

3.5 SHAPES OF MOLECULES

Learning outcomes

Candidates should be able to:

- state and explain the shapes of, and bond angles in, molecules by using VSEPR theory, including as simple examples:
 - CO₂ (linear, 180°)
 - BF₃ (trigonal planar, 120°)
 - CH₄ (tetrahedral, 109.5°)
 - NH₃ (pyramidal, 107°)
 - H₂O (non-linear, 104.5°)
 - PF₅ (trigonal bipyramidal, 120° and 90°)
 - SF₆ (octahedral, 90°)
- predict the shapes of, and bond angles in, molecules and ions analogous to those specified in 3.5.1

VSEPR theory

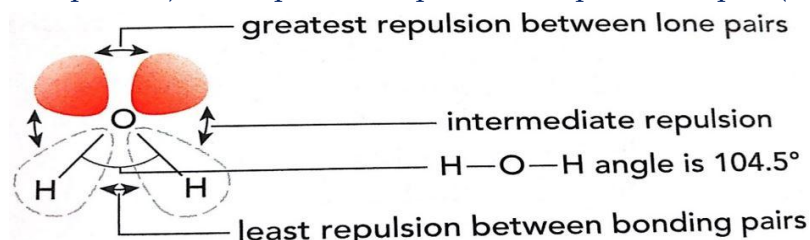
Because all electrons have the same (negative) charge, they repel each other when they are close together. So, a pair of electrons in the bonds surrounding the central atom in a molecule will repel other electron pairs. This repulsion forces the pairs of electrons apart until the repulsive forces are minimized.

The shape and bond angles of a covalently bonded molecule depend on:

- the number of pairs of electrons around each atom
 - whether these pairs are lone pairs or bonding pairs.
- The valence shell electrons are the electrons in the main outer shell.
- Pairs of electrons repel each other because they have the same charge.
- A lone pair of electrons repel each other more than a bonded pair of electrons.
- Repulsion between multiple and single bonds is treated the same as for repulsion between single bonds. Repulsions between pairs of double bonds are greater.
- The shape of a molecule can be deduced using this theory, with the most stable shape being that which minimises the forces of repulsion.

The order of repulsion is:

lone pair-lone pair (most repulsion) > lone pair-bond pair > bond pair-bond pair (least repulsion).



[BF₃](#)

- Beryllium oxide reacts with hydrochloric acid to form molecules of BeCl₂. Deduce the bond angle in BeCl₂.

[1]

- At 1000°C, aluminium chloride exists as AlCl₃(g). State the bond angle in AlCl₃(g).

[1]

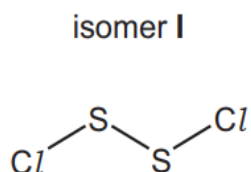
3. When gallium is heated in excess chlorine, gallium trichloride, GaCl_3 , is made.
Draw the shape of the gallium trichloride molecule and suggest the $\text{Cl}-\text{Ga}-\text{Cl}$ bond angle. [2]
4. Silicon shows the same type of bonding and structure as diamond.
Silicon reacts with magnesium to form Mg_2Si .
Solid Mg_2Si reacts with dilute hydrochloric acid to form gaseous SiH_4 and a solution of magnesium chloride.
Predict the shape of the SiH_4 molecule. [1]
5. Suggest the shape of a molecule of H_2S . [1]
6. A molecule of SCl_2 contains two $\text{S}-\text{Cl}$ covalent bonds.
(i) Complete the dot-and-cross diagram in Fig. 2.1 to show the arrangement of the outer electrons in a molecule of SCl_2 .
Use $\times$ to show electrons from the chlorine atoms.
Use $\bullet$ to show electrons from the sulfur atom.
-
- (ii) Predict the shape of, and bond angle in, a molecule of SCl_2 by using VSEPR theory. [2]

shape bond angle

7. Predict the shape of the SCl_2 molecule. [1]

8. Suggest the bond angle in a molecule of CS_2 . [1]

9. Suggest a value for the Cl-S-S bond angle in isomer I.



Explain your answer. [2]

10. I_2 reacts with NH_3 to form NI_3 .
Predict the shape of a molecule of NI_3 . Explain your answer.

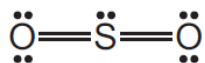
shape

explanation

..... [2]

11. NCl_3 is a yellow liquid that can be used to bleach flour.
Predict the shape of the NCl_3 molecule and the Cl-N-Cl bond angle. [1]

1. The structure of the sulfur dioxide molecule is shown.



What is the shape of the sulfur dioxide molecule?

