# Topic 4: Chemical bonding and structure

4.1 Ionic bonding and structure

U1	Positive ions (cations) form by metals losing valence electrons.
U2	Negative ions (anions) form by non-metals gaining electrons.
U3	The number of electrons lost or gained is determined by the electron configuration of the atom.
U4	The ionic bond is due to electrostatic attraction between oppositely charged ions.
U5	Under normal conditions, ionic compounds are usually solids with lattice structures.
A1	Deduction of the formula and name of an ionic compound from its component ions, including polyatomic ions.
A2	Explanation of the physical properties of ionic compounds (volatility, electrical conductivity and solubility) in terms of their structure.

Ionic bonding

Ionic bonding occurs between elements that have a large difference in electronegativity (typically larger than 1.8). The atom with the low electronegativity (the metal) loses an electron and becomes a **cation**. The atom with the high electronegativity (the non-metal) gains the electron and becomes an **anion**. As a result there is an **electrostatic attraction**(not a real bond)between the two ions.
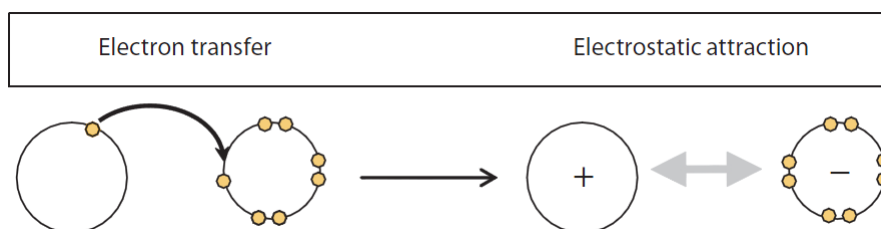
In NaCl, for example, chlorine already has noble gas configuration (it is in the form of diatomic molecules), but the energy given out when the ionic lattice is formed is sufficient to break the bond in the chlorine molecule to give atoms. Each sodium atom gives an electron to a chlorine atom. In the lattice each cation is surrounded by 6 anions and vice versa.

Ionic bonding only happens when a electron transferred from a metal to a non-metal
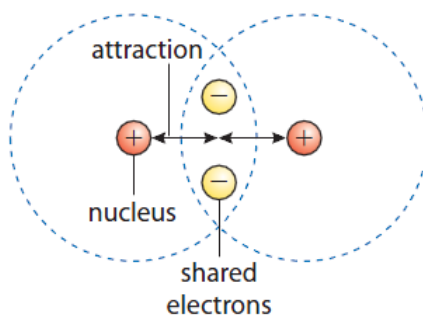
Properties of ionic compounds

- Dissolve in water (ions are free to move, so it conducts electricity)
- Molten ionic compound conducts electricity (ions are free to move)
- In solid state, ionic compound doesn't conduct electricity because ions are not free
- High melting point (in solid state ionic compound has **giant lattice structure**)
- Electronegativity difference ranges from 4 to 1.8

4.2 Covalent bonding

|	
U1	Describe the covalent bond as the electrostatic attraction between a pair of electrons and positively charged nuclei.
U2	Describe how the covalent bond is formed as a result of electron sharing.
U3	Deduce the Lewis (electron dot) structures of molecules and ions for up to four electron pairs on each atom.
U4	State and explain the relationship between the number of bonds, bond length and bond strength.
A1	Predict whether a compound of two elements would be covalent from the position of the elements in the periodic table or from their electronegativity values.

Covalent bonding

In a covalent bond, the electrons are shared and attracted electrostatically by both positive nuclei resulting in a directional bond between the two atoms to form a molecule. Generally the difference in electronegativity has to be less than 1.8 for covalent bonding. It's the overlap of orbitals and the attraction between the nucleus and shared paired of electrons.

Lewis structures

In Lewis structures, lone pairs of electrons can be depicted by two crosses, two dots or a line. A bond can be shown as a line (or double line for double bonds).
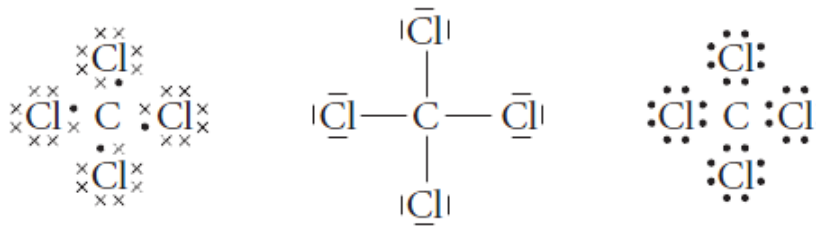

