SHAPES OF MOLECULES

Molecules and ions possess two types of electron pairs:

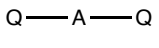
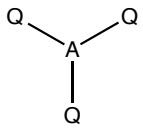
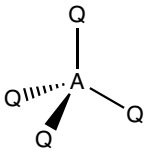
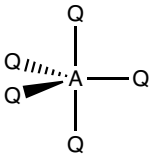
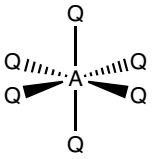
- **Bonding pairs** (the two shared electrons in a covalent bond)
- **Lone pairs** (two electrons in a pair not involved in bonding – also known as **non-bonding pairs**).

These electron pairs will repel each other as far as possible.

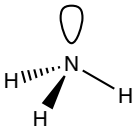
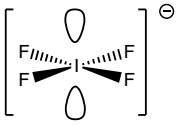
The shape of any molecule or ion is a consequence of the number of electron pairs which repel each other as far as possible.

Lone pairs are more compact than bonding pairs. This means that lone pairs repel more than bonding pairs. This reduces the bond angles to a small extent.

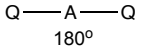
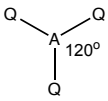
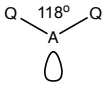
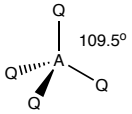
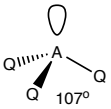
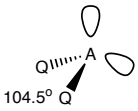
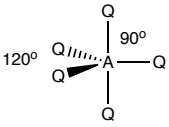
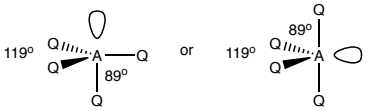
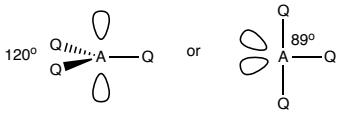
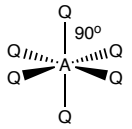
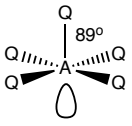
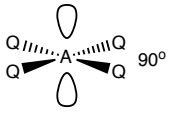
There are five basic shapes that you have to know, and all other shapes are based on these.

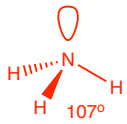
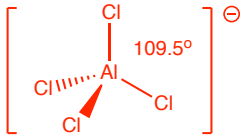
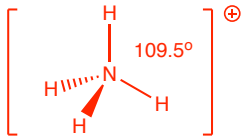
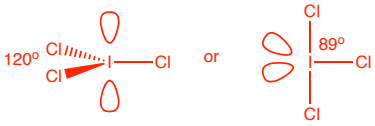
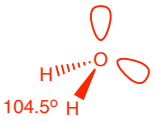
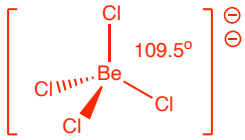
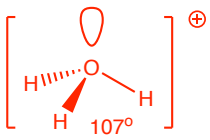
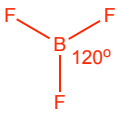
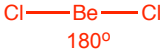
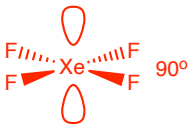
number of electron pairs*	2 pairs	3 pairs	4 pairs	5 pairs	6 pairs
shape					
name of shape	linear	trigonal planar	tetrahedral	trigonal bipyramidal	octahedral
bond angle	180º	120º	109.5º	120º, 90º	90º

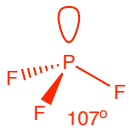
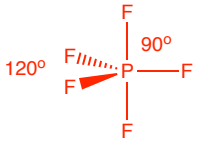
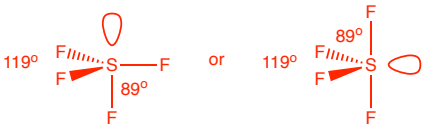
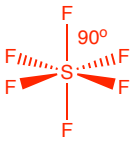
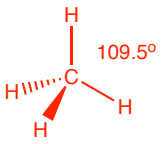
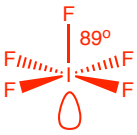
(* double bond counts as one pair for this)

