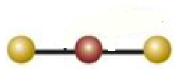
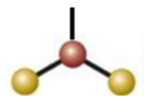
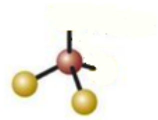
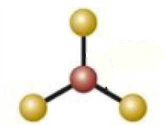
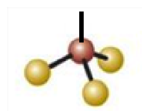
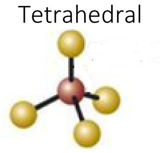
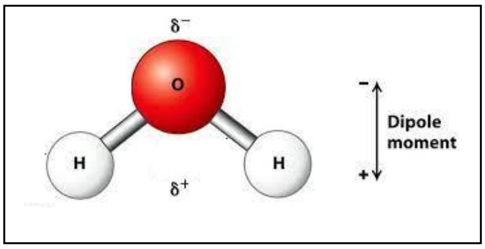
Molecular shapes

The shapes of molecules can be derived from their Lewis dot structures by using the VSEPR (Valence Shell Electron Pair Repulsion) model. Simply put, this model states that electron pairs will repel each other in 3D space so as to be as far from each other as possible.

Step 1 Draw an electron dot diagram of all the bonds in the molecule.
Step 2 Identify the central atom by drawing a Lewis dot diagram.
Step 3 Count the number of bonding and non-bonding pairs of electrons around the central atom.
The table below gives an indication on how to predict the shape.
Step 4 Separate all the pairs of electrons surrounding the central atom as far apart from each other as possible. Don't forget we are working in 3 dimensional space. Treat a double bond as a single bond for the purposes of repulsion.
Step 5 Identify the shape of the molecule looking only at the location of the atoms.

Number of atoms around the central atom.	Number of electron pairs around the central atom	Shape
2	2	Linear 
2	3	Bent or "V"shape 
2	4	Bent or "V"shape 
3	3	Trigonal planar 
3	4	Triangular pyramid 
4	4	Tetrahedral 

Now another thing that we must consider about molecules is the question of symmetry. Symmetrical molecules are said to be non-polar.

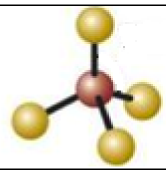
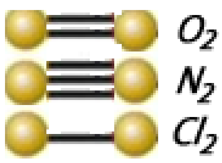
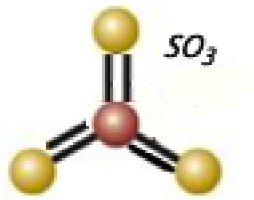
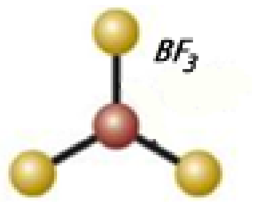


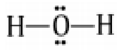
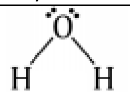
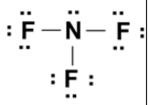
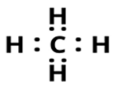
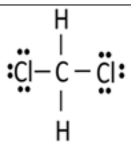
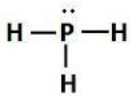
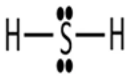
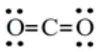
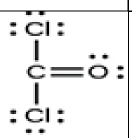
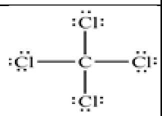
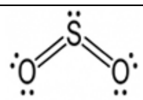
What is a polar molecule?

