

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.


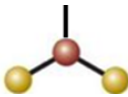

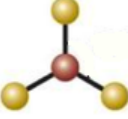
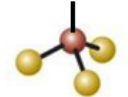

Step 2 Identify the central atom by drawing a Lewis dot diagram.

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.

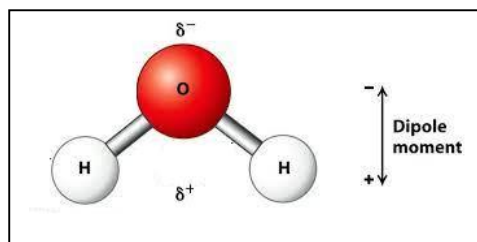
Step 5 Identify the shape of the molecule looking only at the location of the atoms.

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 has a slight positive charge.

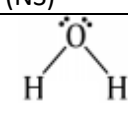


These slight charges are written as δ^+ or δ^- .

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 ₂ O	$\text{H}-\ddot{\text{O}}-\text{H}$	4 electron pairs (Tetrahedral shape)	V-shape		P
NF ₃					
CH ₄					
CH ₂ Cl ₂					
PH ₃					
SH ₂					
CO ₂					
COCl ₂					
CCl ₄					
SO ₂					

Formula	Lewis dot structure	Intra-molecular bonding	Indicate the polarity of the polar molecules
H ₂ O	$\text{H}-\ddot{\text{O}}-\text{H}$	Polar covalent	
O ₂			
CH ₄			Non-polar
CH ₂ O ₂			
PH ₃			
SH ₂			
COH ₂			
NH ₃			
CCl ₄			
CH ₃ COOH			
NOH			

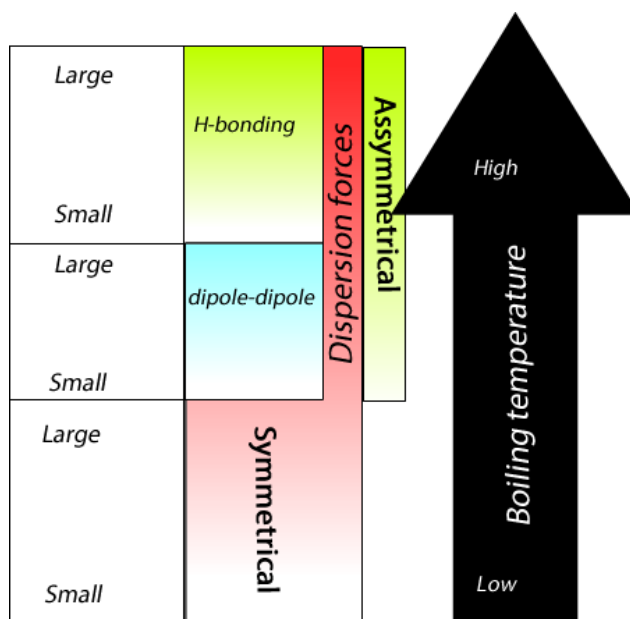
Predicting the strength of intermolecular bonding

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.

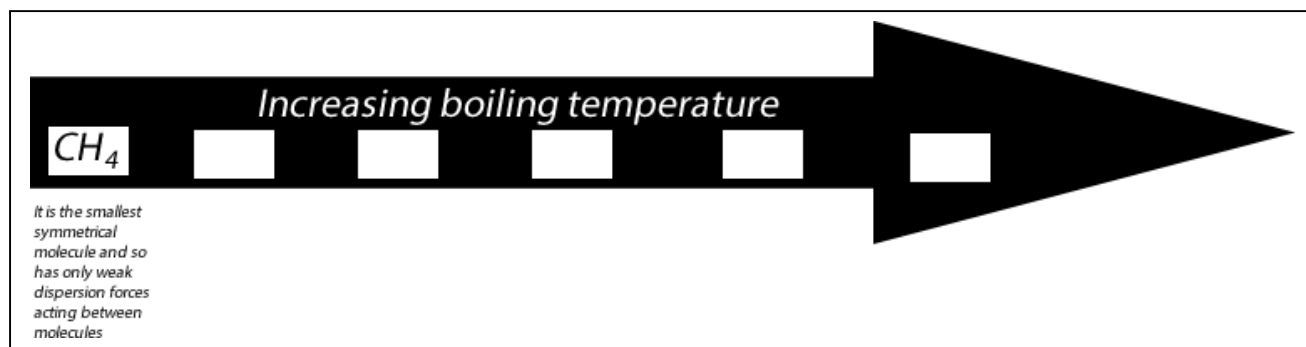


- similar sized asymmetrical molecules have intermolecular forces composed of dipole-dipole and dispersion forces. The red coloured bar, representing dispersion forces extend all the way to all type of molecules indicating the presence of dispersion forces in all molecules no matter their symmetry.

- 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.

- SO₂
- CO₂
- SH₂
- H₂O
- CH₄
- C₂H₆



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.



Shape _____

- b. What is the shape of each molecule?



Shape _____

- c. What are the inter molecular forces acting between molecules of :

NH_3 _____

NF_3 _____

- 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.