Properties of covalent compounds

- Low melting point (smaller structure, except SiO_2)
- Doesn't form giant structure (except SiO_2)
- Insulation of electricity (no free electrons)
- Form simple molecules

Polar bonds

When the atoms are different the more electronegative atom exerts a greater attraction for the electron pair, becoming more electron rich resulting in a polar bond. Bigger difference in electronegativities means a more polar bond. Polar bond ranges from 1.8 – 0.7 electronegativity difference.
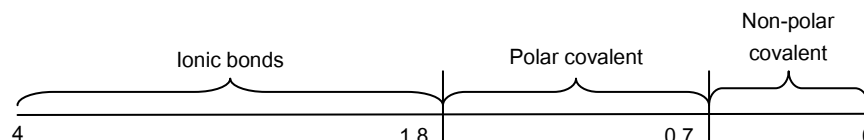
Bond strength and bond length

- Triple is the stronger than a double bond but short than a double bond. Shorter bonds are stronger.

- Bond length is a measure of the distance between two nuclei. Bond strength is described in terms of bond enthalpy. Multiples bonds have a greater number of shared electrons and so have a stronger force of electrostatic attraction between the bonded nuclei. Thus there is a greater pulling power on the nuclei, bringing them closer together, resulting in bonds that are shorter and stronger than single bonds.

4.3   Covalent structures

|	
U1	Lewis (electron dot) structures show all the valence electrons in a covalently bonded species.
U2	The "octet rule" refers to the tendency of atoms to gain a valence shell with a total of 8 electrons.
U3	Some atoms, like Be and B, might form stable compounds with incomplete octets of electrons.
U4	Resonance structures occur when there is more than one possible position for a double bond in a molecule.
U5	Shapes of species are determined by the repulsion of electron pairs according to VSEPR theory.
U6	Carbon and silicon form giant covalent/network covalent structures.
A1	Deduction of Lewis (electron dot) structure of molecules and ions showing all valence electrons for up to four electron pairs on each atom.
A2	The use of VSEPR theory to predict the electron domain geometry and the molecular geometry for species with two, three and four electron domains.
A3	Prediction of bond angles from molecular geometry and presence of non-bonding pairs of electrons.
A4	Prediction of molecular polarity from bond polarity and molecular geometry.
A5	Deduction of resonance structures, examples include but are not limited to C_6H_6, CO_3^{2-} and O_3.
A6	Explanation of the properties of giant covalent compounds in terms of their structures.

Extended Octet

The exceptions to the octet rule are:

- small atoms like B and Be form stable molecules with fewer than eight electrons (an **incomplete octet**)

- atoms of elements in the third period and below may expand their octet by using d orbitals in their valence shell. This arrangement is possible because the d orbitals available in the valence shell of these atoms have energy values relatively close to those of the p orbitals.
- In period 3, after phosphorus, we can see **extended octet** happening, due to an empty d-orbital where electrons can be excited to.

Resonance

Delocalisation is a characteristic of **π bonds** where there is more than one possible position for a double bond within a molecule (when there are **resonance structures**).
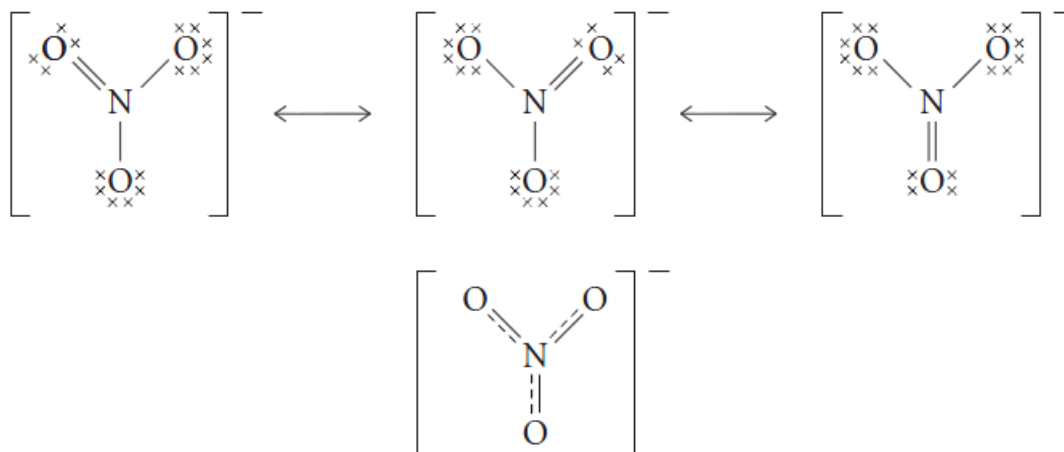
Properties caused by delocalisation

