

Structure 2.2

IB CHEMISTRY SL

<p>25 Mn Manganese 54.938045</p>	<p>16 S Sulfur 32.065</p>	<p>J</p>	<p>6 C Carbon 12.0107</p>	<p>2 He Helium 4.002602</p>	<p>25 Mn Manganese 54.938045</p>
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Structure 2.2.1 and 2.2.2

Understandings:

- A covalent bond is formed by the electrostatic attraction between a shared pair of electrons and the positively charged nuclei (2.2.1).
- The octet rule refers to the tendency of atoms to gain a valence shell with a total of 8 electrons (2.2.1).
- Single, double and triple bonds involve one, two and three shared pairs of electrons respectively (2.2.2).

Learning outcomes:

- Deduce the Lewis formula of molecules and ions for up to four electron pairs on each atom (2.2.1).
- Explain the relationship between the number of bonds, bond length and bond strength (2.2.2).

Additional notes:

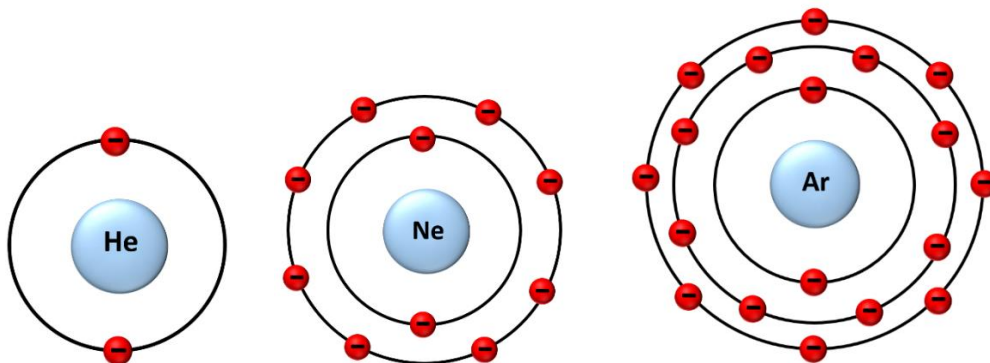
- Lewis formulas (also known as electron dot or Lewis structures) show all the valence electrons (bonding and non-bonding pairs) in a covalently bonded species.
- Electron pairs in a Lewis formula can be shown as dots, crosses or dashes.
- Molecules containing atoms with fewer than an octet of electrons should be covered.
- Organic and inorganic examples should be used.

Linking questions:

- Structure 1.3 Why do noble gases form covalent bonds less readily than other elements?
- Structure 2.1 Why do ionic bonds only form between different elements while covalent bonds can form between atoms of the same element?
- Reactivity 2.2 How does the presence of double and triple bonds in molecules influence their reactivity?

The octet rule

- The octet rule states that atoms are stable with eight electrons in their valence shells with the electron configuration of a noble gas.
- The electron configurations of noble gases He, Ne and Ar are shown below.



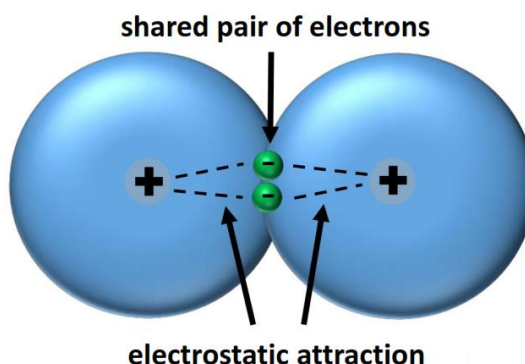
- Noble gases are stable because they have full valence shells.
- Atoms can achieve the electron configuration of a noble gas by either sharing electrons (covalent bonding) or by losing or gaining electrons (ionic bonding).

Exceptions to the octet rule

- Hydrogen and helium are stable with 2 electrons in their valence shell.
- Beryllium is stable with 4 electrons in its valence shell.
- Boron is stable with 6 electrons in its valence shell.
- Elements in period 3 onwards can hold more than 8 electrons in their outer shells (expanded octets).

Covalent bonding

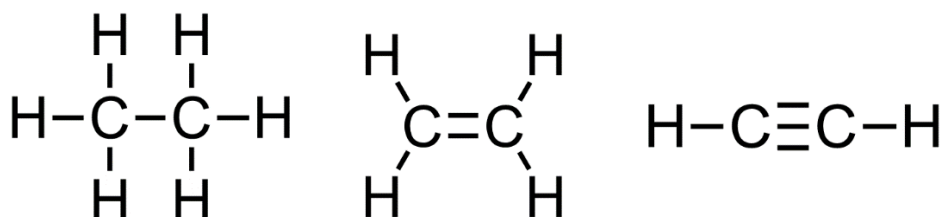
- A covalent bond is the electrostatic attraction between positive nuclei and shared pairs of bonding electrons.
- A covalent bond is an intramolecular bond (bond within a molecule).
- Covalent bonding occurs between non-metal elements only.
- The electronegativity difference between atoms is between 0.0 and 1.7 units.



