Shapes of Molecules part 1

[Click here for shapes part 2]

VSEPR (Valence Shell Electron Pair Repulsion Theory)

You may not have heard of the VSEPR abbreviation but it is worth knowing, as it is a good reminder of the theory behind this topic: valence shell = **outer shell** and therefore **outer electrons**. And everything is based on **electrons repelling** each other.

> the reason any molecule adopts its' shape is to **minimise repulsion**

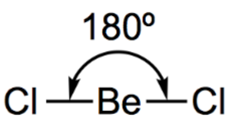
Classic exam question….why does a molecule adopt a particular shape? The electrons position themselves as far apart as possible to **minimize repulsion** → the shapes shown below.

The repulsion is between **electrons** in bonds (bonding pairs), between **lone pairs** or between lone pairs **and** bonding pairs.

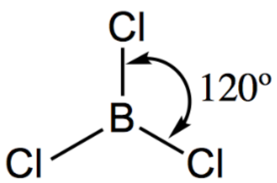
Basic Shapes

I have listed the 7 basic shapes below plus their bond angles. You have to know these. You must know these….you just HAVE to know these! This is the starting point to the whole topic and makes life so much easier if you can recall them on demand. They use a lot of these examples in multiple choice questions, so you can gain some really cheap marks. How many times have they used NH_3!

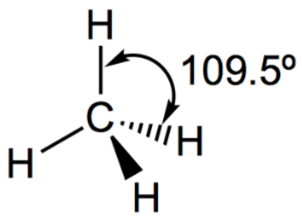
Linear: $BeCl_2$



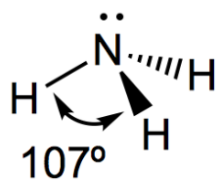
Trigonal Planar: BCl_3



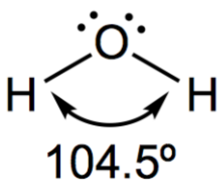
Tetrahedral: CH_4



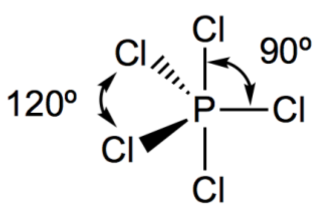
Trigonal Pyramidal (or pyramidal): NH_3



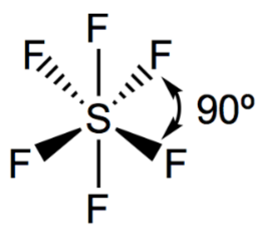
Bent or non-linear: H_2O



Trigonal Bipyramidal: PCl_5



Octahedral: SF_6



✓ These are the common examples, of course there are others you could use instead. But I would stick to these as they are straight out the marking schemes.

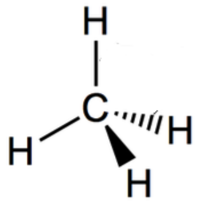
✓ In most of examples we are trying to get 8 electrons around the central atom to satisfy the "octet" rule. But look out for boron which only has **6 electrons** around it (very unusual) and also larger elements like phosphorus which has **10 electrons** around it or sulphur with **12**.

Using the list

We can make the list a bit more user friendly. And this is will be the basis for working out shapes of molecules that are not on the list. The aim is to work out:

how many **bonding pairs** (bonds) and how many **lone pairs** there are

CH_4



We firstly look at what group the **central atom** is in (the atom in the middle) i.e. carbon**.....group 4 → 4 outer electrons**. This means there are 4 electrons on carbon *available* to form bonds.

✓ I am ignoring hydrogen. Assume that the atoms on the "outside" contribute one electron each to a bond no matter what group it's in.

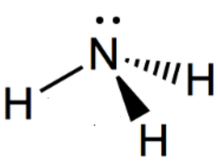
✓ If you are unclear on any of this, just think of dot and cross diagrams. You take one electron from carbon and one from hydrogen to form a bond. That's all we are doing here.

Now, how many bonds is carbon actually making? The formula tells you that! The H_4 part gives it away…it is making **4 bonds**. Therefore all the 4 electrons are **used up** making the 4 bonds….and the important part…. there are **no lone pairs** as all the electrons from carbon are used up making the 4 bonds:

4 bonding pairs and **0 lone pairs**

✓ This is what you are aiming to get to every single time you do these questions.

NH_3



Nitrogen is in **group 5 → 5 outer electrons.** We can see from the formula that there are only 3 bonds. So only 3 of the nitrogen electrons are being used in bonds, therefore **two electrons must be left over**…..and 2 electrons = 1 pair….so we have **one lone pair**.