- intermediate bond lengths and strengths (between single and double)
- **greater stability**: delocalisation spreads electrons as far from each other as possible making the molecule more stable (electrons are not available for chemical reaction)
- electrical conductivity in metals and graphite

Co-ordinate bond (Dative bond)

- Type of bonding involves giving out lone pairs of electrons
- One atom share its 2 electrons together to another atom, which electron contribution is 0
- Arrows are used to shown the co-ordinate bonds (**dative bonds**)
- Example: carbon monoxide with triple bond (two covalent and one dative bond)
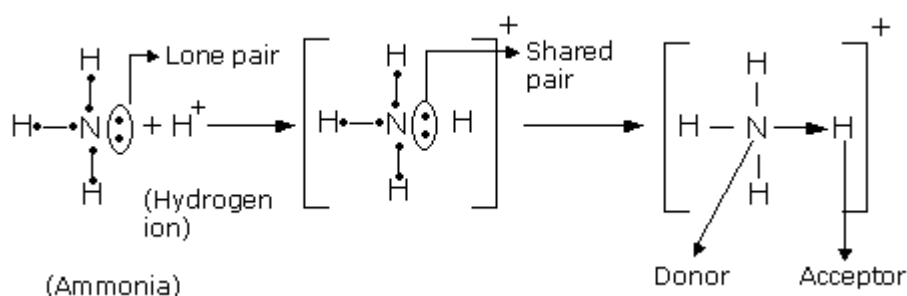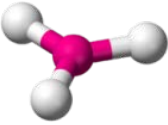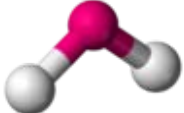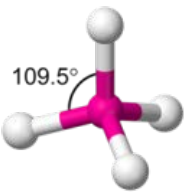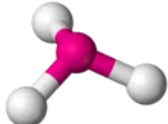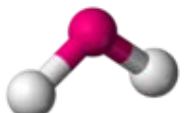

VSEPR theory

VSEPR (valence shell electron pair repulsion) theory states that pairs of electrons arrange themselves so that they are as far apart from each other as possible.
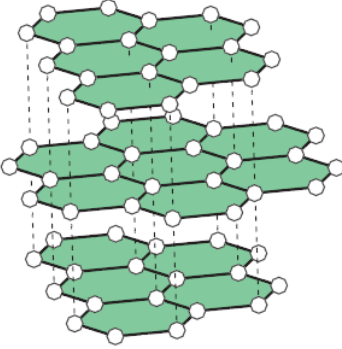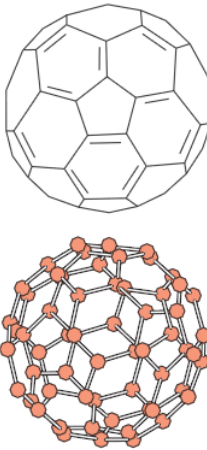
Each molecule has bond pairs of lone pairs of electron, where they can be found is called electron dense region or **charged centres**. Charged centres are indentified only around centre atoms. Depending on how many charged centre, we can figure out the geometry of electron pair distribution; therefore, we can then find the actual shape of molecules.
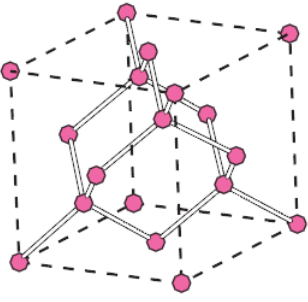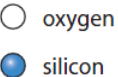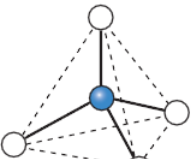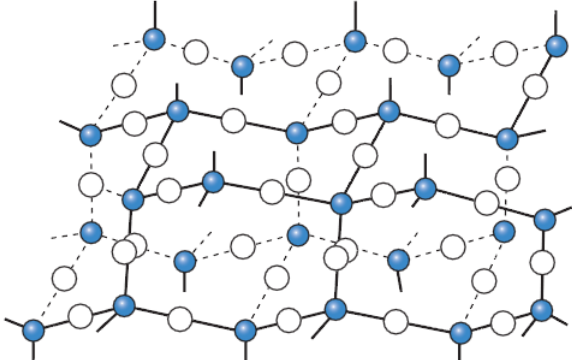
Bond pairs have more space to move due to overlap of orbitals so the repulsion between them is relatively low. However, lone pairs have less space because they are restricted to the certain orbital, so the repulsion between them is larger. Due to this, whenever lone pair presents, it takes more space so will push bond pairs closer. Therefore, for every one lone pair presents, **2.5°** will be reduced from the main angle.

Lone pair electrons don't account for the shape of the molecules.

