

Mastering Chemistry

- Book 2C
- Topic 6 Microscopic
World II



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23.1 The octet rule (p.2)

- ◆ Most of the covalent compounds that you will meet in the course are compounds of hydrogen, carbon, nitrogen and oxygen.
- ◆ You can see in Table 23.1 that atoms of these elements combine so as to obtain 8 electrons in the outermost shells (or 2 electrons for the lighter elements close to helium).
- ◆ This tendency to acquire the electronic arrangements of atoms of noble gases is termed the **octet rule** (八隅體規則).



23.1 The octet rule (p.2)

▶ **Table 23.1** Electron diagrams of molecules that obey the octet rule

Covalent compound	Electron diagram (showing electrons in the outermost shells only)
Methane (CH ₄)	
Ammonia (NH ₃)	
Water (H ₂ O)	



23.2 Molecules not obeying the octet rule (p.2)

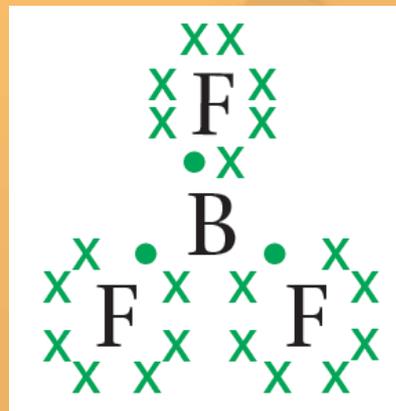
There are a number of molecules that do not obey the octet rule. For example,

- ◆ a molecule in which the central atom does not have enough electrons in the outermost shell to achieve an octet;
- ◆ a molecule in which the central atom has an expanded octet (i.e. more than 8 electrons) in its outermost shell.

23.2 Molecules not obeying the octet rule (p.2)

Molecules with a central atom not having enough electrons

- ◆ A boron atom has 3 outermost shell electrons.
- ◆ When forming a compound such as **boron trifluoride**, BF_3 (三氟化硼), a boron atom shares a pair of electrons with each of three fluorine atoms.
- ◆ The boron atom has only 6 electrons in its outermost shell. It does not achieve an octet.

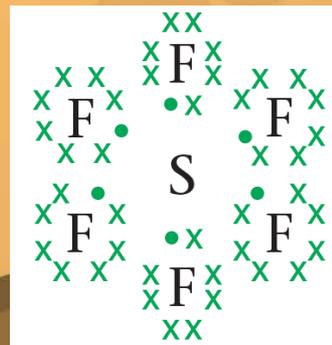
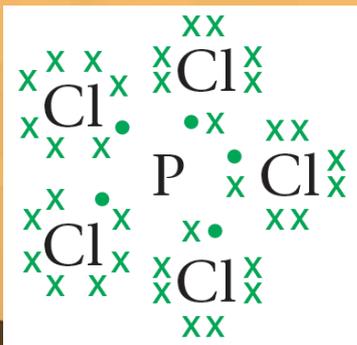




23.2 Molecules not obeying the octet rule (p.2)

Molecules with a central atom having an expanded octet

- Central atoms of both **phosphorus pentachloride**, PCl_5 (五氯化磷) and **sulphur hexafluoride**, SF_6 (六氟化硫) molecules have an expanded octet.
- The outermost shells of atoms of the elements phosphorus and sulphur in Period 3 of the Periodic Table can hold up to 18 electrons. Atoms of elements in Period 2 do not form compounds with more than 8 electrons in their outermost shells because the second electron shell can only hold up to 8 electrons.





23.2 Molecules not obeying the octet rule (p.2)

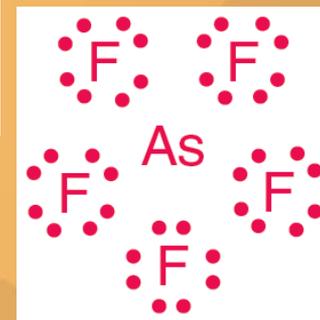
- ◆ Hence nitrogen trichloride (NCl_3) is known to exist but nitrogen pentachloride (NCl_5) is not known to exist. However, both **phosphorus trichloride**, PCl_3 (三氯化磷) and phosphorus pentachloride (PCl_5) are known to exist.



23.2 Molecules not obeying the octet rule (p.2)

Practice 23.1

In each of the following fluorides, the central atom is underlined.



a) Draw an electron diagram for each of the fluorides above, showing electrons in the *outermost shells* only.

b) In which fluorides do the central atoms NOT have an octet structure?





23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

- ◆ Because of similar (negative) charge, electron pairs repel each other. The electron pairs in the outermost shell of an atom will experience the least repulsion when they are as far apart from one another as possible.
- ◆ This applies to both bond pairs and lone pairs. This simple principle allows you to predict the shapes of simple covalent molecules. The theory is called the **valence shell electron pair repulsion theory** (價層電子對相斥學說).
- ◆ Valence shell = the outermost electron shell



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

You are going to determine in this section the shapes of simple molecules containing only single covalent bonds. Follow the steps below:

- 1 Draw an electron diagram of the molecule and count the number of electron pairs in the outermost shell of the central atom.
- 2 Determine the arrangement of the electron pairs around the central atom. These electron pairs stay as far apart as possible so as to minimise repulsion.
- 3 State the shape of the molecule based on the positions of the atoms around the central atom.



