2B – Bonding and shapes of molecules

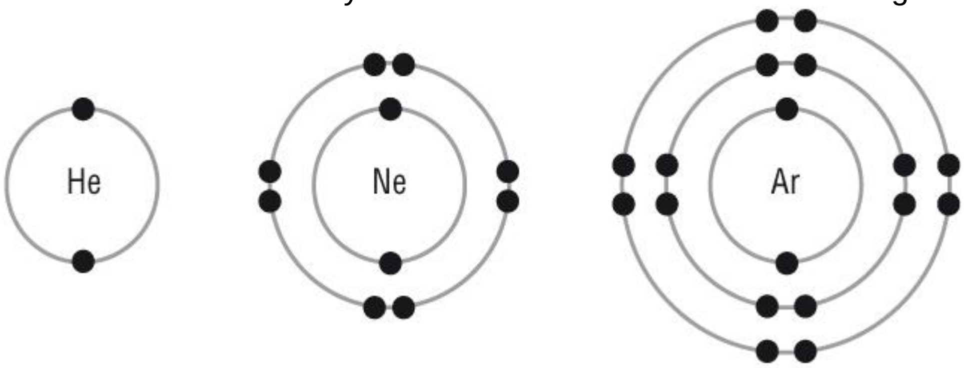
An introduction to chemical bonds

Group 0 - The Noble gases:

- make up 1% of the air.
- Ne used in lights for advertising.
- Ar used in filament bulbs
- Kr used in lasers
- Xe used in headlight bulbs
- He / Ne do not form any compounds
- Others form compounds with great difficulty

Electron configuration:

- These are the only elements that have the electron configuration to exist as single atoms:



He atom
$1s^2$

Ne atom
$1s^2 2s^2 2p^6$

Ar atom
$1s^2 2s^2 2p^6 3s^2 3p^6$

- They have full outer shells and the electrons are paired with opposite spins fulfilling the '**octet rule**'.

Bonding:

- All other elements on the periodic table will combine by sharing or transferring electrons in order to fill their outer shell.
- The atoms, when combined **tend to** have the noble gas configuration - fulfilling the '**octet rule**', although there are some exceptions

Chemical bonding:

- The **Periodic Table** is made up of **2 types of elements**.

Metals + Non - metals

- This means there are **3 types of bonding** in which the atoms of the elements can combine:

Type of Bonding	Which types of atoms combine	Electrons
Ionic	**Metal + Non-metal**	**Transferred: Metal → Non-metal**
Covalent	**Non-metal + Non-metal**	**Shared: Between the atoms**
Metallic	**Metal + Metal**	**Shared: Between <u>all</u> atoms**

Questions: p49, 1 / p73, 12 /

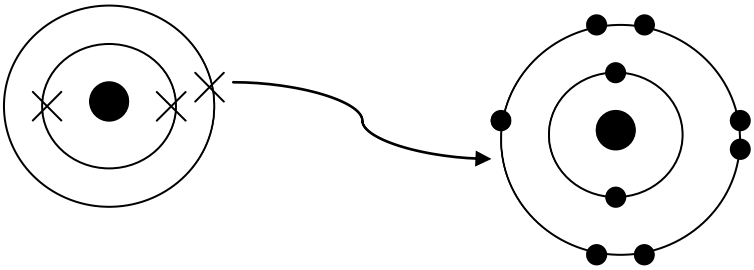
Ionic Bonding

Ionic bonding results from the electrostatic attraction between oppositely charged ions.

- Metals become positive ions (cations) electrons are removed.
- Non-metals become negative ions (anions) electrons are gained.
- Electrons are transferred from metal atoms to non-metal atoms. Both will have full outer shells.
- In an ionic compound the ions are held in place by strong forces of attraction between oppositely charged ions (and repulsion between like charged ions).
- Attraction outweighs repulsion and the forces are balanced.

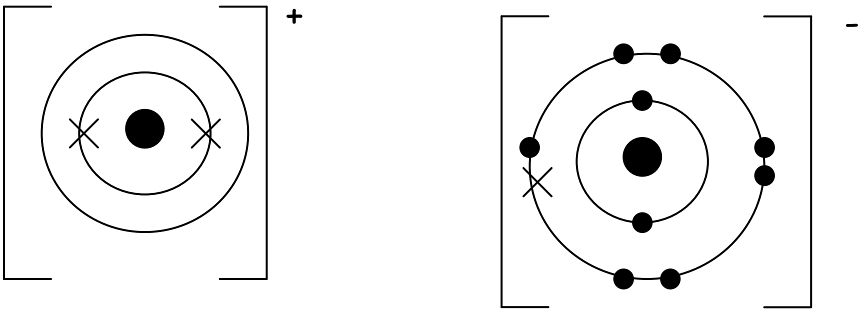
Lithium Fluoride:

- **Metals** form **positive** ions which we call **cations**.
- **Non - metals** form **negative** ions which we call **anions**.
- Dot and cross diagrams is a means of electron counting.