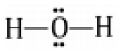
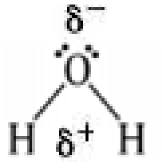
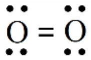
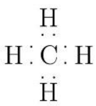
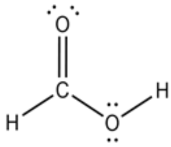
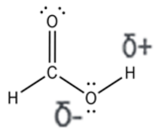
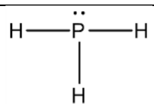
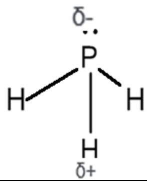
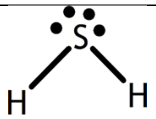
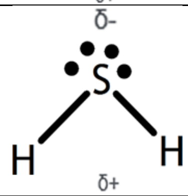
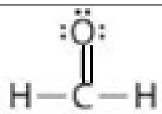
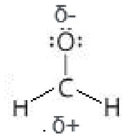
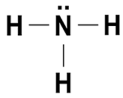
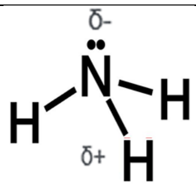
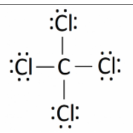
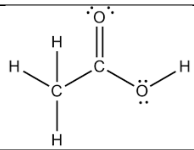
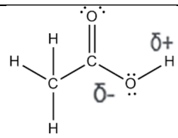
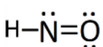
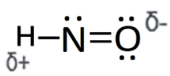
It is a molecule where the bonding electrons are not evenly distributed within the molecule due to electronegativity difference between the bonding atoms. This creates poles with a slight positive or negative charge as shown on the right. The molecule is said to have a dipole moment, as shown on the right. Small, negative charges occur on the surface of the molecule where the more electronegative atoms are. In the case of water, the oxygen carries the slight negative charge while the end with the hydrogen atoms is has a slight positive charge.

These slight charges are written as δ+ or δ-.

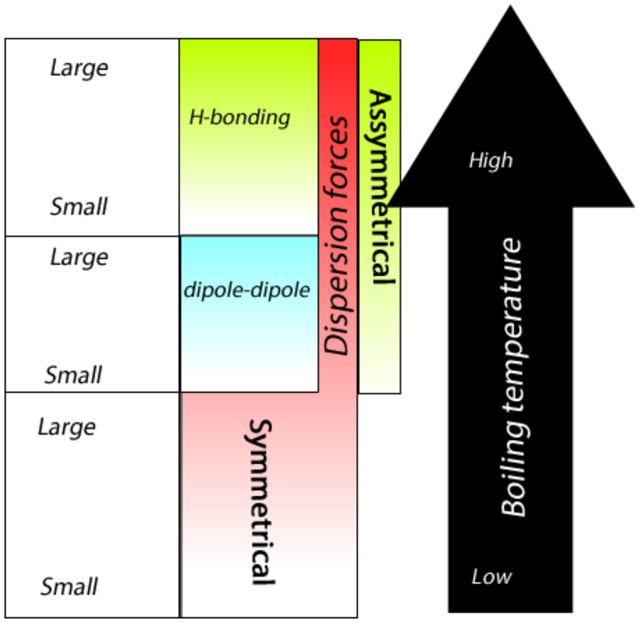
symmetrical molecules are said to be non-polar and asymmetrical molecules are said to be polar.
The table below shows some examples of non-polar molecules.

CH_4 CCl_4 SiF_4 or any other molecule with four identical atoms around the central atom in a tetrahedral arrangement	
CO_2 SO_2 The two identical atoms on either side of the central atom form a symmetrical arrangement.	
O_2 Cl_2 N_2 etc.	
SO_3 BF_3	 
Hydrocarbons	

Formula	Lewis dot structure	Number of pairs of electrons around the central atom	Shape	Symmetrical (s) Non-symmetrical (NS)	Polar (P) non-polar (NP)
H_2O		4 electron pairs (Tetrahedral shape)	V-shape		P
NF_3		4 electron pairs (Tetrahedral shape)	Triangular pyramid	NS	P
CH_4		4 electron pairs (Tetrahedral shape)	Tetrahedral	S	NP
CH_2Cl_2		4 electron pairs (Tetrahedral shape)	Tetrahedral	NS	P
PH_3		4 electron pairs (Tetrahedral shape)	Triangular pyramid	NS	P
SH_2		4 electron pairs (Tetrahedral shape)	"V"shape	NS	P
CO_2		2 electron pairs as each double bond is considered one for the purpose of repulsion	Linear	S	NP
$COCl_2$		Three electron pairs as the double bond is considered one for the purpose of repulsion	Trigonal planar	NS	P
CCl_4		4 electron pairs (Tetrahedral shape)	Tetrahedral	S	NP
SO_2		3 electron pairs as each double bond is considered one for the purpose of repulsion	"V"shape	NS	P