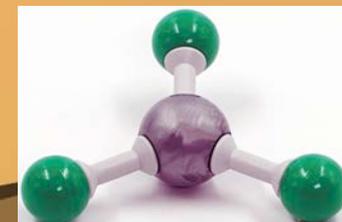
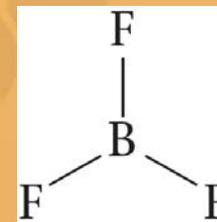
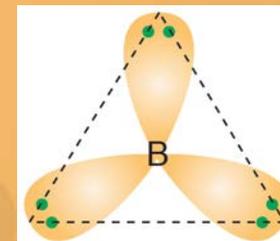
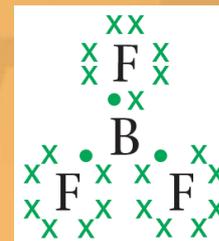
Valence shell electron pair repulsion theory [Ref.](#)



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Molecule with three electron pairs in the outermost shell of the central atom— BF_3

- ◆ In a **boron trifluoride molecule**, there are three bond pairs in the outermost shell of the central boron atom.
- ◆ These three electron pairs stay as far apart as possible and a **trigonal planar** (平面三角的) arrangement results.
- ◆ Hence the boron trifluoride molecule has a trigonal planar shape, with the fluorine atoms at the corners and the boron atom in the centre.

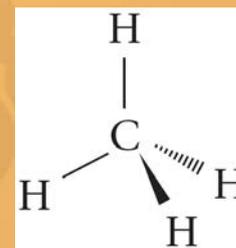
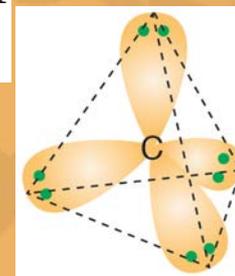
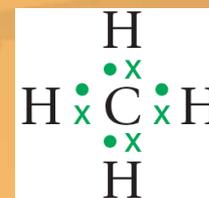




23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Molecule with four electron pairs in the outermost shell of the central atom—**CH₄, NH₃ and H₂O**

- ◆ In a **methane molecule**, there are four bond pairs in the outermost shell of the central carbon atom.
- ◆ The four bond pairs stay as far apart as possible. And a **tetrahedral** (四面體的) arrangement results.
- ◆ Hence the methane molecule has a tetrahedral shape, with the hydrogen atoms at the corners and the carbon atom in the centre.



bond lying on the page

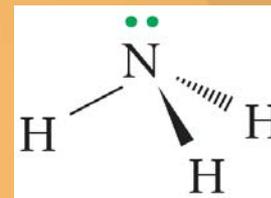
bond coming out of the page

bond going into the page



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

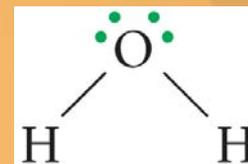
- ◆ In an **ammonia molecule**, there are four electron pairs in the outermost shell of the central nitrogen atom — three bond pairs and one lone pair.
- ◆ These electron pairs stay as far apart as possible and a tetrahedral arrangement results.
- ◆ As there are only three hydrogen atoms bonded to the nitrogen atom, the ammonia molecule is **trigonal pyramidal (三角錐體的)** in shape, with a nitrogen atom at the apex and hydrogen atoms at the three corners of its base.





23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

- ◆ In a **water molecule**, there are also four electron pairs in the outermost shell of the central oxygen atom — two bond pairs and two lone pairs.
- ◆ These electron pairs adopt a tetrahedral arrangement again.
- ◆ However, as there are only two hydrogen atoms bonded to the oxygen atom, the shape of the molecule is bent or **V-shaped (V形的)**.

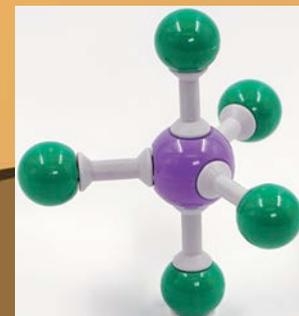
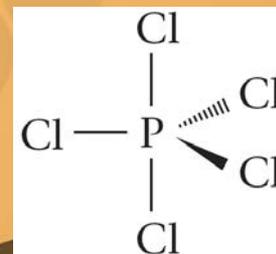
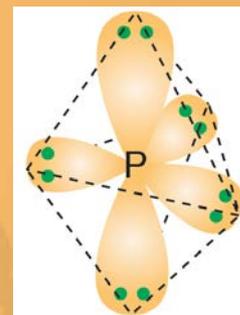
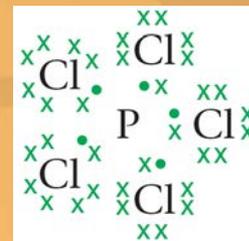




23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Molecule with five electron pairs in the outermost shell of the central atom— PCl_5

- ◆ In a **phosphorus pentachloride molecule**, there are five bond pairs in the outermost shell of the central phosphorus atom.
- ◆ These bond pairs stay as far apart as possible and a **trigonal bipyramidal (三角雙錐體的)** arrangement results.
- ◆ Hence the phosphorus pentachloride molecule is trigonal bipyramidal in shape, with the chlorine atoms at the corners and the phosphorus atom in the centre.

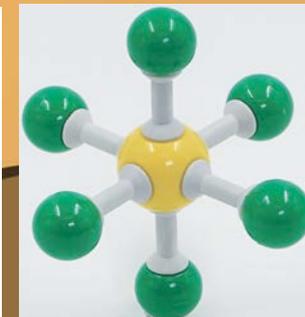
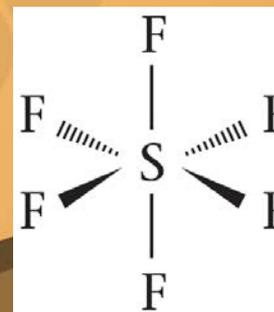
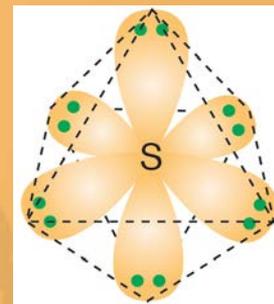
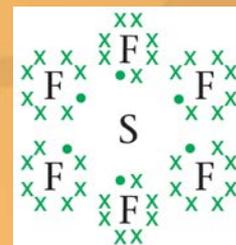




23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Molecule with six electron pairs in the outermost shell of the central atom— SF_6

- ◆ In a **sulphur hexafluoride molecule**, there are the six bond pairs in the outermost shell of the central sulphur atom.
- ◆ These bond pairs stay as far apart as possible and an **octahedral** (八面體的) arrangement results.
- ◆ Hence the sulphur hexafluoride molecule has an octahedral shape, with the fluorine atoms at the corners and the sulphur atom in the centre.