- Both nuclei are attracted to the shared pair of bonding electrons.
- The electrostatic attraction between the nuclei and shared pair of bonding electrons is the covalent bond.

Single, double and triple bonds

- Single bonds are longer and weaker, triple bonds are shorter and stronger.

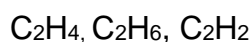


- The carbon-to-carbon bonds in C_2H_6 are longer and weaker than those in C_2H_2 .

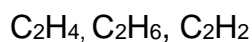
Bond	Number of shared electrons	C to C bond strength (kJ mol^{-1})	C to C bond length (10^{-12} m)
Single	2	347	153
Double	4	614	134
Triple	6	839	120

Exercises:

1. Describe a covalent bond.
2. Where on the periodic table would you find elements that bond by covalent bonding?
3. Arrange the following in order of increasing carbon to carbon bond strength (weakest first).



4. Arrange the following in order of decreasing carbon to carbon bond length (longest first),



Bond order

- Bond order is the number of bonds between a pair of atoms.
- Single bonds have a bond order of 1, double bonds have a bond order of 2 and triple bonds have a bond order of 3.
- The higher the bond order, the stronger (and shorter) the bond.
- Polyatomic ions such as CO_3^{2-} and NO_3^- and molecules such as benzene, C_6H_6 , can have fractional bond orders.
- Bond order can be calculated by dividing the sum of the individual bond orders by the number of bonding groups in the molecule or ion.

Example: Calculate the bond order of the bonds in the nitrate ion, NO_3^- .

Lewis formulas (Lewis structures)

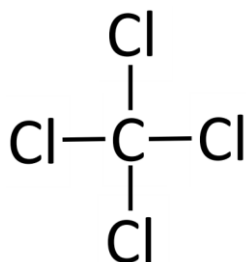
- Lewis formulas show all the valence electrons in a molecule; the bonding electrons and the lone pairs of electrons (non-bonding electrons).

How to determine a Lewis formula

- Calculate the number of valence electrons in the molecule.
- Calculate the number of electrons each atom needs to complete its octet.
- Subtract 1 from 2 – this will give you the number of bonding electrons in the molecule.
- Draw the skeletal structure of the molecule with the least electronegative atom at the center.
- Complete the octets of the atoms in the molecule.

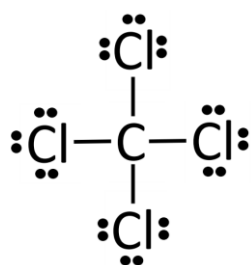
Example – CCl₄ (carbon tetrachloride)

- Total number of valence electrons = $4 + (4 \times 7) = 32$
- Number of valence electrons needed for each atom to complete its octet (5×8) = 40
- $40 - 32 = 8$ bonding electrons
- Skeletal formula:



One single bond = 2 electrons (total 8 bonding electrons).

- Complete the octets of all the atoms in the molecule.



Do a final check that all electrons are accounted for. It should match with the number in part 1 (32).

Exercises:

1. Draw Lewis formulas for the following molecules.

a) Cl_2

b) HCl

c) CH_3Cl

d) CF_4

e) PF_3

f) BF_3

g) BeCl_2

h) N_2H_4

i) H_2O

j) CH_3OH

k) CO

l) C_2H_4

j) HCN

2. Draw Lewis formulas for the following ions.

a) Cl^-

b) NH_4^+

c) OH^-

3. Which molecules contain an incomplete octet of electrons?

Structure 2.2.3

Understandings:

- A coordination bond is a covalent bond in which both the electrons of the shared pair originate from the same atom.

Learning outcomes:

- Identify coordination bonds in compounds.

Additional notes:

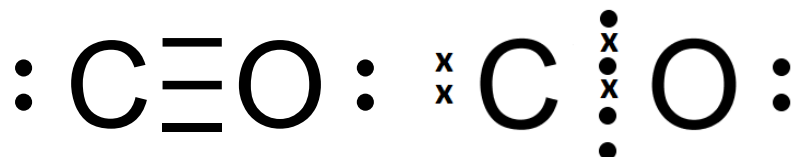
- Include coverage of transition element complexes (HL).

Linking questions:

- Reactivity 3.4 (HL) Why do Lewis acid–base reactions lead to the formation of coordination bonds?