Formula	Lewis dot structure	Intra-molecular bonding	Indicate the polarity of the polar molecules
H_2O		Polar covalent	
O_2		Pure covalent	Non-polar
CH_4		Polar covalent	Non-polar
CH_2O_2		Polar covalent	
PH_3		Polar covalent	
SH_2		Polar covalent	
COH_2		Polar covalent	
NH_3		Polar covalent	
CCl_4		Polar covalent	Non-polar
CH_3COOH		Polar covalent	
NOH			

Predicting the strength of intermolecular bonding



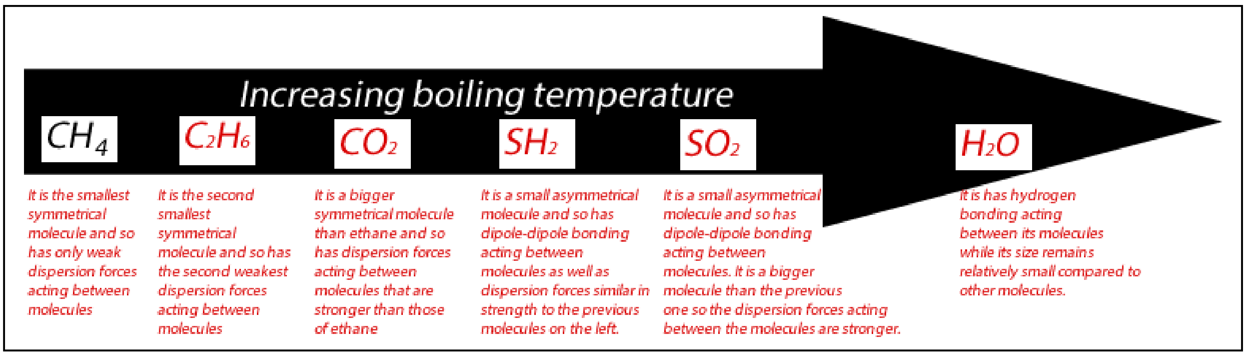
The boiling point of a pure molecular substance is a good indicator of the strength of the intermolecular bonds.

On the right is a diagram that may be useful in sorting similar sized molecules according to boiling temperature.
The diagram on the right attempts to show that:
- the intermolecular forces acting between symmetrical molecules are dispersion forces only. These forces however can be very strong if the molecule is large enough and that is why it extends all the way to the top. So a large symmetrical molecule can have a higher boiling temperature than a smaller molecule that exhibits hydrogen bonding.

- similar sized asymmetrical molecules have intermolecular forces composed of dipole-dipole and dispersion forces. The red coloured bar, representing dispersion forces extend all the way to all type of molecules indicating the presence of dispersion forces in all molecules no matter their symmetry.

- Dispersion forces can be significant and can produce strong intermolecular forces that can rival hydrogen bonding for very large molecules.

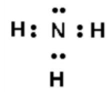
Use the diagram to place the following molecules in increasing order of melting point. Give your reason for the selection, the first one is done for you as an example.
SO_2
CO_2
SH_2
H_2O
CH_4
C_2H_6



Inter molecular bonding

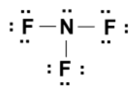
1. Consider the two molecules NF_3 and NH_3.
   a. Draw Lewis dot diagrams for both molecules in the space provided on the right.
   b. What is the shape of each molecule?

   NH_3

   Shape – *Triangular pyramid*

   NF_3

   Shape - *Triangular pyramid-*

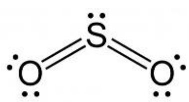
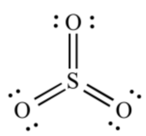
   c. What are the inter molecular forces acting between molecules of :
   NH_3 ____*hydrogen-bonding, dispersion forces*
   NF_3 ____ *dipole-dipole bonding, dispersion forces*

   d. Ammonia (NH_3) and nitrogen trifluoride (NF_3) are both gasses at room temperature. Ammonia boils at a temperature of -33.34 °C while NF_3, which is a bigger molecule, boils at
   -129 °C. Explain why.
   NF_3 has intermolecular forces composed of dipole-dipole and dispersion forces. NH_3 has stronger intermolecular forces composed of hydrogen bonding as well as weaker dispersion forces.