23.3 Shapes of simple molecules containing only single covalent bonds (p.5)



Building 'balloon' molecules



Building ball-and-stick models of molecules



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Practice 23.2

1 Chemists are able to predict the shape of a simple molecule from the number of electron pairs in the outermost shell of the central atom. Explain how this enables chemists to predict the shape.

Pairs of electrons repel.

The shape is determined by the number of bond pairs and the number of lone pairs of electrons around the central atom.



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

2 In each of the following molecules, the central atom is underlined.

- hydrogen sulphide (H_2S)
- phosphine (PH_3)
- silicon tetrachloride (SiCl_4)

For each molecule,

- a) draw an electron diagram (showing electrons in the *outermost shells* only);
- b) determine the number of electron pairs in the outermost shell of the central atom;
- c) draw a three-dimensional structure;
- d) state its shape.



23.3 Shapes of simple molecules containing only single covalent bonds (p.5)

Molecule	Electron diagram (showing electrons in the outermost shells only)	Number of electron pairs in the outermost shell of the central atom	Three-dimensional structure	Shape
H ₂ S		4		bent / V-shaped
PH ₃		4		trigonal pyramidal
SiCl ₄		4		tetrahedral



23.4 Shapes of simple molecules containing multiple covalent bonds (p.11)

- ◆ When it comes to predicting the shape of a molecule, electrons making up a multiple covalent bond are treated collectively as one group of electrons.

Carbon dioxide molecule

- ◆ In a carbon dioxide molecule, you can consider the carbon atom as being surrounded by two electron groups.
- ◆ The two electron groups repel each other and stay as far apart as possible. This gives the carbon dioxide molecule a **linear** (線形的) shape, with all the three atoms aligned in a straight line.

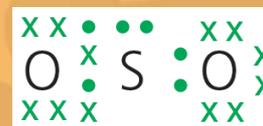




23.4 Shapes of simple molecules containing multiple covalent bonds (p.11)

Practice 23.3

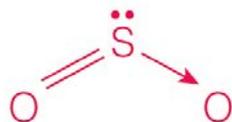
The electron diagrams of two molecules are shown below (showing electrons in the *outermost shells* only).



For each molecule,

- draw a three-dimensional structure;
- state and explain its shape.

SO₂



bent or V-shaped

Consider the sulphur atom as being surrounded by three electron groups.

The three electron groups repel each other and stay as far apart as possible to minimise repulsion and a trigonal planar shape results.

HCN



linear shape

Consider the carbon atom as being surrounded by two electron groups.

The two electron groups repel each other and stay as far apart as possible to minimise repulsion.

This gives the molecule a linear shape.



23.5 Relationship between the number of electron pairs in the outermost shells of central atoms and shapes of simple molecules (p.12)

Table 23.2 Relationship between the number of electron pairs in the outermost shells of central atoms and shapes of simple molecules

Total number of electron pairs	Number of bond pairs	Number of lone pairs	Shape	Example
2	2	0	linear	CO ₂
3	3	0	trigonal planar	BF ₃
4	4	0	tetrahedral	CH ₄
4	3	1	trigonal pyramidal	NH ₃
4	2	2	bent or V-shaped	H ₂ O
5	5	0	trigonal bipyramidal	PCl ₅
6	6	0	octahedral	SF ₆

DSE 2012 Paper 1A Q12 DSE 2016 Paper 1A Q21



Key terms (p.15)

octet rule	八隅體結構	trigonal pyramidal	三角錐體的
boron trifluoride	三氟化硼	bent	角形的
phosphorus pentachloride	五氯化磷	V-shaped	V形的
sulphur hexafluoride	六氟化硫	trigonal bipyramidal	三角雙錐體的
phosphorus trichloride	三氯化磷	octahedral	八面體的
valence shell electron pair repulsion theory	價層電子對相斥學說	linear	線形的
trigonal planar	平面三角的	buckminsterfullerene	布克碳
tetrahedral	四面體的	fullerene	富勒烯



Summary (p.16)

- 1 A molecule whose central atom not having enough electrons in its outermost shell to achieve octet or having an expanded octet (i.e. more than 8 electrons) in its outermost shell does not obey the octet rule. Examples are BF_3 , PCl_5 and SF_6 .



Summary (p.16)

2 The following table summarises the relationship between the number of electron pairs in the outermost shells of central atoms and shapes of simple molecules.