Coordination bonds

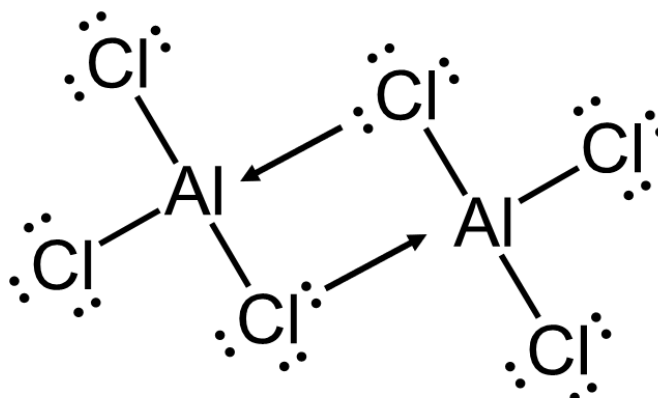
- A coordination bond is a covalent bond in which one atom contributes both the bonding electrons to the bond.
- Carbon monoxide (CO) has a triple covalent bond between the carbon and oxygen atoms – one of these bonds is a coordination bond where both the bonding electrons come from the oxygen atom.



- Other molecules and ions that have coordination bonds are H_3O^+ , NH_4^+ and Al_2Cl_6 .
- Draw the Lewis structures of CO, H_3O^+ and NH_4^+ in the boxes below.

CO	H_3O^+	NH_4^+

- Al_2Cl_6 is a dimer formed between two molecules of AlCl_3 .



Structure 2.2.4

Understandings:

- The valence shell electron pair repulsion (VSEPR) model enables the shapes of molecules to be predicted from the repulsion of electron domains around a central atom.

Learning outcomes:

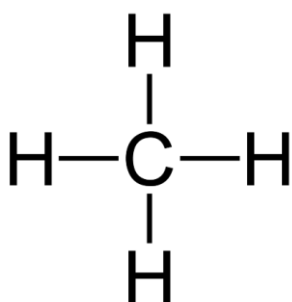
- Predict the electron domain geometry and the molecular geometry for species with up to four electron domains.

Additional notes:

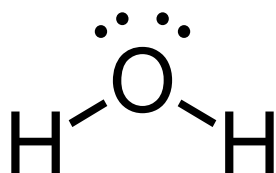
- Include predicting how non-bonding pairs and multiple bonds affect bond angles.

VSEPR theory

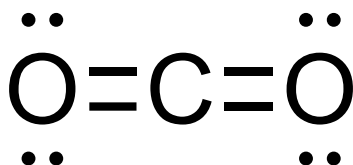
- Valence shell electron pair repulsion theory is used to predict the geometry (shape) of molecules.
- Electron pairs (bonds or lone pairs) repel each other and spread apart as far as possible.
- The term electron domain is used to refer to bonds or lone pairs of electrons (non-bonding electrons) around an atom in a molecule.
- Single bonds, double bonds, triple bonds and lone pairs of electrons (non-bonding electrons) count as one electron domain.



How many electron domains are there around the carbon atom?



How many electron domains are there around the oxygen atom?



How many electron domains are there around the carbon atom?

The order of repulsion between electron domains is as follows:

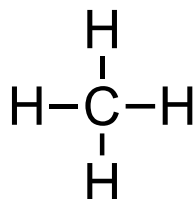
lone pair – lone pair > lone pair – bonding domain > bonding domain – bonding domain

most repulsion

least repulsion

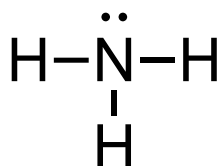
Molecules with four electron domains

- Four bonding domains, zero non-bonding domains



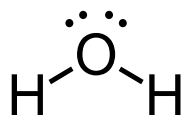
electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
4	4	0	tetrahedral	tetrahedral	109.5°

- Three bonding domains, one non-bonding domain



electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
4	3	1	tetrahedral	trigonal pyramidal	107.8°

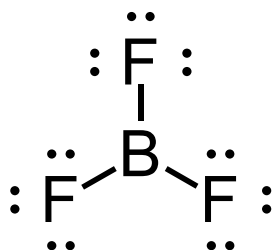
- Two bonding domains, two non-bonding domains



electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
4	2	2	tetrahedral	bent	104.5°

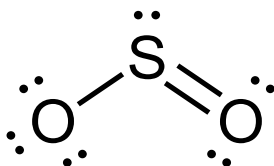
Molecules with three electron domains

- Three bonding domains, zero non-bonding domains



electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
3	3	0	trigonal planar	trigonal planar	120°

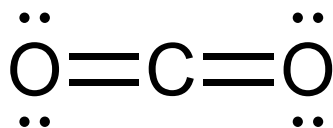
- Two bonding domains, one non-bonding domain



electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
3	2	1	trigonal planar	bent	<120°

Molecules with two electron domains

- Two bonding domains, zero non-bonding domains



electron domains	bonding domains	non-bonding domains	electron domain geometry	molecular geometry	bond angle
2	2	0	linear	linear	180°

Exercise: Determine the molecular geometry and bond angles in the following molecules:

a) HCN

b) PH₃

c) CH₂Cl₂

d) Cl₂O

e) C₂H₂

f) BF₃

g) BeH₂

h) H₂S

Structure 2.2.5

Understandings:

- Bond polarity results from the difference in electronegativities of the bonded atoms.

