

# **SHAPES OF MOLECULES**

# SHAPES OF MOLECULES

## CONTENTS

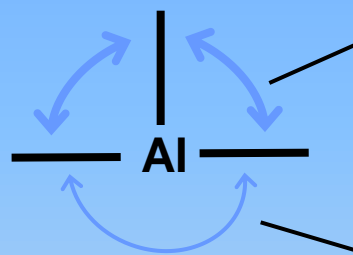
- **Prior knowledge**
- **Electron pair repulsion theory**
- **The regular molecular shapes**
- **Shapes of molecules with lone pairs**
- **Shapes of ions**
- **Molecules with double bonds**
- **Other examples**
- **Test questions**
- **Check list**



# ELECTRON PAIR REPULSION THEORY

**“THE SHAPE ADOPTED BY A SIMPLE MOLECULE OR ION IS THAT WHICH KEEPS REPULSIVE FORCES TO A MINIMUM”**

Molecules contain covalent bonds. As covalent bonds consist of a pair of electrons, each bond will repel other bonds.

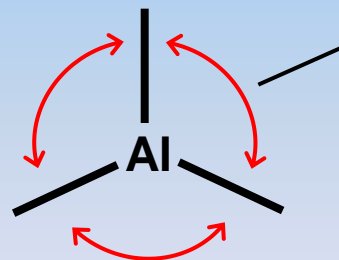


Bonds are **closer together** so **repulsive forces are greater**

Bonds are **further apart** so **repulsive forces are less**

Bonds will therefore push each other as far apart as possible to reduce the repulsive forces.

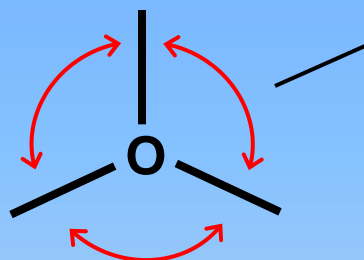
Because the repulsions are equal, the bonds will also be equally spaced



All bonds are **equally spaced** out as far apart as possible

# ELECTRON PAIR REPULSION THEORY

**“THE SHAPE ADOPTED BY A SIMPLE MOLECULE OR ION IS THAT WHICH KEEPS REPULSIVE FORCES TO A MINIMUM”**



All bonds are equally spaced out as far apart as possible to give minimum repulsive forces

Because of the equal repulsive forces between bond pairs, most simple molecules, (ones with a central atom and others bonded to it), have standard shapes with equal bond angles.

However, the presence of lone pairs on the central atom affects the angle between the bonds and thus affects the shape.

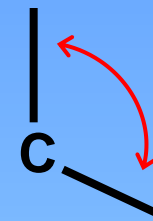
MOLECULES WITHOUT LONE PAIRS

MOLECULES WITH LONE PAIRS

# REGULAR SHAPES

Molecules, or ions, possessing **ONLY BOND PAIRS** of electrons fit into a set of standard shapes. **All the bond pair-bond pair repulsions are equal.**

All you need to do is to count up the number of bond pairs and choose one of the following examples...



A covalent bond will repel another covalent bond

<b>BOND PAIRS</b>	<b>SHAPE</b>	<b>BOND ANGLE(S)</b>	<b>EXAMPLE</b>
2	LINEAR	180°	BeCl <sub>2</sub>
3	TRIGONAL PLANAR	120°	AlCl <sub>3</sub>
4	TETRAHEDRAL	109.5°	CH <sub>4</sub>
5	TRIGONAL BIPYRAMIDAL	90° & 120°	PCl <sub>5</sub>
6	OCTAHEDRAL	90°	SF <sub>6</sub>

# BERYLLIUM CHLORIDE



**Beryllium - has two electrons to pair up**

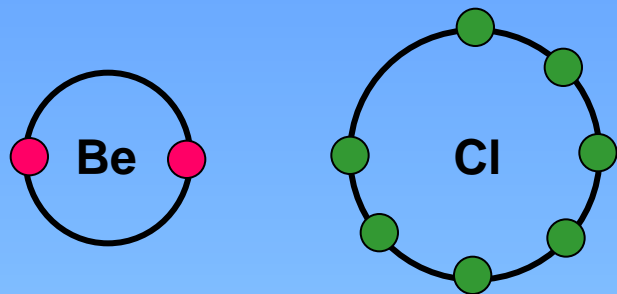
**Chlorine - needs 1 electron for 'octet'**

**Two covalent bonds are formed**

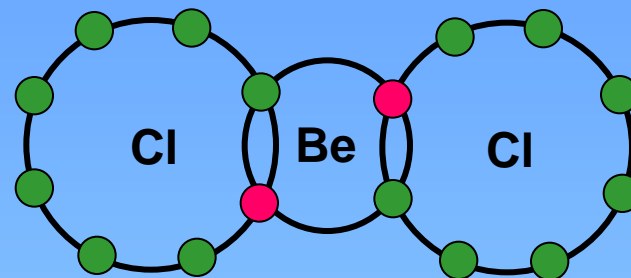
**Beryllium still has an incomplete shell**



# BERYLLIUM CHLORIDE



Beryllium - has two electrons to pair up  
Chlorine - needs 1 electron for 'octet'