Total number of electron pairs	Number of bond pairs	Number of lone pairs	Shape	Example
2	2	0	linear	CO ₂
3	3	0	trigonal planar	BF ₃
4	4	0	tetrahedral	CH ₄
4	3	1	trigonal pyramidal	NH ₃
4	2	2	bent or V-shaped	H ₂ O
5	5	0	trigonal bipyramidal	PCl ₅
6	6	0	octahedral	SF ₆



Unit Exercise (p.17)

Note: Questions are rated according to ascending level of difficulty (from 1 to 5):



question targeted at level 3 and above;



question targeted at level 4 and above;



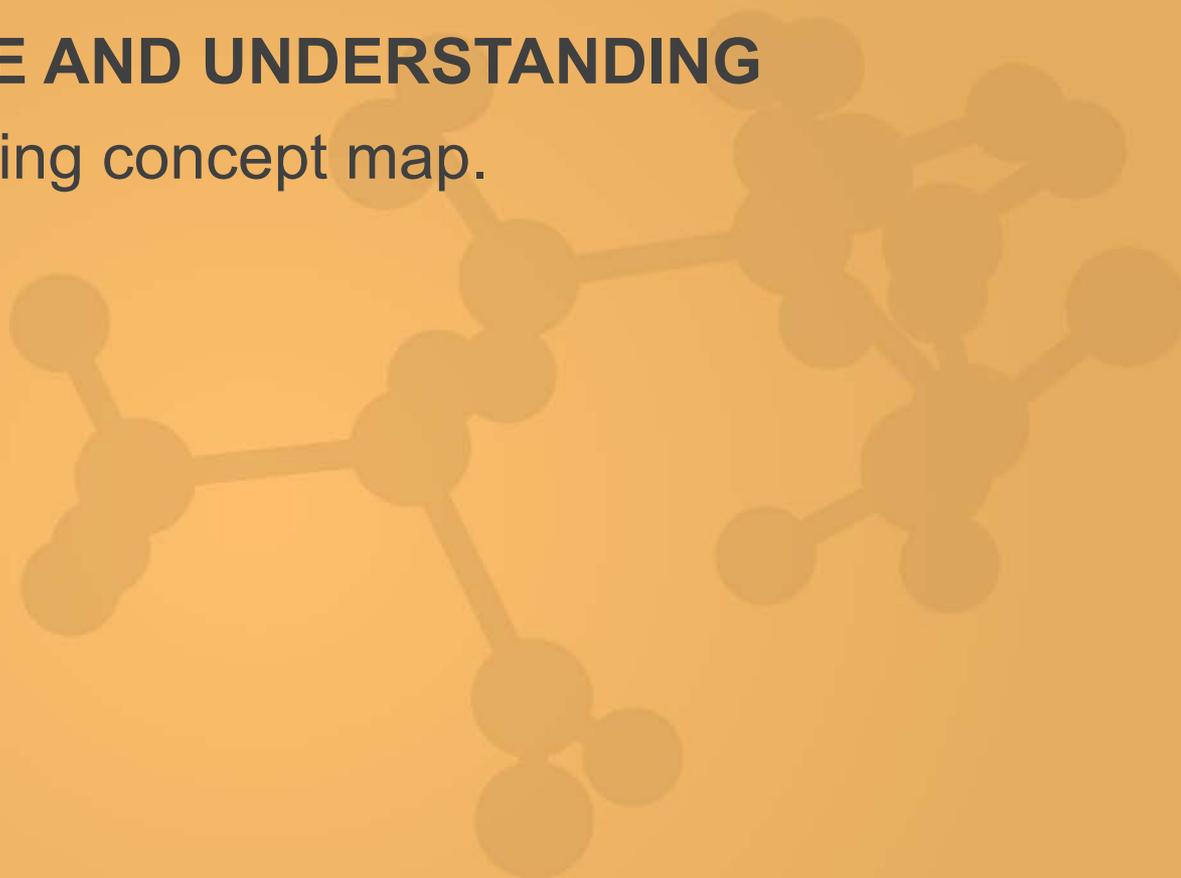
question targeted at level 5.

' * ' indicates 1 mark is given for effective communication.

Unit Exercise (p.17)