Learning outcomes:

- Deduce the polar nature of a covalent bond from electronegativity values.

Additional notes:

- Bond dipoles can be shown either with partial charges or vectors.
- Electronegativity values are given in the data booklet.

Linking questions:

- Structure 2.1 What properties of ionic compounds might be expected in compounds with polar covalent bonding?

Polar covalent bonds

- Polar covalent bonds occur between atoms that have a difference in electronegativity.

Difference in electronegativity	Polar or non-polar covalent bond	Example
0	non-polar (pure) covalent bond	Cl-Cl
0.1– 0.4	non-polar (weakly polar) covalent bond	C-H
0.5 –1.7	polar covalent bond	C-F

- Bond polarity can be shown by a vector arrow or by δ^+ and δ^- as shown below.



Exercises:

- Draw a diagram showing the bonding polarity in HF (hydrogen fluoride).

2. For each bond, find the difference in electronegativity and classify as either pure covalent, non-polar covalent or polar covalent. Draw bond dipoles or partial charges on each atom.

Bond	Pure covalent, non-polar covalent or polar covalent	Bond dipoles
Br-Br		
C-Cl		
C-I		
C-O		
N-F		
H-F		

Structure 2.2.6

Understandings:

- Molecular polarity depends on both bond polarity and molecular geometry.

Learning outcomes:

- Deduce the net dipole of a molecule or ion by considering bond polarity and geometry.

Additional notes:

- Examples should include species in which bond dipoles do and do not cancel each other.

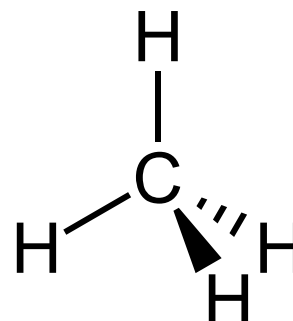
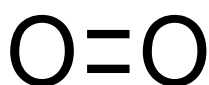
Linking questions:

- Structure 3.2 (HL) What features of a molecule make it “infrared (IR) active”?

Polar and non-polar molecules

The polarity of a molecule depends on two factors:

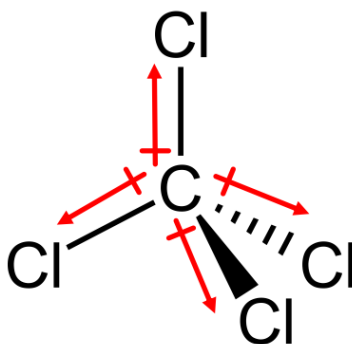
- The presence of polar bonds within the molecule.
- The shape (geometry) of the molecule.



- O_2 , N_2 and CH_4 are non-polar molecules.
- O_2 and N_2 are diatomic; both atoms have the same electronegativity.
- CH_4 has non-polar bonds.

Non-polar molecule with polar bonds

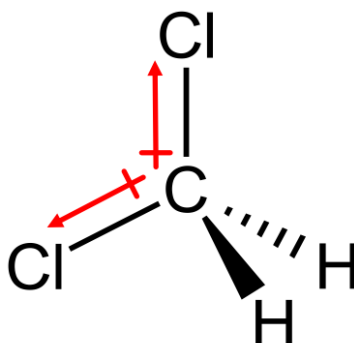
- CCl_4 is a non-polar molecule that has polar bonds.



- The bond polarities cancel out, therefore, the molecule has no net-dipole moment.

Polar molecules

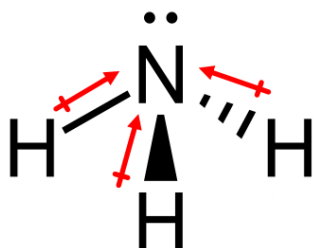
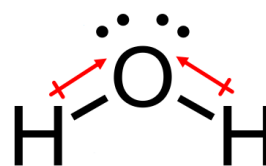
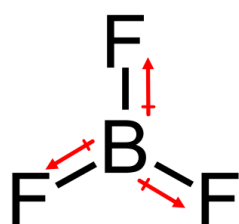
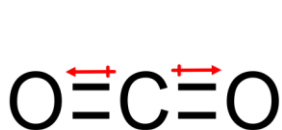
- CH_2Cl_2 is a polar molecule.



- The bond polarities do not cancel out, therefore, it has a net-dipole moment.

Exercises:

1. Outline the two factors that determine the polarity of a molecule.
2. Explain how a molecule can have polar bonds but overall have no net-dipole moment (is a non-polar molecule).
3. Determine if the molecules below are polar or non-polar, giving a reason.



Structure 2.2.7

Understandings:

- Carbon and silicon form covalent network structures.

Learning outcomes:

- Describe the structures and explanation of the properties of silicon, silicon dioxide and carbon's allotropes: diamond, graphite, fullerenes and graphene.

