NCEA Chemistry 3.4

Particles, Substances and Thermochemistry AS 91390

Achievement Criteria

This achievement standard involves describing properties of atoms, molecules, and ions, and thermochemical principles.

Properties of particles will be limited to:

- ☐ electron configuration of atoms and ions of the first 36 elements (using *s,p,d* notation)
- ☐ periodic trends in atomic radius, ionisation energy, and electronegativity, and comparison of atomic and ionic radii
- ☐ Lewis structures and shapes (up to six electron pairs about the central atom for molecules and polyatomic ions, including those with multiple bonds), polarity of molecules
- ☐ Attractive forces between atoms, ions, and molecules. These will include ionic bonds, covalent bonds, and intermolecular attractions due to temporary dipoles and permanent dipoles (including hydrogen bonding).

Properties of substances will be limited to:

- ☐ melting point, boiling point and solubility
- ☐ enthalpy and entropy changes associated with spontaneity in chemical reactions (entropy calculations are not required)

Thermochemical principles will include

- ☐ specific heat capacity
- ☐ $\Delta_c H^\circ$, $\Delta_f H^\circ$, $\Delta_r H^\circ$, $\Delta_{vap} H^\circ$, $\Delta_{sub} H^\circ$, and $\Delta_{fus} H^\circ$
- ☐ Hess's Law including application of $\Delta_r H = \sum \Delta_f H((\text{products}) - \sum \Delta_f H(\text{reactants}))$ and related calculations.

Atomic Structure

Atomic and Mass number

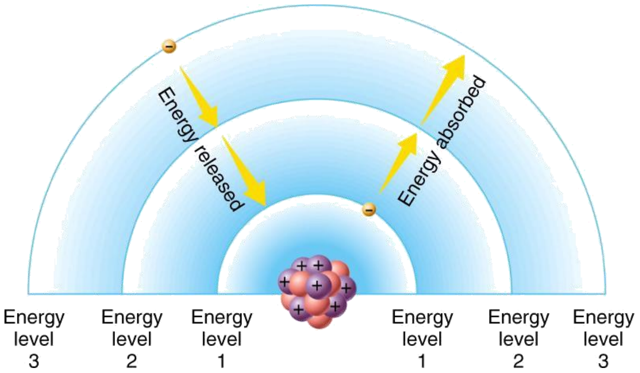
The atomic number is unique for each element. A neutral atom has the same number of electrons as protons. The periodic table is arranged in order of an elements atomic number and the mass number is the total number of protons and neutrons together.

Electrons orbit a nucleus of an atom at fixed energy levels.

An electron can only be found in a fixed energy level around a nucleus.

A ball bouncing down a flight of stairs provides an analogy for energy levels of electrons because a ball can only rest on each step, not between steps.

An electron can move up an energy level if energy is absorbed, such as light or heat. When the electron moves back down to its lowest possible level the energy is released again, often in the form of light.

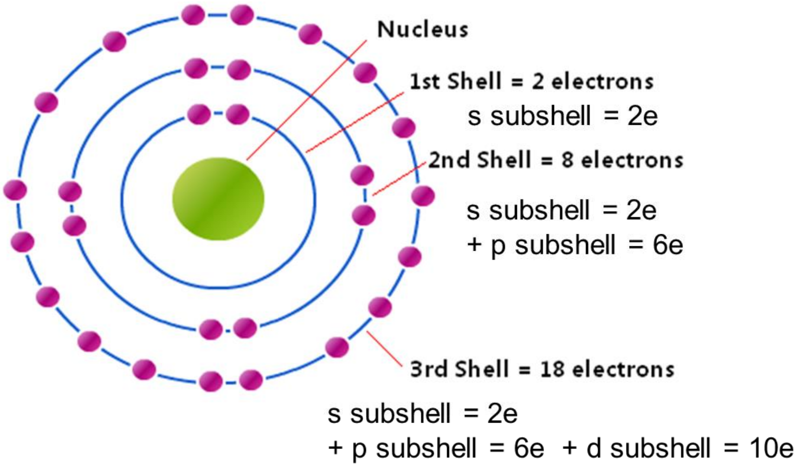


Electron orbitals

The major energy levels (shell) split into subshells. Each sub shell level made up of one or more atomic orbitals.

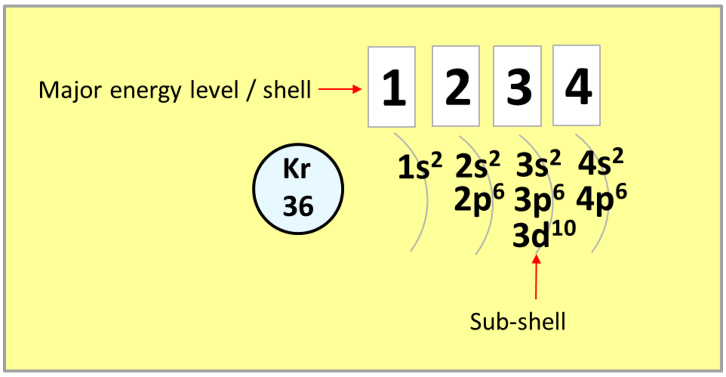
An Orbital is an area of space with high probability of finding a particular electron pair. Electrons orbit in pairs spinning opposite directions

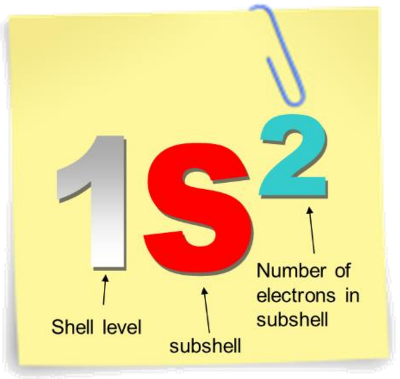
- ☐ s subshell = 1 pair (2e)
- ☐ p subshell = 3 pairs (6e)
- ☐ d subshell = 5 pairs (10e)



Electron Configuration notation

The arrangement of the electrons around the nucleus is known as its configuration. The sub shells are numbered according to the major shell/energy level they are in.

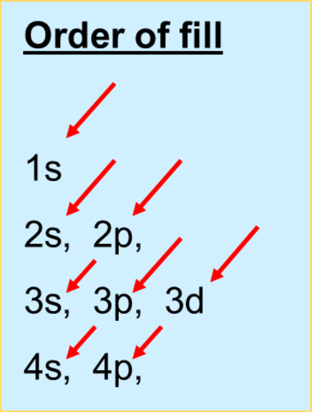




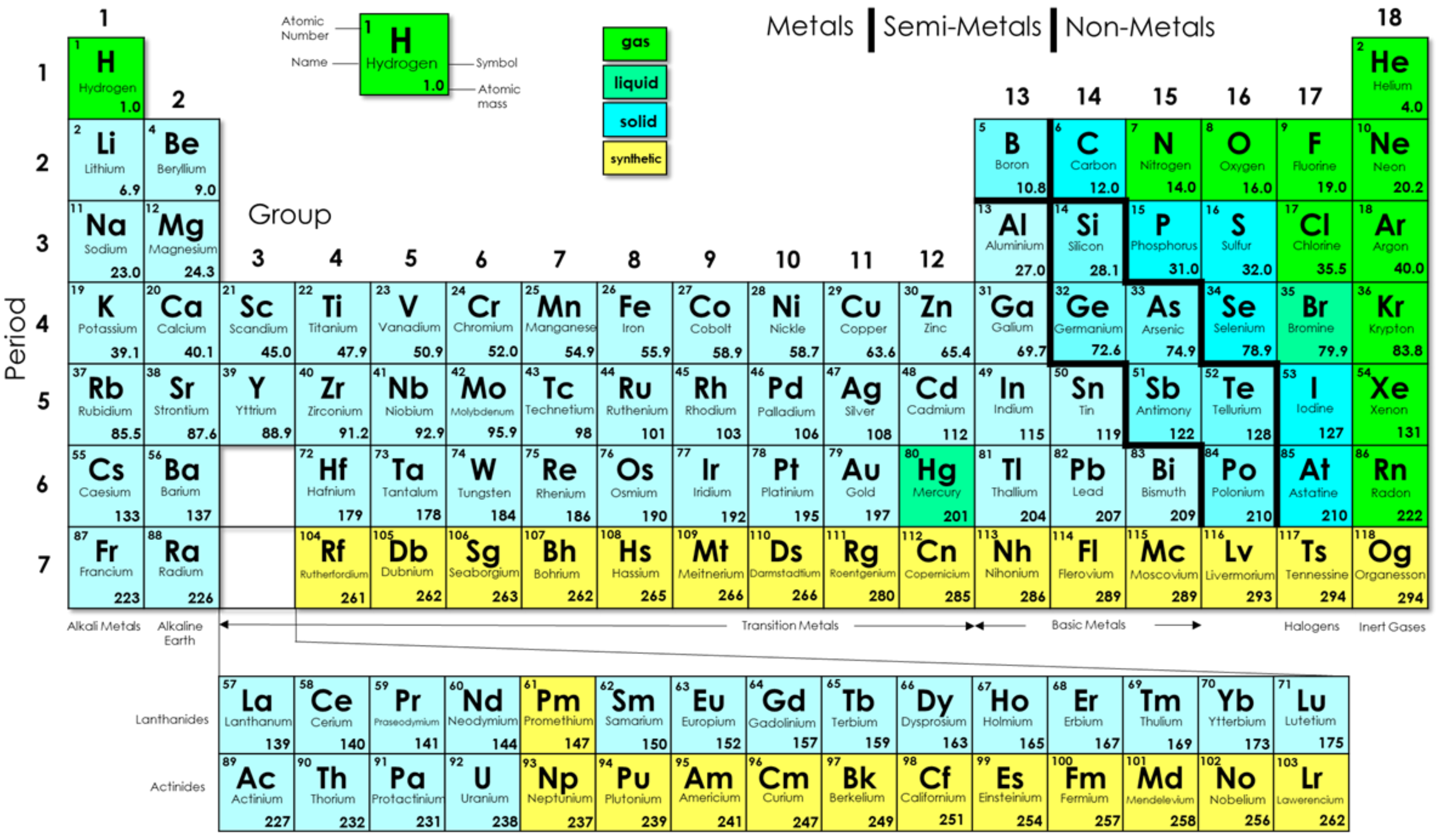
Order of fill

Electrons always fill the shells with the lowest energy level first. (The Aufbau principle) Even though the subshells are filled according to energy level, the notation is still written out in order.
$1s^2,2s^2,2p^6,3s^2,3p^6,3d^{10},4s^2,4p^6$…

1. All of the orbitals hold up to 2 electrons, which make up a pair (s1,p3,d5).
2. The electron pairs spin in opposite directions indicated with arrows
3. Electrons fill up orbitals with lower energy levels first
4. The most stable (lower energy) arrangement is for the sublevels to be filled with a single electron first (with the same direction spin) before pairing electrons. (Hund's rule) Place electrons singly first showing upwards arrow. [Extension]