Number of charge centres	Geometrical arrangement of charge centres	Number of bonding pairs	Number of non-bonding pairs	Shape and angle	Visual aid
2	linear	2	0	linear 180°	
2	linear	1	1	Linear 180°	
3	Triangular planar	3	0	Triangular planar 120°	
3	Triangular planar	2	1	V-shaped 117.5°	
4	tetrahedral	4	0	tetrahedral 109.5°	109.5°
4	tetrahedral	3	1	Triangular pyramidal 107°	
4	tetrahedral	2	2	v-shaped 104.5°	

Carbon allotropes, silicon and silicon dioxide

Diamond	Graphite	C_{60} fullerene
sp^3 hybridization	sp^2 hybridization	sp^2 hybridization
each C forms 4 single bonds	each C forms 3 single bonds	each C forms 2 single bonds and 1 double
tetrahedral structure	parralel layers of hexagon	one 'ball' contains 60 C atoms
hardest substance, high m.p. and b.p.	layer silde over each other – lubricant; high b.p. and m.p.; goode conductor of electricity	conductor of electricity, low m.p. and b.p.; can be used as lubricant

| Silicon	Silicon dioxide

SiO$_4$ tetrahedron

quartz |

Polarity

The prerequisite of polar molecules is polar covalent bonds (electronagetivity difference 1.8-0.7)

Polar bonds will result in a denser region of electron cloud closer to an atom, creating a **dipole moments**.

'

molecular
dipole moment
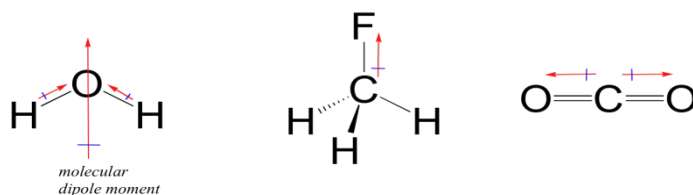
If dipole moments cancel out, the molecule is non-polar, if not, this molecule is polar.
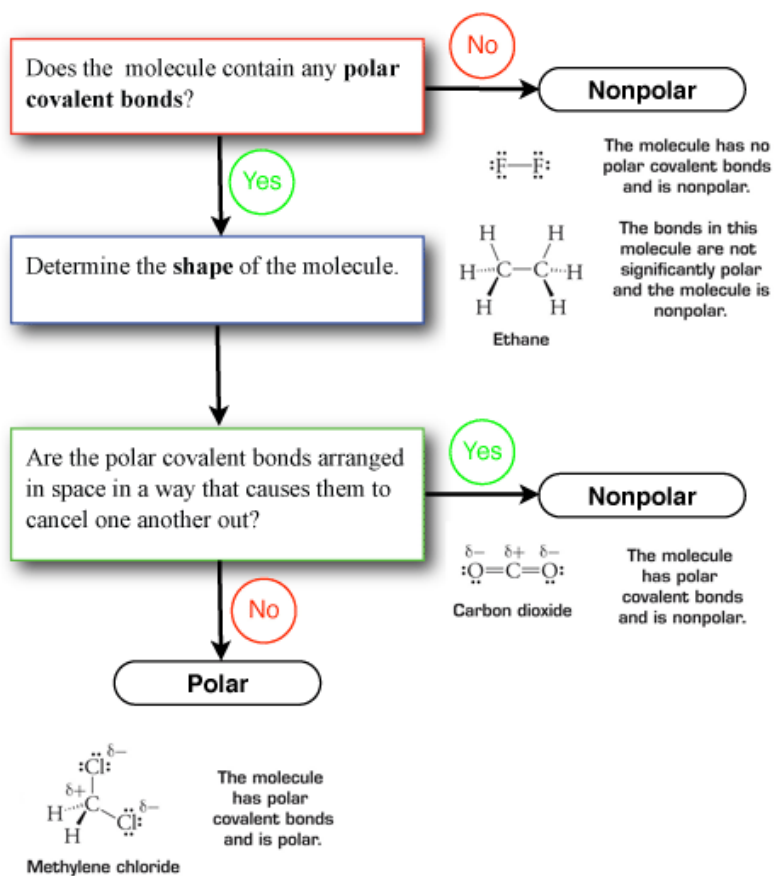
Number of charge centres	Geometrical arrangement of charge centres	Number of bonding pairs	Number of non-bonding pairs	Shape and angle	Polarity (one type of atom)
2	linear	2	0	linear 180°	Non-polar
2	linear	1	1	Linear 180°	Non-polar
3	Triangular planar	3	0	Triangular planar 120°	Non-polar
3	Triangular planar	2	1	V-shaped 117.5°	polar
4	tetrahedral	4	0	tetrahedral 109.5°	Non-polar
4	tetrahedral	3	1	Triangular pyramidal 107°	Polar
4	tetrahedral	2	2	V-shaped 104.5°	Polar
5	Triangular bipyramidal	5	0	Triangular bipyramidal 90°,120°	Non-polar
5	Triangular bipyramidal	4	1	See saw 117.5°,87.5°	Polar
5	Triangular bipyramidal	3	2	T-shape 90°	Polar
5	Triangular bipyramidal	2	3	Linear 180°	Non-polar
6	Octahedral	6	0	Octahedral 90°	Non-polar
6	Octahedral	5	1	Square pyramidal 87.5°	Polar
6	Octahedral	4	2	Square planar 90°	Non-polar
6	Octahedral	3	3	T-shape 90°	Polar
6	Octahedral	2	4	Linear 90°	Non-polar