Additional notes:

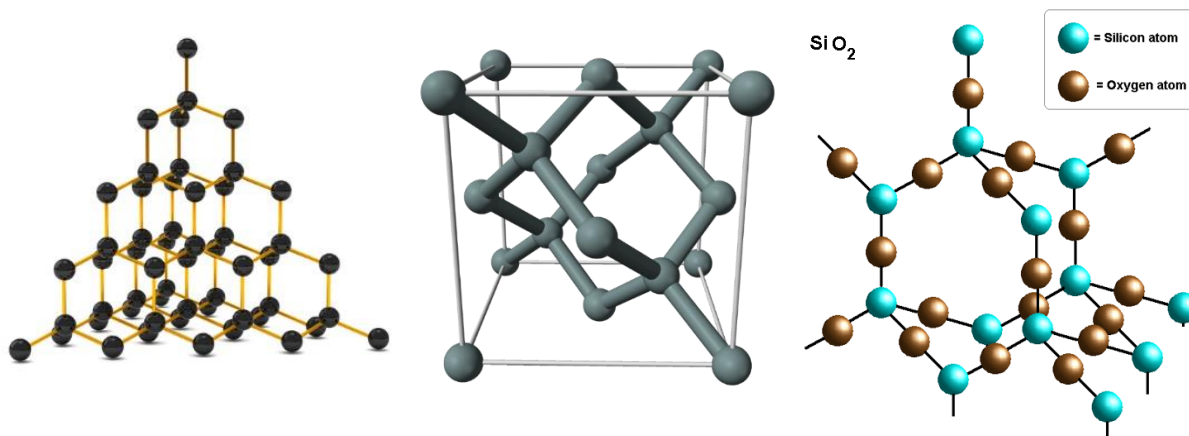
- Allotropes of the same element have different bonding and structural patterns, and so have different chemical and physical properties.

Linking questions:

- Structure 3.1 Why are silicon–silicon bonds generally weaker than carbon–carbon bonds?

Giant covalent structures

- Giant covalent structures do not form discrete molecules.
- Examples include diamond, Si and SiO₂



- Giant covalent structures do not conduct electricity (no free moving electrons).
- They are insoluble in polar and non-polar solvents.
- They have high melting and boiling points due to the strong covalent bonds between atoms.
- They are very hard substances.

Exercises:

1. Classify the following covalent compounds as simple molecular or giant covalent based on their properties:

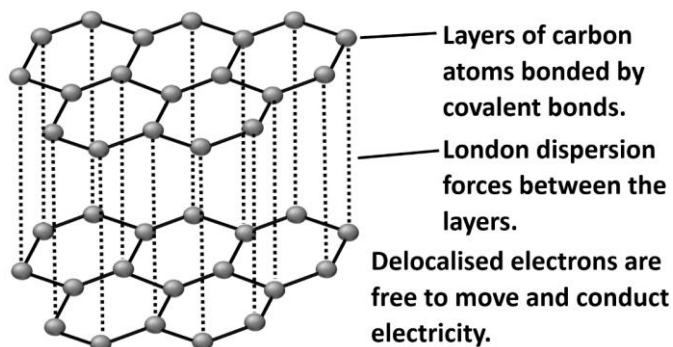
Property	Simple molecular	Giant covalent
High melting and boiling point		
Insoluble in polar and non-polar solvents		
Liquids and gases under standard conditions		
Do not form discrete molecules		
Poor electrical conductors		
Soluble in polar or non-polar solvents		
Form discrete molecules		
Very hard substances		

2. Explain the following properties of the covalent compounds.
 - a. Pentane (C_5H_{12}) is insoluble in water but soluble in hexane (C_6H_{14}).
 - b. Diamond does not conduct electricity.
 - c. CO_2 is a gas under standard conditions.
 - d. SiO_2 has a melting point of $1600\text{ }^\circ C$

Allotropes of carbon

- Allotropes are different forms of the same element in the same physical state.
- Carbon has 4 allotropes – graphite, diamond, Fullerene C₆₀ and graphene.
- Different bonding within the structures gives the allotropes different properties.

Graphite



- Graphite has a layered structure.
- The layers are held together by weak intermolecular forces.
- The layers can slide over one another (because of weak intermolecular forces).
- Each carbon atom is bonded to 3 other carbon atoms.
- The bond angle between carbon atoms is 120°, trigonal planar.
- Graphite is a good conductor of electricity because of the delocalised electrons that are free to move within the structure.

Diamond



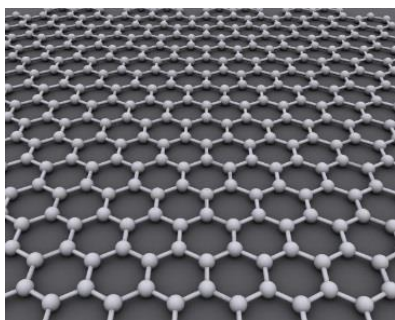
- Giant covalent structure.
- High melting and boiling point.
- Very hard (strong covalent bonds between atoms).
- Each carbon is bonded to 4 other carbon atoms.
- Bond angle is 109.5°, tetrahedral.
- Does not conduct electricity (no delocalised electrons).
- Used in jewellery and for cutting glass.