Periodic Table

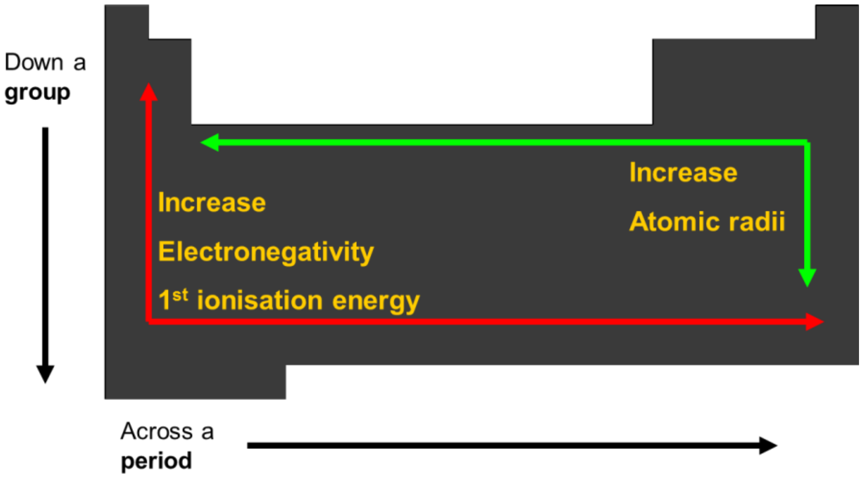


Period	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18
1	1 H Hydrogen 1.0																	2 He Helium 4.0
2	3 Li Lithium 6.9	4 Be Beryllium 9.0											5 B Boron 10.8	6 C Carbon 12.0	7 N Nitrogen 14.0	8 O Oxygen 16.0	9 F Fluorine 19.0	10 Ne Neon 20.2
3	11 Na Sodium 23.0	12 Mg Magnesium 24.3											13 Al Aluminium 27.0	14 Si Silicon 28.1	15 P Phosphorus 31.0	16 S Sulfur 32.0	17 Cl Chlorine 35.5	18 Ar Argon 40.0
4	19 K Potassium 39.1	20 Ca Calcium 40.1	21 Sc Scandium 45.0	22 Ti Titanium 47.9	23 V Vanadium 50.9	24 Cr Chromium 52.0	25 Mn Manganese 54.9	26 Fe Iron 55.9	27 Co Cobolt 58.9	28 Ni Nickle 58.7	29 Cu Copper 63.6	30 Zn Zinc 65.4	31 Ga Gallium 69.7	32 Ge Germanium 72.6	33 As Arsenic 74.9	34 Se Selenium 78.9	35 Br Bromine 79.9	36 Kr Krypton 83.8
5	37 Rb Rubidium 85.5	38 Sr Strontium 87.6	39 Y Yttrium 88.9	40 Zr Zirconium 91.2	41 Nb Niobium 92.9	42 Mo Molybdenum 95.9	43 Tc Technetium 98	44 Ru Ruthenium 101	45 Rh Rhodium 103	46 Pd Palladium 106	47 Ag Silver 108	48 Cd Cadmium 112	49 In Indium 115	50 Sn Tin 119	51 Sb Antimony 122	52 Te Tellurium 128	53 I Iodine 127	54 Xe Xenon 131
6	55 Cs Caesium 133	56 Ba Barium 137		72 Hf Hafnium 179	73 Ta Tantalum 178	74 W Tungsten 184	75 Re Rhenium 186	76 Os Osmium 190	77 Ir Iridium 192	78 Pt Platinum 195	79 Au Gold 197	80 Hg Mercury 201	81 Tl Thallium 204	82 Pb Lead 207	83 Bi Bismuth 209	84 Po Polonium 210	85 At Astatine 210	86 Rn Radon 222
7	87 Fr Francium 223	88 Ra Radium 226		104 Rf Rutherfordium 261	105 Db Dubnium 262	106 Sg Seaborgium 263	107 Bh Bohrium 262	108 Hs Hassium 265	109 Mt Meitnerium 266	110 Ds Darmstadtium 266	111 Rg Roentgenium 280	112 Cn Copernicium 285	113 Nh Nihonium 286	114 Fl Flerovium 289	115 Mc Moscovium 289	116 Lv Livermorium 293	117 Ts Tennessine 294	118 Og Organesson 294

Lanthanides	57 La Lanthanum 139	58 Ce Cerium 140	59 Pr Praseodymium 141	60 Nd Neodymium 144	61 Pm Promethium 147	62 Sm Samarium 150	63 Eu Europium 152	64 Gd Gadolinium 157	65 Tb Terbium 159	66 Dy Dysprosium 163	67 Ho Holmium 165	68 Er Erbium 167	69 Tm Thulium 169	70 Yb Ytterbium 173	71 Lu Lutetium 175
Actinides	89 Ac Actinium 227	90 Th Thorium 232	91 Pa Protactinium 231	92 U Uranium 238	93 Np Neptunium 237	94 Pu Plutonium 239	95 Am Americium 241	96 Cm Curium 247	97 Bk Berkelium 249	98 Cf Californium 251	99 Es Einsteinium 254	100 Fm Fermium 257	101 Md Mendelevium 258	102 No Nobelium 256	103 Lr Lawerencium 262

Periodic trends

Periodic trends can be seen in atoms and ions as you move across a period and down a group. The trends investigated will include Atomic and ionic radii (distance from the centre of the nucleus to the valence energy level), electronegativity and the 1st ionisation energy.

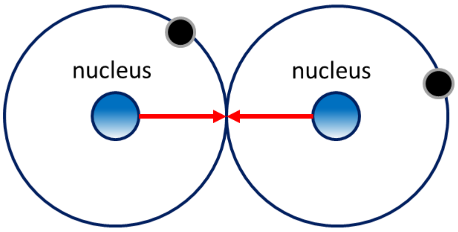


Atomic Radii

Atomic Radii is affected by two main factors:

(1) Nuclear charge (number of protons): The stronger the pull the electrons have to the protons with electrostatic attraction, then the smaller the size of the atom radii. The most important factor is nuclear charge – atoms are neutral and as the number of protons increases, the number of electrons increases at the same rate. The more electrons in the valence shell, because of an increased number of equivalent protons, the more they will be pulled in tighter and therefore show smaller atomic radii.

(2) Number of energy levels: The greater the number of energy levels the larger the atomic radii. Electrons repel each other (electron-electron repulsion) and spread out to maximum distance in each energy level. The internal energy levels "shield" and reduce electrostatic attraction of the valence electrons to the protons. Note that the addition of another electron does not result in a fractional decrease in the electrostatic attraction to any given electron, but it does increase the electron-electron repulsion, so an overall decrease in nett attractive force.



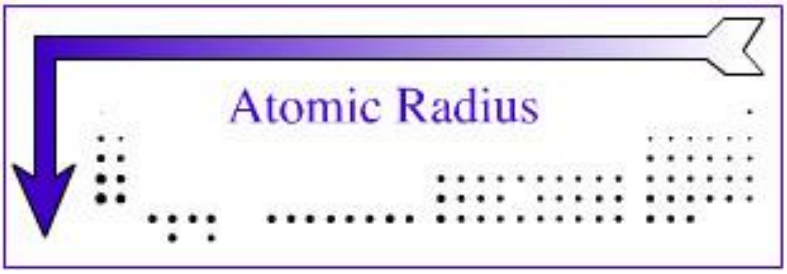
Atomic radius is half the distance between the nuclei of two bonded atoms

Atomic Radii Trends

Across the period the Atomic radii decreases E.g., Li → Ne in period 2

As the nuclear charge increases across the period, so does the electrostatic attraction and so outer electrons are pulled closer to nucleus. The electron repulsions are balanced by the nuclear charge attractions, and as the nuclear charge gets larger, so the electrons get closer together.

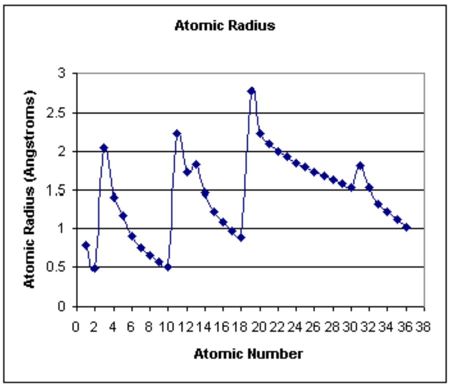
Addition of another electron does increase the electron-electron repulsion, but this is over come with increased nuclear charge which effectively increases the nett attractive force



Down the group the Atomic radii increases E.g. Li → Fr in group one

Electrons are being added to successive shells and both charge on nucleus and electron repulsion increase in step to "cancel each other out". However, successive shells are further from the nucleus therefore, there is a subtle increase in atomic radii and an overall decrease in Net electrostatic attraction.

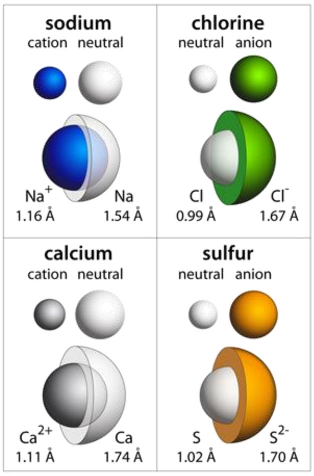
Addition of another electron does not result in a fractional decrease in the electrostatic attraction "shielding" to any given electron, but it does increase the electron-electron repulsion, which effectively reduces the nett attractive force

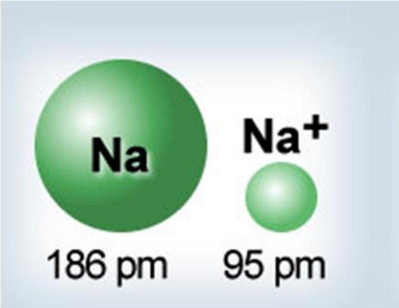
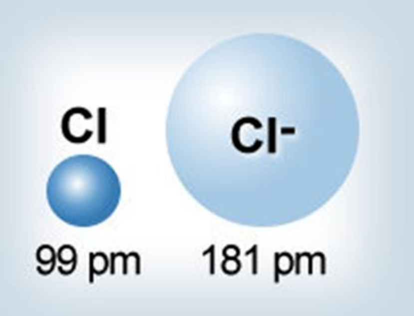


Ionic Radii

Cations (metal ions) are smaller in radii than their atoms. The outside energy level of electrons are removed but the nuclear charge (number of protons) remains the same creating a smaller radii than the atom

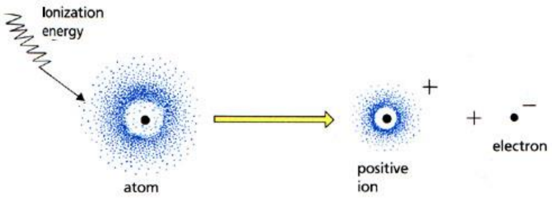
Anions (non-metal ions) are larger in radii than their atoms. Extra electrons are added to the outside valance shell that have to be accommodated for and there is no change to the nuclear charge. Electron-electron repulsion spreads the electrons out further creating larger radii than the atom.



Cations i.e. Na to Na^+	Anions i.e. Cl to Cl^-
The inter-electronic repulsion experienced by the electron cloud of the cation is less than the neutral atom, and since both species have the same amount of nuclear charge, the net electrostatic attractive force on the electron cloud in the cation is greater than the neutral atom resulting in a smaller cation size.  	The inter-electronic repulsion experienced by the electron cloud of the cation is greater than the neutral atom, and since both species have the same amount of nuclear charge, the net electrostatic attractive force on the electron cloud in the cation is less than the neutral atom resulting in a larger anion size. 

1st ionisation energy Trends

The first ionisation energy is the energy required to remove one mole of electrons from the outside valance shell of 1 mole of atoms in a gaseous state.



An Ionisation equation can be written as: (M representing an atom)

$M \rightarrow M^+ + e^-$ $\Delta H = + kJ$ as this is always an endothermic reaction

If the ionisation energy is high, that means it takes a lot of energy to remove the outermost electron. If the ionisation energy is low, that means it takes only a small amount of energy to remove the outermost electron.

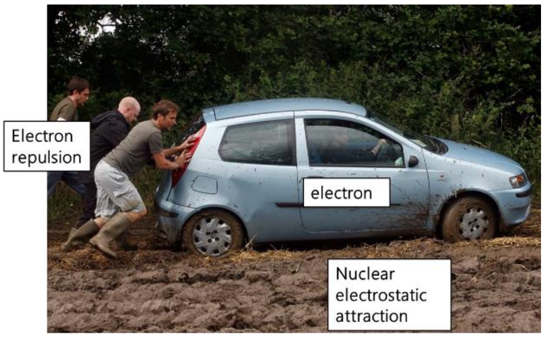
Ionisation energy is affected by two factors:

(1) Nuclear charge: As it increases, there is a stronger pull to the electrons by electrostatic attraction.

(2) Number of energy levels: Electrons in a lower energy level are much closer to the nucleus and thus have much stronger net electrostatic attraction to it. Electrons in a lower energy level shell have electron repulsion but are closer together. Electrons in higher energy level shells are experience less net electrostatic attraction to the nucleus, as they are further away.

1st ionisation energy Analogy

In order to remove an electron from an atom you need to overcome the nuclear attraction of its protons holding it around order. This can be shown by the mud that the car is stuck in. The more mud (nuclear attraction) the more energy to remove the car (electron). However, other electrons in the atom are repelling the electron to be removed – so the more people pushing the car (electron repulsion) the easier it is to extract the car (electron)



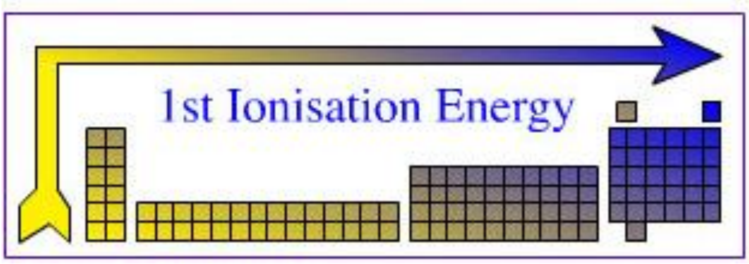
1st ionisation energy Trends

Across a period the 1st ionisation energy increases

As the nuclear charge increases, the Net attraction between the nucleus and the electrons increases and it requires more energy to remove an electron from the outermost energy level and that means there is a higher ionisation energy. As you go across the periodic table, nuclear charge is the most important consideration. Therefore, going across the periodic table, there should be an increase in ionisation energy because of the increasing nuclear charge.