PART I KNOWLEDGE AND UNDERSTANDING

1 Complete the following concept map.

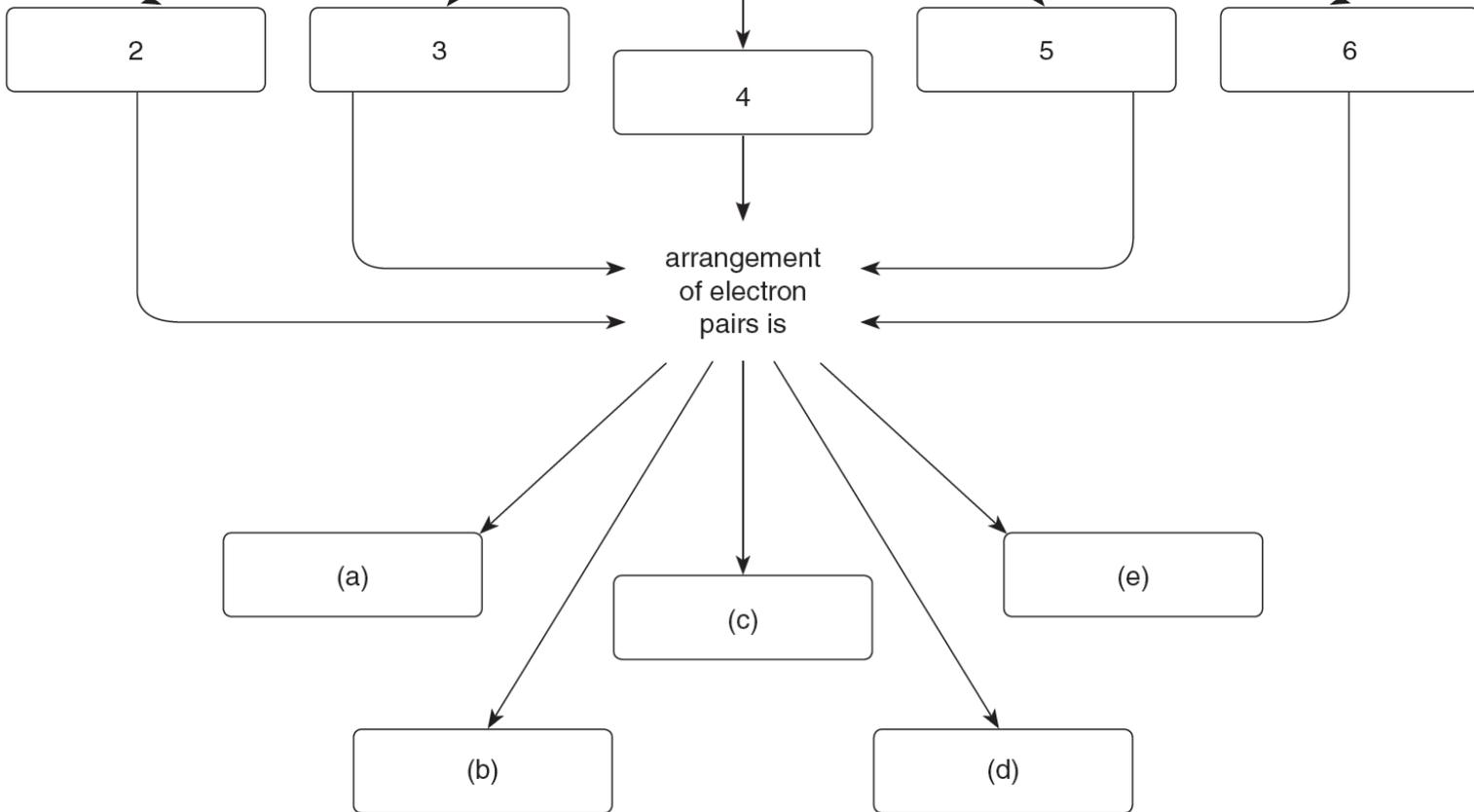




shape of molecule

- a) linear
- b) trigonal planar
- c) tetrahedral
- d) trigonal bipyramidal
- e) octahedral

if the number of electron pairs in the outermost shell of the central atom is



 Unit Exercise (p.17)**PART II MULTIPLE CHOICE QUESTIONS**

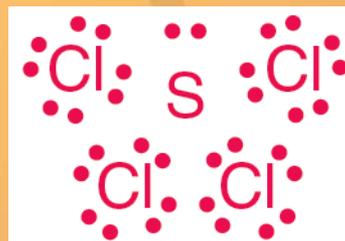
2 Which of the following chemical species does NOT follow the octet rule?

- A K_2O
- B CaO
- C NF_3
- D SCl_4

Answer: D

Explanation:

The electron diagram of SCl_4 is shown below. SCl_4 does NOT follow the octet rule.



(showing electrons in the outermost shells only)



Unit Exercise (p.17)

3 In the species below, the underlined atom is the central atom, and all non-central atoms have an octet electronic arrangement. In which of them does the central atom NOT have an octet electronic arrangement?

- A SF₂
- B CF₂
- C CS₂
- D NCl₃

Answer: B

(HKDSE, Paper 1A, 2015, 11)



Unit Exercise (p.17)