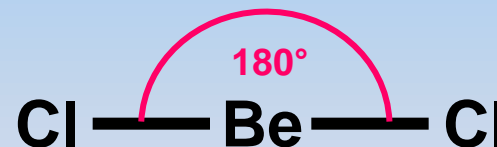


Two covalent bonds are formed  
Beryllium still has an incomplete shell

BOND PAIRS	2
LONE PAIRS	0

BOND ANGLE... **180°**

SHAPE... **LINEAR**

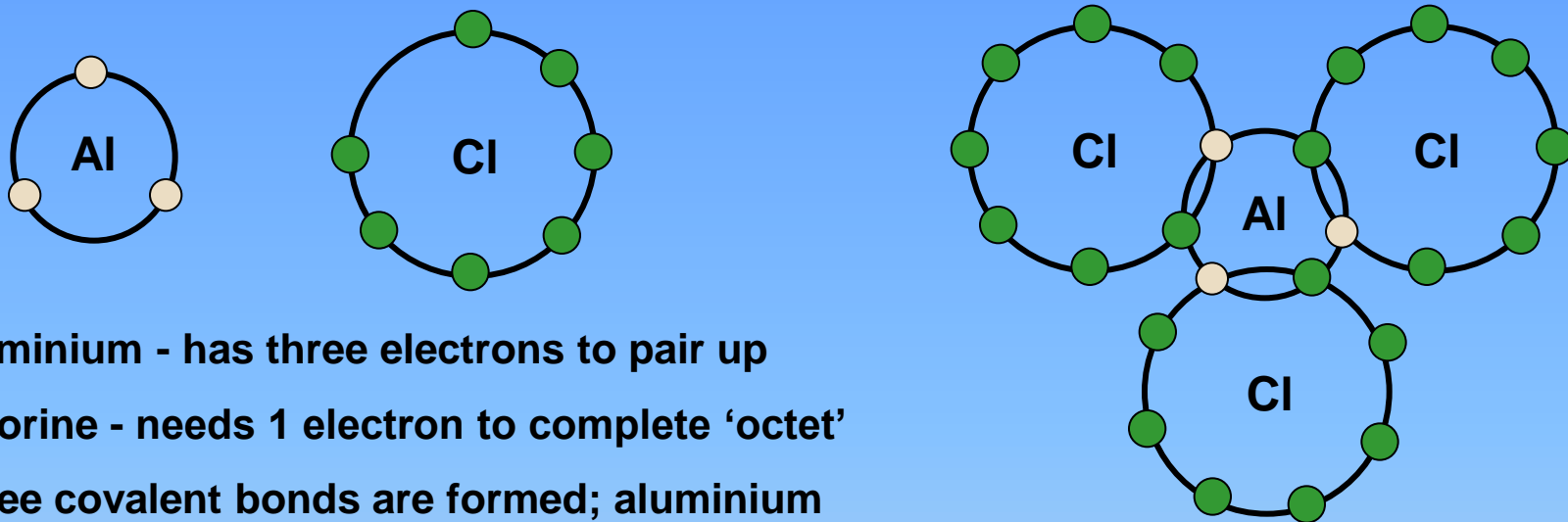


## ADDING ANOTHER ATOM - ANIMATION





# ALUMINIUM CHLORIDE



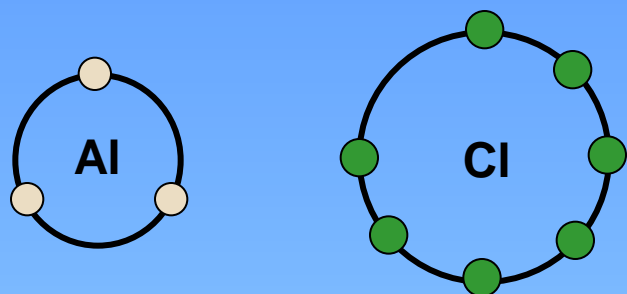
**Aluminium - has three electrons to pair up**

**Chlorine - needs 1 electron to complete 'octet'**

**Three covalent bonds are formed; aluminium still has an incomplete outer shell.**



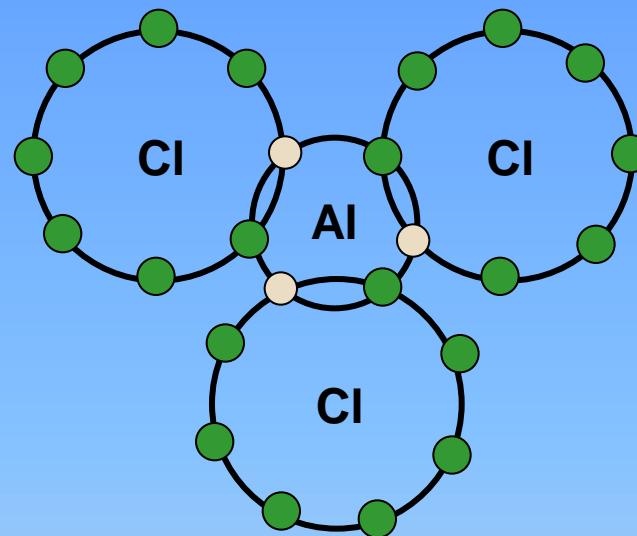
# ALUMINIUM CHLORIDE



Aluminium - has three electrons to pair up

Chlorine - needs 1 electron to complete 'octet'

Three covalent bonds are formed; aluminium still has an incomplete outer shell.

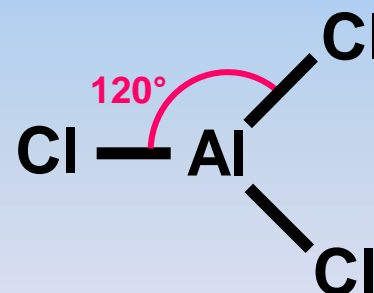


BOND PAIRS 3

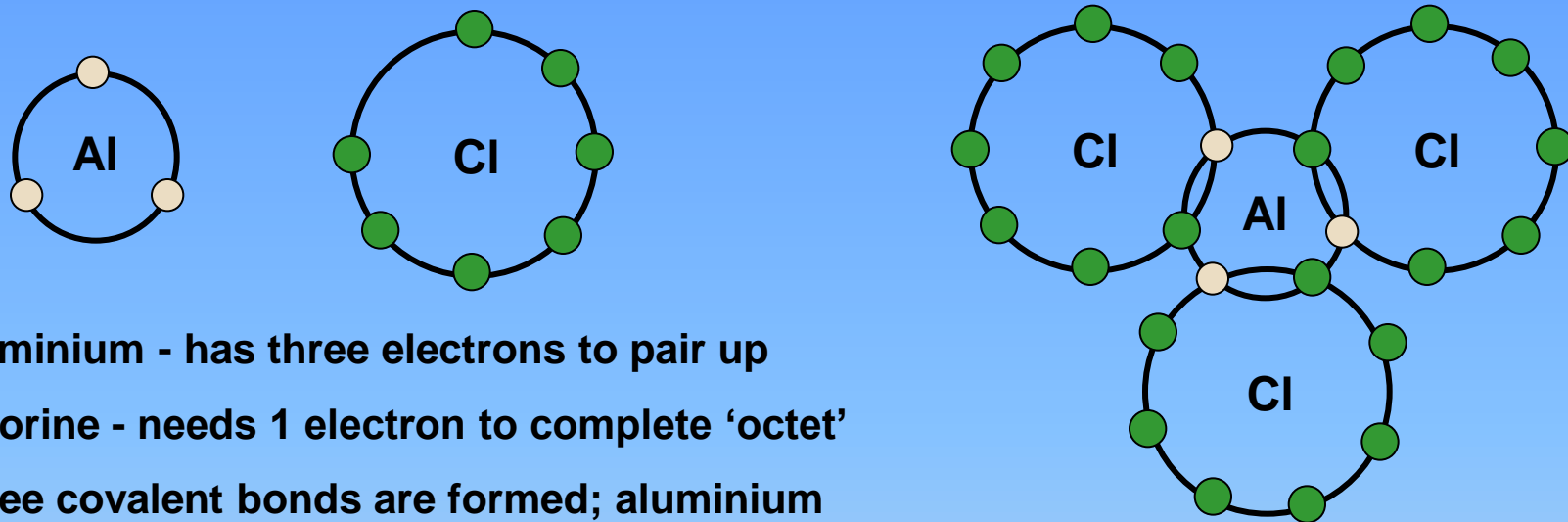
LONE PAIRS 0

BOND ANGLE... **120°**

SHAPE... **TRIGONAL PLANAR**



# ALUMINIUM CHLORIDE



Aluminium - has three electrons to pair up

Chlorine - needs 1 electron to complete 'octet'

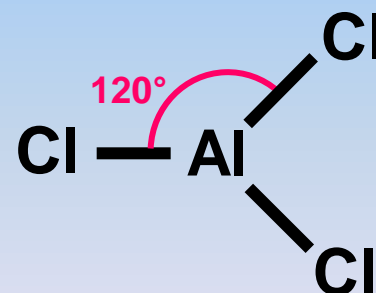
Three covalent bonds are formed; aluminium still has an incomplete outer shell.