A linear

B non-linear

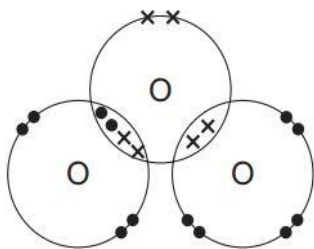
C pyramidal

D tetrahedral

12. Complete the table to name the shape and give the bond angle of each species.

	Name of Shape	Bond angle
CO_2		
NH_3		
H_2O		

2. VSEPR theory should be used in answering this question.
The dot-and-cross diagram for an ozone, O_3 , molecule is shown.



What is the predicted bond angle in this molecule?

- A 107° B 109.5° C 117° D 120°

3. Which row is correct?

	Molecule	total number of pairs of electrons in the valence shell of the central atom	shape
A	CO_2	two	linear
B	BF_3	three	trigonal planar
C	NH_3	four	regular tetrahedral
D	PF_5	six	octahedral

4. Which molecules are planar?

A BCl_3

B NH_3

C PH_3

5. In which pair do the molecules have the same shape as each other?

a. H_2O and CO_2

b. H_2O and SCl_2

c. NH_3 and BH_3

d. SCl_2 and $BeCl_2$

6. What are the shapes of the molecules of water and boron trifluoride?

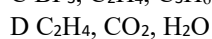
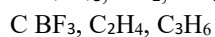
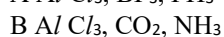
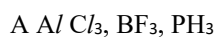
	H_2O	BF_3
A	linear	pyramidal
B	linear	trigonal
C	non-linear	pyramidal
D	non-linear	trigonal

7. Which of the following molecules and ions have a regular trigonal planar shape?

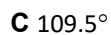


- a. all of them b. only I c. I and II d. I and III

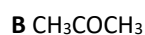
8. In which set do all the molecules have all their atoms arranged in one plane?



9. What is the bond angle in the ammonium ion?



10. Which molecule or ion contains the smallest bond angle?



11. Ammonia reacts with acids to form the ammonium ion.
Which row is correct?

	shape of NH_4^+	bond angle in NH_4^+ / $^\circ$
A	pyramidal	107
B	pyramidal	109.5
C	tetrahedral	107
D	tetrahedral	109.5

12. When ammonia, NH_3 , is dissolved in water, a small concentration of ammonium ions, NH_4^+ , is formed. Which row is correct?

	number of electrons in one ammonium ion	change of the H–N–H angle from ammonia to the ammonium ion
A	8	decreases
B	8	increases
C	10	decreases
D	10	increases

13. Which row is correct?

	shape		bonds present	
	ammonia molecule	ammonium ion	ammonia molecule	ammonium ion
A	pyramidal	regular tetrahedral	σ	σ
B	pyramidal	regular tetrahedral	σ	π
C	regular tetrahedral	pyramidal	σ	σ
D	regular tetrahedral	pyramidal	π	σ

14. Two compounds of boron are sodium borohydride, NaBH_4 , and boron trifluoride, BF_3 . What are the shapes of the borohydride ion and the boron trifluoride molecule?

	borohydride ion	boron trifluoride
A	square planar	pyramidal
B	square planar	trigonal planar
C	tetrahedral	pyramidal
D	tetrahedral	trigonal planar

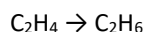
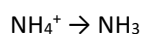
15. AlCl_3 vapour forms molecules with formula Al_2Cl_6 as it is cooled. What happens to the bond angles during the change from AlCl_3 to Al_2Cl_6 ?

- A Some decrease, some remain the same.
 B Some increase, some remain the same.
 C They all decrease.
 D They all increase.