Down a group the 1st ionisation energy decreases

Going down the table, the effect of increased nuclear charge is weighed against the effect of increased electron repulsion, and the number of energy levels becomes the predominant factor. With more energy levels, the outermost electrons (the valence electrons) are further from the nucleus and are not so strongly attracted to the nucleus, and therefore there is a reduction in net electrostatic attraction. Thus, the ionisation energy of the elements decreases as you go down the periodic table because it is easier to remove the electrons. The more stable elements have higher ionisation energies.



[Extension] All bonding is electrostatic and is characterised by Coulombs Law ($F = kQq/r^2$) which is an inverse square law so distance from nucleus really does matter

Electronegativity

Electronegativity is the tendency of an atom to attract bonding electrons from another atom. Higher electronegativity values mean a higher tendency to attract electrons. Atoms with high electronegativity are strong oxidants (gain electrons).

Electronegativity is affected by two factors:

(1) Nuclear charge: As an atoms nuclear charge increases, there is a stronger pull on electrons of another atom by electrostatic attraction.

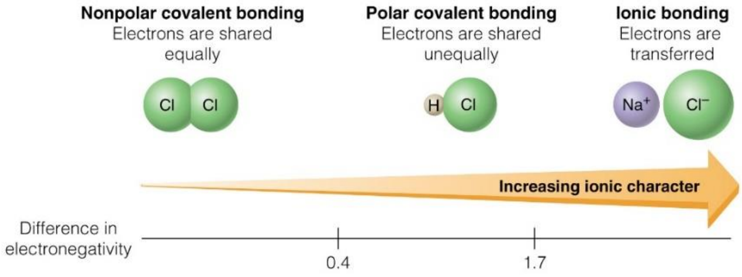
(2) Number of energy levels: the more energy levels an atom has the lower the net electrostatic attraction and the radii of the atom is larger. Because this then creates a bigger distance between 'neighbouring' atoms, Electrons from other atoms experience less electrostatic attraction to the nucleus of another atom. Therefore an atom in the same group has less electronegativity than an atom above it with less energy levels(Even though it has more nuclear charge)

Ionic – covalent bond continuum due to electronegativity

Bond types between atoms can depend on the electronegativity of the atoms. Rather than discrete categories, molecules fall along a continuum.

If there is little difference in electronegativity between two atoms then they tend to form a covalent bond with no polarity difference. A greater electronegativity difference creates a polar bond with uneven "sharing" of valance electrons.

If the electronegativity is even greater then there will be a complete transfer of electron from one atom (Metal) to another atom (non-metal) and ions will form that are held together with an ionic bond.



Electronegativity Trends

Across a Period the electronegativity increases   E.g. Li → Ne

The atoms have increased "pulling power" as the nuclear charge is increasing. Electrons are held tighter to the nucleus and there is a greater net electrostatic attraction. This allows another atom to be closer and it has a stronger attraction to electrons from that atom, so electronegativity increases.

Down a group the electronegativity decreases   E.g. Li → Fr

Both nuclear attraction and electron repulsion increase in step, but with an overall decrease in Net electrostatic attraction. However, as successive shells increase atomic radii, then the electrostatic attraction of the nucleus to other atoms' electrons decreases, so atoms have less electronegativity as you move down a group.

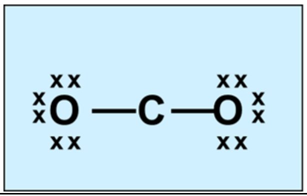
Periodic trends Summary

	Electronegativity	1st ionisation energy	Atomic radii
Across a Period	The greater the nuclear charge, the easier it is to obtain more electrons from other atoms > more p+ to pull with INCREASES	As the nuclear charge is larger it requires more energy to remove an electron as they are held tighter (and closer) to the nucleus INCREASES	Across a period the energy level numbers stay the same but proton numbers increase pulling more at the valence electrons DECREASES
Down a group	The larger the number of energy levels the less net electrostatic attraction so the less ability an atoms has to remove the valance electrons of another atom DECREASES	As the energy level numbers increase the easier it is to remove electrons as the valence electrons are further from the 'pull' of the protons and more electron repulsion by other electrons in inner energy levels DECREASES	Down a group the energy levels become further away from the nucleus therefore the valence electrons repel more, less effected by protons, taking up more space and increasing the size INCREASES

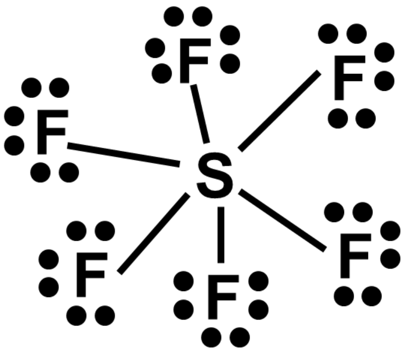
Lewis Diagrams

G Lewis devised a system of drawing covalent molecules showing arrangement of atoms and valence electrons – both those involved in bonding and those that are not (called lone pairs). Electrons in inner shells are not involved in bonding. These diagrams are called Lewis diagrams (or structures) The Lewis diagram is drawn so that each atom has eight electrons associated with it (except for hydrogen, which has two). This is the *octet rule*.

Lewis Diagrams – Steps to drawing

1. Calculate valence electrons of all atoms. If the molecule is an ion, then subtract the charge from the total electrons and place the charge outside of square brackets of the Lewis diagram at the end. *Example carbon dioxide.* C = 4 O = 6 O = 6 16 CO_2	2. Write down number of pairs of electrons. 16 / 2 = 8 pairs
3. Place atom with least filled valence shell in the centre with the other atoms arranged around the outside (periphery) O C O	4. Bond all atoms together (either x or - = one pair of electrons) O—C—O 8 pairs – 2 pairs = 6 pairs remaining
5. Place remaining e- pairs around the periphery atoms so each has 4 pairs (including bond pair) around it.  6 pairs – 6 pairs = 0 pairs remaining	6. If there are any remaining pairs place them around the outside of the central atom.
7. Rearrange non-bonded pairs into bonded pairs if the central atom does not have 4 pairs around it.	

Expanded Octet



SF_6 creates a molecule that has 6 bonded F atoms around the central S atom.

Third row elements (e.g., Al, Si, P, S, and Cl) often have <u>more</u> than four valence shell orbitals filled with non-bonding Pairs and/or Bond Pairs; this is called "expanded Octet". Obviously, elements from the fourth and higher rows can also exhibit "expanded valence". EXAMPLE Phosphorus, electron configuration. 2, 8, 5 can form up to five covalent bonds.

E.g. phosphorus pentachloride

P + 5Cl ➔ PCl_5

Expanded Octet - Rule of orbitals – exceptions to the rule [Extension]

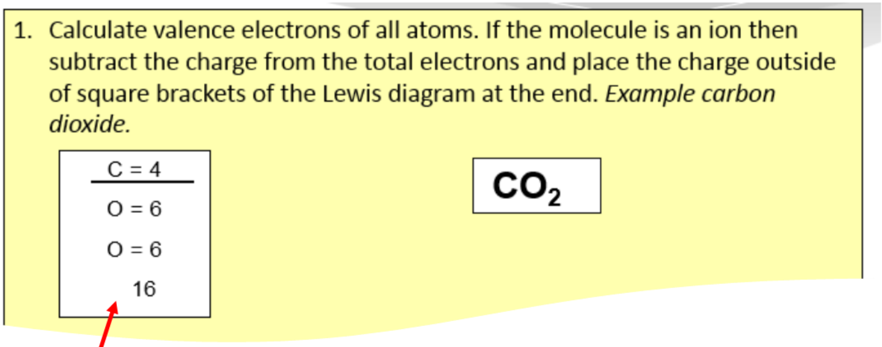
If there are extra non-bonding Pairs of electrons left after all of the periphery atoms are filled in accordance with the *octet rule* then they are placed around the central atom(s) according to the Rule of Orbitals. *The Rule of Orbitals*: the total number of non-bonding pairs and bond pairs (NBP+BP) associated with an atom cannot exceed the number of Valence Shell Orbitals (VSO = n^2, where n is the row of the Periodic Table in which that atom resides).

n = 1 (H): maximum VSE pairs (NBP+BP) = VSO = 1;

n = 2 (B, C, N, O, F): maximum VSE pairs (NBP+BP) = VSO = 4 ("octet rule")

n = 3 ((Al, Si, P, S, Cl): maximum VSE pairs (NBP+BP) = VSO = 9 etc.

Lewis Diagrams of ions



1. Calculate valence electrons of all atoms. If the molecule is an ion then subtract the charge from the total electrons and place the charge outside of square brackets of the Lewis diagram at the end. *Example carbon dioxide.*

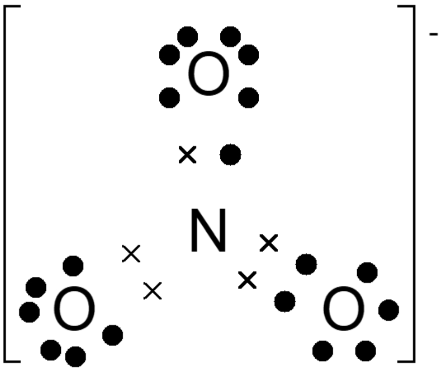
C = 4
O = 6
O = 6
16

CO_2

In step 1. For negative ions, add extra e- to valence electrons
For positive ions remove e- from valence electrons

e.g. for nitrate NO_3^-

Put bracket around ion and show charge.

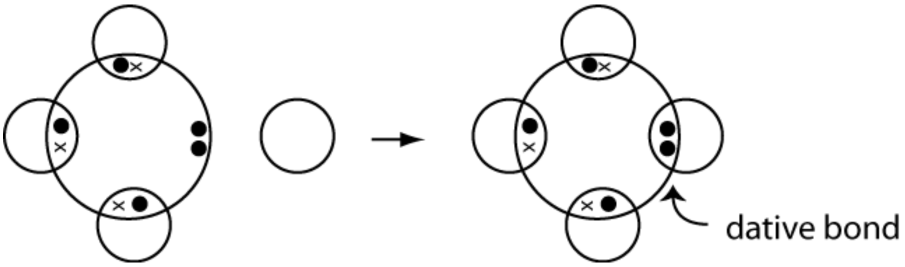


Dative Bonds

A dative bond occurs when one atom donates both electrons to form a single covalent bond.

E.g., an ammonium ion is made from an ammonia molecule and a hydrogen ion.

NH_3 + H^+ → NH_4^+



Bonding the atoms

Often, the formula is written to indicate connectivity.

For example: HCN = H bonded to C, C bonded to N, H and N are not bonded.
CH_3OCH_3 = three H bonded to C1, C1 bonded to O, O bonded to C2, C2 bonded to three H.
CH_3CH_2OH = three H bonded to C1, C1 bonded to C2, C2 bonded to two H and O, O bonded to H.

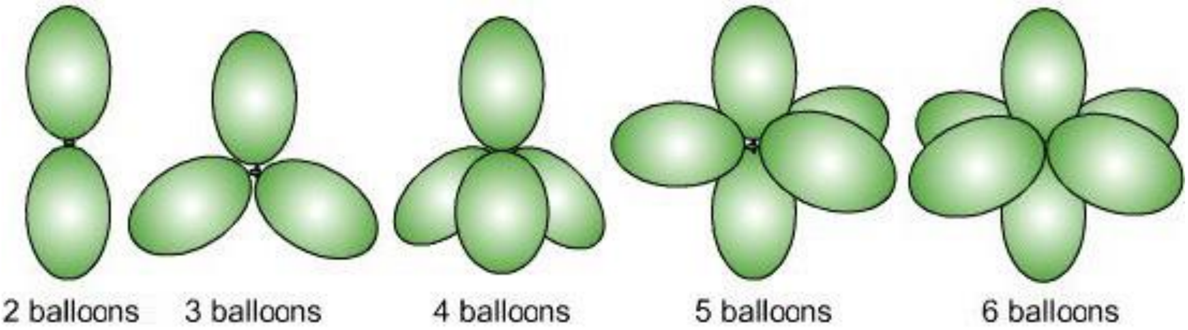
Otherwise, as a general rule, the *least electronegative* elements are central, the *most electronegative* elements are peripheral

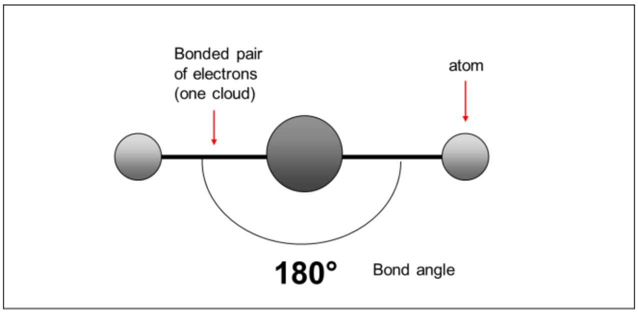
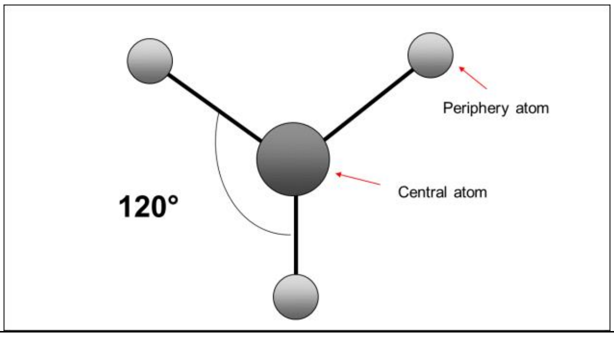
Molecular Shapes

Valence Shell Electron Pair Repulsion Theory - electrons repel and therefore regions of negative charge move as far apart from each other as possible around a central atom. (Used to predict molecular shape.)