BOND PAIRS 3

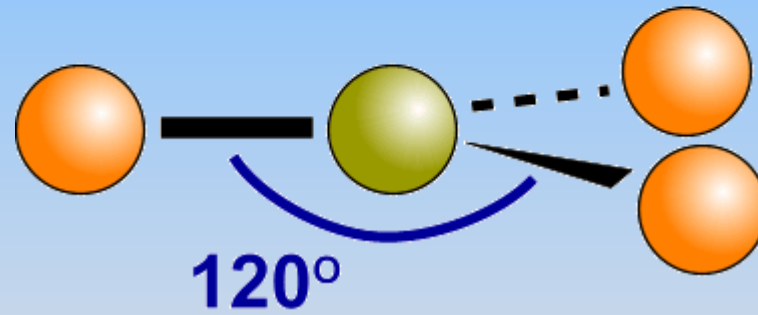
LONE PAIRS 0

BOND ANGLE... **120°**

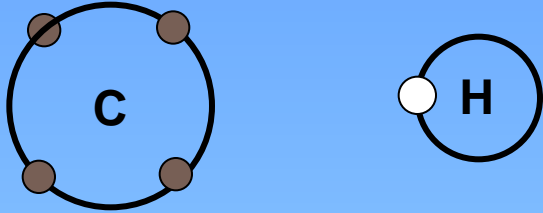
SHAPE... **TRIGONAL PLANAR**



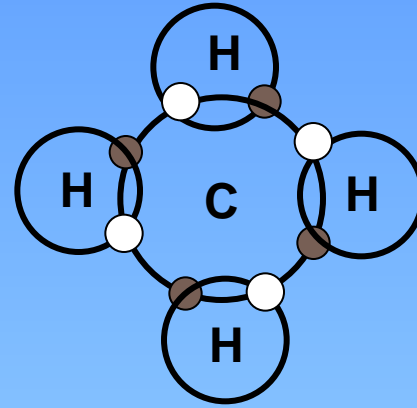
## ADDING ANOTHER ATOM - ANIMATION



# METHANE



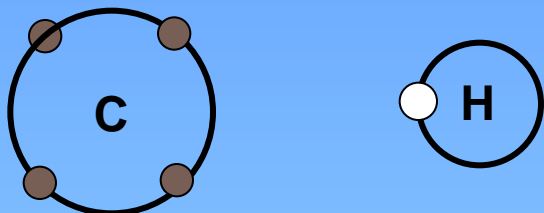
**Carbon - has four electrons to pair up**  
**Hydrogen - 1 electron to complete shell**



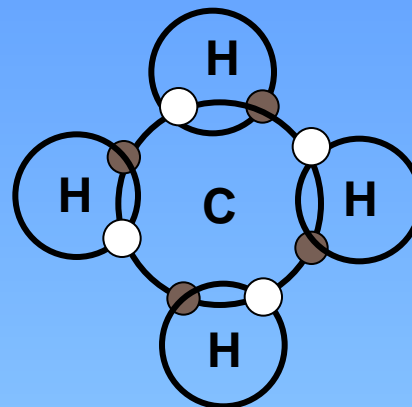
**Four covalent bonds are formed**  
**C and H now have complete shells**



# METHANE



Carbon - has four electrons to pair up  
Hydrogen - 1 electron to complete shell

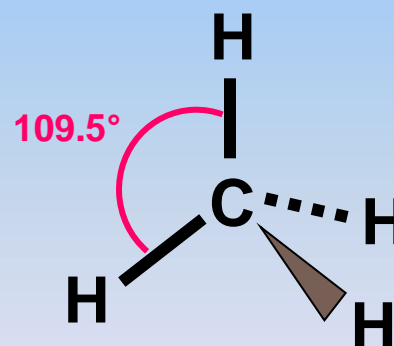


Four covalent bonds are formed  
C and H now have complete shells

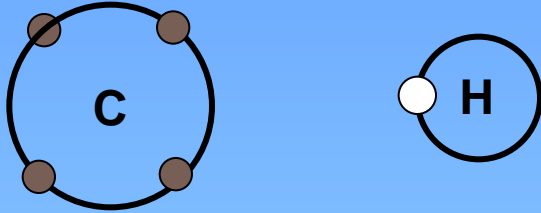
**BOND PAIRS**                      4  
**LONE PAIRS**                    0

BOND ANGLE... **109.5°**

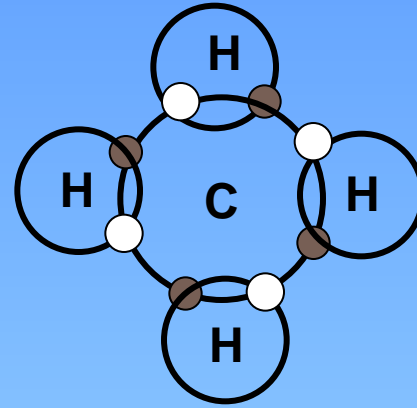
SHAPE... **TETRAHEDRAL**



# METHANE



Carbon - has four electrons to pair up  
Hydrogen - 1 electron to complete shell



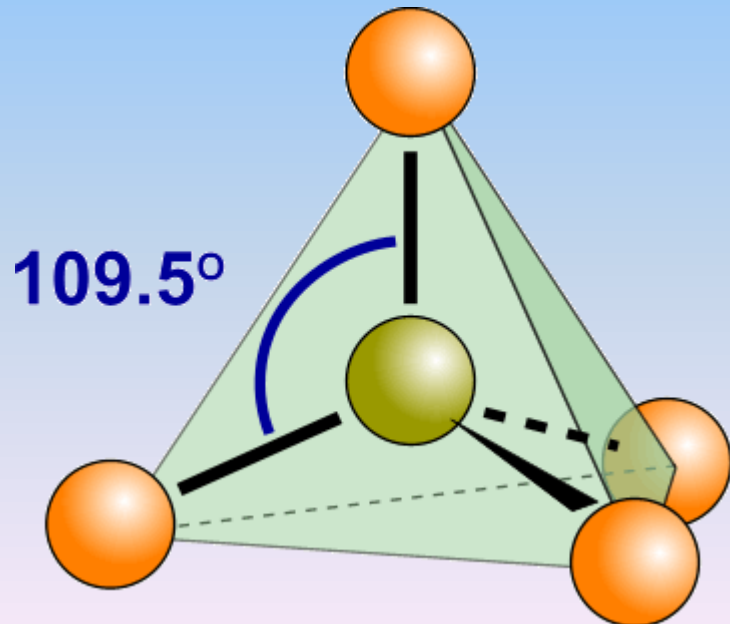
Four covalent bonds are formed  
C and H now have complete shells

BOND PAIRS 4

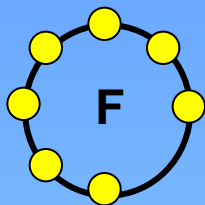
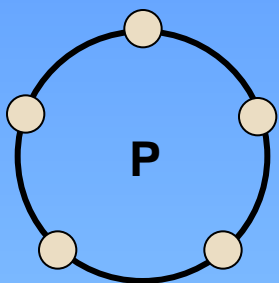
LONE PAIRS 0

BOND ANGLE... **109.5°**

SHAPE... **TETRAHEDRAL**



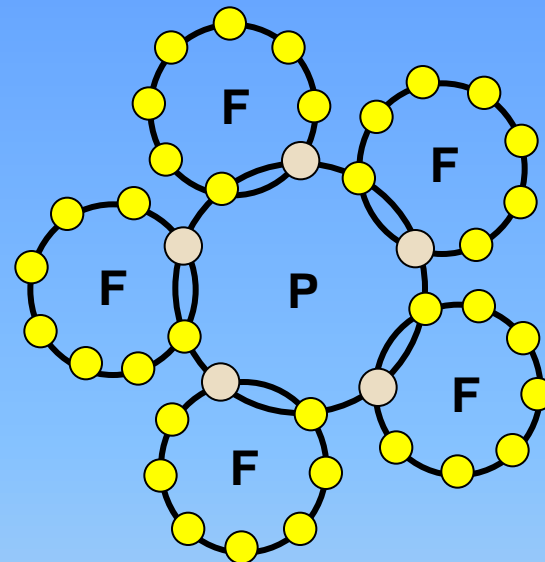
# PHOSPHORUS(V) FLUORIDE



**Phosphorus - has five electrons to pair up**

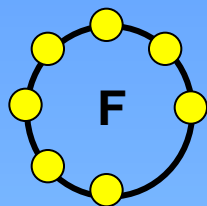
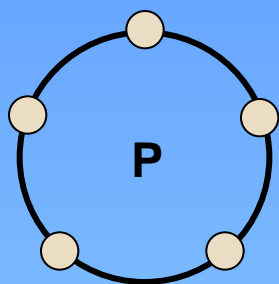
**Fluorine - needs one electron to complete 'octet'**