4.4   Intermolecular forces

U1	Intermolecular forces include London (dispersion) forces, dipole-dipole forces and hydrogen bonding.
U2	The relative strengths of these interactions are London (dispersion) forces <dipole-dipole forces < hydrogen bonds.
A1	Deduction of the types of intermolecular force present in substances, based on their structure and chemical formula.
A2	Explanation of the physical properties of covalent compounds (volatility, electrical conductivity and solubility) in terms of their structure and intermolecular forces.

Dipole-dipole force (all polar molecules)

Dipole-dipole occurs because polar molecules are attracted to each other by electrostatic forces. It is stronger that Van der Waals' but weaker than H-bonding.

### Hydrogen bonding (only in polar molecules with –OH and –NH group)

Hydrogen bonding occurs when hydrogen is bonded directly to a small highly electronegative element, such as fluorine, oxygen or nitrogen. As the electron pair is drawn from the hydrogen atom, it has a small relative charge and therefore attracts a lone pair from a neighbouring molecule. Hydrogen bonds are not real bonds, they are just attraction between molecules.

London dispersion force (all molecules)

Electrons can at any one moment be unevenly spread. This produces **temporary induced dipoles**. These can induce another dipole in neighbouring molecules. This force is called the **London** force. Number of electrons and size of molecules affects the magnitude of London force due to larger electron region.

Strength of intermolecular forces

1. Hydrogen bonding
2. Dipole-dipole
3. London dispersion force
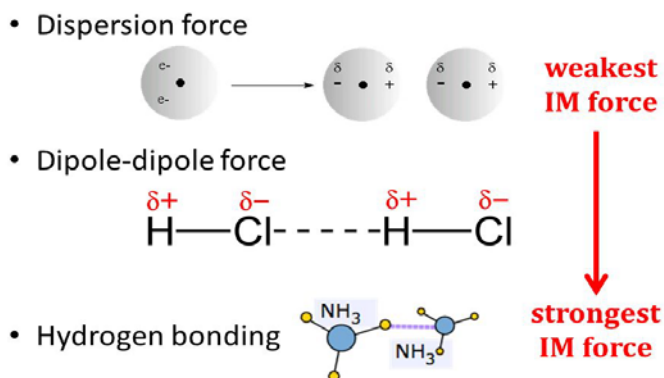
IMFs & boiling points and melting points

The stronger the intermolecular forces, the harder it is to separate the molecules i.e. the more energy it takes which corresponds to a higher temperature, so the stronger the IMFs, the higher the boiling point and melting point. Distillation can happen due to difference in intermolecular forces between molecules.

IMFs & solubility

Polar substances dissolve in polar solvent and non-polar substances dissolve in non-polar solvent. This is because the intermolecular forces of solute and solvent matches. The solution therefore will be homogenous.

IMFs & vapour pressure

Weaker intermolecular force will result in higher vapour pressure. This is because the liquid cannot hold particles together due to weak intermolecular forces, so particles leave the liquid, leading to more particles presented in form of gas, creating larger pressure. Also, higher vapour pressure leads to low boiling and melting point.

4.5   Metallic bonding

U1	A metallic bond is the electrostatic attraction between a lattice of positive ions and delocalized electrons.
U2	The strength of a metallic bond depends on the charge of the ions and the radius of the metal ion.
U3	Alloys usually contain more than one metal and have enhanced properties.

A1	Explanation of electrical conductivity and malleability in metals.
A2	Explanation of trends in melting points of metals.
A3	Explanation of the properties of alloys in terms of non-directional bonding.