1. Draw the electron dot diagram
2. Count the electron pairs (regions of negative charge) around the central atom. (Double and triple bonds may be considered as single charge regions)
3. Consider the shape the charge regions repel to.
4. Name the shape formed by the bonded atoms.

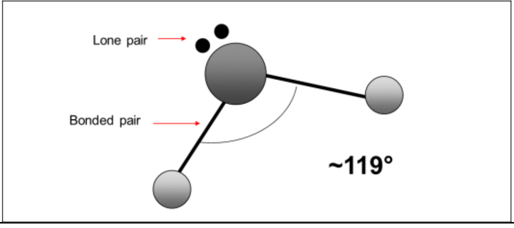
Repelling power of charge regions:
Triple bond > double bond > lone pair > single bond



Molecular Shapes – two regions of charge Since regions of electrons are negatively charged, they repel each other as far apart as possible. Two regions arrange themselves on opposite sides of the central atom to form a linear shape. The bond angle will be 180°. The bonded regions form a linear shape. 	Molecular Shapes – three regions of charge (0 non-bonding pairs) Three regions of negative charge will cause a bond angle of 120° as they repel each other. All the atoms still lie on a flat plane (like a sheet of paper) to form a trigonal planar shape. The bonded negative regions form a trigonal planar shape. (Or triangular planar) 

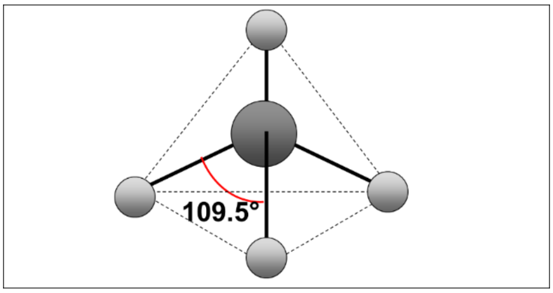
Molecular Shapes – three regions of charge (1 non-bonding pair)

When one of the regions of electrons is a *non-bonding pair*, it will have a slightly greater push to the bonded pairs. This is because the lone pair are only orbiting around one positive nucleus and their negative charge is less 'neutralised' than if they had another nucleus to orbit around. The regions of negative charge repel to a trigonal planar shape. The bond angle between the remaining pairs is approximately 120° (119 °).
The final shape formed by the atoms is called bent.



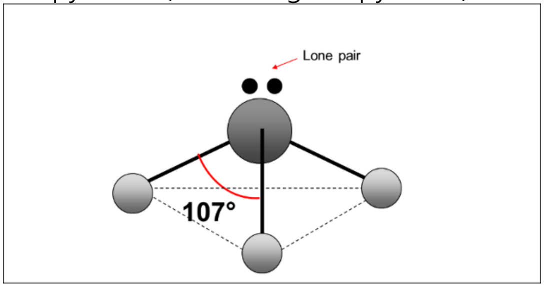
Molecular Shapes – four regions of charge (0 non-bonding pairs)

When four regions of negative charge are around a central atom, they repel each other into a 3-dimensional shape. The bond angle is now 109.5°. This is because it is a sphere divided into 4 rather than a circle.
This shape formed is tetrahedral.



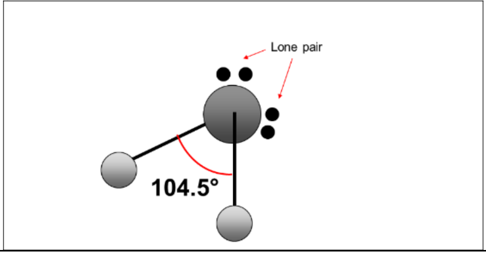
Molecular Shapes – four regions of charge (1 non-bonding pair)

The four regions of negative charge still occupy a 3-dimensional tetrahedral shape. (The non-bonding pair, however, exerts a stronger repulsion to the remaining bonded pairs). The bond angle is 109.5° (107° actually)
The final shape the bonded atoms form is a trigonal pyramid (or a triangular pyramid)



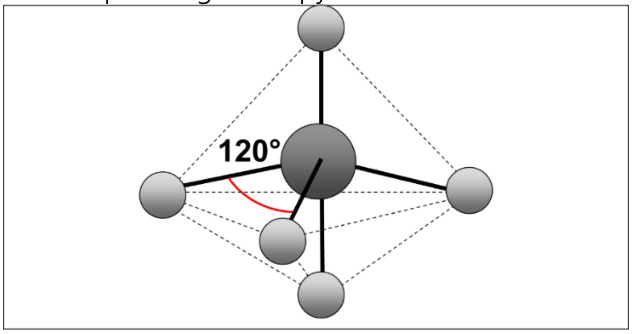
Molecular Shapes – four regions of charge (2 non-bonding pairs)

The four regions of negative charge repel each other to a (warped) tetrahedral shape. However, the two non-bonding pairs create a much stronger repulsion than one lone pair and the bond angle between the remaining bonded pairs is smaller again at approximately 105° (compared to 119° of the bent shape with only three regions of negative charge). The final shape the bonded atoms form is called Bent.



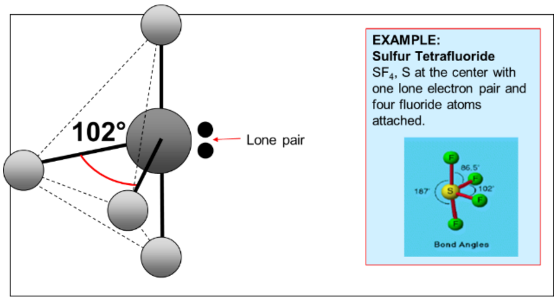
Molecular Shapes – five regions of charge (0 non-bonding pairs)

When five regions of negative charge are around a central atom, they repel each other into a 3-dimensional shape. The bond angle is now 120°.
The central atom has 3 central regions of negative charge that are 120° apart and 1 region above and below, 180° apart
This shape is trigonal bipyramid.



Molecular Shapes – five regions of charge (1 non-bonding pairs)

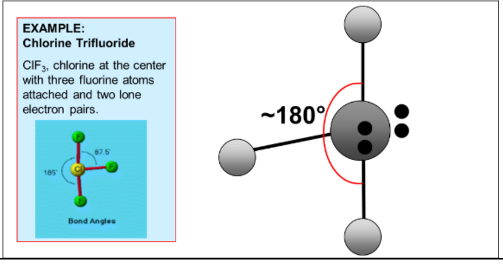
When five regions of negative charge are around a central atom, they repel each other into a trigonal bi-pyramid shape. The bond angle is now 102°. One of the central regions is a non-bonding pair.
The overall shape formed from bonded regions is a see-saw.



EXAMPLE:
Sulfur Tetrafluoride
SF_4, S at the center with one lone electron pair and four fluoride atoms attached.

Molecular Shapes – five regions of charge (2 non-bonding pairs)

When five regions of negative charge are around a central atom, they repel each other into a trigonal bi-pyramid shape. The bond angle is slightly less than 180° between the two upright regions of negative charge. Two regions of negative charge in the form of non-bonding pairs exist around the central atom.
The final shape formed by bonded negative charge regions is T-shaped.

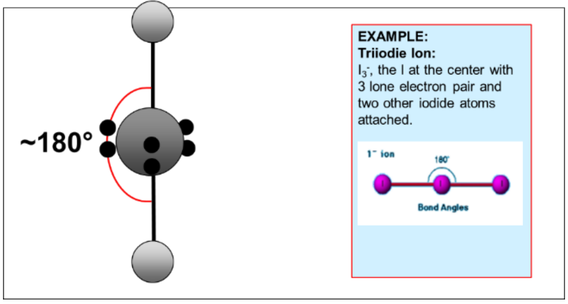


EXAMPLE:
Chlorine Trifluoride

ClF_3, chlorine at the center with three fluorine atoms attached and two lone electron pairs.

Molecular Shapes – five regions of charge (1 non-bonding pairs)

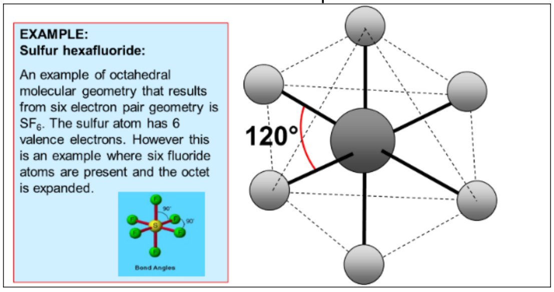
When five regions of negative charge are around a central atom, they repel each other into a trigonal bi-pyramid shape. The bond angle is now slightly less than 180°. Three regions around the central atom are in the form of non-bonding pairs.
The final shape created by bonded regions of negative charge is linear.



EXAMPLE:
Triiodie Ion:
I_3^-, the I at the center with 3 lone electron pair and two other iodide atoms attached.

Molecular Shapes – six regions of charge (0 non-bonding pairs)

When six regions of negative charge are around a central atom, they repel each other into an octahedral shape. The bond angle is now 120° between the central regions of negative charge. Two regions of negative charge are vertical of the central atom at approximately 180 °
The shape the bonded regions of negative charge form is also an octahedral shape.

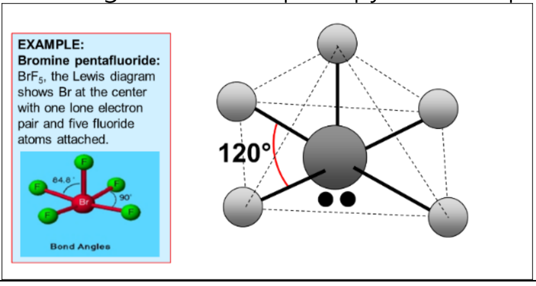


EXAMPLE:
Sulfur hexafluoride:

An example of octahedral molecular geometry that results from six electron pair geometry is SF_6. The sulfur atom has 6 valence electrons. However this is an example where six fluoride atoms are present and the octet is expanded.

Molecular Shapes – six regions of charge (1 non-bonding pair)

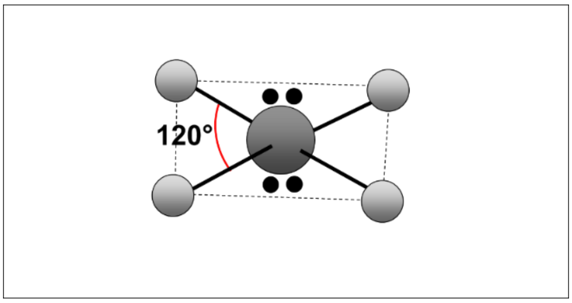
When six regions of negative charge are around a central atom, they repel each other into an octahedral shape. The bond angle is now 120° between the central regions of negative charge. Unlike the five regions of charge that loses the horizontal atoms first to non-bonding pairs, the 6-region shape loses its vertical atoms first to lone pairs.
The shape the remaining bonded regions of negative charge form is a square pyramid shape.