**Five covalent bonds are formed; phosphorus can make use of d orbitals to expand its 'octet'**





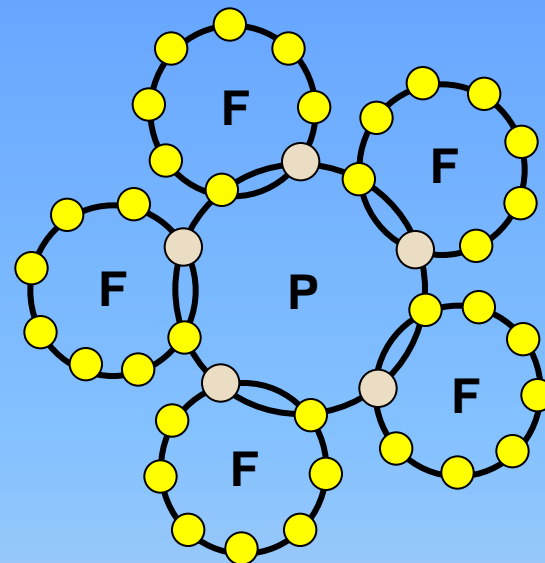
# PHOSPHORUS(V) FLUORIDE



Phosphorus - has five electrons to pair up

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Five covalent bonds are formed; phosphorus can make use of d orbitals to expand its 'octet'

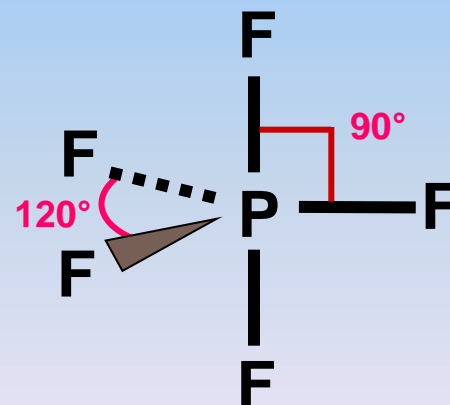


BOND PAIRS 5

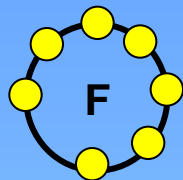
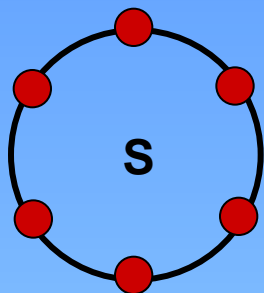
LONE PAIRS 0

BOND ANGLE... **120° & 90°**

SHAPE... **TRIGONAL BIPYRAMIDAL**



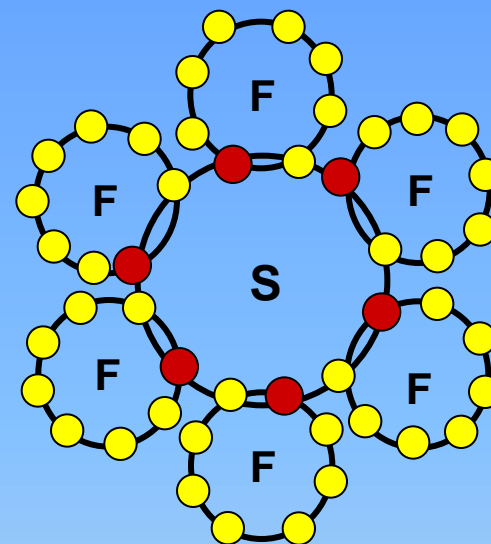
## SULPHUR(VI) FLUORIDE



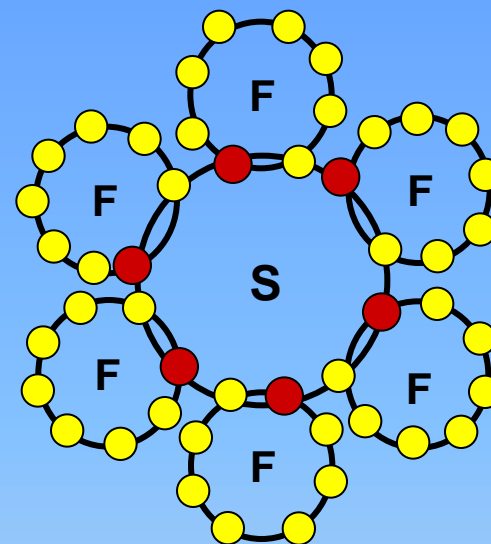
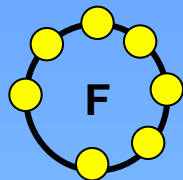
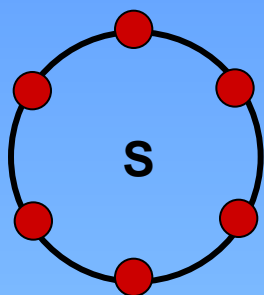
**Sulphur - has six electrons to pair up**

**Fluorine - needs one electron to complete 'octet'**

**Six covalent bonds are formed; sulphur can make use of d orbitals to expand its 'octet'**



# SULPHUR(VI) FLUORIDE



Sulphur - has six electrons to pair up

Fluorine - needs one electron to complete 'octet'

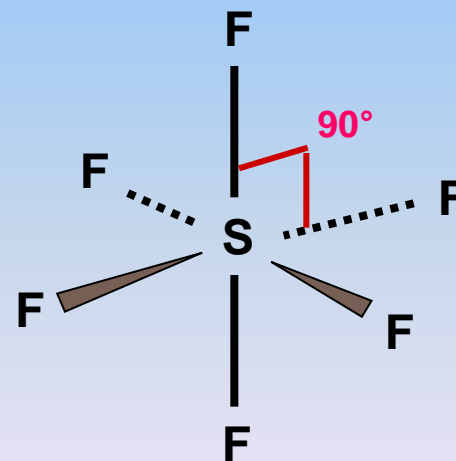
Six covalent bonds are formed; sulphur can make use of d orbitals to expand its 'octet'

**BOND PAIRS**                      6

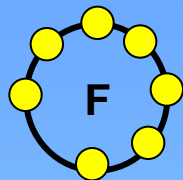
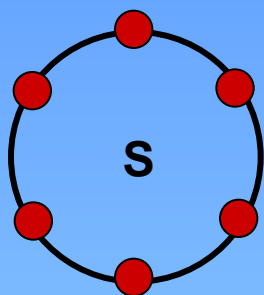
**LONE PAIRS**                      0