Metallic bonding

In the metal, the valence electrons detached from atoms creating a sea of electrons. A **metallic bond** is the attraction between positive metal ions and electron cloud. It can be described as "metal ions surrounded by a cloud of delocalised electrons (a sea of electrons)"

Properties of metals

- Metals are good conductors of heat and electricity because they contain mobile charges (free electrons)
- Metals are malleable and ductile because the layers of cations can slide over each other without breaking more bonds than are made.
- Metals have high melting point and boiling point due to strong forces between positive ions and electrons.

Bonding		Properties
Metallic bonding		high melting point, good conductor
Macromolecular covalent		high melting point, poor conductor (except graphite)
Simple covalent	Weak IMFs	low melting/boiling points
	Strong IMFs	higher melting/boiling points

Some polar covalent molecules, however, in conditions where they can ionise will conduct electricity. For example, HCl dissolved in water (hydrochloric acid) is an electrical conductor.

Strength of metallic bonding

- Radius of the ion (larger radius means electrostatic attraction is in larger distance, weaker bonding)
- Charge of the ion (higher the charge, strong the attraction)

Trends in melting point & boiling point

- In group 17, from F_2 to I_2, melting point gets larger. This is because atoms have larger size and more electrons, so the London dispersion forces become stronger. Stronger IMF leads to higher melting point.
- In group 1, from Li to Fr, melting point gets smaller. This is because atoms have larger size, so the electrostatic attraction is in the larger distances. IMF gets smaller, leading to decreasing melting point.
- In period 2, from N_2 to F_2, melting point decrease. This because the atom size gets smaller, leading to smaller London dispersion forces (however, electron number increases but with less effect); thus, it result in lower melting point.

Alloys

Mixture of metal, is a kind of metallic solution

Transition metals always form alloys because they have closer atomic radius.

In general, alloys have **poor electricity and heat** conductivity than pure metal. This is because their size is different, so the **flow of electrons** is blocked.

Topic 14: Chemical bonding and structure (HL)

## 14.1   Further aspects of covalent bonding and structure

U1	Covalent bonds result from the overlap of atomic orbitals. A sigma bond (σ) is formed by the direct head-on/end-to-end overlap of atomic orbitals, resulting in electron density concentrated between the nuclei of the bonding atoms. A pi bond (π) is formed by the sideways overlap of atomic orbitals, resulting in electron density above and below the plane of the nuclei of the bonding atoms.
U2	Formal charge (FC) can be used to decide which Lewis (electron dot) structure is preferred from several. The FC is the charge an atom would have if all atoms in the molecule had the same electronegativity. FC = (Number of valence electrons)-½(Number of bonding electrons)-(Number of non-bonding electrons). The Lewis (electron dot) structure with the atoms having FC values closest to zero is preferred.
U3	Exceptions to the octet rule include some species having incomplete octets and expanded octets.
U4	Delocalization involves electrons that are shared by/between all atoms in a molecule or ion as opposed to being localized between a pair of atoms.
U5	Resonance involves using two or more Lewis (electron dot) structures to represent a particular molecule or ion. A resonance structure is one of two or more alternative Lewis (electron dot) structures for a molecule or ion that cannot be described fully with one Lewis (electron dot) structure alone.
A1	Prediction whether sigma (σ) or pi (π) bonds are formed from the linear combination of atomic orbitals.
A2	Deduction of the Lewis (electron dot) structures of molecules and ions showing all valence electrons for up to six electron pairs on each atom.
A3	Application of FC to ascertain which Lewis (electron dot) structure is preferred from different Lewis (electron dot) structures.
A4	Deduction using VSEPR theory of the electron domain geometry and molecular geometry with five and six electron domains and associated bond angles.
A5	Explanation of the wavelength of light required to dissociate oxygen and ozone.
A6	Description of the mechanism of the catalysis of ozone depletion when catalysed by CFCs and NOx.

Sigma (σ) bonds

Sigma bonds result from axial (**head-on**) overlap of s, p and hybrid orbitals in different combinations.

Pi (π) bonds

Pi bonds result from **sideways overlap** of parallel orbitals and consist of two regions of electron density (two overlaps). Pi bonds are weaker than sigma bonds as their electron density is further from the positive charge of the nucleus.
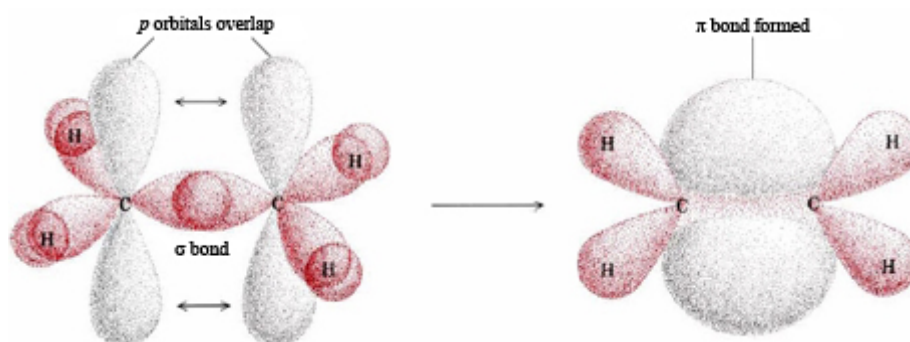

Double and triple bonds

Double bonds consist of one sigma bond and one pi bond. Triple bonds consist of one sigma and two pi bonds. The first bond formed is always **sigma bond**.