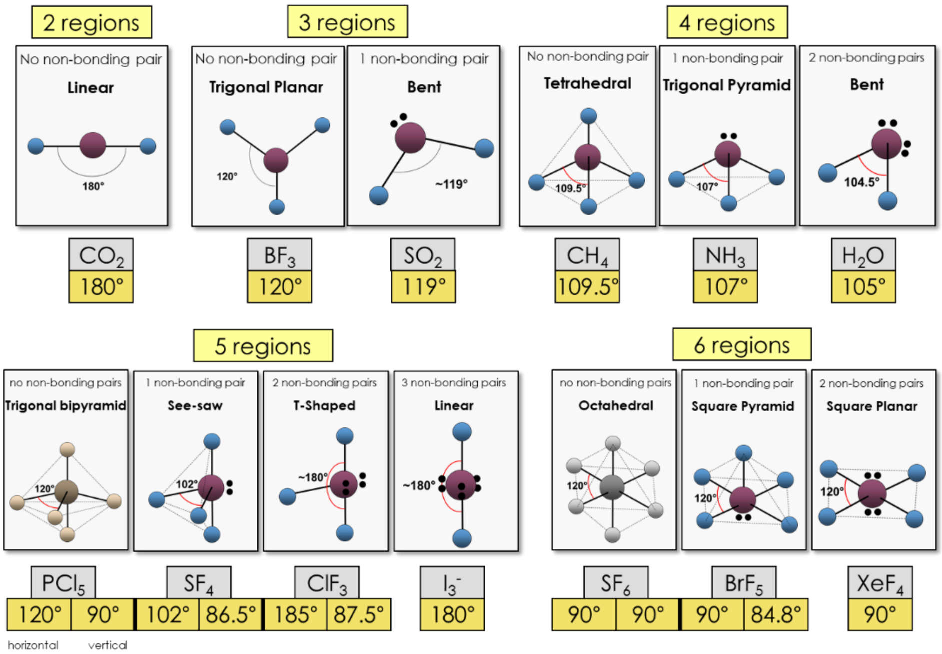


EXAMPLE:
Bromine pentafluoride:
BrF_5, the Lewis diagram shows Br at the center with one lone electron pair and five fluoride atoms attached.

Molecular Shapes – six regions of charge (2 non-bonding pairs)

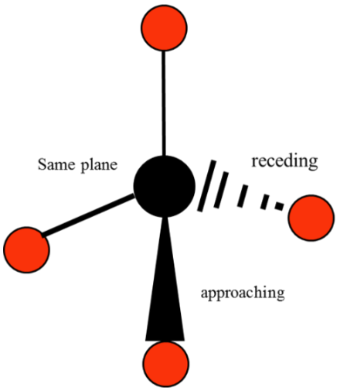
When six regions of negative charge are around a central atom, they repel each other into an octahedral shape. The bond angle is now 120° between the central regions of negative charge. Unlike the five regions of charge that loses the horizontal atoms first to non-bonding pairs, the 6-region shape loses its two vertical atoms, which are replaced by non-bonding pairs.
The shape the remaining bonded regions of negative charge form is a square planar shape.





Drawing Shapes

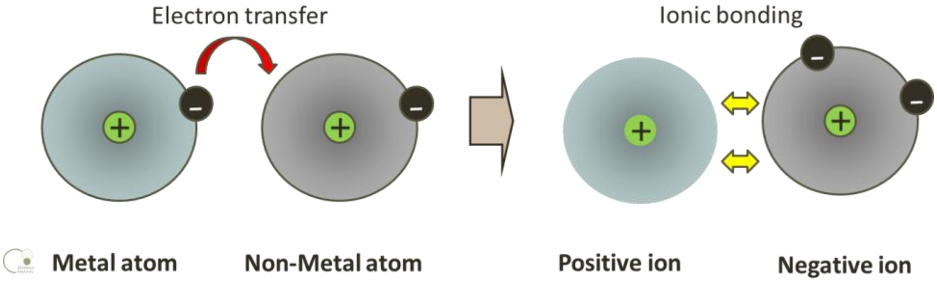
1. Atom on same plane as central atom – straight solid line
2. Atom receding from central atom – lines starting large and getting smaller
3. Atom approaching from central atom – solid triangle starting small and getting larger



Bonding

Ionic Bonding is where one atom completely takes valence electrons from another to form ions and the resulting negative and positive ions hold together with electrostatic attraction. This type of bonding occurs when a metal and non-metal react and there is a transfer of electrons to form ions.

The ions then combine in a set ratio to form a neutral compound with negative and positive charges balanced out.



Strength of Ionic Bonds

Two factors are involved with determining the strength of ionic bonds.

The first is the charge of the ions. A 2+ and 2- (e.g. MgO) bond will be much stronger than a + and – (e.g. KCl) ionic bond.

Secondarily is the distance between the ions. The closer the ions, the stronger the electrostatic bond.

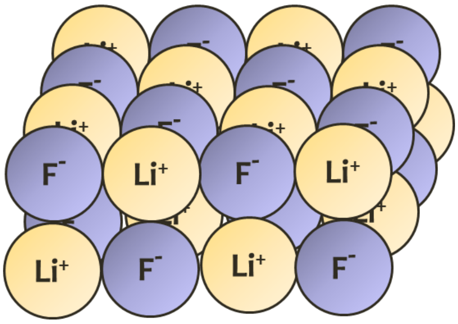
Ionic compounds are the product of chemical reactions between metal and non-metal ions

Some compounds are ionic compounds, since they are made up of cations and anions.

The Anion (F) takes the electrons off the Cation (Li) so their outer energy levels have a stable 8 electrons each.

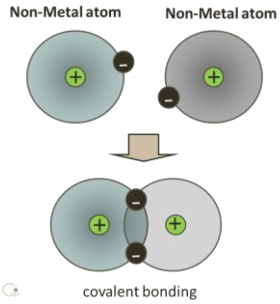
Anions and Cations have a strong electrostatic attraction for each other so they bond together as a compound.

Compounds are neutral substances. For ionic compounds, the charges of the positive ions are balanced by the charges of the negative ions.



Covalent Bonding

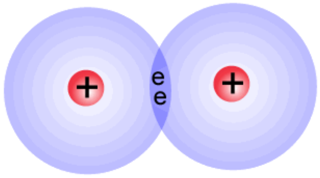
Covalent Bonding occurs when electrons are shared between neighbouring atoms. No ions are formed and there is no transfer of electrons. The compound formed is neutral with no charge. When the electronegativity is similar between atoms then the electrons will be shared evenly creating a non-polar molecule. If there is a significant electronegativity difference then dipoles will be created when the electrons orbit for a greater time around the more electronegative atom. This will create a polar molecule.



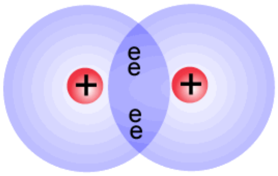
The valance electrons are involved in bonding. These electrons orbit in pairs. The negative charge of the electron pair will attract the positively charged nuclei of other atoms, and this holds the atoms together in a molecule. The electron pair must lie between the nuclei for the attraction to outweigh the repulsion of the two nuclei. This ‘sharing’ of electrons between atoms creates a covalent bond – giving both atoms the stability of a full outer shell. Covalent bonds are normally formed between pairs of non-metallic atoms.

Some covalent bonds involve only one pair of electrons and are known as single bonds. Other covalent bonds can involve two pairs of electrons; double bonds and three pairs of electrons; triple bonds.

Only one pair of electrons holding the nuclei together

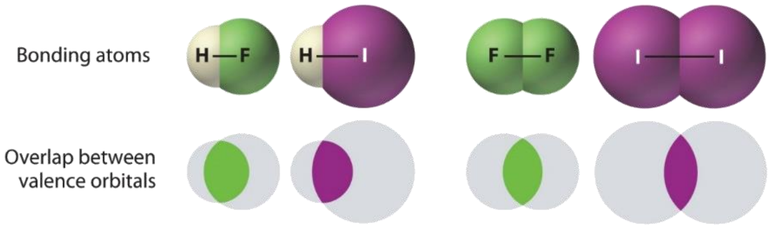


Two pair of electrons hold the nuclei tighter and closer



All covalent bonds are strong and they require a large amount of energy to ‘break’ the bond.

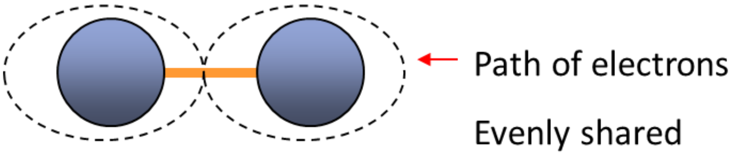
[Extension] However, some covalent bonds are stronger than others are. The greater the overlap of valence orbitals (the area the valence electrons orbit the nucleus) the stronger the bond.



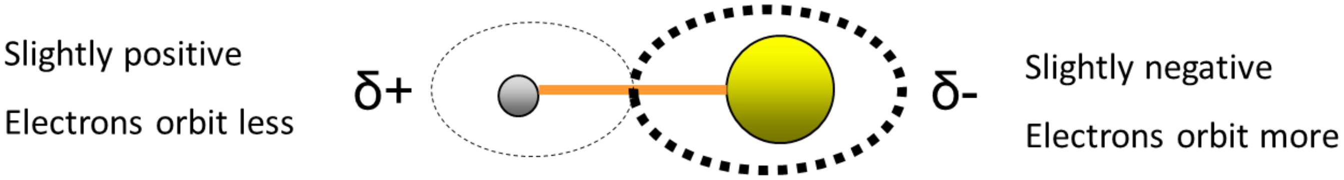
(a) H–F versus H–I **(b) F–F versus I–I**

Polarity and dipoles

If two identical atoms are bonded together then they have exactly the same amount of attraction to the shared electrons in the bonded pair. This is because their electronegativity is the same. This becomes a non-polar molecule with non-polar bonds. The whole molecule is also non-polar because there is no electronegativity difference and the valence electrons orbit each atom evenly. Example - Iodine molecule I_2



If two different types of atoms are bonded together then they will exert different levels of attraction for the orbiting electrons. That is because they may have different numbers of electron shells and different numbers of protons in their nucleus. This will cause an electronegativity difference and a dipole will form. These bonds become polar bonds. Example – hydrochloric acid HCl



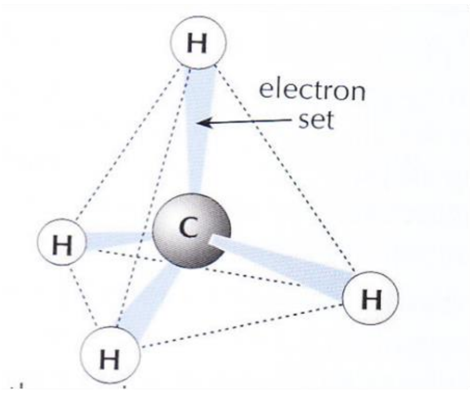
If two different atoms are bonded they form a polar bond, as there is an electronegativity difference and the valence electrons spend more time around the atom with the higher electronegativity value (that atom becomes slightly negative) The atom that the valence electrons spend less time around becomes slightly positive.

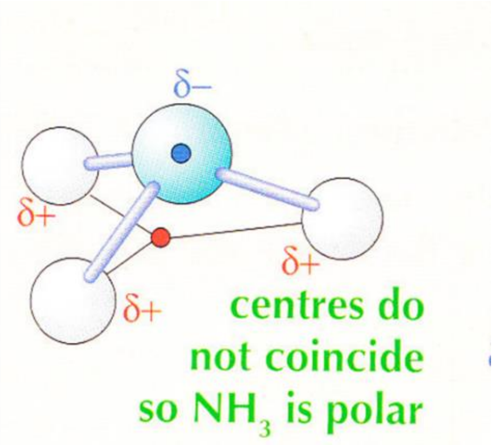
Symmetry and Polarity

The polarity of a molecule with polar bonds depends upon whether the molecule is symmetrical or not.

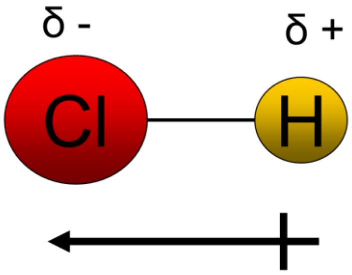
A symmetrical molecule (one where the centres of peripheral atoms coincide) becomes a non-polar molecule – as the dipoles and thus the charges balance out

An unsymmetrical molecule (one where the centre of peripheral atoms do not coincide) is a polar molecule.





Dipoles may also be shown as an arrow, with a cross, +ve, at the tail. The arrowhead is the –ve end. The more electronegative atom forms the negative end and the less electronegative atom forms the positive end.



Solubility

The solubility of a substance is the amount of that substance that will dissolve in a given amount of solvent. Solubility is a quantitative term. Solubility's vary depending on the solvent and the solute. The terms soluble and insoluble are relative. Some substances can be sparingly soluble where only the minutest percentage dissolves. For a solute to dissolve the attraction to the solvent molecules must be stronger than the bonds holding the atoms/molecules of the solute together.

Dissolving and Polarity

Polar substances dissolve polar substances.

E.g., Water, being polar attracts the molecules of other polar substances (e.g. HCl) and will dissolve them.

Polar substances will not dissolve non-polar substances.