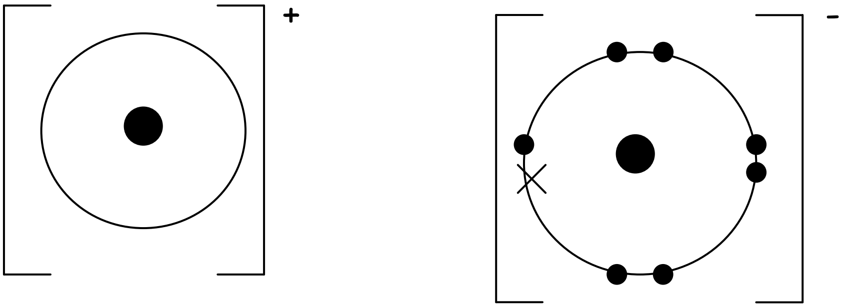
Li F

Becomes



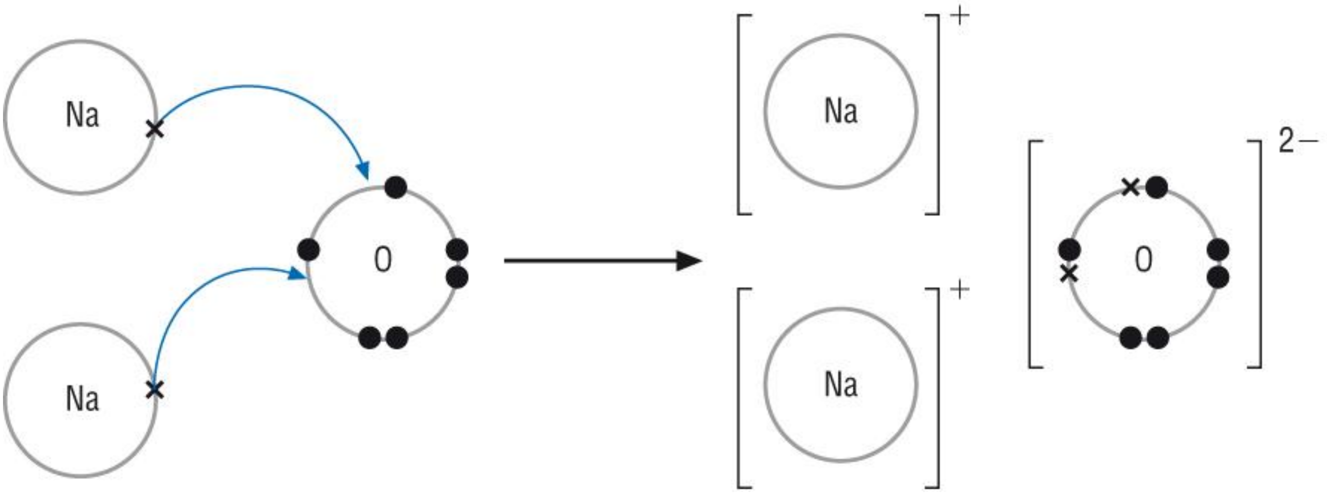
Li^+ F^-

However we only show the ions and only the outer shells:-



Li^+ F^-

Sodium oxide:



- Na atom loses 1e to empty its outer shell

2Na → $2Na^+$ + $2e^-$

$1s^2 2s^2 2p^6 3s^1$ → $1s^2 2s^2 2p^6$

- O atom must gain 2e to fill its outer shell

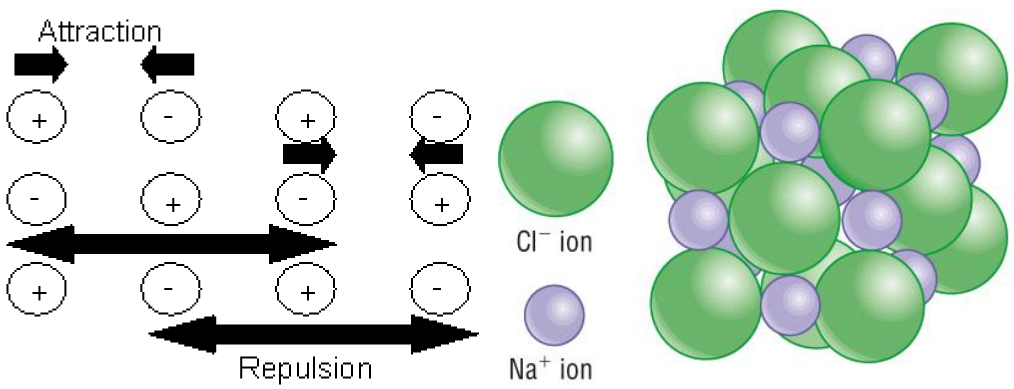
O + $2e^-$ → O^{2-}

$1s^2 2s^2 2p^4$ → $1s^2 2s^2 2p^6$

- This means that 2 Na atoms must lose 1e each = 2e to give O its 2e's needed to fill its outer shell.