4 Which of the following molecules has a planar shape?

A BF_3

B PF_3

C CF_4

D SF_6

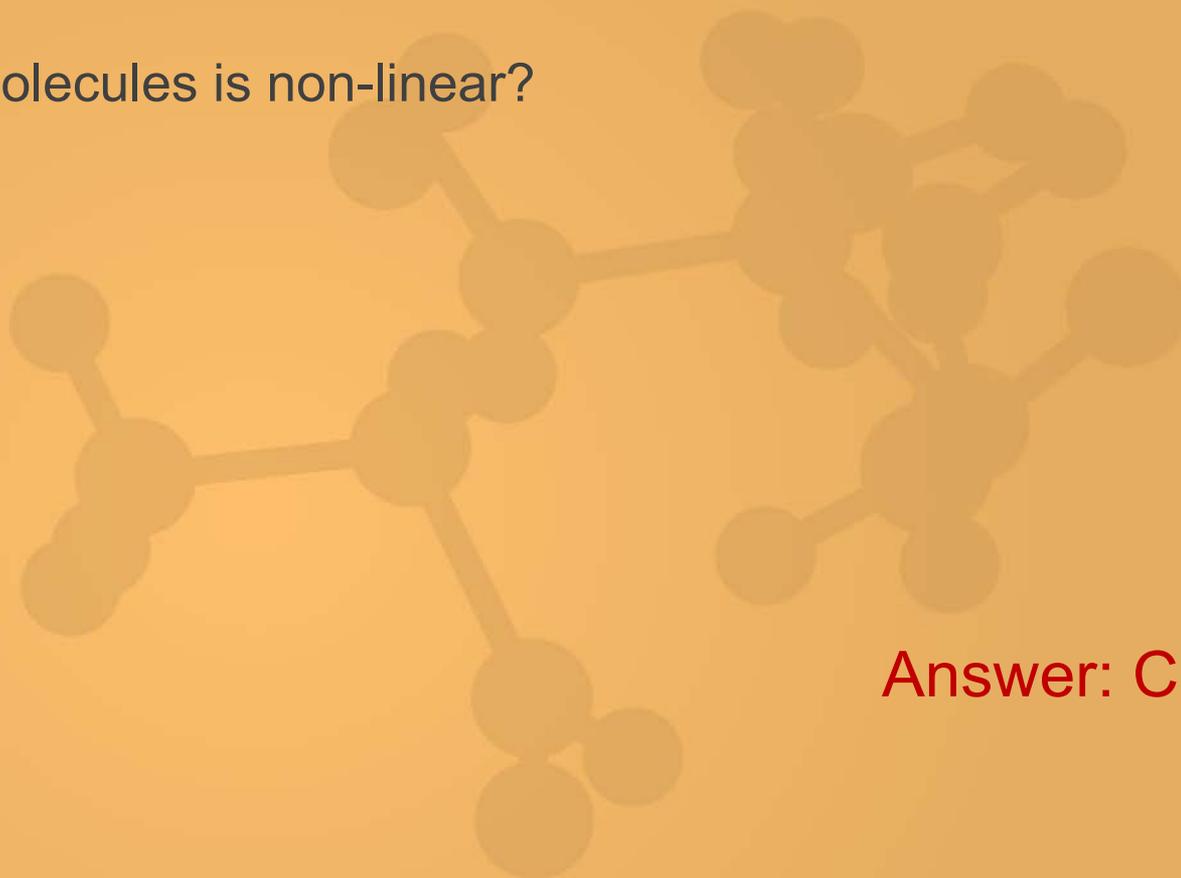
Answer: A



Unit Exercise (p.17)

5 Which of the following molecules is non-linear?

- A CO_2
- B HCN
- C H_2O
- D HCl



Answer: C



Unit Exercise (p.17)

6 Which of the following structures is expected to have three bond pairs and one lone pair in the outermost shell of the central atom?

A Square

B Trigonal planar

C Trigonal pyramidal

D Octahedral

Answer: C



Unit Exercise (p.17)

7 Which of the following chemical species does NOT have a pyramidal shape?

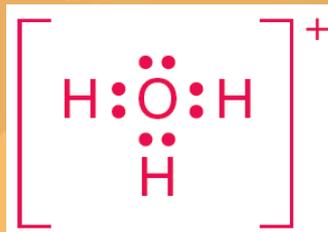


- A BF_3
- B NCl_3
- C H_3O^+
- D PH_3

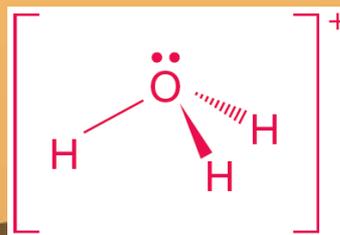
Answer: A

Explanation:

Option C — The electron diagram of H_3O^+ is shown below.



(showing electrons in the outermost shells only) H_3O^+ has a pyramidal shape.





Unit Exercise (p.17)

8 In which of the following pairs do the molecules have an identical shape?

A BCl_3 , PCl_3

B BF_3 , NF_3

C CCl_4 , CH_4

D CO_2 , H_2

Answer: C

Explanation:

Both CCl_4 and CH_4 have a tetrahedral shape.



Unit Exercise (p.17)

9 Which of the following molecules is NOT planar?

A BH_3

B COCl_2

C HCHO

D PF_3

Answer: D



Unit Exercise (p.17)

10 Which of the following molecules have non-octet structures?



(1) NO_2

(2) PBr_3

(3) BCl_3

A (1) and (2) only

B (1) and (3) only

C (2) and (3) only

D (1), (2) and (3)

Answer: B

(HKDSE, Paper 1A, 2014, 22)



Unit Exercise (p.17)

11 Which of the following molecules have a similar shape?

(1) BCl_3

(2) NH_3

(3) PF_3

A (1) and (2) only

B (1) and (3) only

C (2) and (3) only

D (1), (2) and (3)

Answer: C

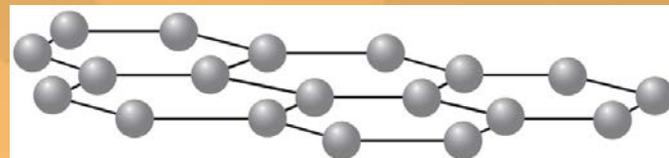
(HKDSE, Paper 1A, 2016, 21)



Unit Exercise (p.17)



12 Graphene is an individual single layer of graphite. Part of its structure is shown below:



the structure of graphene

Which of the following statements about graphene are correct?

- (1) It is a strong material.
- (2) It is a non-conductor of electricity.
- (3) It has a high melting point.

Answer: B

Explanation:

- A (1) and (2) only
- B (1) and (3) only
- C (2) and (3) only
- D (1), (2) and (3)

- (1) Graphene is strong because it has a giant covalent structure. It is difficult to break the strong covalent bonds between the atoms.
- (2) Graphene can conduct electricity because it has delocalised electrons.
- (3) A lot of heat is needed to break the strong covalent bonds between the carbon atoms during melting. Thus, graphene has a high melting point.

 Unit Exercise (p.17)**PART III STRUCTURED QUESTIONS**

- 13 Suggest a reason why phosphorus can form both PCl_3 and PCl_5 while nitrogen can only form NCl_3 .

Phosphorus can form compounds with more than 8 electrons in the outermost shell of its atom. /

Nitrogen CANNOT form compounds with more than 8 electrons in the outermost shell of its atom. (1)



Unit Exercise (p.17)

14 For each of the following molecules,

- draw an electron diagram, showing electrons in the *outermost shells* only;
- draw a three-dimensional structure;
- give its shape.





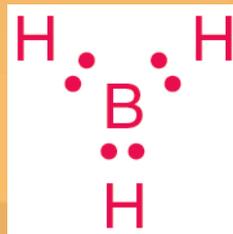
Unit Exercise (p.17)

Molecule	Electron diagram (showing electrons in the outermost shells only)	Three-dimensional structure	Shape
CCl ₄	 (1)	 (1)	tetrahedral (1)
NCl ₃	 (1)	 (1)	trigonal pyramidal (1)
CO ₂	 (1)	 (1)	linear (1)
H ₂ O	 (1)	 (1)	bent / V-shaped (1)

 Unit Exercise (p.17)

15 Borane (BH_3) is a reactive compound that has been used as a rocket propellant.

a) Draw the electron diagram of a borane molecule, showing electrons in the outermost shells only.



b) Predict the shape of a borane molecule. Explain why BH_3 has this shape.