E.g. Water, (polar) has a stronger attraction to itself than to non-polar molecules (e.g. cyclohexane) and will not dissolve them.

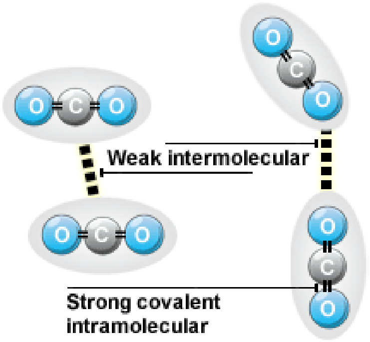
Non-polar substances dissolve non-polar substances.

E.g., Non-polar solvents (like cyclohexane) attract non-polar solutes (like napthalene) by the same weak Van der Waals forces they attract themselves by and so will dissolve non-polar solutes.

Weak Intermolecular Forces

Weak intermolecular forces of attraction occur between molecular solids. There are three kinds of Weak Intermolecular Force:

- ☐ Instantaneous dipole (ID) – temporary dipole – all molecules have this type
- ☐ Permanent dipole (PD) – permanent dipole – only polar molecules have this type in addition to ID-ID
- ☐ Hydrogen bonding (HB) – permanent dipole – molecules with H bonded to O, N or F have this type of bonding



Note the distinction:

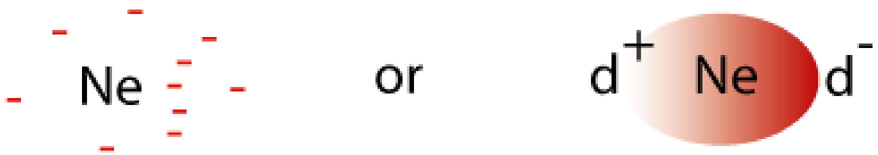
Intra-molecular Forces: the strong bonding forces within a molecule. I.e. the covalent bonds holding the molecule together.
Inter-molecular Forces: the weak bonding forces between molecules due to the attractions between partial charges.

Instantaneous dipole (ID – ID) Attractions

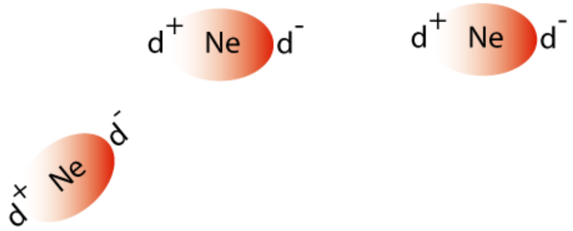
The inert gases (group 18) are monatomic, and must be non-polar, yet the atoms attract together to form liquids and freeze to form solids. Likewise, non-polar molecules like cyclohexane condense and freeze. This suggests that some kind of bonding force operates between non-polar monatomic elements or non-polar molecules.

Instantaneous/temporary Dipole

In any monatomic element or molecule, the electrons are moving rapidly. At any one instant, the arrangement of electrons about the nucleus will not be symmetric. This creates an instantaneous dipole (ID).



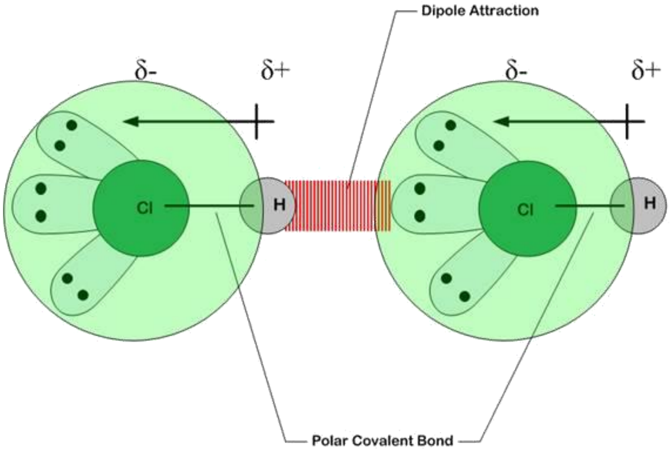
An atom with an ID will attract electrons in a neighbouring atom. This causes an induced dipole in this atom. The instantaneous dipole atom then attracts the induced dipole atom.



Permanent dipole (PD – PD) Attractions

Polar molecules have an imbalance of charge caused by an electronegativity difference between its constituent atoms. The weak molecular force always involves instantaneous dipole but in small molecules, permanent dipole will play a larger part in the bonding.

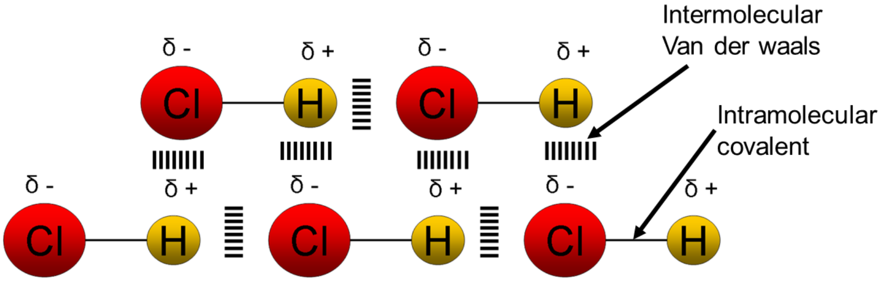
The slightly negative end of one molecule will be attracted to the slightly positive end of another molecule. The higher strength of the PD-PD bonding means that polar molecules will have a higher boiling/melting point to non-polar molecules (with only ID-ID bonding) of similar molar mass.



Permanent Dipole (PD – PD) Attractions and melting point

The weakness of PD – PD bonding is revealed by the low melting points of PD molecular solids, by comparison with other types of solids, but it is still stronger than ID-ID bonding alone of a similar molar mass.

E.g.	hydrogen chloride (PD – PD)	-114 °C
	Acetone (PD – PD)	-95 °C
	NaCl (ionic)	801 °C
	Copper (metallic)	1085 °C



Molecules that have side chains do not “pack” together so well as single chain molecules so cannot get as close to other molecules – all things being equal straight chained versions of molecules tend to have higher MP and BP

Strength of ID-ID attractions compared with PD-PD

ID – ID attractions increase in strength as the number of electrons in the atom or molecule increase. See trend He – Xe. Increasing MPs show increasing force of intermolecular bonds.

Small molecules that have ‘ID-ID only’ have lower MPs than small molecules with both PD-PD and ID-ID, indicating that ‘ID-ID only’ is a weaker bond than ‘PD-PD + ID-ID’. e.g.

When both ID-ID and PD-PD are present in a series of compounds, which has the greater influence on MP?

ID-ID increase down this series due to increasing number of electrons per molecule. However, PD-PD increase going up series due to increasing electro-negativity difference between the atoms in the molecules.

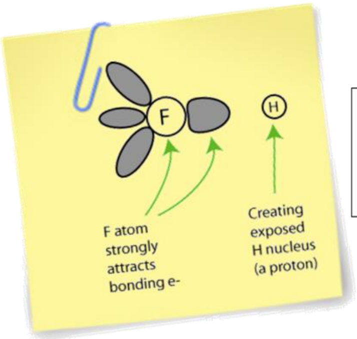
As MPs increase, going down the series it seems that increasing ID-ID is making the stronger contribution to inter-molecular forces. For polar molecules with higher numbers of electrons such as HI, ID-ID makes a stronger contribution to intermolecular forces than PD-PD.

	Ne	MP (°C)
HCl	18	-114
HBr	36	-87
HI	54	-51

Hydrogen Bonding

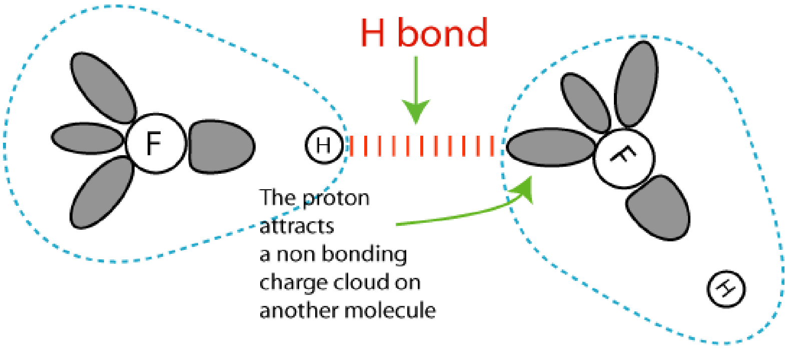
This is a special type of PD – PD bonding. It occurs when hydrogen is bonded to N, O or F. Since these are the three most electronegative elements and since they have very small atoms, (which concentrates their charge), they have a strong polarising effect on the covalent bond with hydrogen. Hydrogen, having no inner electron shells, is left as an exposed proton. Very strong dipoles are created/

This proton, being very small indeed, exerts a strong attraction to a non-bonding pair of electrons on a neighbouring molecule.



This proton, being very small indeed, exerts a strong attraction to a non-bonding pair of e- on a neighbouring molecule.

The hydrogen bond is around 10% of the strength of a covalent bond, and is the strongest of the three types of intermolecular attraction.



Hydrogen Bonding of Water

The high surface tension of water is explained by the presence of a hydrogen-bonded network of water molecules at the surface. This network is sufficiently strong to enable a needle to be floated on the surface of the water.

H bonding gives ice a network tetrahedral structure (like diamond). When ice melts, this partially collapses, and molecules move closer together so water is denser. (Density - water = 1.0 g cm^{-3} Density - ice = 0.92 g cm^{-3}) In contrast, most molecular solids expand on melting.

Non-Polar Temporary (Instantaneous) dipole ID - ID	Polar Permanent dipole +Instantaneous dipole PD – PD + ID - ID	Polar (H-O, H-N, H-F) Hydrogen Bonding + Instantaneous dipole HB – HB + ID - ID
The (...) molecular solid is non-polar and so the only intermolecular forces would be due to temporary dipole interactions. This type of intermolecular bonding is the weakest of the three so these molecular solids will have the lowest boiling point. Generally as the molar mass increases, there are more electrons and more instantaneous dipole-dipole interactions so all things being equal, the boiling points would increase.	The (.....) molecular solid is polar and contains both Permanent dipole and instantaneous dipole interactions. The permanent dipole is generally the stronger force and will be the dominant force found in the molecular solid and therefore these substances tend to have a higher boiling point than the non-polar substances. The instantaneous dipole forces will become more significant if the molar mass of the molecule becomes greater.	The (...) molecular solid has the highest boiling point of the three. This is because it has hydrogen bonds, which are very strong intermolecular forces. The electronegativity difference between the H-.... Bond creates a very polar molecule, which takes a lot of energy to break the intermolecular bond between molecules hence a high boiling point. These molecular substances also contain instantaneous dipoles, which only become significant when the molar mass is large.

Enthalpy

Enthalpy and Enthalpy Change (ΔH)

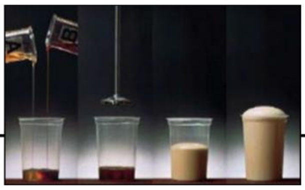
Enthalpy (or Heat Content) is the energy in a substance due to kinetic energy of particles and potential energy in chemical bonds. Enthalpy change (ΔH) is the difference in enthalpy of products H_P and reactants H_R

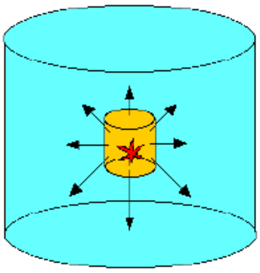
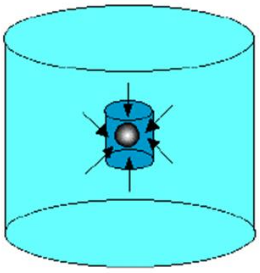
$\Delta H \quad = \quad H_P \; - \; H_R$

Enthalpy Changes

H_p (products) and H_r (reactants) cannot be measured directly. We can measure Enthalpy change (ΔH) by measuring energy.

Endothermic and Exothermic

Released to surroundings (Exothermic Reactions)	Absorbed from surroundings (Endothermic Reactions)
	

Exothermic Reactions	Endothermic Reactions
These are reactions where heat energy is released into the surroundings. Surroundings gain heat energy. (Increase in temperature) Products will have less energy than reactants. ΔH is NEGATIVE (-)	These are reactions where heat energy is absorbed from the surroundings. Surroundings lose heat energy. (Decrease in temperature) Products will have more energy than reactants. ΔH is POSITIVE (+)
	

Exothermic reaction examples

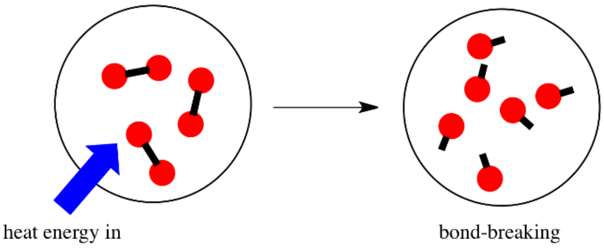
Any combustion reaction is exothermic. The bonds holding the atoms of fuel molecules together (usually consisting of carbon and hydrogen atoms) release a lot of energy in the form of light and heat when they are broken. The total energy holding the bonds together in the products are less than the total energy in the reactions and the difference is released.