Giant ionic lattices

- The dot and cross diagrams only show what happens in order to form the ions but in an ionic reaction lots of metal atoms lose electrons to non-metal atoms forming ions.
- This means that each ion will attract oppositely charged ions in all directions.
- The ions are held in place by strong forces of attraction between oppositely charged ions (and repulsion between like charged ions).
- Forces are non-directional and are therefore arranged in giant lattice structures (hence crystals):

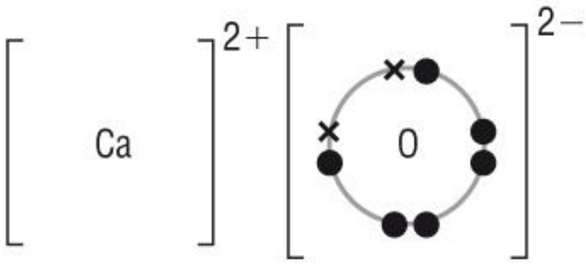


- Each sodium ion is surrounded by 6 chloride ions (and vice versa).
- These crystals (ionic compounds) have **high melting and boiling points** due to this.
- Magnesium oxide has a similar structure to sodium chloride but the electrostatic attraction in magnesium oxide is greater due to the higher charges on the ions.

- This means that the melting and boiling point of magnesium oxide 3125K is greater than sodium chloride 1074K.
- **Brittle** as they cleave along a plane of ions.

Further examples of ionic bonding:

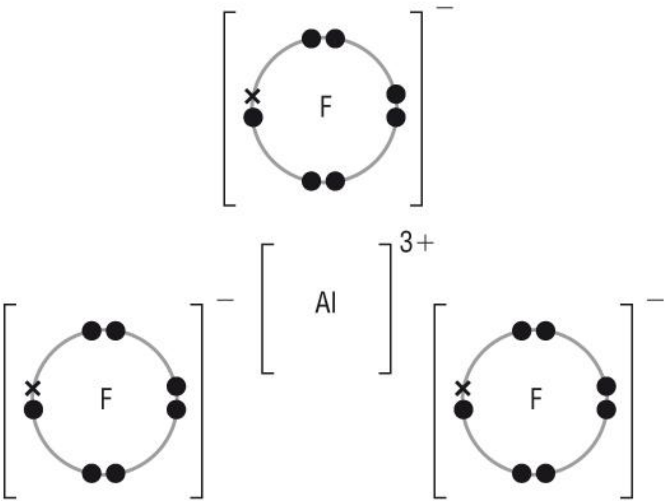
CaO



$Ca \rightarrow Ca^{2+} + 2e^-$

$O + 2e^- \rightarrow O^{2-}$

AlF_3



$Al \rightarrow Al^{3+} + 3e^-$

3 times: $F + e^- \rightarrow F^-$

Questions: p51, 1-2 / p73, 3

<u>Ions and the Periodic Table</u>

Predicting charges:

- It is possible to predict the charges of elements using the Periodic Table:

Group	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**0**
No e's in outer shell	**1**	**2**	**3**	**4**	**5**	**6**	**7**	**Full**
No electrons lost gained	**Lose 1**	**Lose 2**	**Lose 3**	**x**	**Gain 3**	**Gain 2**	**Gain 1**	**x**
Charge on ion	**1+**	**2+**	**3+**	**x**	**3-**	**2-**	**1-**	**x**

- Be, B, C and Si do not usually form ions as too much energy is required.