Working out shapes (single bonds only)	NH_3	IF_4^-
1) Count the number of electrons on the central atom. If the species is charged, add or remove electron(s) to account for the charge.	N is in group 5 so has 5 outer shell electrons	I is in group 7 so has 7 outer shell electrons; however the species is 1– and so there is one extra electron, so there are 8 outer shell electrons.
2) Each atom forms one bond to the central atom using one of the central atom's electrons. How many electrons are left and so how many lone pairs are there?	3 of the 5 electrons are used in the bonds to N this leaves 2 other electrons which make 1 lone pair	4 of the 8 electrons are used in the bonds to I this leaves 4 other electrons which make 2 lone pairs
3) How many electron pairs altogether?	3 bonding pair + 1 lone pair = 4	4 bonding pair + 2 lone pair = 6
4) What is the shape based on?	4 electron pairs mean the shape is based on a tetrahedron	6 electron pairs mean the shape is based on a octahedron
5) Take into account the lone pairs	3 of the 4 pairs are bonds so the shape based on the bonds is trigonal pyramidal.  bond angle 107° (Bond angles will be slightly less than the normal tetrahedral bond angle due to the extra repulsion from the lone pair.)	4 of the 6 pairs are bonds so the shape based on the bonds is square planar (the lone pairs get as far apart as possible and go on opposite sides).  bond angle 90° (As the lone pairs are opposite each other, the extra repulsions cancel each other out)

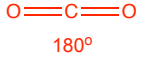
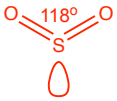
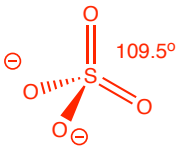
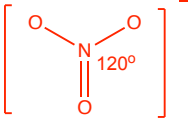
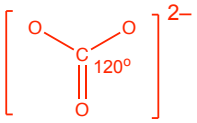
This table shows common shapes, including those where there are lone pairs.

total number of electron pairs	**number of bonding pairs**	**number of lone pairs**	**shape**	
2	2	0		linear
3	3	0		trigonal planar
	2	1		bent (V-shape)
4	4	0		tetrahedral
	3	1		trigonal pyramidal
	2	2		bent (V-shape)
5	5	0		trigonal bipyramidal
	4	1		trigonal pyramidal or see-saw
	3	2		trigonal planar or T-shape
6	6	0		octahedral
	5	1		square pyramid
	4	2		square planar

Species	Number of outer shell electrons (corrected for any charge)	Number of bonding pairs	Number of lone pairs	Sketch of shape & bond angles	Name of shape
NH_3	5	3	1		trigonal pyramidal
$AlCl_4^-$	4	4	0		tetrahedral
NH_4^+	4	4	0		tetrahedral
ICl_3	7	3	2		trigonal planar or T-shape
H_2O	6	2	2		bent (V-shape)
$BeCl_4^{2-}$	4	4	0		tetrahedral
H_3O^+	5	3	1		trigonal pyramidal
BF_3	3	3	0		trigonal planar
$BeCl_2$	2	2	0		linear
XeF_4	8	4	2		square planar

Species	Number of outer shell electrons (corrected for any charge)	Number of bonding pairs	Number of lone pairs	Sketch of shape & bond angles	Name of shape
PF_3	F	3	1		trigonal pyramidal
PF_5	5	5	0		trigonal bipyramidal
SF_4	6	4	1		trigonal pyramidal or see-saw
SF_6	6	6	0		octahedral
CH_4	4	4	0		tetrahedral
IF_5	7	5	1		square pyramid

Extension task Here are some harder examples (these contain double bonds – each double bond effectively acts as one bonding pair). Sketch, name the shape give bonds angle(s).

	CO_2	SO_2	SO_4^{2-}	NO_3^-	CO_3^{2-}
Sketch & bond angle(s)					
Name	linear	bent (V-shape)	tetrahedral	trigonal planar	trigonal planar