Shapes of Molecules part 2

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More difficult shapes

Example: ClF_3

Firstly identify the central atom, which is of course **chlorine**.

Group 7 → 7 outer electrons and that it makes **3 single bonds** to the fluorine atoms.

Lone pairs: we have **4 electrons** left over → **2 lone pairs**

3 bonding pairs and **2 lone pairs**

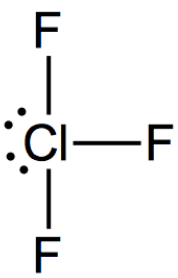
What shape is it based on?

From part 1, we had a nice table with all the combinations of bonding pairs and lone pairs. Well, this combination does not appear in the table….hmmmm.

There are **3 bonds plus 2 lone pairs**, which makes **"5"** in total. From the table, we know that 5 is usually trigonal bipyramidal. So this is what we base our shape on and draw something shape similar to this.

✓ It's exactly the same theory when going from CH_4 → NH_3 → H_2O

So, we simply remove two bonds from a normal trigonal bipyramidal shape and put in two lone pairs instead:

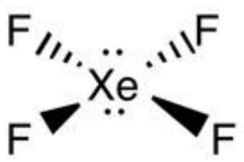


This isn't the easiest example but it demonstrates all the points you need to be able to do.

The bond angles will be reduced slightly from the normal 90° and 120° due to the lone pairs, but it is ok to draw it as shown. Again, the bond angle reduction is the same theory as we looked at before.

✓ Don't worry about the names of shapes like this. You aren't expected to know them, just how to get the shape and approximate bond angles. Also, if you put the lone pairs somewhere else, you should get the marks still.

Example: XeF_4



Another unusual one is a **square planar** shape. It is based on octahedral (6 things surrounding the central atom) but with 2 of the bonds replaced by lone pairs.

An example that has appeared a few times is XeF_4 (all bond angles are 90°).

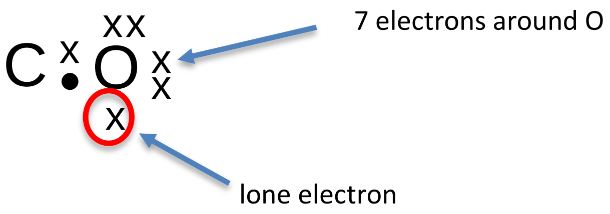
4 bonding pairs and **2 lone pairs**

Ions

Up to now we have not really paid much attention to the atoms on the 'outside' of the molecule, we have been looking at the central atom. But you have to be careful especially when oxygen is on the outside.

The problem with oxygen

If an oxygen atom only forms **one bond** to a central atom, this would leave only has **7 electrons** around it….it needs 8. And one of the electrons is **not paired** up, which would make it a radical!



Oxygen usually forms two bonds and the above is the reason why. That's why CO_2 has two double bonds and not two single bonds.

This might seem like common sense and you probably know that oxygen forms two bonds but when faced with drawing an ion like NO_3^- or SO_4^{2-}, students have no idea what to do and often draw one bond from oxygen to the central atom.

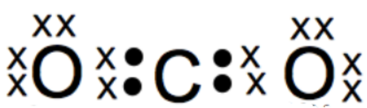
Solving the oxygen problem

There are three possible solutions to this problem:

1. form a double bond between oxygen and the central atom.

If you form a double bond to an oxygen, then the problem is solved. Oxygen contributes two electrons to the bond and therefore there are 4 outer electrons left.

You will be familiar with this in CO_2. As was mentioned above, both bonds are C=O.



2. 'give' oxygen an extra electron i.e. form an ion with a charge.

A 1- charge means an **extra electron** has been given to **one** of the oxygen atoms. A 2- charge means one electron has been given to **two** different oxygen atoms.

✓ Oxygen is not the only example this could apply to but it is by far the most common atom used in these examples.

✓ There are examples of ions with a 1+ charge. In this case we are probably not talking about oxygen. A very well known example is NH_4^+. The + charge means an **electron has been removed** to ensure an even number of outer electrons.

3. form a dative covalent bond.

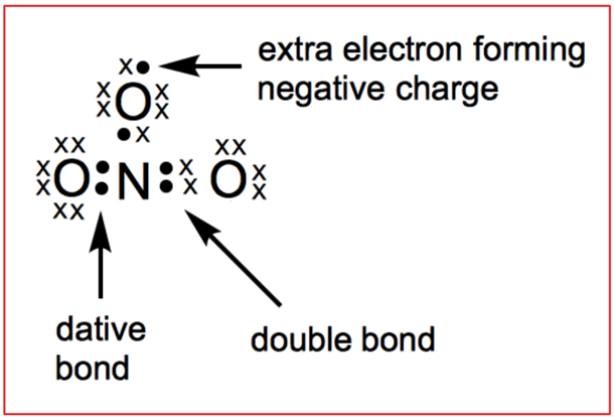
This is an alternative to forming a double bond. Instead of one atom contributing one electron, it will contribute two electrons. This also solves the outer electron problem.