Transitions metals:

- These elements can usually form more than one ion:

Element	**Charge on ion / oxidation number**					
Mn	**2+**	**3+**	**4+**	**5+**	**6+**	**7+**
Roman numeral	**II**	**III**	**IV**	**V**	**VI**	**VII**

- The charge / oxidation number of the ion is written as a roman numeral:

Iron (II) Fe^{2+} Copper (II) Cu^{2+}

Molecular ions (common ions)

- Groups of covalently bonded atoms can also gain and lose electrons.
- These are called molecular (or common ions)

1+		1-		2-		3-	
Ammonium	NH_4^+	**Hydroxide**	OH^-	**Carbonate**	CO_3^{2-}	**phosphate**	PO_4^{3-}
		Nitrate	NO_3^-	**Sulphate**	SO_4^{2-}		
		Nitrite	NO_2^-	**Sulphite**	SO_3^{2-}		
		Hydrogen carbonate	HCO_3^-	**Dichromate**	$Cr_2O_7^{2-}$		

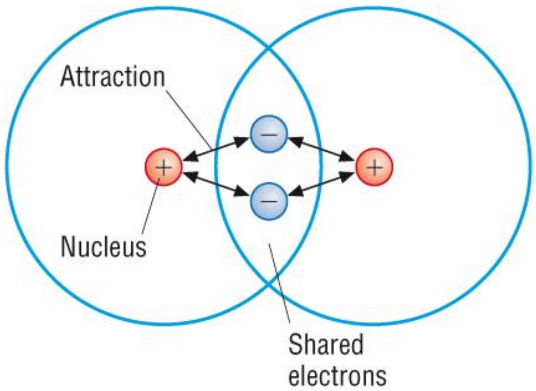
Predicting ionic formula:

- The ions in a chemical formula must **add up to zero**.
- Use subscripts after an ion in a formula to double/triple that ion so the sum=0. eg. $CuCl_2$
- If you are double/tripling ions that consist of more than one element (molecular ions) brackets must be used. eg. $Ca\mathbf{(}OH\mathbf{)}_2$
- If Roman numeral numbers follow a transition metal ion in brackets, that tells you the positive charge on that transition metal ion.

Sodium Chloride -	Na^+ Cl^-	Write the ions with charges
	1+ : 1-	Write the ratio of the charges
		Multiply up if necessary to = 0
	NaCl	Bring together omitting the charges
Copper (II) Chloride	Cu^{2+} Cl^-	Write the ions with charges
	2+ : 1- (x2)	Write the ratio of the charges
	Cu^{2+} : Cl^-_2	Multiply up if necessary to =0
	$CuCl_2$	Bring together omitting the charges
Calcium Hydroxide	Ca^{2+} OH^-	Write the ions with charges
	2+ : 1- (x2)	Write the ratio of the charges
	Ca^{2+} : $(OH^-)_2$	Multiply up if necessary to =0
	$Ca(OH)_2$	Bring together omitting the charges

Questions p53, 1-3 / p73, 4

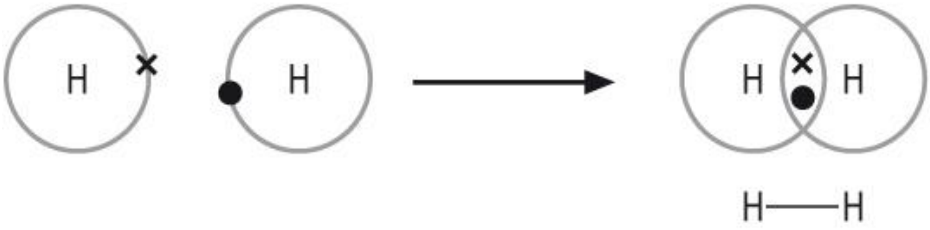
<u>Covalent Bonding</u>



- These occur between 2 or more non metals. As neither will donate, they have to share.
- Attraction comes between the positive nucleus and the negative electrons that are shared between them.
- In each case the outer shell has to be filled (reach the noble gas configuration).

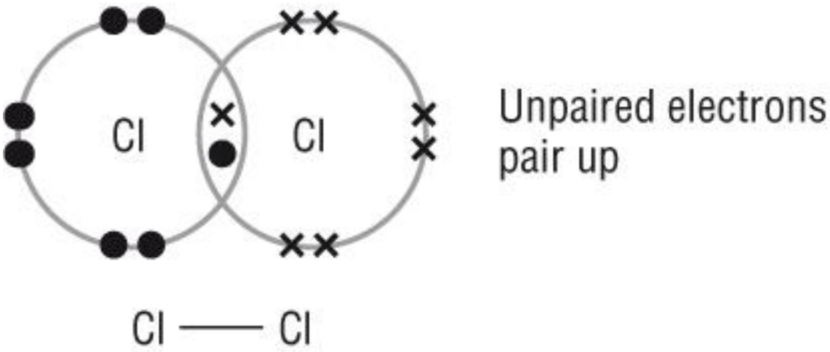
Octet rule (more accurately - full shell rule)
Single covalent bonds

- The single outer shell electrons are involved in a covalent bond.
- Each hydrogen has 1 single unpaired electron in its outer shell.
- Each hydrogen contributes 1 electron to the covalent bond = 2 electron.
- The electrons in a covalent bond are in between the 2 atoms therefore they are directional.