Trigonal planar shape (1)

In a BH_3 molecule, there are three bond pairs in the outermost shell of the central boron atom. These three electron pairs stay as far apart as possible to minimise repulsion and a trigonal planar arrangement results. (1)

 Unit Exercise (p.17)

16 Carbon disulphide (CS_2) is a volatile, flammable liquid which is produced in small quantities in volcanoes.

a) Draw the electron diagram of a carbon disulphide molecule, showing electrons in the *outermost shells* only.



b) Predict and explain the shape of the molecule.

Linear shape (1)

Consider the carbon atom as being surrounded by two electron groups. The two groups repel each other and stay as far apart as possible to minimise repulsion and a linear arrangement results. (1)



Unit Exercise (p.17)

17 Sulphur can form sulphur difluoride (SF_2) and sulphur hexafluoride (SF_6).

a) Draw an electron diagram of each fluoride, showing electrons in the *outermost shells* only.

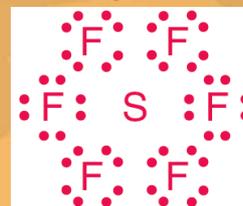
Electron diagram of SF_2 :



(1)

(showing electrons in the outermost shells only)

Electron diagram of SF_6 :



(1)

(showing electrons in the outermost shells only)

b) Explain whether sulphur is obeying the octet rule in each fluoride.

Sulphur in SF_2 obeys the octet rule.

Sulphur in SF_6 does NOT obey the octet rule.

There are 12 electrons in the outermost shell of the sulphur atom. (1)



Unit Exercise (p.17)

- c) Draw the three-dimensional structure of the SF₂ molecule and state the shape of the molecule.



(1)

Bent or V-shaped (1)

- d) The SF₆ molecule has an octahedral shape. Explain why.

The six bond pairs in the outermost shell of the central sulphur atom stay as far apart as possible to minimise repulsion. (1)



Unit Exercise (p.17)

18 Chlorine forms the molecules CH_2Cl_2 , CCl_4 and PCl_5 .



a) Identify which of the molecules has a central atom with non-octet electronic arrangement. Explain your answer.

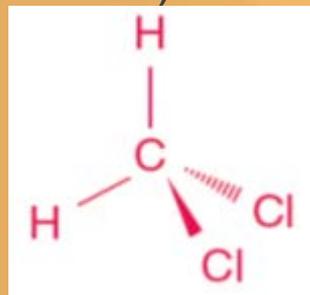


There are 10 electrons in the outermost shell of the central phosphorus atom. (1)

b) i) Use your understanding of electron pair repulsion, draw the three-dimensional structure of each molecule.

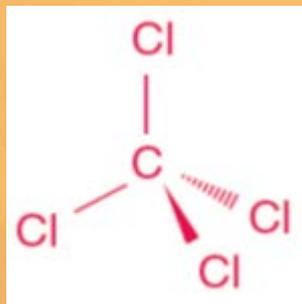
Include all lone pair(s) of electrons that can influence the structure.

ii) Name the shape of each molecule.



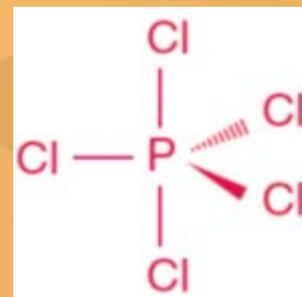
(1)

Tetrahedral (1)



(1)

Tetrahedral (1)



(1)

Trigonal bipyramidal (1)

 Unit Exercise (p.17)

19 This question is about the fluorides BF_3 , NF_3 and OF_2 .

a) Name the shape of a BF_3 molecule.

Trigonal planar shape (1)

b) The shape of a NF_3 molecule is similar to that of a NH_3 molecule.
Explain why it is so.

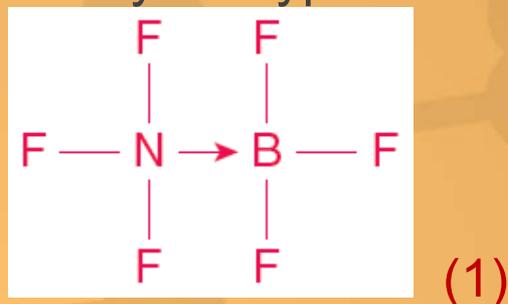
The nitrogen atoms in both NF_3 and NH_3 have three bond pairs of electrons and one lone pair of electrons in the outermost shell.

The repulsion between these electron pairs causes both NF_3 and NH_3 to adopt a trigonal pyramidal shape. (1)



Unit Exercise (p.17)

- c) Draw a diagram to show the bonding in the single product of the reaction between BF_3 and NF_3 . Identify the type of bond that forms between these two molecules.



Dative covalent bond (1)

- d) Draw the three-dimensional structure of an OF_2 molecule. Explain why the molecule has this structure.

The four electron pairs in the outermost shell of the central oxygen atom adopt a tetrahedral arrangement. (1)

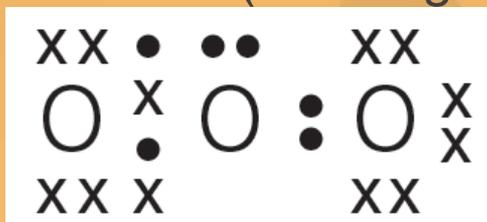
However, as there are only two fluorine atoms bonded to the oxygen atom, the shape of the molecule is bent or V-shaped. (1)





Unit Exercise (p.17)

20 Ozone (O_3) is a much less stable triatomic form of oxygen. The electron diagram of ozone is shown below (showing electrons in the *outermost shells* only).