2. Place the following molecules in increasing order of boiling temperature. Give reasons for your choices. CO_2, SH_2, SiH_4, CH_4
   Since the molecules CO_2, SiH_4 and CH_4 are symmetrical the intermolecular forces are solely made up of dispersion forces and are relatively small. Hence we arrange them in order of size CH_4, SiH_4, CO_2. SH_2 on the other hand is an asymmetrical molecule that, as well as dispersion forces has dipole-dipole bonding acting.

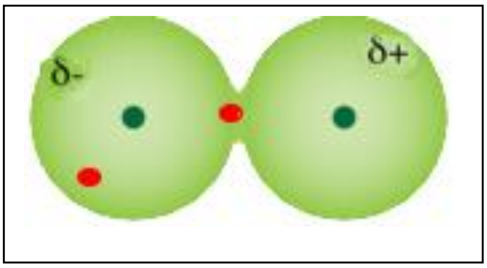
   CH_4, SiH_4, CO_2, SH_2

3. The boiling temperature of SO_2 is -10.1 °C while SO_3 has a boiling temperature of 45°C.
   a. Complete the table below.

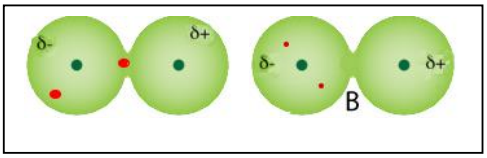
Molecule	Lewis dot diagram	Shape	Polarity (polar, non-polar)
SO_2		*Bent*	*Polar*
SO_3		*Triangular planar*	*Non-polar*

   b. Explain the difference in boiling temperature.
   SO_2 has intermolecular forces comprised of dipole-dipole and dispersion forces while the intermolecular forces exhibited between the SO_3 molecules are dispersion forces only. Clearly the size of SO_3 plays a role. It has a greater size than SO_2 and hence the dispersion forces acting are greater than the dipole-dipole and dispersion forces of SO_2 combined.

Dispersion forces, dipole-dipole and hydrogen bonding.



1) Consider the image on the right of a hydrogen molecule showing the two electrons in red and the two nuclei in green.
   a. Label the diagram using the following symbols.
   δ- or δ+



   b. In the diagram on the right, label any changes to the electrons, protons and dipoles that will take place in molecule "B" if the hydrogen molecule depicted above was next to it.
   *The instantaneous dipoles on the first hydrogen molecule will induce polarity in the molecule labelled "B". This is known as **induced polarity** and will result in a force of attraction between the two molecules.*

2) Which of the following forms of intermolecular bonding rely ***solely*** on instantaneous dipoles? Circle the correct response and give a reason
   a) dipole-dipole Yes/No Explain
   As well as instantaneous dipoles forming (dispersion forces) the molecule has permanent dipoles that attract each other.

   b) hydrogen bonding Yes/No Explain
   As well as instantaneous dipoles forming (dispersion forces) the molecule has permanent dipoles that attract each other. These dipoles are especially strong when a hydrogen atom is bonded to any one of the following atoms, oxygen, nitrogen or fluorine.
   c) dispersion forces Yes/No Explain
   Dispersion forces come about when electrons move randomly into locations inside the molecule which causes the molecule to develop are instantaneous and temporary dipole.

3) Ammonia has a boiling temperature of -33 °C whereas water boils at 100 °C.
   a. Describe the intramolecular bonding of each molecule
   NH_3 __*Polar covalent*
   H_2o __ *Polar covalent*
   b. Circle the correct response.
   What type of molecule is
   Ammonia Polar / non-polar
   Water Polar / non-polar
   c. Describe the intermolecular bonding of each molecule.
   NH_3 ___*Hydrogen bonding + dispersion forces*
   d. H_2o ___ *Hydrogen bonding + dispersion forces*
   e. Explain the difference in boiling temperature between the two molecules.
   Water is a touch bigger molecule than NH_3 has dispersion forces are slightly greater between the water molecules than between the molecules of NH_3

4. Consider the table on the right which shows the electronegativity of some elements in the periodic table and the diagram below of the HCl and H_2O molecules.