**BOND ANGLE...**    **90°**

**SHAPE...**    **OCTAHEDRAL**



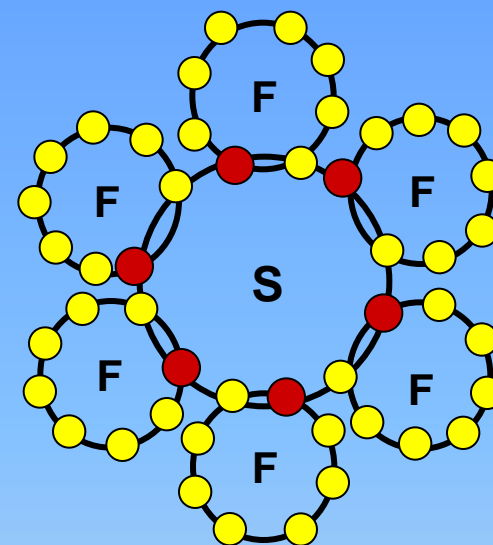
# SULPHUR(VI) FLUORIDE



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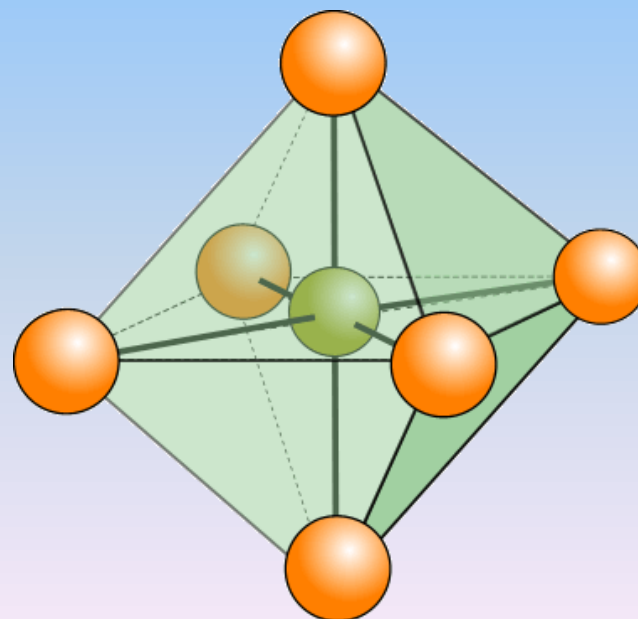


**BOND PAIRS**                      6

**LONE PAIRS**                    0

**BOND ANGLE...**    **90°**

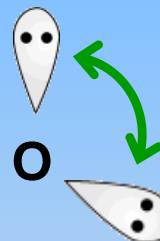
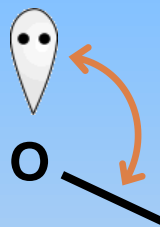
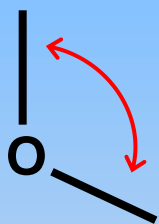
**SHAPE...**    **OCTAHEDRAL**



# IRREGULAR SHAPES

If a molecule, or ion, has lone pairs on the central atom, the shapes are slightly distorted away from the regular shapes. This is because of the extra repulsion caused by the lone pairs.

**BOND PAIR - BOND PAIR < LONE PAIR - BOND PAIR < LONE PAIR - LONE PAIR**



As a result of the extra repulsion, bond angles tend to be slightly less as the bonds are squeezed together.



# AMMONIA



BOND PAIRS	3
LONE PAIRS	1
<b>TOTAL PAIRS</b>	<b>4</b>

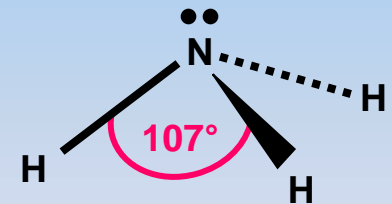
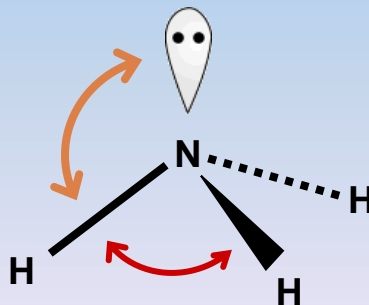
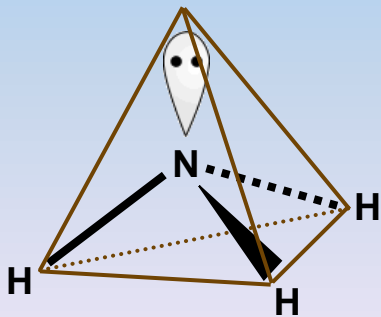
- Nitrogen has five electrons in its outer shell
- It cannot pair up all five - it is restricted to eight electrons in its outer shell
- It pairs up only three of its five electrons
- 3 covalent bonds are formed and a pair of non-bonded electrons is left
- As the total number of electron pairs is 4, the shape is **BASED** on a tetrahedron

# AMMONIA



BOND PAIRS	3
LONE PAIRS	1
<b>TOTAL PAIRS</b>	<b>4</b>

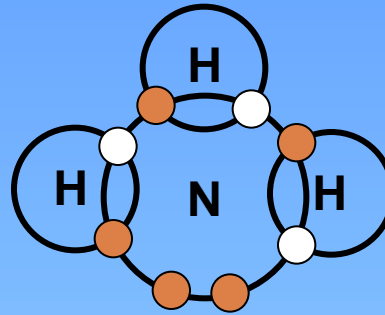
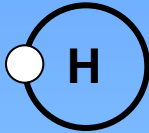
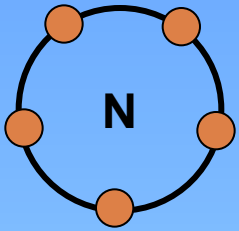
- The shape is based on a tetrahedron but not all the repulsions are the same
- **LP-BP REPULSIONS** > **BP-BP REPULSIONS**
- The N-H bonds are pushed closer together
- Lone pairs are **not included** in the shape



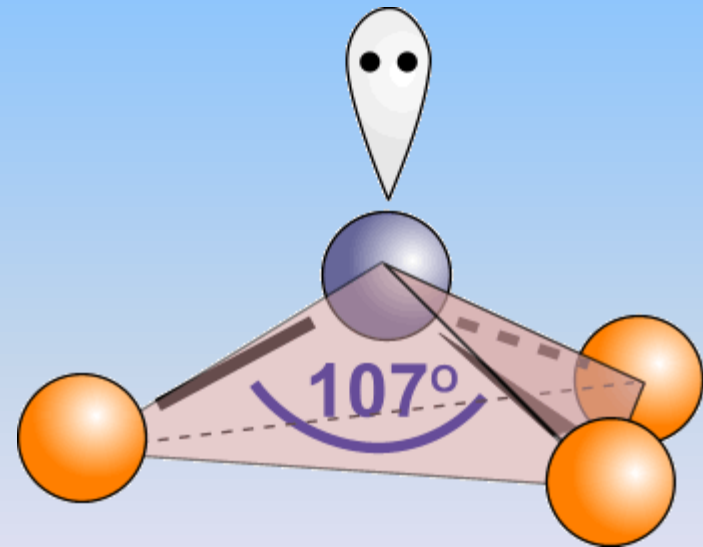
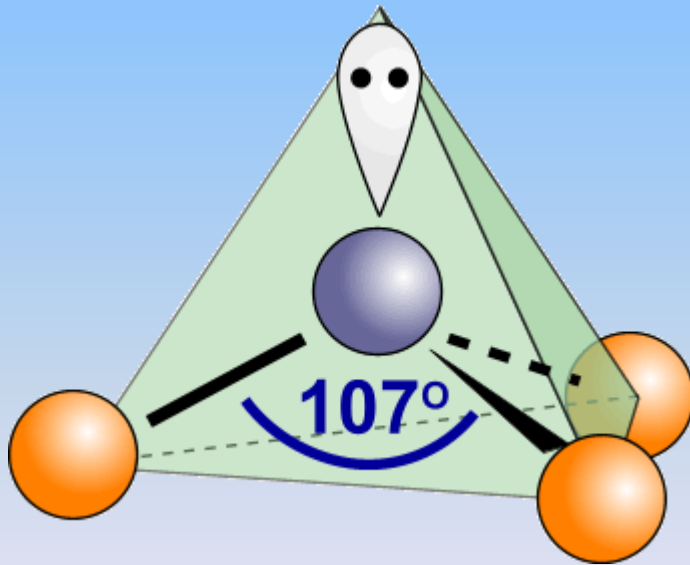
ANGLE... **107°**