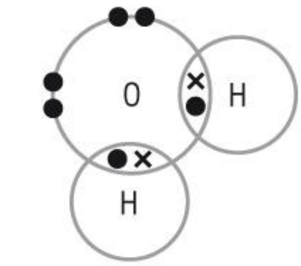


Chlorine:

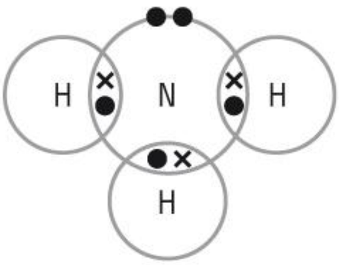
- Each chlorine has 7e in its outer shell.
- Each Cl has 1 unpaired electron in its outer shell.
- Each Cl contributes an electron each = 2e forming 1 single covalent bond:



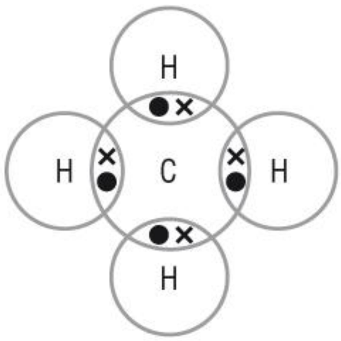
Other examples:



H_2O
2 unpaired electrons
pair up



NH_3
3 unpaired electrons
pair up



CH_4
4 unpaired electrons
pair up

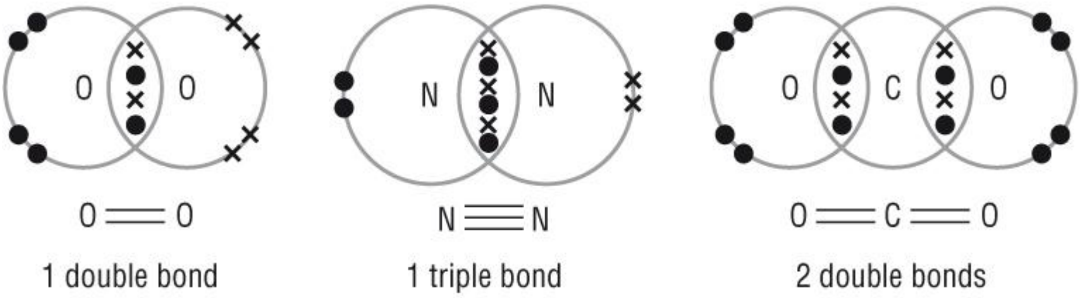
Group	4	5	6	7
Element	C	N	O	F
Electrons in outer shell	4	5	6	7
Lone pairs	0	1	2	3
Unpaired electrons in outer shell	**4**	**3**	**2**	**1**

No of covalent bonds	4	3	2	1

- Lone pairs of electrons are when the paired electrons are not used in a covalent bond.
- They do however give a region of concentrated negative charge.

Multiple covalent bonds

- Some atoms can form more than a single bond, double and triple.
- This depends on how many single unpaired electrons there are in the outer shell:



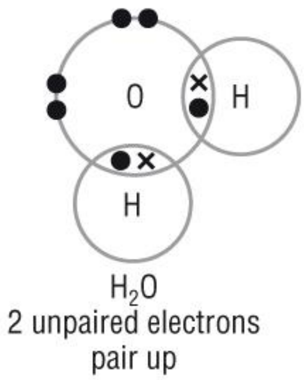
- Each bond is represented by a line:

Questions: 1-2 P55

Further covalent bonds
Dative covalent bonds:

- A covalent bond is when each atom provides 1e each to be shared between them.
- A dative covalent bond is when both of the bonding electrons are provided by the same atom.
- In order for this to happen, an atom or atom in a molecule **must** have a **lone pair of electrons:**

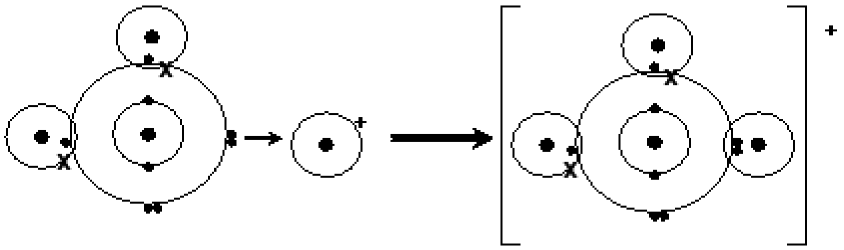
The oxonium ion:



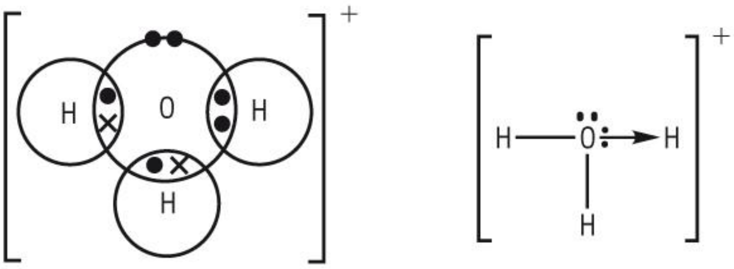
- Water has 2 lone pairs.
- It will react with the hydrogen chloride gas to form the **Oxonium ion**

$$HCl_{(aq)} \quad + \quad H_2O_{(l)} \quad \rightarrow \quad H_3O^+_{(aq)} \quad + \quad Cl^-_{(aq)}$$

- Looking at the atoms for how this molecule is formed:



- A lone pair of electrons from the water molecule is used to forma **dative covalent bond.**
- The bond is indistinguishable from the other covalent bonds but we use an arrow to show that one of the bonds is dative:

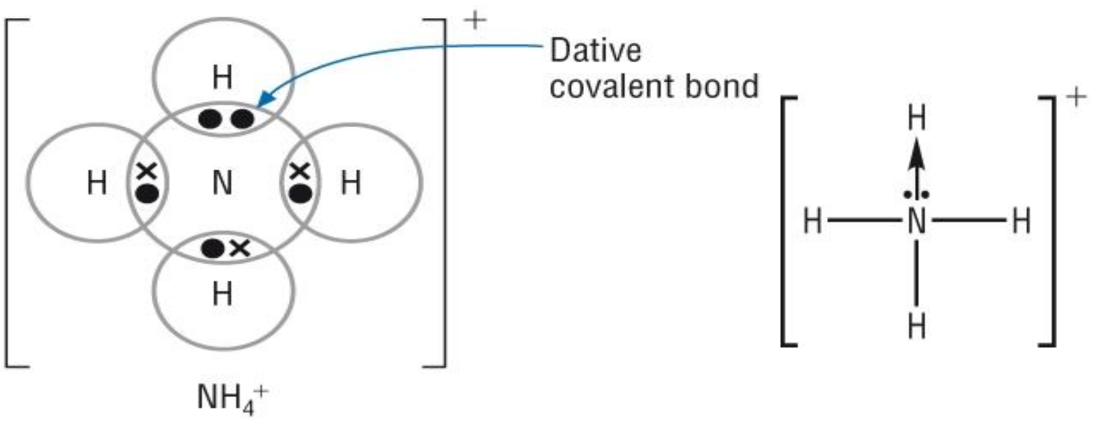


- The **oxonium ion** is responsible for acid reactions and is represented as:

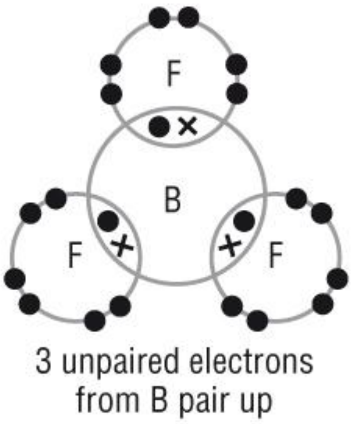
H_3O^+ or $H^+_{(aq)}$

The ammonium ion:

- The same can be done for ammonia. This forms the **ammonium ion:**



Breaking the octet rule:

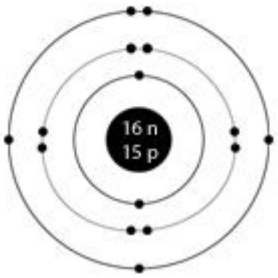
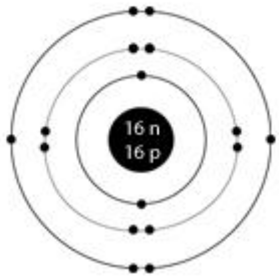
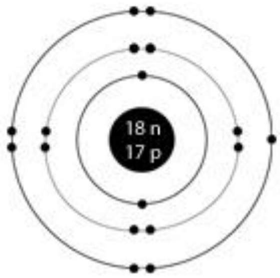


- The problem with this rule is that some atoms do not have enough electrons in their outer shell to form enough covalent bonds to make 8e.
- Boron is in group 3 of the Periodic table. This means it has 3e in its outer shell.
- This means that Boron can only form 3 covalent bonds = 6e in its outer shell:

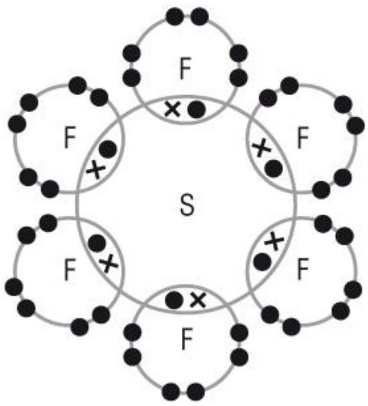
Expanding the octet:

Period 3, the electron shell is much larger and can accommodate more covalent bonds.