NO_3^-

Keeping the above rules in mind we will look at how to draw a few of these ions.

N has **5 outer electrons** and is forming **3 bonds** to the oxygens, which would leave us with a lone pair. But we can't do this as it would give us 3 x N-O single bonds and the lone electron problem we discussed above.

However, there is **one negative charge**, which takes care of one of the oxygen atoms. So, we can have one N-O single bond as long as that oxygen has the negative charge on it. This uses one of the nitrogen electrons, so we have 4 left.



The other two bonds have to be double bonds or one double bond and one dative covalent single bond (both electrons coming from the nitrogen).

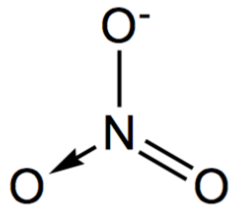
In the Edexcel June 2014 paper they said in the question that nitrogen forms a dative covalent bond, so I would go with that. But if they didn't say that, then you could draw either option, they are both technically correct.

To get the shape from this, just treat it like the examples we did before:

3 bonding pairs and **0 lone pairs**

✓ The double bond is counted as **one** bonding pair still.

So what shape in the basic shapes does this fit? **Trigonal planar**



SO_4^{2-}

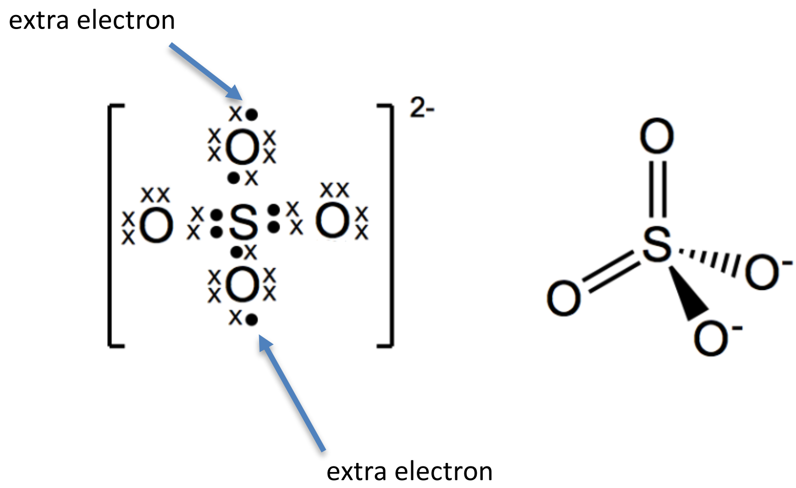
This is similar to the NO_3^- example. You have the outside oxygens again. Sulphur has 6 outer electrons.

There is a 2- charge this time, which means one electron is given to two oxygen atoms. Therefore those oxygens are ok, we can form 2 x S-O single bonds with a negative charge on each oxygen.

We still have 4 electrons left on sulphur. We can't simply do two single bonds as we'll hit the old oxygen problem again. But we could try two double bonds, which would leave us with 0 lone pairs:

4 bonding pairs and **0 lone pairs**

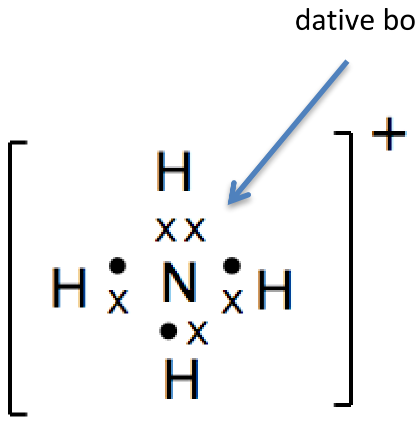
And we now are very familiar that this is **tetrahedral**:



Note that sulphur 12 electrons around it and not 8. This is possible with bigger elements

✓ AQA do tend to get some strange looking ions in questions. Just apply the above theory. If it is a positively charged ion, then they have just **removed an electron** to ensure the electrons are all paired up and that there are 8 electrons around each atom.

NH_4^+



✓ the '+' has occurred due to an electron being **removed** from the 'H' atom at the top. Nitrogen has made a dative bond to the same 'H'. There are 8 electrons around the 'N'.

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