Sigma bond is shorter because head-on overlap happens closer to the nucleus. Pi bond is longer because sideway overlap happens further away from the nucleus.
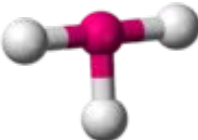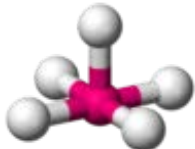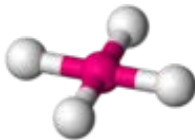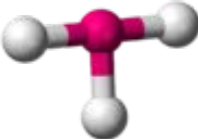
Formal Charge

FC = (Number of valence electrons)-½(Number of bonding electrons)-(Number of non-bonding electrons).

Least formal charge means the most stable atom, suggesting that this kind of structure is correct. If FC is the same, using electro negativity to deduce, more **electronegative** atom carries **negative formal charge.**
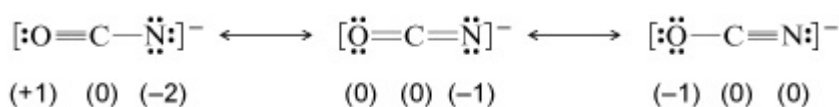
As shown in the molecule [OCN]⁻ above, left configuration has largest formal charge, so it cannot be the correct structure. Middle and the right one have the same formal charge; but oxygen in the right one, as more electronegative atom, has the negative formal charge. So the right one is the correct structure of [OCN]⁻

VSEPR Theory on 5 and 6 charged centre

No. of charge centres	Geometry	No. bonding pairs	No. non-bonding pairs	Bond angles	Shape	Visual aid
5	Triangular bipryramidal	5	0	90° 120°	Triangular bipyramidal	
		4	1	87.5° 117.5°	see saw (distorted tetrahedral)	
		3	2	90°	T-shaped	
		2	3	180°	linear	
6	octahedral	6	0	90°	octahedral	
		5	1	87.5°	square pyramidal	
		4	2	90°	square planar	
		3	3	90°	T-shaped	
		2	4	180°	Linear	

14.2   Hybridisation

Hybridisation

Hybridisation is the process whereby unequal atomic orbitals within an atom mix to form new hybrid atomic orbitals which are the same as each other, but different from the original orbitals. Hybrid orbitals form stronger bonds by allowing greater overlap. Experimental evidence suggests that bonds in an molecule have equal length, which support the idea of hybridisation.
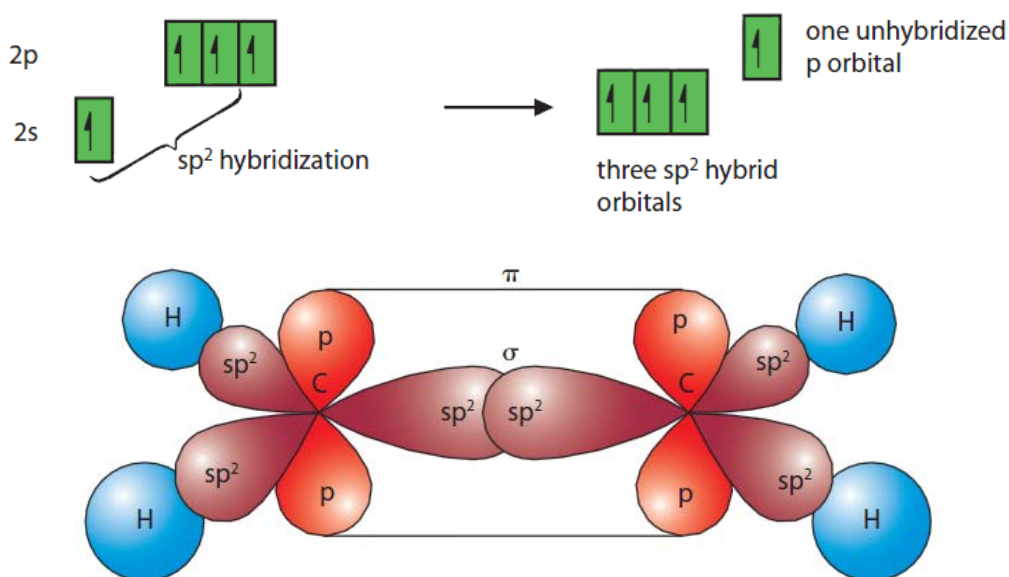
sp^3 hybridisation