- Some atoms are able to have more than 8 electrons in its outer shell when covalently bonding.
- It very much depends on how many of their outer shell electrons are used in bonding / lone pairs:

		
Phosphorous	**Sulphur**	**Chlorine**
If all unpaired electrons are used then there will be **3 covalent bonds** = 6e plus the lone pair of 2e = **8e**	If all unpaired electrons are used then there will be **2 covalent bonds** = 4e plus the 2 lone pair of 2e = **8e**	If all unpaired electrons are used then there will be **1 covalent bond** = 2e plus the 3 lone pair of 6e = **8e**
If the lone pair unpairs then there are 5 unpaired electrons. These will form **5 covalent bonds** = **10e**	If one of the lone pair unpairs then there are 4 unpaired electrons. These will form **4 covalent bonds** = 8e plus the remaining lone pair of 2e = **10e**	If one of the lone pair unpairs then there are 3 unpaired electrons. These will form **3 covalent bonds** = 6e plus the 2 remaining lone pairs of 4e = **10e**
	If both of the lone pairs unpair then there are 6 unpaired electrons. These will form **6 covalent bonds** = **12e**	If 2 of the lone pairs unpair then there are 5 unpaired electrons. These will form **5 covalent bonds** = 10e plus the remaining lone pair of 2e = **12e**
		If all of the lone pairs unpair then there are 7 unpaired electrons. These will form **7 covalent bonds** = **14e**
Group 5 = 3, 5 bonds	**Group 6 = 2, 4, 6 bonds**	**Group 6 = 1, 3, 5, 7 bonds**

- It all depends upon how many electrons are used in bonding.



- All 6 electrons in sulphur have been used to form covalent bonds.
- This makes 12e in the outer shell of sulphur.
- Each of the fluorine's have 8e in their outer shell.

A better rule:

1. **All electrons can be used to form covalent bonds from Period 3 onwards**
2. **The maximum number of bonds = the number of electrons in the outer shell**

Questions: 1-2 P57

Shapes of molecules and ions:

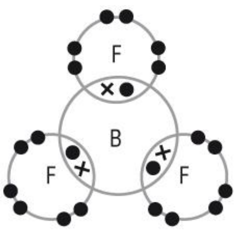
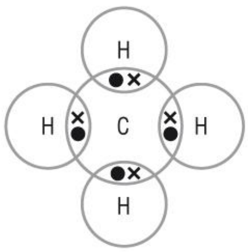
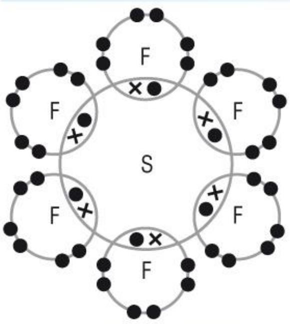
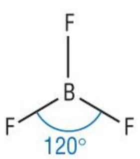
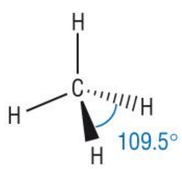
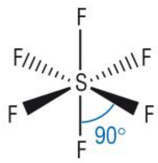
Electron pair repulsion theory:

- The shape of a molecule is wholly determined by the number of electron pairs (or areas) around a central atom.

Bonding pairs & Lone pairs

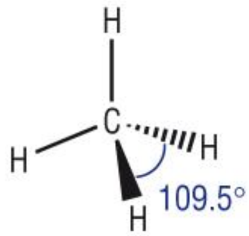
- Electron pairs repel each other as far as possible.
- This repulsion determines the shape and bond angle.

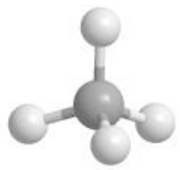
Bonding pairs of electrons

Molecule	BF_3	CH_4	SF_6
Dot-and-cross diagram			
Number of electron pairs around central atom	3	4	6
Shape and bond angles			
Name of shape	Trigonal planar	Tetrahedral	Octahedral

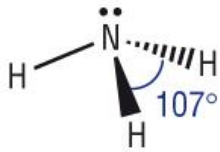
Lone pair electrons:

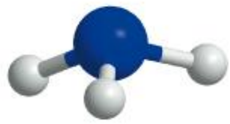
A methane molecule is tetrahedral with bond angles of 109.5 °C.