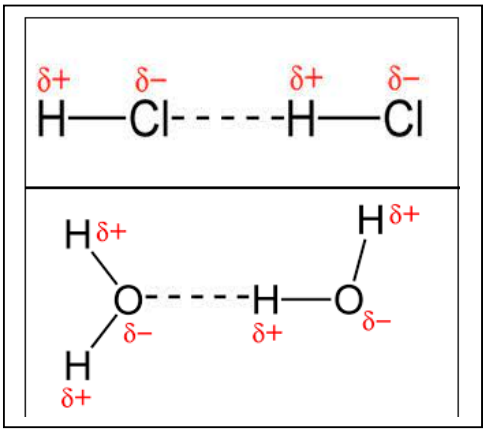
1 H 2.1																
3 Li 1.0	4 Be 1.5											5 B 2.0	6 C 2.5	7 N 3.0	8 O 3.5	9 F 4.0
11 Na 0.9	12 Mg 1.2											13 Al 1.5	14 Si 1.8	15 P 2.1	16 S 2.5	17 Cl 3.0
19 K 0.8	20 Ca 1.0	21 Sc 1.3	22 Ti 1.5	23 V 1.6	24 Cr 1.6	25 Mn 1.5	26 Fe 1.8	27 Co 1.9	28 Ni 1.9	29 Cu 1.9	30 Zn 1.6	31 Ga 1.6	32 Ge 1.8	33 As 2.0	34 Se 2.4	35 Br 2.8
37 Rb 0.8	38 Sr 1.0	39 Y 1.2	40 Zr 1.4	41 Nb 1.6	42 Mo 1.8	43 Tc 1.9	44 Ru 2.2	45 Rh 2.2	46 Pd 2.2	47 Ag 1.9	48 Cd 1.7	49 In 1.7	50 Sn 1.8	51 Sb 1.9	52 Te 2.1	53 I 2.5
55 Cs 0.7	56 Ba 0.9	57 La 1.1	72 Hf 1.3	73 Ta 1.5	74 W 1.7	75 Re 1.9	76 Os 2.2	77 Ir 2.2	78 Pt 2.2	79 Au 2.4	80 Hg 1.9	81 Tl 1.8	82 Pb 1.9	83 Bi 1.9	84 Po 2.0	85 At 2.2
87 Fr 0.7	88 Ra 0.9	89 Ac 1.1														

Increasing →

Decreasing ↓

Electronegativities of the Elements

a. The dotted lines show the bonds formed between molecules of HCl and the bonds formed between molecules of H_2O.



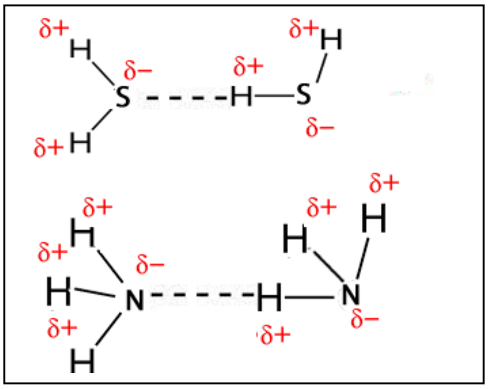
i. Place the following symbols δ+ or δ- in the appropriate place on each molecule.

ii. What type of intermolecular bonding exists between the molecules of:

- HCl _*Dipole-dipole and dispersion forces*
- H_2O _*Hydrogen bonding and dispersion forces*

iii. Explain why the boiling temperature of HCl is -85°C while the boiling temperature of H_2O is 100°C with reference to the table of the electronegativity of elements.
Both HCl and H_2O are small molecules that can produce relatively weak dispersion forces. H_2O, unlike HCl which has dipole-dipole bonding, also exhibits hydrogen bonding. Hydrogen bonding is a particularly strong form of dipole-dipole bonding and as such attracts the molecules of water more strongly hence more energy is needed to break the intermolecular bonds of water than the intermolecular bonds of HCl

b. Consider the diagram on the right. The dotted lines show the bonds formed between molecules of H_2S and the bonds formed between molecules of NH_3.



i. Place the following symbols δ+ or δ- in the appropriate place on each molecule.

ii. What type of intermolecular bonding exists between the molecules of:

- NH_3 __ *Hydrogen bonding and dispersion forces*
- H_2S __*Dipole-dipole and dispersion forces*

iii. Which molecule will have the highest boiling temperature? *NH_3*

Both molecules are relatively small hence the dispersion forces acting between both sets of molecules are relatively weak. NH_3 , unlike H_2S, also exhibits hydrogen bonding which is a strong form of dipole-dipole bonding.

5. Consider the diagrams on the right.

   The red line indicates an intermolecular bond while the black lines indicates a bond between two non-metal atoms.

   You may use any of the three diagrams to label the following.

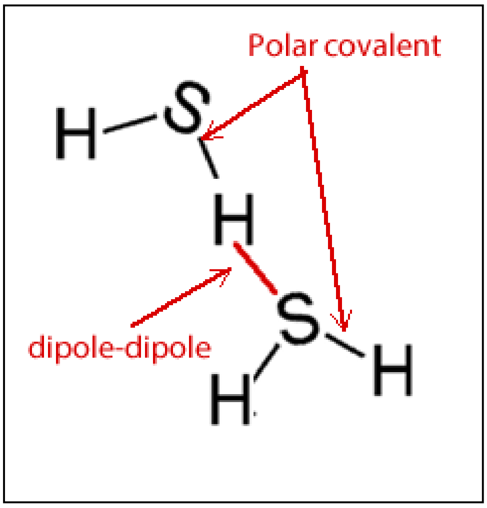
   a. Dispersion forces

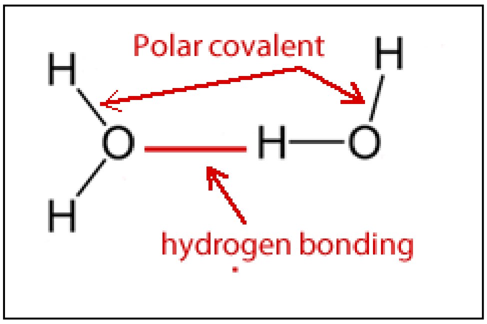
   b. Dipole-dipole bond

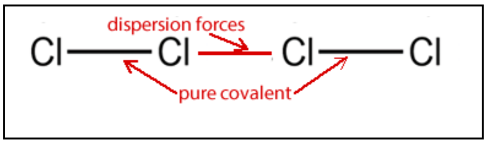
   c. Hydrogen bond

   d. Polar covalent bond

   e. Pure covalent bond

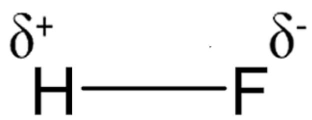




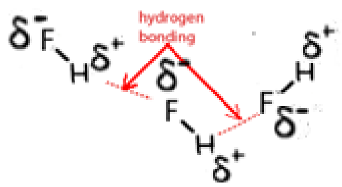


6. Explain why molecules that have a hydrogen atom covalently bonded to either an oxygen, nitrogen or fluorine atom have higher boiling temperatures than similar sized molecules without this type of bond. Use H_2S and HF as examples and draw diagrams to assist in your explanation in the space below.

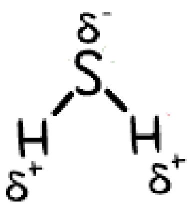
HF



The electronegativity difference between F and H is 1.9 (4.0 – 2.1). The dipoles that are formed are larger than those of SH_2.



H_2S



The electronegativity difference between S and H is 0.4 (2.5 – 2.1). The dipoles that are formed are not as great as those of HF.