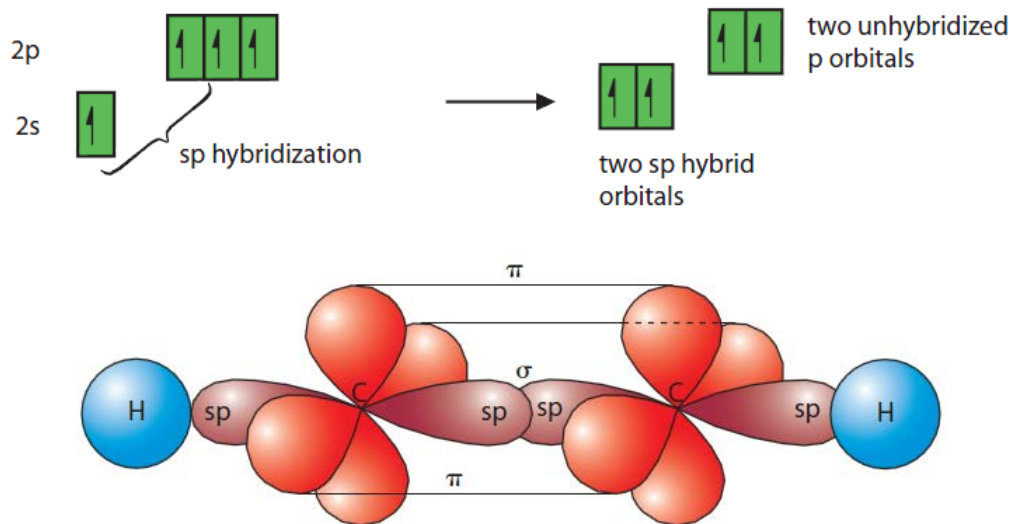When carbon forms four single bonds (e.g. CH_4), it undergoes sp^3 hybridisation:
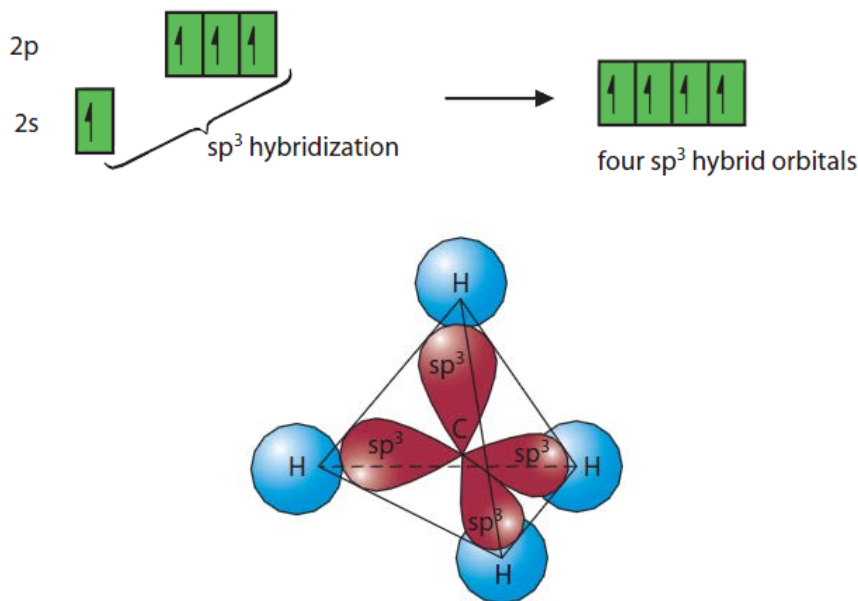
sp^2 hybridisation

When carbon forms a double bond (e.g. C_2H_4), it undergoes sp^2 hybridisation:

sp hybridisation

When carbon forms a triple bond (e.g. C_2H_2), it undergoes sp hybridisation:

Hybridisation and molecular shape

The shape of a molecule can be used to determine the type of hybridisation that has occurred:

- tetrahedral arrangement   ↔ sp^3 hybridised
- planar triangular arrangement   ↔ sp^2 hybridised
- linear arrangement   ↔ sp hybridised

Bond types and hybridisation

Hybridisation only occurs when a sigma bond forms. Pi bonds only form when two **unmixed** orbitals sideway overlap. sp^3 will means 4 sigma bonds formed; sp^2 will means 3 sigma bonds formed; sp will means 2 sigma bonds formed.