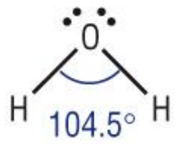


An ammonia molecule is pyramidal with bond angles of 107 °C.





A water molecule is non-linear with a bond angle of 104.5 °C.



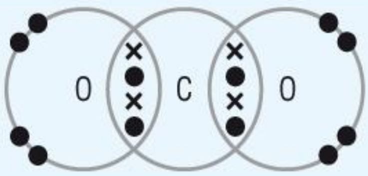
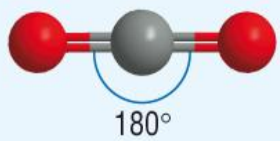
Explanation:

- **Count how many bonding pairs (or areas with double bonds) and lone pair electrons**
- **Pairs of electrons repel other pairs of electrons as far as possible and this determines the shape**
- **Lone pairs are closer to the central atom than bonding pair electrons.**
- **Lone pair electrons will repel other pairs of electrons more than bonding pairs of electrons.**
- **Each lone pair of electrons reduces the bond angle by 2.5^o.**
- **Order of repulsion:**

Lone Pair – Lone Pair > Lone Pair – Bonding Pair > Bonding Pair – Bonding Pair

Molecules with double bonds:

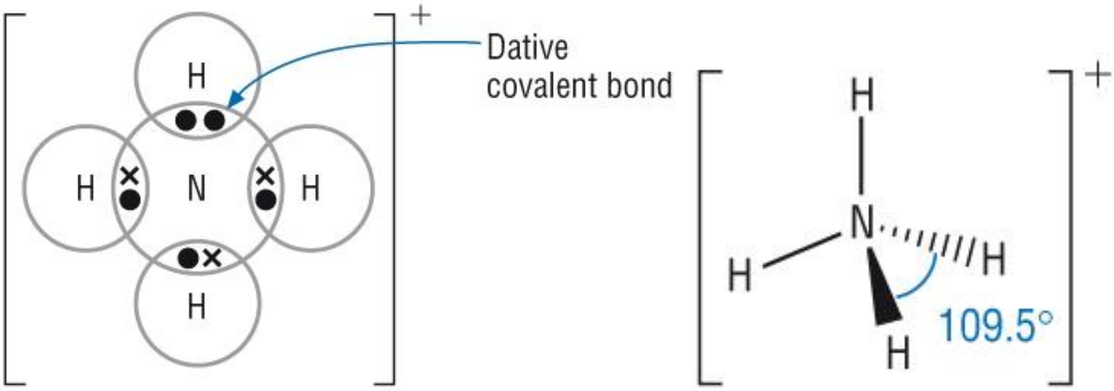
- Double bonds have 4e in one region.
- To work out the shape we have to think in terms of **bonding regions** instead of bonding pairs:

Molecule	Dot-and-cross diagram	Number of bonding regions	Shape and bond angle	Name of shape
CO_2		2		Linear

- CO_2 has **2 bonding regions** which will repel each other as far as possible.
- This will give a **linear** molecule with a bond angle of **180^o**.

Shapes of ions:

- Molecular ions follow the same rules as any molecule, remember the ammonium ion:



NH_4^+

- It is basically the same shape as CH_4 - tetrahedral.

Summary:

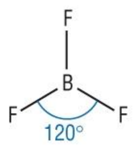
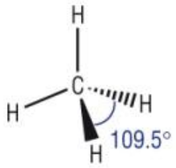
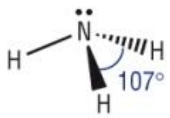
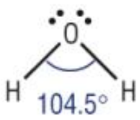
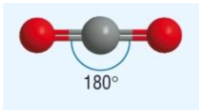
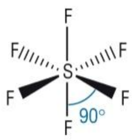
State the number of bonding and lone pairs of electrons

Pairs of electrons repel as far as possible

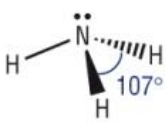
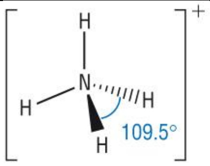
This determines the shape

Lone pairs repel more than bonding pairs as closer to central atom

Each lone pair reducing the bond angle by 2.5^{o} as it is closer to the central atom

3BP (areas)	4BP	3BP / 1LP	2BP / 2LP	2 Areas (4BP)	6BP
					
Trigonal planar	Tetrahedral	Pyramidal	Non - linear	Linear	Octahedral

How does the addition of H+ ion change shape of ammonia (water)

3BP / 1LP		4BP
	The addition of a datively bonded H^+ ion uses the lone pair converting it to a bonding pair (similar for water)	
Trigonal planar		Tetrahedral

Questions: 1-3 P59 / 5, 9 P73