2. Place the following molecules in increasing order of boiling temperature. Give reasons for your choices. CO_2 , SH_2 , SiH_4 , CH_4

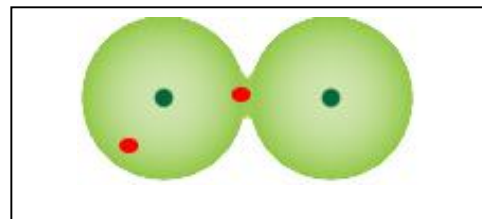
3. The boiling temperature of SO_2 is -10.1°C while SO_3 has a boiling temperature of 45°C .
- a. Complete the table below.

Molecule	Lewis dot diagram	Shape	Polarity (polar, non-polar)
SO_2			
SO_3			

- b. Explain the difference in boiling temperature.

Dispersion forces, dipole-dipole and hydrogen bonding.

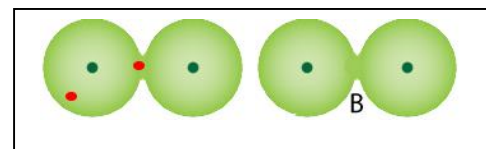
- 1) Consider the image on the right of a hydrogen molecule showing the two electrons in red and the two nuclei in green.



- a. Label the diagram using the following symbols.

δ^- or δ^+

- b. In the diagram on the right, label any changes that will take place on molecule "B" if the hydrogen molecule depicted above was next to it. Explain your reason for the changes and show the location of electrons and dipoles that may or may not form.



- 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

b) hydrogen bonding Yes/No Explain

c) dispersion forces Yes/No Explain

- 3) Ammonia has a boiling temperature of $-33\text{ }^\circ\text{C}$ whereas water boils at $100\text{ }^\circ\text{C}$.

- a. Describe the intramolecular bonding of each molecule

NH_3 _____

H_2O _____

- 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 _____

H_2O _____

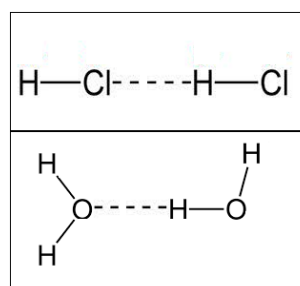
- d. Explain the difference in boiling temperature between the two molecules.

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 H₂O molecules.

1 H 2.1																	Decreasing ↓					
3 Li 1.0	4 Be 1.5	Increasing →																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																				

Electronegativities of the Elements

- a. Consider the image on the right, the dotted lines show the bonds formed between molecules of HCl and the bonds formed between molecules of H₂O.

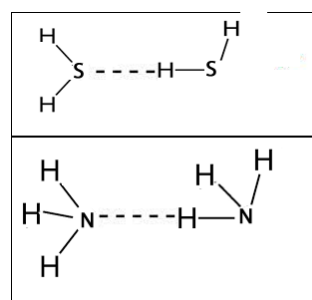


- i. Place the following symbols δ^+ or δ^- in the appropriate place on each molecule.

- ii. What type of intermolecular bonding exists between the molecules of:
- HCl _____
 - H₂O _____

- iii. Explain why the boiling temperature of HCl is -85°C while the boiling temperature of H₂O is 100°C with reference to the table of the electronegativity of elements.

- b. Consider the diagram on the right. The dotted lines show the bonds formed between molecules of H₂S and the bonds formed between molecules of NH₃.



- 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:
- NH₃ _____
 - H₂S _____

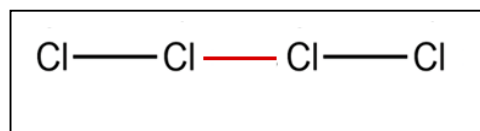
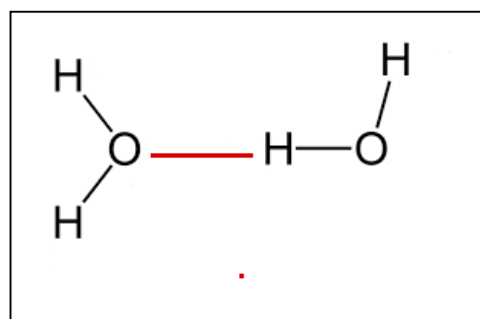
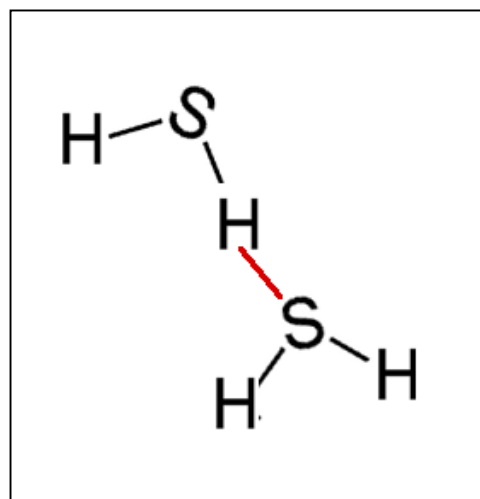
- iii. Which molecule will have the highest boiling temperature?

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.

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.