16. Aluminium chloride exists as Al_2Cl_6 molecules at room temperature. When heated to a high temperature, AlCl_3 molecules are formed. What are the arrangements of the bonding pairs of electrons around the aluminium atom in the two forms of aluminium chloride?

	AlCl_3	Al_2Cl_6
A	planar	planar
B	planar	tetrahedral
C	tetrahedral	tetrahedral
D	tetrahedral	octahedral

17. Two conversions are outlined below.

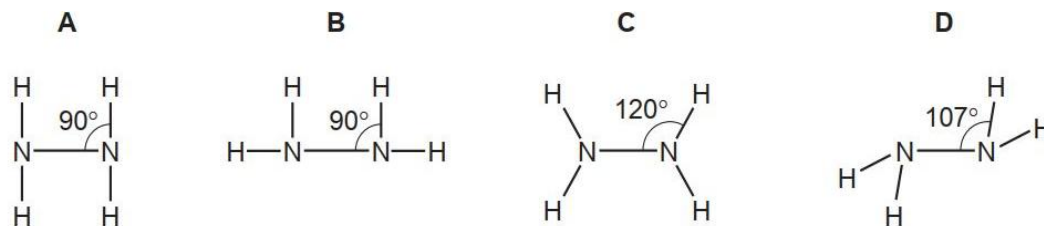


What similar feature do these two conversions have?

- E a lone pair of electrons in the product
 F change in oxidation state of an element

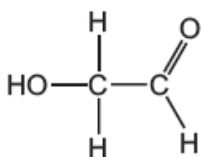
- G decrease in bond angle of the species involved
 H disappearance of a π bond

18. What is the most likely shape of a molecule of hydrazine, N_2H_4 ?



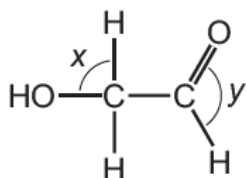
13. Hydroxyethanal, HOCH_2CHO , has been observed in dust clouds near the centre of our galaxy.

hydroxyethanal

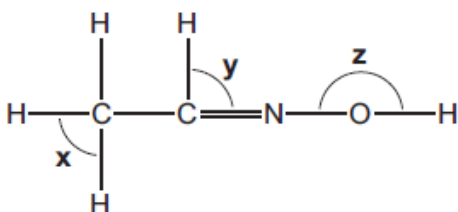


Predict the bond angles labelled x and y in the diagram of hydroxyethanal.

[2]



19. Ethanal reacts with hydroxylamine, NH_2OH , to form the molecule shown.



What is the order of **increasing** bond angle in this structure from smallest to largest?

A z, x, y

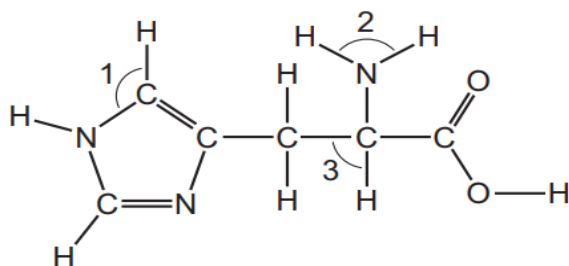
B y, z, x

C x, z, y

D z, y, x

20. Histidine is an amino acid.

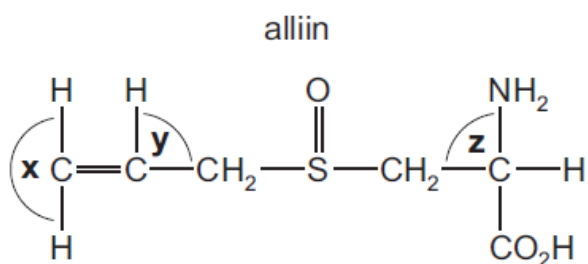
histidine



What are the approximate bond angles 1, 2, and 3?