SHAPE... **PYRAMIDAL**

# AMMONIA

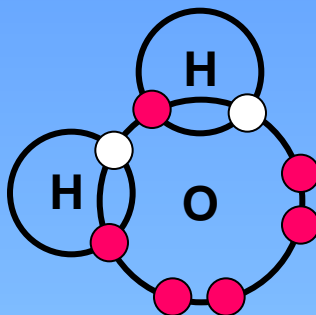
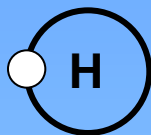
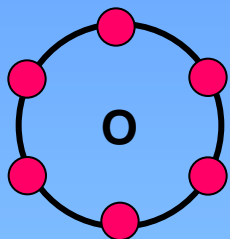


BOND PAIRS	3
LONE PAIRS	1
<b>TOTAL PAIRS</b>	<b>4</b>





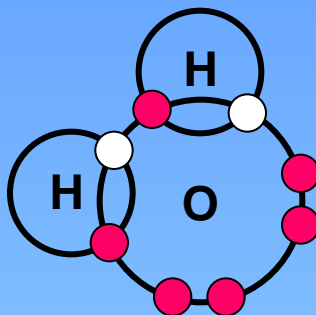
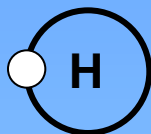
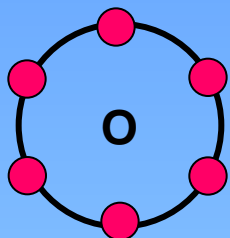
# WATER



BOND PAIRS	2
LONE PAIRS	2
<b>TOTAL PAIRS</b>	<b>4</b>

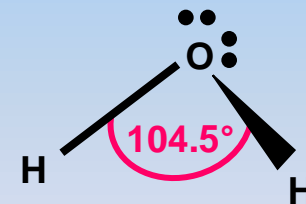
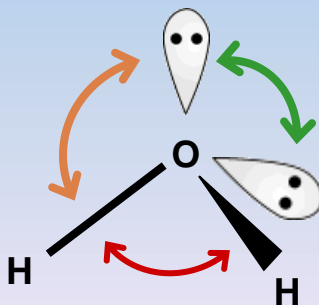
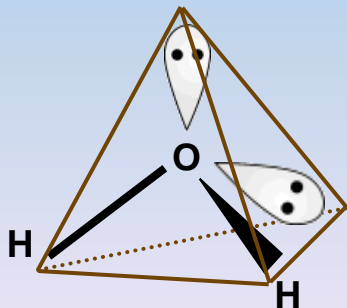
- Oxygen has six electrons in its outer shell
- It cannot pair up all six - it is restricted to eight electrons in its outer shell
- It pairs up only two of its six electrons
- 2 covalent bonds are formed and 2 pairs of non-bonded electrons are left
- As the total number of electron pairs is 4, the shape is **BASED** on a tetrahedron

# WATER



BOND PAIRS	2
LONE PAIRS	2
<b>TOTAL PAIRS</b>	<b>4</b>

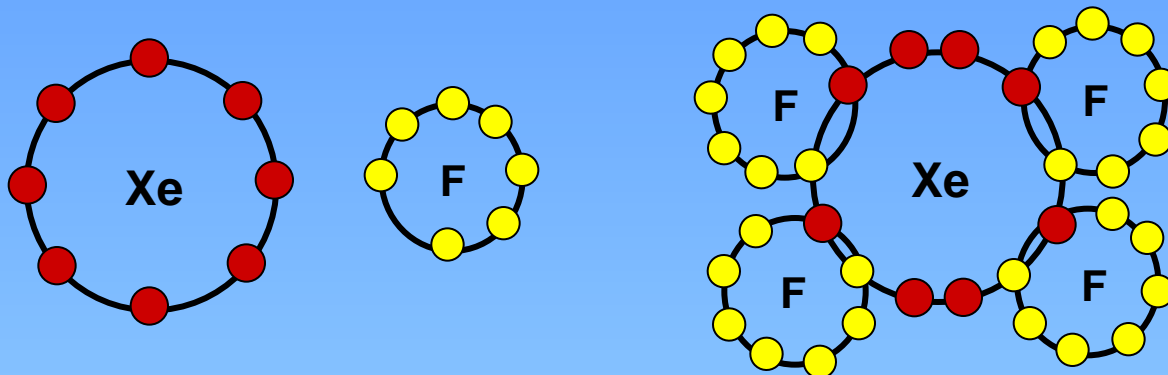
- The shape is based on a tetrahedron but not all the repulsions are the same
- **LP-LP REPULSIONS** > **LP-BP REPULSIONS** > **BP-BP REPULSIONS**
- The O-H bonds are pushed even closer together
- Lone pairs are not included in the shape



ANGLE... **104.5°**

SHAPE... **ANGULAR**

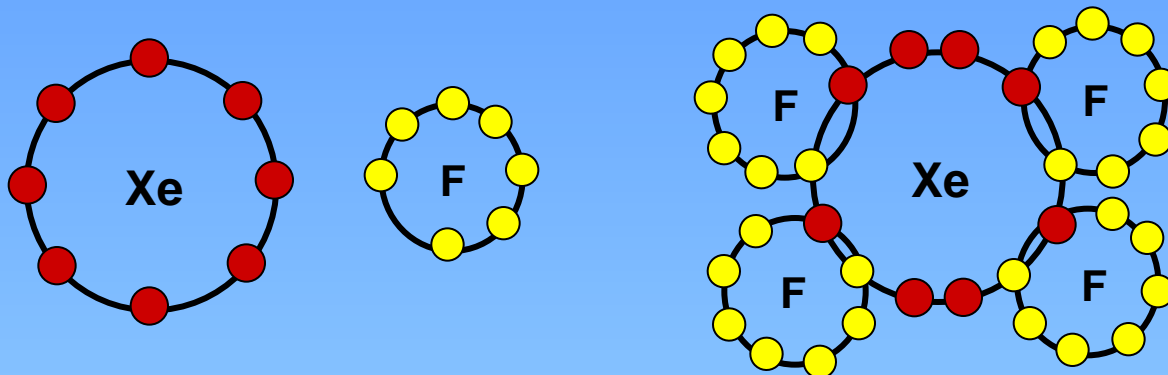
# XENON TETRAFLUORIDE



BOND PAIRS	4
LONE PAIRS	2
<b>TOTAL PAIRS</b>	<b>6</b>

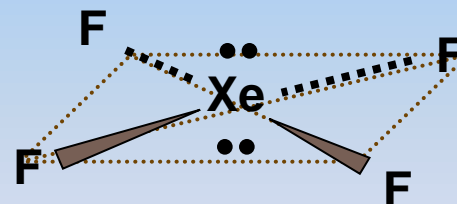
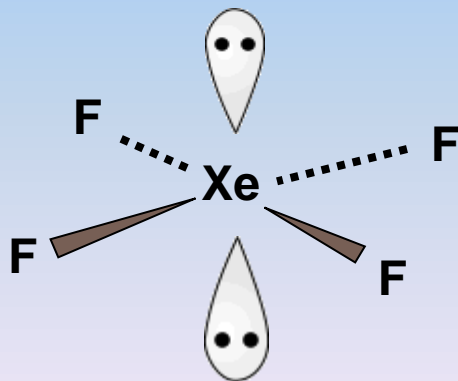
- Xenon has eight electrons in its outer shell
- It pairs up four of its eight electrons
- 4 covalent bonds are formed and 2 pairs of non-bonded electrons are left
- As the total number of electron pairs is 6, the shape is **BASED** on an octahedron

# XENON TETRAFLUORIDE



BOND PAIRS	4
LONE PAIRS	2
<b>TOTAL PAIRS</b>	<b>6</b>

- As the total number of electron pairs is 6, the shape is BASED on an octahedron
- There are two possible spatial arrangements for the lone pairs
- The preferred shape has the two lone pairs opposite each other



ANGLE... **90°**

SHAPE... **SQUARE PLANAR**

# CALCULATING THE SHAPE OF IONS

The shape of a complex ion is calculated in the same way a molecule by...