Forming Bonds - Bonds forming between atoms and molecules release energy therefore bond forming is an exothermic reaction. Bonds are formed to form a stable molecule.

Endothermic reaction examples

Melting ice is an example of an endothermic reaction. The solid ice (water) atoms that are in a fixed pattern are barely moving and need to absorb energy in order to move faster and break the bonds to form water in a liquid state.

Breaking Bonds - Bonds holding atoms and molecules together require the input of energy in order to break them apart therefore breaking of bonds is an endothermic reaction. The input of energy (usually light or heat energy) cause the atoms and molecules to move faster and 'pull away' from each other. Each type of bond has its own specific amount of energy, called bond energy measured in kJ, required to break its bond.

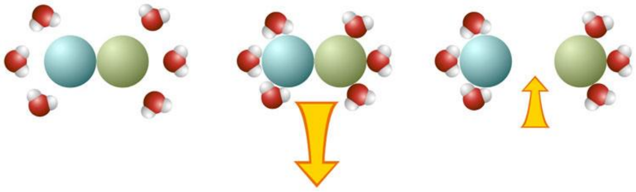


If more energy is required to break the bonds of the reactants than released when the bonds of the products are form then the overall reaction is endothermic.

If less energy is required to break the bonds than is released when the bonds of the products are formed then the overall reaction is exothermic.

Enthalpy in Dissolving

If more energy is released when water bonds to the solute than it takes to separate the solute, the dissolving is exothermic and the temperature increases. An example is adding a strong acid (such as sulfuric acid) or base (such as sodium hydroxide)



Enthalpy Diagrams

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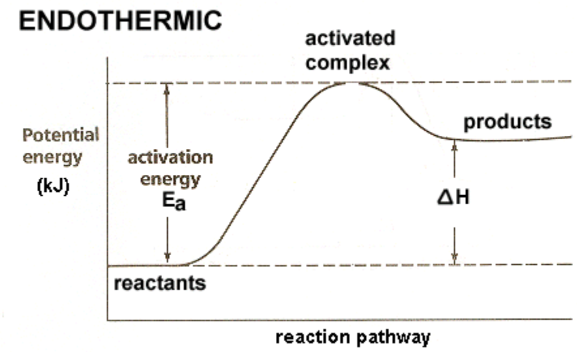

An endothermic reaction will absorb energy and the products will be at a higher enthalpy than the reactants.
The reaction system will feel cool to the touch as heat energy is taken from the surroundings, including your skin, and used to break bonds in the molecules.
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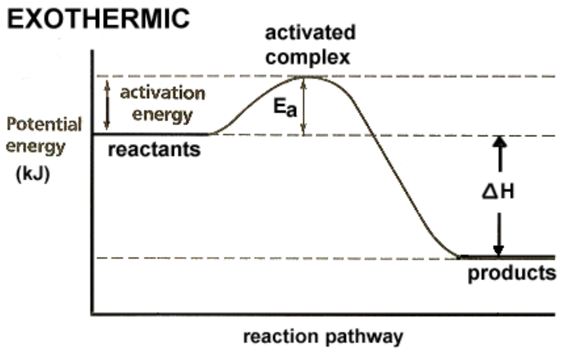

An exothermic reaction will release energy and the products will be at a lower enthalpy level than the reactants.
The reaction system will feel will feel hot to the touch as the energy is released as heat energy.
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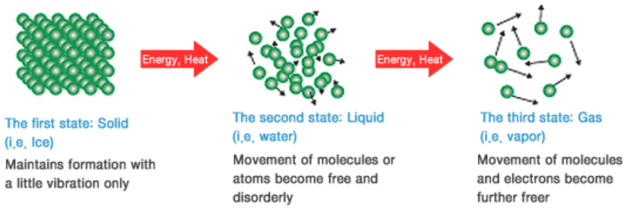
Enthalpy in Changes of State

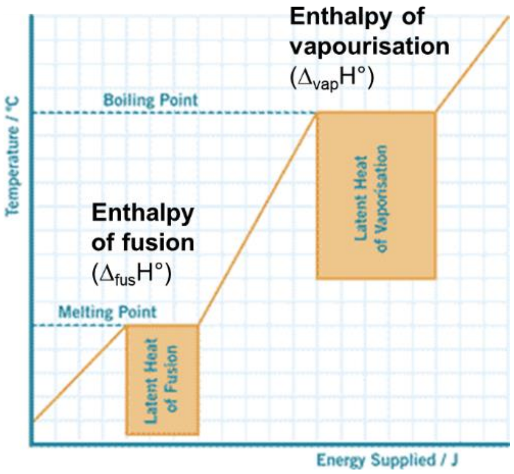
Solid particles are packed closely and only vibrate in a fixed position. Liquid particles are also packed closely but the particles move around more. Gas particles have a lot of space between them and move around quickly. Kinetic energy causes particles to move. The more kinetic energy a particle has the faster it moves. Kinetic energy can be added to a particle by adding heat energy (and heats up). The heat energy is then transformed into the kinetic energy. Kinetic energy can also be lost from a particle, which slows it down, when it changes back into heat energy and is lost (and cools).



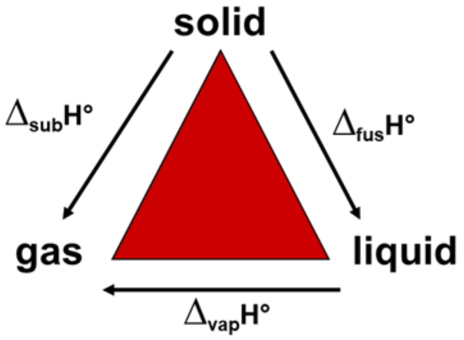
Changing states

When heat energy is added to a solid substance at a particular temperature called the melting point, it will change state into a liquid. Prior to this point, a rise in heat energy will also show a rise in temperature. At the melting point, the heat energy will be used to break the bonds in a solid – an endothermic reaction called latent heat of fusion- rather than show a temperature increase.

The same occurs at the boiling point from a liquid to a gas – an endothermic reaction called latent heat of vaporisation.



Enthalpy of fusion ($\Delta_{fus}H^\circ$)	1 mole solid to liquid state
Enthalpy of vaporisation ($\Delta_{vap}H^\circ$)	1 mole liquid to gas state
Enthalpy of sublimation ($\Delta_{sub}H^\circ$)	1 mole solid to gas state



Other definitions of Enthalpy

Standard Enthalpy of combustion (Δ_cH°)

"The enthalpy change when one mole of an element or compound reacts completely with oxygen under standard conditions."

Standard Enthalpy of formation (Δ_fH°)

"The enthalpy change when one mole of a substance is formed from its constituent elements under standard conditions."

Standard Enthalpy of reaction (Δ_rH°) for any given reaction.

"The enthalpy change when products are formed from their constituent reactants under standard conditions."

Standard conditions

Measurements depend on conditions. When measuring an enthalpy change you will get different values under different conditions. For example, the enthalpy change of a particular reaction will be different at different temperatures, different pressures or different concentrations of reactants.

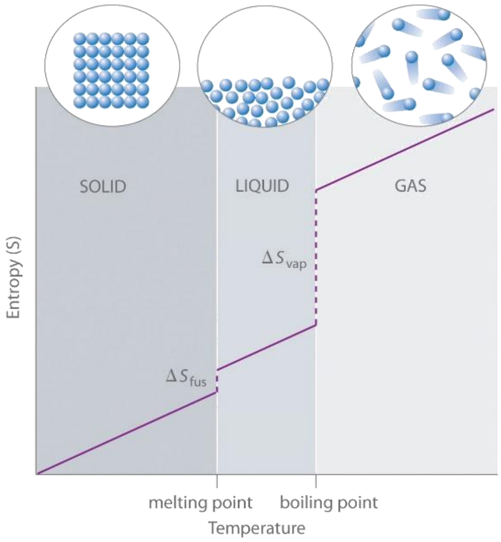
The values for enthalpy are given for standard conditions, indicated by the superscript θ

Standard conditions include:

- ☐ Temperature of 25°C
- ☐ Atmospheric pressure conditions of 1 ATM
- ☐ Concentration of 1 mole per Litre

Entropy

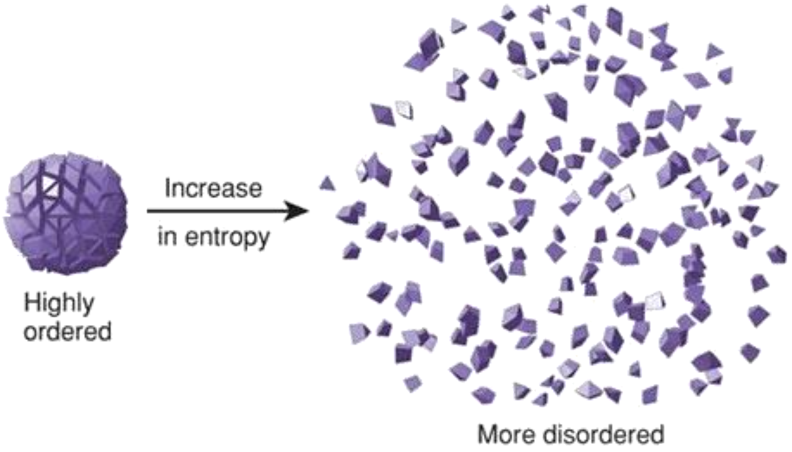
Entropy is the measure of the disorder of a system, usually denoted by the letter S. A highly ordered system has low entropy. Entropy is the measure of the disorder of a thermodynamic system.
Disorder increases then as a result the entropy of a system increases.
Molecules in the gaseous state have greater entropy than liquid state because there is less "order" in gaseous molecules. Gas molecules move in random chaos without any restrictions. Therefore, going from liquid to gas you have increased the entropy of the system. Molecules in the liquid state have a greater entropy then those in the solid state. Molecules in the solid state are almost fixed in one spot. They are highly ordered and so liquid molecules have more disorder.
So melting increases entropy of a system.



Entropy as a measure of disorder

The majority of spontaneous reactions are exothermic due to a natural tendency towards “minimum enthalpy”. Some endothermic reactions do occur spontaneously because of a different tendency towards “maximum entropy”. Entropy increases the “disorderedness” of a system. For example, there is more “disorder” when a solid melts or a liquid boils or a solid dissolves into a solution.

$\Delta S = S_{final} - S_{initial}$ A positive $+\Delta S$ means Entropy has increased



A reaction will be spontaneous if it results in the enthalpy decreasing and the entropy increasing. A reaction will not occur spontaneously if the enthalpy increases and the entropy decreases.

When the entropy and enthalpy oppose each other (they are both positive or both negative) then an equilibrium situation occurs. The overall result depends on the relative magnitude of the two tendencies.

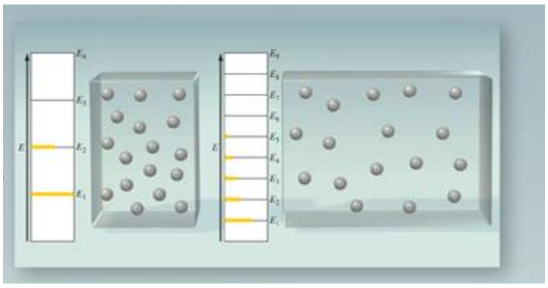
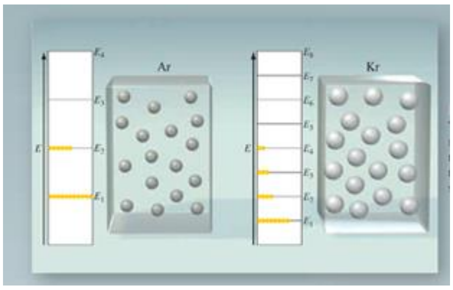
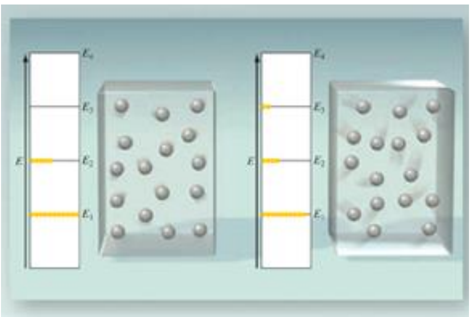
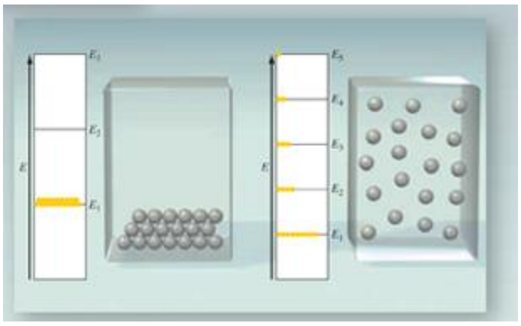
Entropy in solid, liquid and gas

Kinetic energy increases with increasing temperature so the entropy factor becomes more important at higher temperatures. This is why equilibrium constants, K_c, (which measure the equilibrium position), change with temperature.