3 bonding pairs and **1 lone pair**

Doing it quicker!

Above might seem a bit long winded. But with time you can do this very quickly. All you are doing is working out how many lone pairs it has as you can see from the formula how many bonds it has.

CH_4…I can see immediately it has 4 bonds. So how many lone pairs, if an?. All I do is match the number of bonds to the group number….carbon is group 4 and there are 4 bonds…therefore there are no electrons "unused" and therefore no lone pairs.

NH_3….there are 3 bonds but nitrogen is group 5 therefore there must be 2 electrons left over → 1 lone pair.

If you think about it….you can do this exceptionally quickly. All we are really doing is:

group number – the number of bonds → lone pairs

✓ Just be careful. Remember **2 electrons = ONE pair**….just like socks…or gloves.

We can then do the same for ALL the 7 molecules in the magic list above to form a table:

Shape Name	Bonding Pairs	Lone Pairs	Total
Linear	2	0	2
Trigonal Planar	3	0	3
Tetrahedral	4	0	4
Pyramidal	3	1	4
Bent	2	2	4
Trigonal Bipyramidal	5	0	5
Octahedral	6	0	6

✓ I put a "total" column in the table. This is not needed except when looking at the progression in bond angles from CH_4 → NH_3 → H_2O. I have written more on this at the end of this tutorial.

Shapes of other molecules

The best part is now you can work out the shape of ANY molecule, more or less. We just need to do as we did above and then one final step….

compare the number of bonding pairs and lone pairs to those in the table above → **shape name**

H_2S

Exactly the same as we did above….sulphur is **group 6 → 6 outer electrons**. We can see it is only making **2 bonds**. Therefore we must have 4 electrons remaining → **2 lone pairs**.

2 bonding pairs and **2 lone pairs**

Now look at the table above…which shape has 2 bonding pairs and 2 lone pairs? Bent…therefore H_2S is the same shape as H_2O. Easy! Reallllllyyy reaallllyyy easy.

PCl_3

Phosphorus is in **group 5 → 5 outer electrons**. It is making **3 bonds**, therefore we must have **one lone pair:**

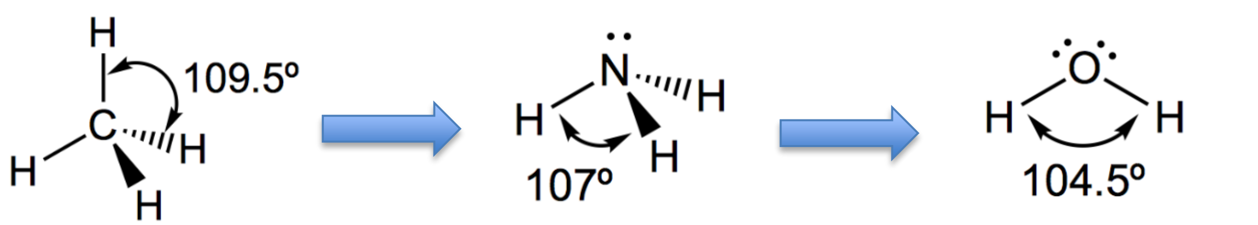
3 bonding pairs and **1 lone pair**

So again, look at the table above…it's pyramidal. It becomes really boring after a while. Same old shapes!

Reduction in bond angles

An extremely common question is to ask about the progression in bond angles from CH_4 → NH_3 → H_2O…which is 109.5° → 107° → 104.5°.

✓ If you call it 109 or 109.5, it's fine. Doesn't have to be THAT accurate.



4 bonding pairs
0 lone pairs

3 bonding pairs
1 lone pair

2 bonding pairs
2 lone pairs

Why? It's the introduction of lone pairs. The **lone pairs cause more repulsion** and forces the electrons in bonds to move further away from the lone pairs → reduction in bond angle.

Tetrahedral is the “big daddy” in this progression. 109.5° is the starting point. The NH_3 and H_2O shapes are based on tetrahedral as the have “4 things” in total (see table further up the page). But the lone pairs as I mentioned cause this angle to reduce slightly. Alongside this, **the name must change**.

The names come from the bond angle. As soon as the angle changes, the name changes

One step further…CH_4 only has repulsion between electrons in bonds. NH_3 has the extra repulsion of the lone pair and the electrons in bonds. H_2O has even more repulsion as the lone pairs repel each other as well.

Lone pair:lone pair repulsion > lone pair:bonding pair repulsion > bonding pair:bonding pair repulsion

This could apply to more complicated examples as well, which we will look at in part 2. It’s not always just the above progression.

Click here for shapes part 2