites**

There are many useful resources on the internet for this topic, including animated diagrams and free software for drawing and viewing molecules. Here are three!

http://wunmv.wustl.edu/EduDev/Vsepr
http://www.spusd.k12.ca.us/chemmybear/shapes.html
http://www.chem.ufl.edu/~myers/chm2045/shapes.htm

## Practice Questions

Examination questions on this topic usually form one part of a complete question and ask for the dot and cross diagram of a molecule/ion along with its shape and bond angles. The molecules below have all been asked in AS and A2 specimen questions.

1. For each of the molecules/ions below
   (i) draw its dot-cross diagram
   (ii) sketch its shape
   (iii) show its bond angles
   (iv) give the name of the shape

   (a) $H_2S$
   (b) $CHCl_3$
   (c) $F_2O$
   (d) $PF_5$
   (e) $PCl_6^-$
   (f) $SiCl_4$
   (g) HCN
   (h) $POCl_3$
   (i) $BeF_2$
   (j) $PCl_3$

   (3 marks each)

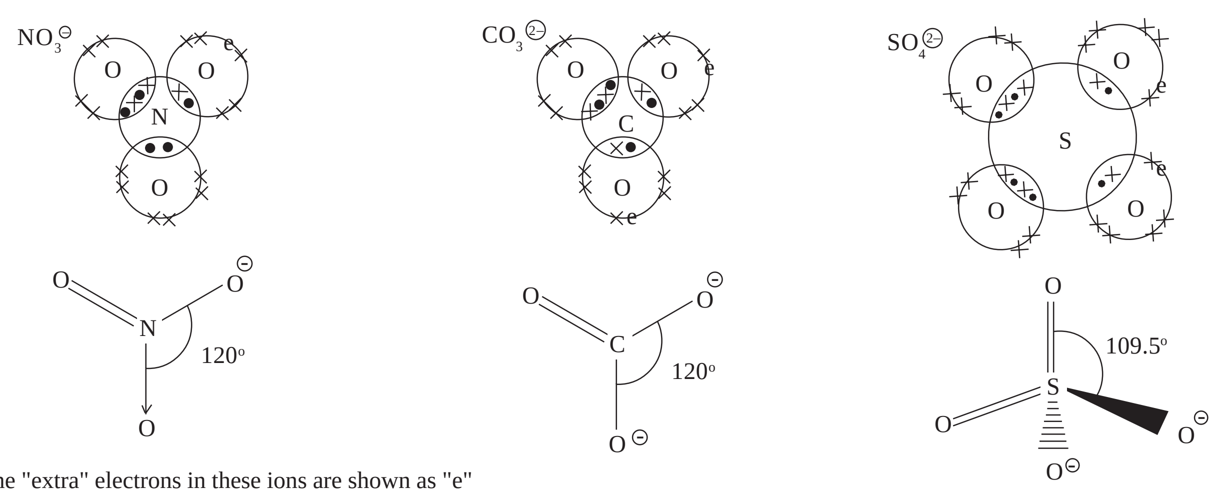
2. Explain, using a dot-cross diagram, why $XeF_4$ has a square planar structure.

   (4 marks)

3. What factors affect the shape of a molecule?

   (3 marks)

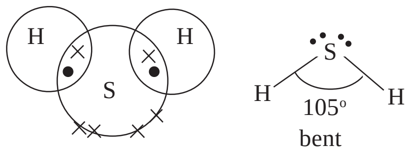
**Fig 4. Shapes of anions** - ***Remember all the bond angles are equal!***




NB: the "extra" electrons in these ions are shown as "e"

**Answers**
marks:- (1) dot-cross (1) shape (1) bond angles

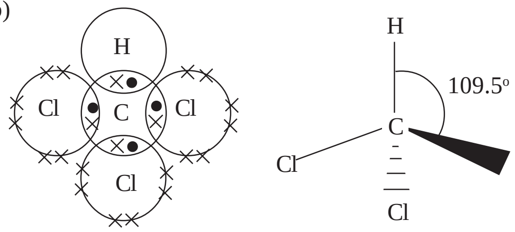
1. (a)




bent

(3)