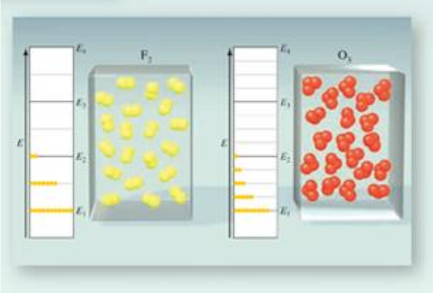
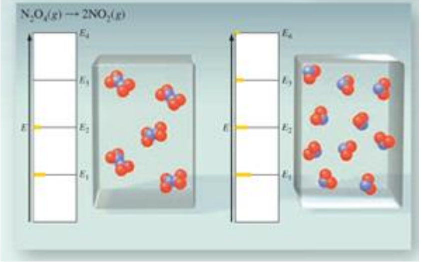
For example in the case of melting ice, the tendency to minimum enthalpy favours the ice phase (less kinetic energy) whereas the tendency to maximum entropy favours the liquid phase (more randomness). Above the melting point of ice, the entropy factor dominates (as it increases with temperature) so spontaneous melting occurs. Below the melting point, the enthalpy factor dominates so spontaneous freezing occurs.

Entropy increases as temperature increases because more kinetic energy means molecules are more disorderly.
Entropy increases in a reaction if the reaction produces more product molecules than it contains reactant molecules especially if you are going from a solid to a liquid or to a gas. Entropy increases when solutions are formed from pure liquids or pure solids. Because there is greater disorder in aqueous solutions then liquids that are pure or solids that are pure.
The entropy of the universe equals the entropy of system + entropy of surrounding
ΔS universe always increases.

Factors that influence the Entropy of a system

Volume increase causes an increase in entropy. With an increase in volume, there are more energy levels available therefore, energy can be dispersed more. 	Molar Mass increase causes an increase in entropy. With an increase in mass, there are more energy levels available therefore, energy can be dispersed more. 
Temperature increase causes an increase in entropy. With an increase in temperature, the molecules have greater kinetic energy making more energy levels available therefore, energy can be dispersed more. 	Phase Change from solid to liquid to gas causes an increase in entropy. With an increase in mobility of particles from solid to liquid to gas there are many more possible arrangements of particles therefore increasing randomness. 

Factors that influence the Entropy of a system

Greater complexity of molecules causes an increase in entropy. With an increase in complexity of molecules, there are an increased number of ways it can rotate and vibrate between each atom therefore increasing randomness.  	An increase in the number of moles in a reaction causes an increase in entropy. With an increase in the number of moles in a chemical reaction, the number of different arrangements of molecules increases therefore increasing randomness. 

Enthalpy of Reaction using calorimetry

To measure enthalpy changes, the reaction it is carried out in an insulated container (such as a polystyrene cup) and the temperature change (in °C) is measured. Using this temperature change, ΔT, and the value of the specific heat capacity, c, the amount of heat energy (q) transferred to the mass m of substance (usually water) can be calculated using the expression

$$q = m\ c\ \Delta T$$

The specific heat capacity of the water is 4.18 J $°C^{-1}$ g^{-1}.

Every 1mL of water can be taken as 1g due to its density

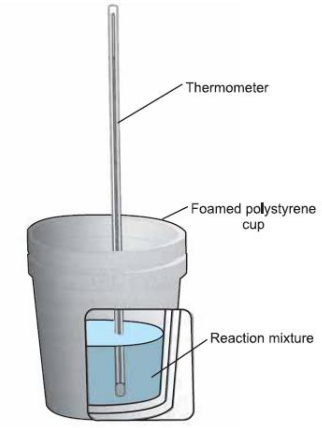


Fig. 6.8 Calorimeter for measuring heat changes at constant pressure (atmospheric pressure).

1. Calculate the mass of reactants – record in grams (one ml liquid = one gram)

2. Measure the temperature of the reactants and the temperature of the products and calculate ΔT (°C)

3. Calculate q using formula above Note: q will be in J and need to be converted to kJ for next step

Using Q to calculate enthalpy of reaction ($\Delta_r H°$)

Enthalpy of reaction $\Delta_r H°$ can be calculated from heat energy (q) in the previous step if the number of moles of one of the reactants is known, or calculated.

$\Delta_r H° = -q / n$

Note that the q is negative and will need to be converted to kJ

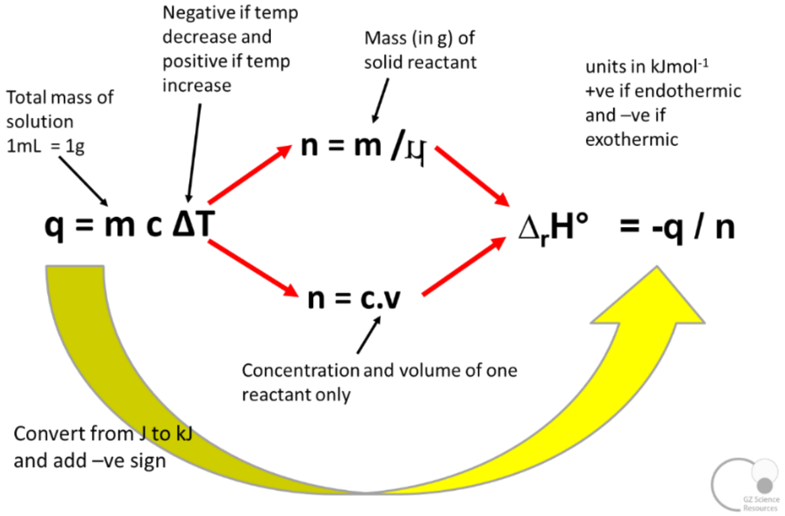
Moles (n) can be calculated from either mass of one of the reactants

$n = m / M$ M= molar mass ($gmol^{-1}$)   m = mass (g)

Or from the concentration and volume of one of the reactants

$n = c.v$ c = concentration ($molL^{-1}$)   v = volume (L)

Using Q to calculate enthalpy of reaction ($\Delta_r H°$) Summary



Calculations using $\Delta_f H^o$ Values

The standard enthalpy of any reaction can be obtained by subtraction of the standard enthalpies of formation of reactants from those of the products.

$$\Delta_r H^o = \sum n\, \Delta_f H^o_{products} - \sum n\, \Delta_f H^o_{reactants}$$

Where n is the stoichiometric coefficient of each substance in the reaction equation.

Example

Using the standard heats of formation of $CO_2(g)$, $H_2O(l)$, and $C_6H_{12}O_6(s)$, calculate the standard enthalpy of combustion of glucose.

$\Delta_f H^o(C_6H_{12}O_6,\ s) = -1268\ \text{kJ mol}^{-1}$

$\Delta_f H^o(CO_2,\ g) = -394\ \text{kJ mol}^{-1}$

$\Delta_f H^o(H_2O,\ l) = -286\ \text{kJ mol}^{-1}$

$\Delta_f H^o(O_2,\ g) = 0\ \text{kJ mol}^{-1}$

Note - Start by writing an equation for the combustion of 1 mole of glucose.

$$C_6H_{12}O_6(s) + 6O_2(g) \rightarrow 6CO_2(g) + 6H_2O(l)$$

$$\Delta_r H^o = \sum n\Delta_f H^o_{\text{products}} - \sum n\Delta_f H^o_{\text{reactants}}$$

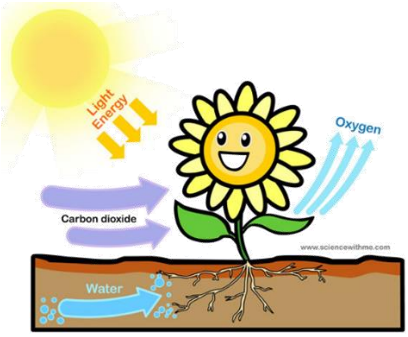
$$\Delta_r H^o = (6 \times -394 + 6 \times -286) - (1 \times -1268 + 6 \times 0) = -2812\ \text{kJ mol}^{-1}$$

Hess’s law

If an overall reaction can be broken down into a series of two or more steps, then the corresponding overall enthalpy of reaction is the sum of the enthalpies of the individual reaction steps. None of the steps needs to be a reaction that can be carried out in the laboratory.

The energy difference depends only on the difference in energy between the reactants and products, not on the reaction path taken.

Application of Hess's law



The process of photosynthesis is an endothermic process in which energy from the sun is trapped and stored in the bonds of glucose.

$6CO_{2(g)} + 6H_2O_{(l)} \rightarrow C_6H_{12}O_{6(aq)} + 6O_{2(g)} \quad \Delta rH° = +2808 \text{ kJ mol}^{-1}$

It is difficult reaction to measure enthalpy change so using the principal of Hess's law we can more easily measure the enthalpy change for the reverse reaction, the combustion of glucose (i.e. the process of respiration). The difference between reactants and products will be the same – we only need to reverse the sign from exothermic to endothermic

$C_6H_{12}O_{6(aq)} + 6O_{2(g)} \rightarrow 6CO_{2(g)} + 6H_2O_{(l)} \quad \Delta rH° = -2808 \text{ kJ mol}^{-1}$

Steps to calculating enthalpy of reaction Hess's Law

Example: calculate $\Delta_f H°$ (C_3H_8)

Step 1. Write out equation for reaction to calculate

$3C_{(s)} + 4H_{2(g)} \rightarrow C_3H_{8(g)} \quad \Delta_f H° = ?$

Step 2.Use given equations and rearrange until they match equation

1. $C_{(s)} + O_{2(g)} \rightarrow CO_{2(g)} \quad \Delta_c H° = -394\text{Kjmol}^{-1}$

Can multiply all by 3. Multiply enthalpy as well

$\underline{3C_{(s)}} + 3O_{2(g)} \rightarrow 3CO_{2(g)} \quad \Delta_c H° = 3(-394\text{Kjmol}^{-1})$

2. $H_{2(g)} + \frac{1}{2} O_{2(g)} \rightarrow H_2O_{(l)} \quad \Delta_c H° = -286\text{Kjmol}^{-1}$

$\underline{4H_{2(g)}} + 2O_{2(g)} \rightarrow 4H_2O_{(l)} \quad \Delta_c H° = 4(-286\text{Kjmol}^{-1})$

3. $C_3H_{8(g)} + 5O_{2(g)} \rightarrow 4H_2O_{(l)} + 3CO_{2(g)} \quad \Delta_c H° = -2220\text{Kjmol}^{-1}$

Can reverse so molecules on same side. Reverse enthalpy sign

$4H_2O_{(l)} + 3CO_{2(g)} \rightarrow \underline{C_3H_{8(g)}} + 5O_{2(g)} \quad \Delta_c H° = +2220\text{Kjmol}^{-1}$

Step 3. Cancel out any molecules on either side.

$\underline{3C_{(s)}} + \cancel{3O_{2(g)}} \rightarrow \cancel{3CO_{2(g)}} \quad \Delta_c H° = 3(-394\text{Kjmol}^{-1})$

$\underline{4H_{2(g)}} + \cancel{2O_{2(g)}} \rightarrow \cancel{4H_2O_{(l)}} \quad \Delta_c H° = 4(-286\text{Kjmol}^{-1})$

$\cancel{4H_2O_{(l)}} + \cancel{3CO_{2(g)}} \rightarrow \underline{C_3H_{8(g)}} + \cancel{5O_{2(g)}} \quad \Delta_c H° = +2220\text{Kjmol}^{-1}$

Step 4. Ensure remaining molecules match reaction equation

$3C_{(s)} + 4H_{2(g)} \rightarrow C_3H_{8(g)}$

Step 5. Add up enthalpies

$\Delta_f H° = 3(-394\text{Kjmol}^{-1}) + 4(-286\text{Kjmol}^{-1}) + +2220\text{Kjmol}^{-1}$

$= -106\text{Kjmol}^{-1}$