Explain why an ozone molecule is V-shaped.

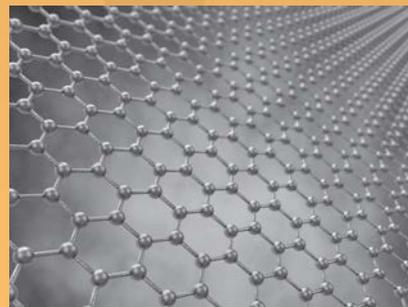
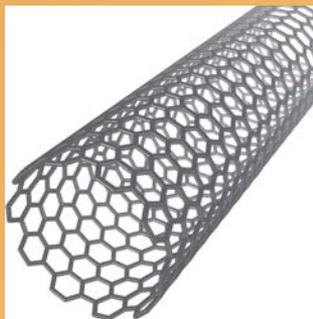
There are two electron groups and one lone pair in the outermost shell of the central oxygen atom. The three groups of electron stay as far apart as possible to minimise repulsion and a trigonal planar arrangement results.

(1)

However, as there are only two oxygen atoms bonded to the central oxygen atom, the shape of the molecule is bent or V-shaped.

 Unit Exercise (p.17)

21 Carbon atoms are used to make nanotubes.



The left figure shows that carbon atoms in a nanotube are bonded like a single layer of atoms in graphite.

The right figure shows the structure of a single layer of graphite.

a) Suggest why carbon nanotubes are used as lubricants.

Weak forces exist between carbon nanotubes. (1)

Carbon nanotubes can slide past each other easily. (1)

b) Explain why graphite can conduct electricity.

There are delocalised electrons in graphite. (1)

(AQA GCSE (Higher Tier), Additional Science, Unit C2, Jun. 2014, 5(a)–(b))

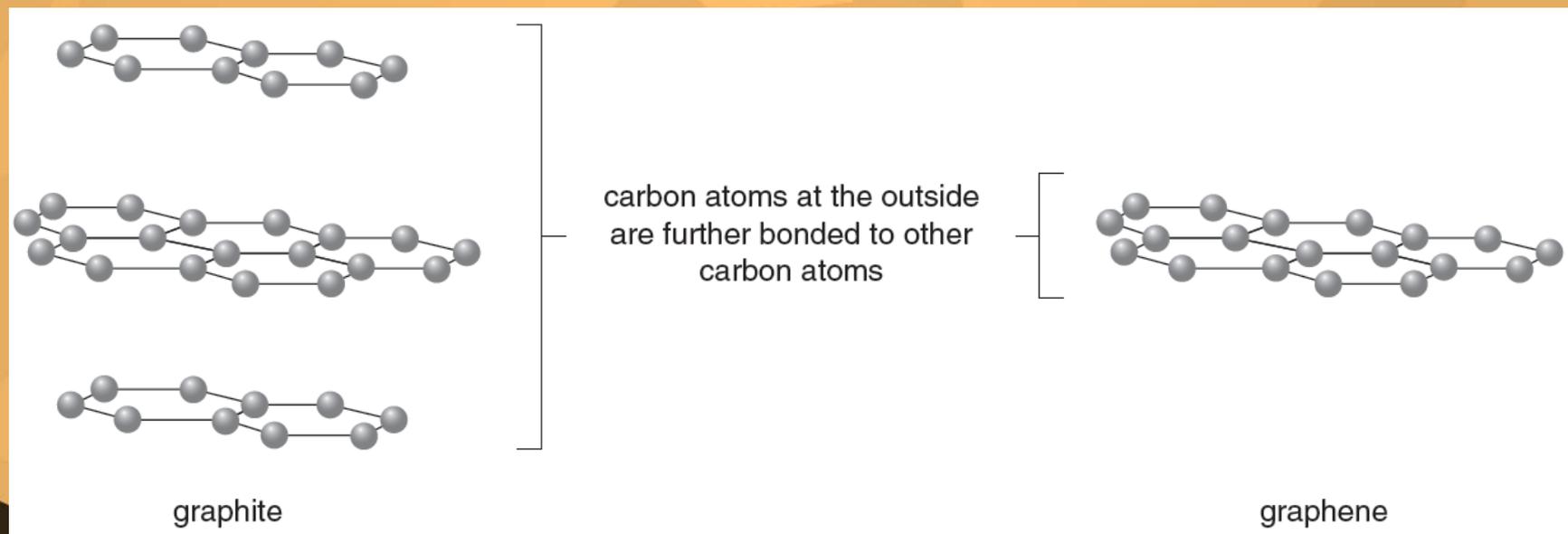
 Unit Exercise (p.17)

22 The 2010 Nobel Prize for Physics was awarded for the discovery of a new material called graphene. It consists of a single layer of carbon atoms obtained from graphite.



Graphene is a good conductor of electricity and very strong. It has a high melting point.

The structures of graphite and graphene are shown below:





Unit Exercise (p.17)

a) Explain why graphene can conduct electricity.

In graphene, each carbon atom is covalently bonded to three neighbouring carbon atoms. An unbonded outermost shell electron is present in each carbon atom. These unbonded electrons can move throughout the structure. Thus, graphene can conduct electricity. (1)

b) Explain why graphene has a high melting point.

Graphene has a giant covalent structure.

To melt graphene, lots of strong covalent bonds between atoms have to be broken. A lot of heat is needed. (1)

c) Scientists believe that graphene can replace steel in making cars. Apart from the consideration about its strength, suggest ONE reason why graphene can be a better material than steel in making cars.

Any one of the following:

- Graphene has a lower density. (1)
- Graphene is not easily corroded / is chemically inert. (1)