- calculating the number of electrons in the outer shell of the central species \*
- pairing up electrons, making sure the outer shell maximum is not exceeded
- calculating the number of bond pairs and lone pairs
- using ELECTRON PAIR REPULSION THEORY to calculate shape and bond angle(s)

- \* the number of electrons in the outer shell depends on the charge on the ion
- \* if the ion is positive you remove as many electrons as there are positive charges
- \* if the ion is negative you add as many electrons as there are negative charges

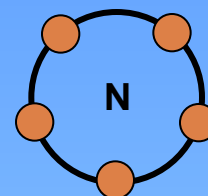
e.g. for  $\text{PF}_6^-$  add one electron to the outer shell of P

for  $\text{PCl}_4^+$  remove one electron from the outer shell of P

**EXAMPLE**

**SHAPES OF IONS**

Draw outer shell electrons of central atom



## EXAMPLE

# SHAPES OF IONS

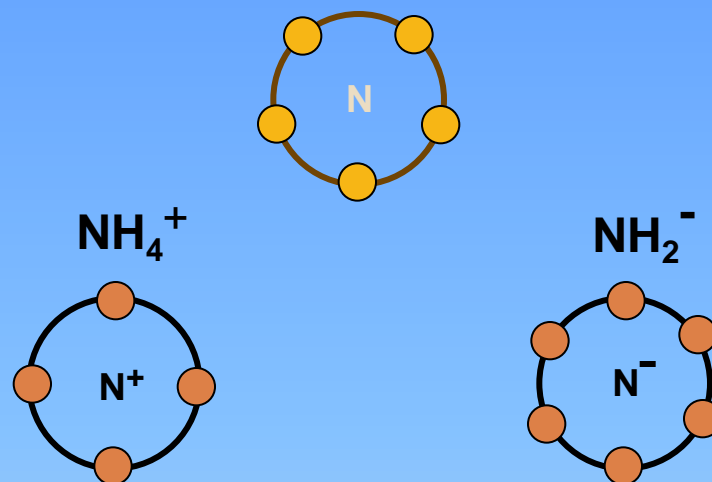
Draw outer shell electrons of central atom

For every positive charge on the ion,  
remove an electron from the outer shell...

For every negative charge add an electron  
to the outer shell...

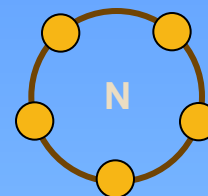
for  $\text{NH}_4^+$  remove 1 electron

for  $\text{NH}_2^-$  add 1 electron



**EXAMPLE****SHAPES OF IONS**

Draw outer shell electrons of central atom

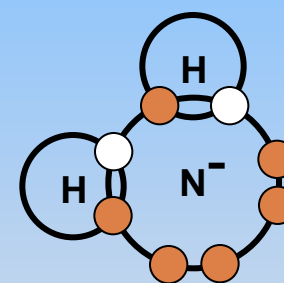
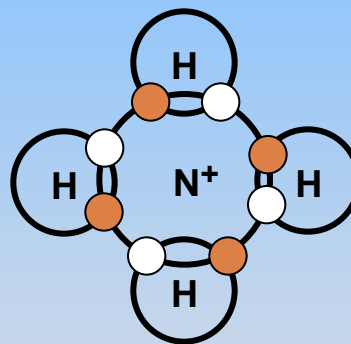
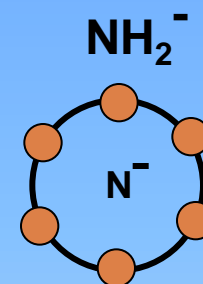
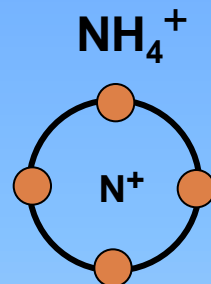


For every positive charge on the ion, remove an electron from the outer shell

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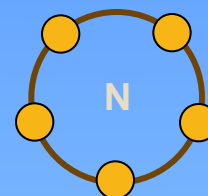


Pair up electrons in the usual way



**EXAMPLE****SHAPES OF IONS**

Draw outer shell electrons of central atom

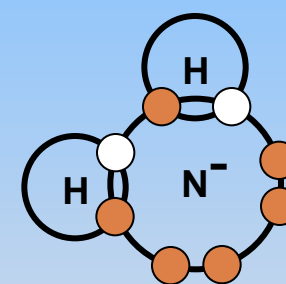
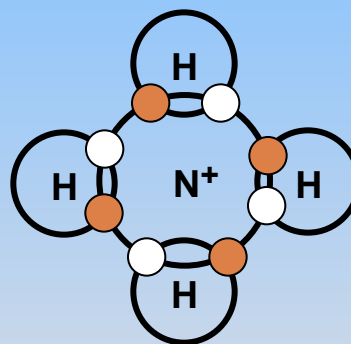
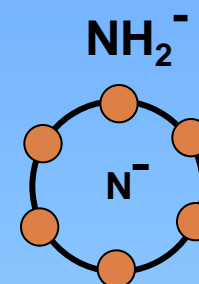
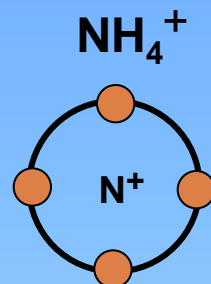


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Pair up electrons in the usual way

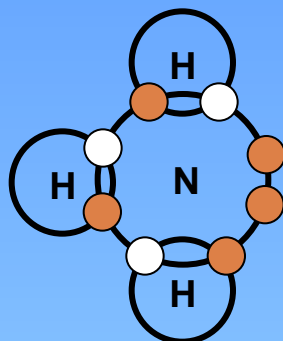
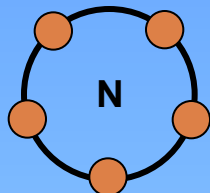
Work out shape and bond angle(s) from number of bond pairs and lone pairs.