Fullerene C₆₀

- Each carbon atom is bonded to 3 other carbon atoms.
- Structure consists of 12 pentagons and 20 hexagons.
- Poor electrical conductor (better than diamond but worse than graphite).



Graphene



- Each carbon atom is bonded to 3 other carbon atoms.
- Bond angle between carbon atoms is 120° .
- Very good heat and electrical conductivity.
- Very thin (one layer thick) but very strong.

Allotropes of carbon and their uses

Allotrope	Uses
Graphite	dry lubricant, electrode rods, pencils
Diamond	jewellery, tools for cutting glass
Fullerene C ₆₀	lubricant, nanotubes
Graphene	lightweight, thin, flexible, yet durable display screens, electric/photronics circuits, solar cells

Exercises:

1. Outline why graphite is a good conductor of electricity but diamond is not.
2. Give one reason for the high melting and boiling point of diamond.
3. State and explain the bond angles of graphite and diamond.
4. Explain why graphite is a very soft substance.

Structure 2.2.8 and 2.2.9

Understandings:

- The nature of the force that exists between molecules is determined by the size and polarity of the molecules.
- Intermolecular forces include London (dispersion), dipole-induced dipole, dipole–dipole and hydrogen bonding.
- Given comparable molar mass, the relative strengths of intermolecular forces are generally: London (dispersion) forces < dipole–dipole forces < hydrogen bonding.

Learning outcomes:

- Deduce the types of intermolecular force present from the structural features of covalent molecules.
- Explain the physical properties of covalent substances to include volatility, electrical conductivity and solubility in terms of their structure.

Additional notes:

- The term “van der Waals forces” should be used as an inclusive term to include dipole–dipole, dipole- induced dipole, and London (dispersion) forces.
- Hydrogen bonds occur when hydrogen, being covalently bonded to an electronegative atom, has an attractive interaction on a neighbouring electronegative atom.

Linking questions:

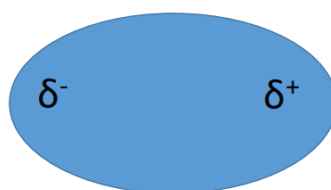
- Structure 1.5 To what extent can intermolecular forces explain the deviation of real gases from ideal behaviour?
- Structure 3.2 To what extent does a functional group determine the nature of the intermolecular forces?

Intermolecular forces

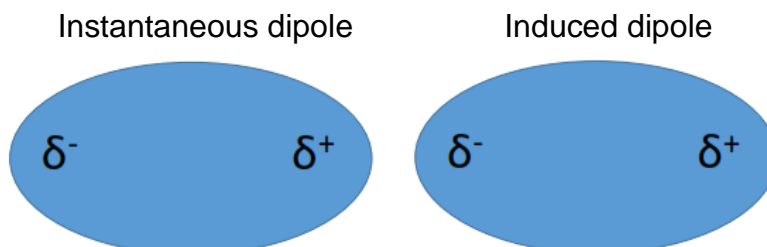
- Intermolecular forces are forces of attraction between molecules.
- The three types of intermolecular force are:
London dispersion forces, dipole-dipole forces and hydrogen bonding.
- London dispersion forces, dipole-induced dipole and dipole-dipole forces are collectively known as van der Waals forces.

London dispersion forces

- London dispersion forces are the weakest type of intermolecular force.
- They exist between all atoms or molecules (both polar and non-polar).
- Due to the constant motion of electrons, an atom or molecule can develop a temporary (instantaneous) dipole.



- An instantaneous dipole in one molecule can cause an induced dipole in a nearby molecule.



- London dispersion forces have a significant effect on the physical properties of molecules, such as boiling point.

Exercises:

1. State the types of intermolecular forces that are van der Waals forces.

2. Outline the formation of London dispersion forces.

Boiling point of the halogens

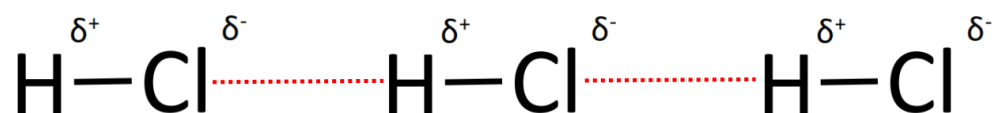
	Molar mass (g mol ⁻¹)	Boiling point (°C)
F ₂	30.8	-188
Cl ₂	70.9	-34.0
Br ₂	160	58.0
I ₂	254	193

- The boiling points of the halogens increase as their molar masses increase.
- The strength of London dispersion forces increases with increasing molar mass.
- Stronger London dispersion forces result in a higher boiling point (more energy is required to overcome the attractive forces between molecules).