(b)




tetrahedral

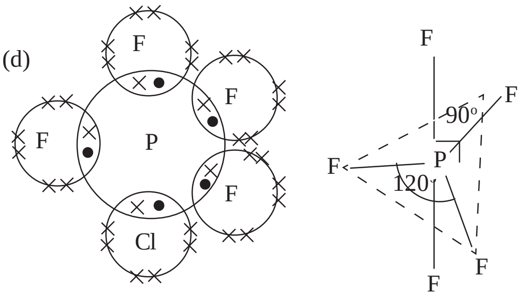
(3)

(c)


bent

(3)

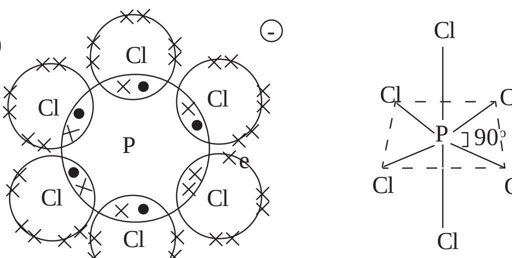
(d)




trigonal bipyramidal

(3)

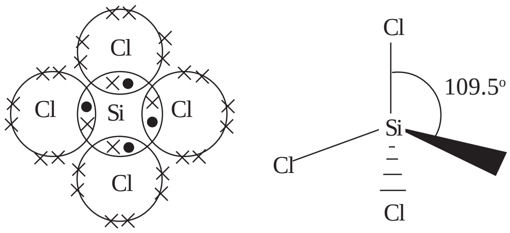
(e)




octahedral

(3)

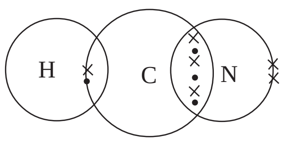
(f)

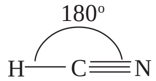



tetrahedral

(3)

(g)

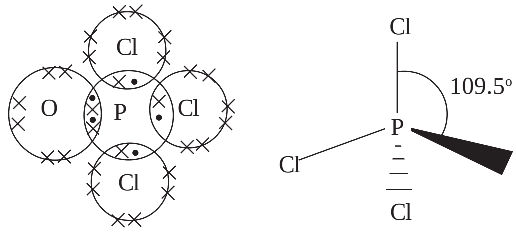



linear

(3)

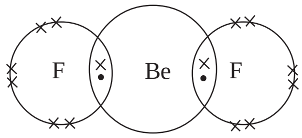
(h)

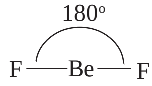



(3)

tetrahedral

(i)

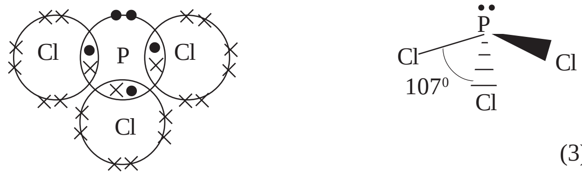



linear

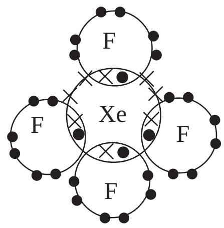
(3)

(j)



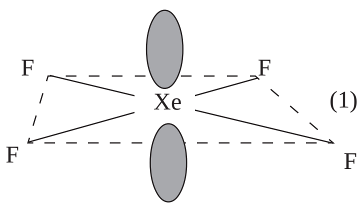

(3)

2.




(1)

Around the central Xe atom there are 6 electron pairs - 2 lone pairs and 4 bond pairs (1)
6 pairs give an **octahedral** shape.(1) Lone-pairs repel more than bond-pairs, so the lone-pairs position themselves away form each other on opposite sides




(1)

3. The factors are
   (a) the number of electron pairs in total (1)
   (b) how many are bond-pairs and how many are lone-pairs (1)
   (c) lone-pairs repel more than bond-pairs. (1)

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