**BOND PAIRS 4**  
**LONE PAIRS 0**  
**TETRAHEDRAL**  
**H-N-H 109.5°**

**BOND PAIRS 2**  
**LONE PAIRS 2**  
**ANGULAR**  
**H-N-H 104.5°**

REVIEW

SHAPES OF IONS

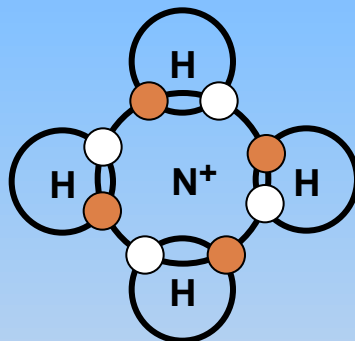
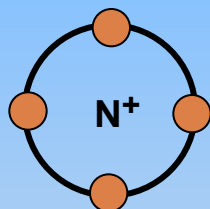
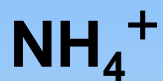


BOND PAIRS 3

PYRAMIDAL

LONE PAIRS 1

H-N-H  $107^\circ$

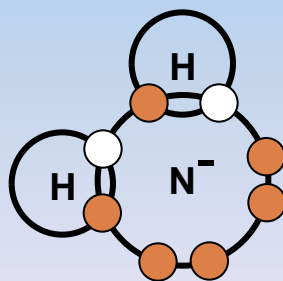
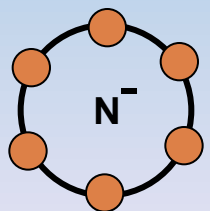


BOND PAIRS 4

TETRAHEDRAL

LONE PAIRS 0

H-N-H  $109.5^\circ$



BOND PAIRS 2

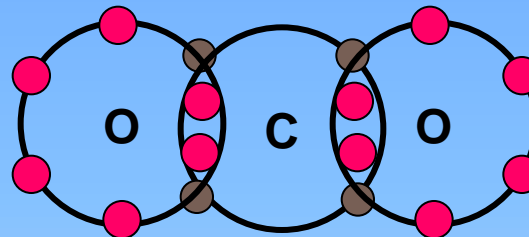
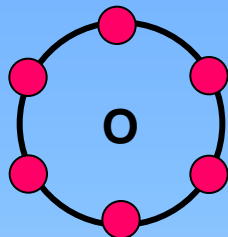
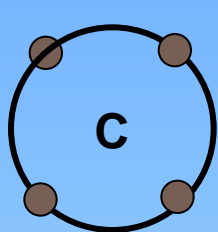
ANGULAR

LONE PAIRS 2

H-N-H  $104.5^\circ$

## MOLECULES WITH DOUBLE BONDS

The shape of a compound with a double bond is calculated in the same way.  
A double bond repels other bonds as if it was single e.g. carbon dioxide



Carbon - needs four electrons to complete its shell

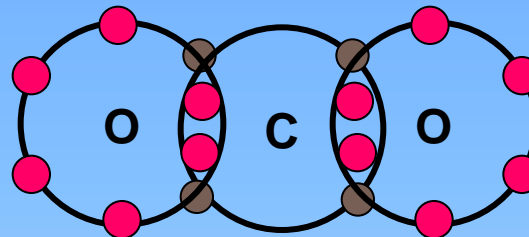
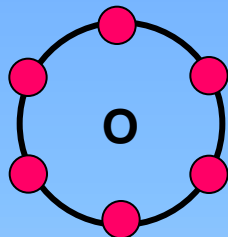
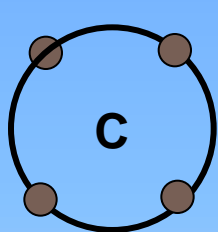
Oxygen - needs two electron to complete its shell

The atoms share two electrons  
each to form two double bonds



# MOLECULES WITH DOUBLE BONDS

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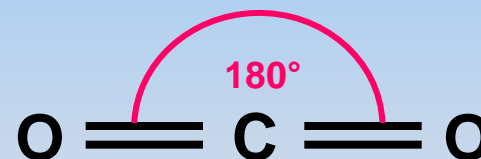
Oxygen - needs two electron to complete its shell

The atoms share two electrons each to form two double bonds

DOUBLE BOND PAIRS      2

LONE PAIRS              0

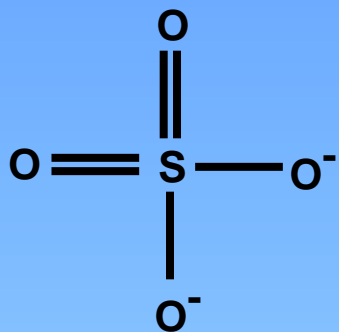
Double bonds behave exactly as single bonds for repulsion purposes so the shape will be the same as a molecule with two single bonds and no lone pairs.



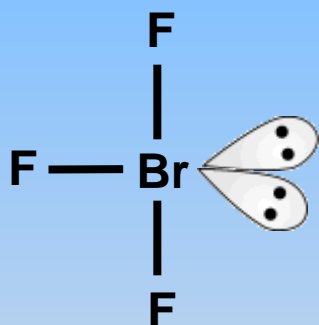
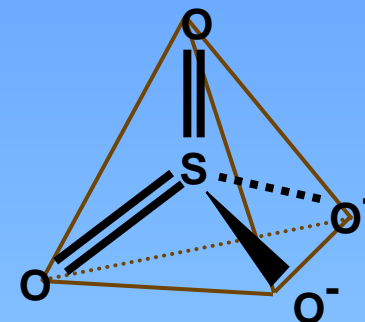
BOND ANGLE... 180°

SHAPE... **LINEAR**

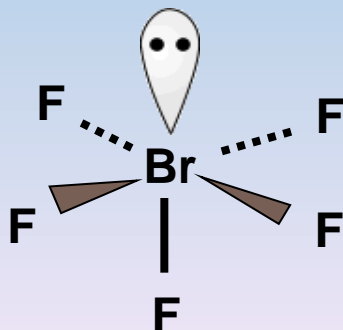
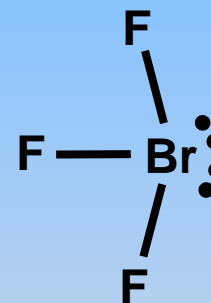
## OTHER EXAMPLES



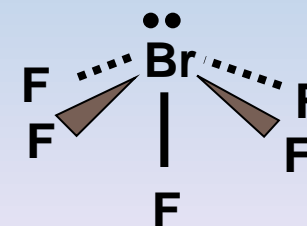
**BOND PAIRS** 4  
**LONE PAIRS** 0  
**TETRAHEDRAL**  
**ANGLE**  $109.5^\circ$



**BOND PAIRS** 3  
**LONE PAIRS** 2  
**'T' SHAPED**  
**ANGLE**  $<90^\circ$



**BOND PAIRS** 5  
**LONE PAIRS** 1  
**'UMBRELLA'**  
**ANGLES**  $90^\circ <90^\circ$



# TEST QUESTIONS

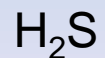
For each of the following ions/molecules,

state the number of bond pairs

state the number of lone pairs

state the bond angle(s)

state, or draw, the shape



# TEST QUESTIONS

ANSWER

For each of the following ions/molecules,

state the number of bond pairs

state the number of lone pairs

state the bond angle(s)

state, or draw, the shape

$\text{BF}_3$	3 bp	0 lp	$120^\circ$	trigonal planar	boron pairs up all 3 electrons in its outer shell
$\text{SiCl}_4$	4 bp	0 lp	$109.5^\circ$	tetrahedral	silicon pairs up all 4 electrons in its outer shell
$\text{PCl}_4^+$	4 bp	0 lp	$109.5^\circ$	tetrahedral	as ion is +, remove an electron in the outer shell then pair up
$\text{PCl}_6^-$	6 bp	0 lp	$90^\circ$	octahedral	as the ion is -, add one electron to the 5 in the outer shell then pair up
$\text{SiCl}_6^{2-}$	6 bp	0 lp	$90^\circ$	octahedral	as the ion is 2-, add two electrons to the outer shell then pair up
$\text{H}_2\text{S}$	2 bp	2 lp	$92^\circ$	angular	sulphur pairs up 2 of its 6 electrons in its outer shell - 2 lone pairs are left