Exercise: Explain why the boiling points of the halogens increase down the group.

Dipole-dipole forces

- Dipole-dipole forces occur between polar molecules that have a permanent dipole.
- They are the second strongest type of intermolecular force.
- There is an electrostatic attraction between the partial positive charge in one molecule and the partial negative charge on another.
- The dipole-dipole attractions between HCl molecules are shown below.

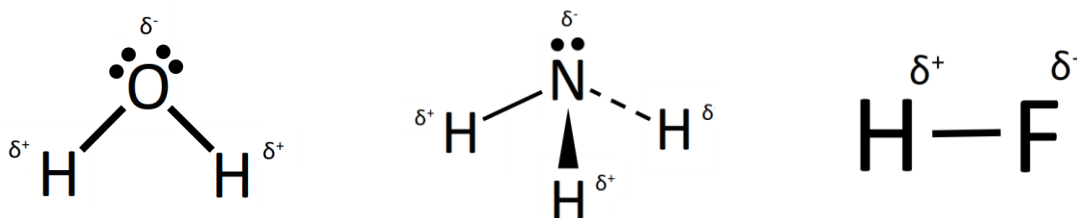


Exercises:

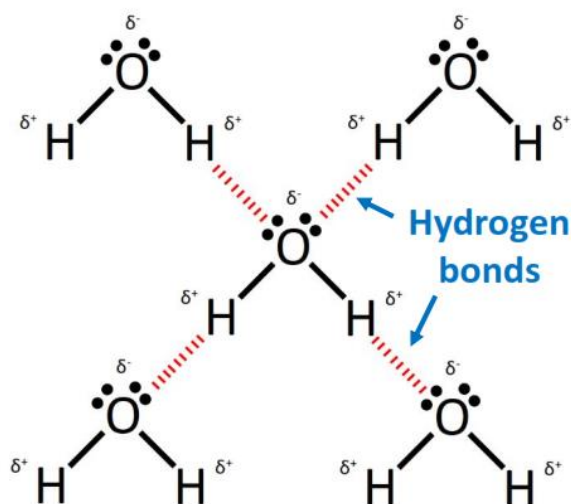
1. State the type of molecules that dipole-dipole forces occur between.
2. Outline the formation of the dipole-dipole forces in HCl.

Hydrogen bonding

- Hydrogen bonding occurs when a hydrogen atom is bonded to either a nitrogen, oxygen or fluorine atom.
- It is the strongest type of intermolecular force.
- Example of compounds that have hydrogen bonding between their molecules are H₂O, NH₃ and HF.



- Hydrogen bonds between water molecules are shown below. These are responsible for the high boiling point of water.

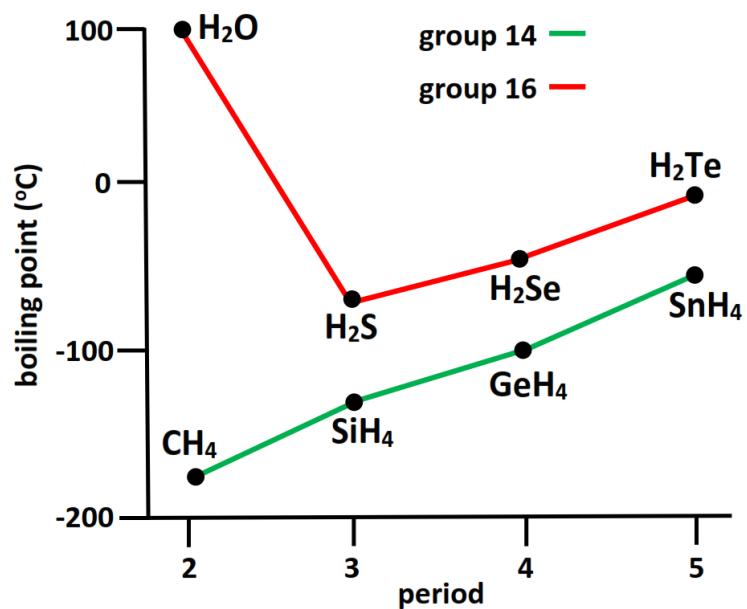


- The hydrogen bond is between the partial positive charge on the hydrogen atom and the partial negative charge on the oxygen atom
- Water has a much higher boiling point compared to other molecules with similar molar masses because of the effect of hydrogen bonding.

Exercises:

1. Which groups of atoms are necessary for the formation of a hydrogen bond?
2. Outline the formation of a hydrogen bond between water molecules.

Boiling points of group 14 and group 16 hydrides



Exercise: From the above graph, describe and explain the trend in boiling point of the group 14 and group 16 hydrides.

Exercises:

1. Arrange the following in terms of increasing strength.

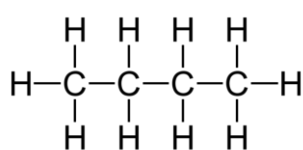
Hydrogen bonding London dispersion forces Dipole-dipole forces

2. Identify the **strongest** type of intermolecular forces in the following molecules.

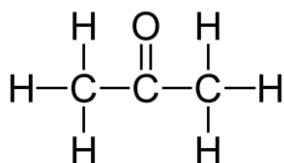
- | | |
|---------------------|----------------------------------|
| a) Cl ₂ | f) CH ₃ Cl |
| b) HCl | g) H ₂ O |
| c) HF | h) CH ₃ OH |
| d) CH ₄ | i) C ₂ H ₆ |
| e) CCl ₄ | j) NH ₃ |

3. Explain why, at room temperature, F₂ and Cl₂ are gases, Br₂ is a liquid and I₂ is a solid.

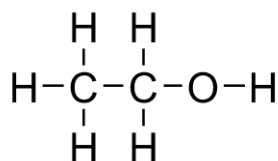
4. The structures of butane, propanone, and ethanol can be seen below. They have similar molar masses, but different boiling points. Explain the difference in boiling point between the three molecules.



butane B.P. -1°C



propanone B.P. 56°C



ethanol B.P. 78°C

Structure 2.2.10

Understandings:

- Chromatography is a technique used to separate the components of a mixture based on their relative attractions involving intermolecular forces to mobile and stationary phases.

Learning outcomes:

- Explain, calculate and interpret the retardation factor values, RF.

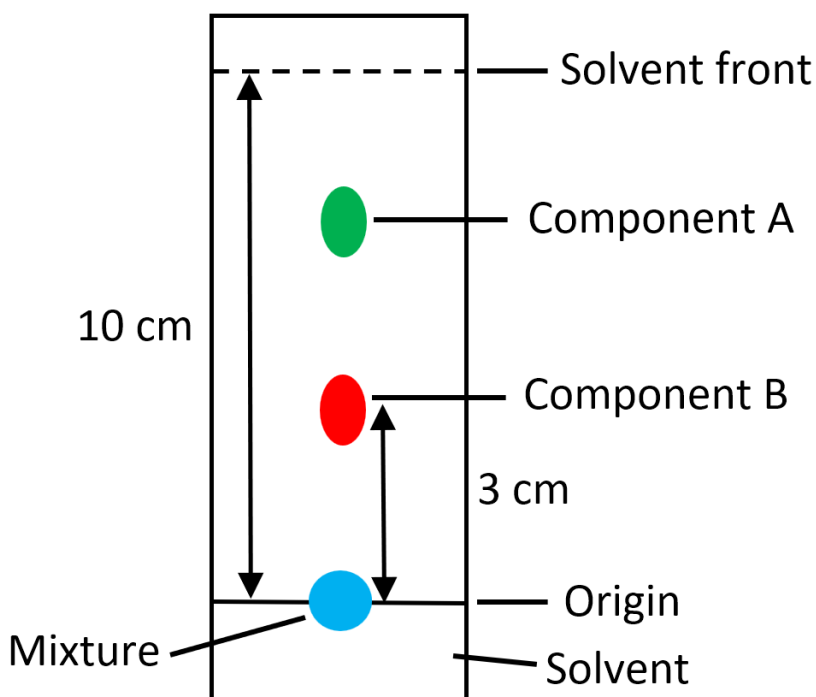
Additional notes:

- The use of locating agents is not required.
- The operational details of a gas chromatograph or high-performance liquid chromatograph will not be assessed.

Chromatography

- Chromatography is a separation technique used to separate a mixture of solutes in a solvent.
- A small sample of the mixture is spotted near the bottom of a piece of filter paper (known as the origin).
- The filter paper is suspended in a solvent with the spot above the level of the solvent.
- As the solvent rises up the filter paper by capillary action, the components of the mixture will distribute themselves between two phases – the stationary phase (the filter paper) and the mobile phase (the solvent).
- This distribution is determined by the strength of the intermolecular forces experienced by the components of the mixture in each phase.
- If the component forms stronger intermolecular forces with the stationary phase it will not travel as far up the paper.
- Conversely, a component that forms stronger intermolecular forces with the mobile phase will travel further up the paper.

Example: On the chromatogram shown, component A forms stronger intermolecular forces with the mobile phase than component B and travels further up the paper. Component B forms stronger intermolecular forces with the stationary phase and does not travel as far up the paper.



Calculating the retardation factor, R_f

- The components of the mixture can be identified by calculating the retardation factor, R_f .
- The retardation factor is calculated by dividing the distance moved by the component by the total distance moved by the solvent (known as the solvent front).

$$R_f = \frac{\text{distance moved by component}}{\text{distance moved by solvent front}}$$

- **Example:** in the chromatogram shown above, component B travels 3 cm and the solvent front is 10 cm. The retardation factor is:

$$R_f = \frac{3 \text{ cm}}{10 \text{ cm}} = 0.3$$

- This R_f value can be compared to the R_f values of known substances and the components of the mixture can be identified.