	1	2	3
A	109.5°	107°	90°
B	120°	107°	109.5°
C	120°	120°	90°
D	120°	120°	109.5°

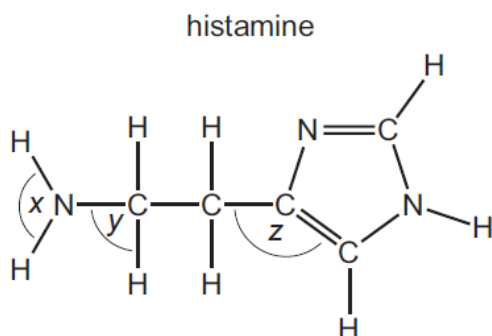
21. The structural formula of alliin is shown.



What are the approximate bond angles **x**, **y** and **z** in a molecule of alliin?

	x	y	z
A	90°	90°	109°
B	120°	109°	90°
C	120°	120°	109°
D	180°	109°	109°

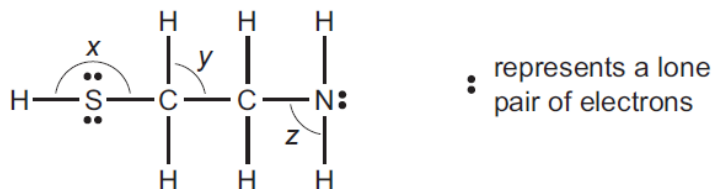
22. The structure of the hormone histamine is shown.



Which row contains the bond angles **x**, **y** and **z** in histamine in the correct order from the smallest to the largest?

	smallest bond angle	→	largest bond angle
A	x	y	z
B	y	x	z
C	y	z	x
D	z	y	x

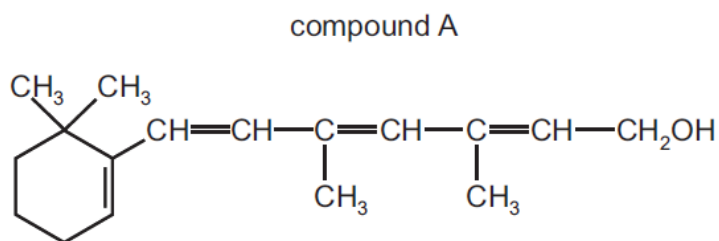
23. Three bond angles are labelled on the molecule shown.



What is the order of decreasing size of the bond angles x , y and z ?

largest	Smallest		
A	X	y	z
B	X	z	y
C	Y	z	x
D	Z	y	x

24. The structure of compound A is shown.



Some of the carbon atoms in compound A have a tetrahedral arrangement of bonds.
Some of the carbon atoms in compound A have a trigonal planar arrangement of bonds.
How many carbon atoms are there of each type?

	tetrahedral	trigonal planar
A	5	12
B	8	8
C	9	6
D	9	8

25. Which statement about the Cl-N=O molecule is correct?

- A Each molecule contains one Sigma and two Pi bonds
- B It is a non-polar molecule.
- C It is a linear molecule.
- D The nitrogen atom is sp^2 hybridised.

26. Phosphorus forms two chlorides. Phosphorus(III) chloride, PCl_3 , is a covalent liquid. Phosphorus(V) chloride is an ionic solid. One of the ions present is $[\text{PCl}_4]^+$.
What is the shape of the PCl_3 molecule and the $[\text{PCl}_4]^+$ ion?

	PCl_3	$[\text{PCl}_4]^+$
A	pyramidal	square planar
B	pyramidal	tetrahedral
C	tetrahedral	square planar
D	trigonal planar	tetrahedral

27. Which molecules contain at least one bond angle of 120° ?

1 C₂H₄

2 PF₅

3 NC₃

28. Which molecule does **not** have any 90° or 180° bond angles?

A C₂H₆

B CO₂

C PF₅

D SF₆

29. Which shape is correctly predicted by VSEPR theory?

	number of bonded electron pairs	number of lone pairs	shape
A	2	2	linear
B	2	2	tetrahedral
C	3	1	pyramidal
D	3	1	trigonal planar

14. An excess of Cl₂ reacts with phosphorus to form PCl₅.

PCl₅ is a simple molecule in the gas phase.

It also exists in a solid form as two ions, PCl₄⁺ and PCl₆⁻.

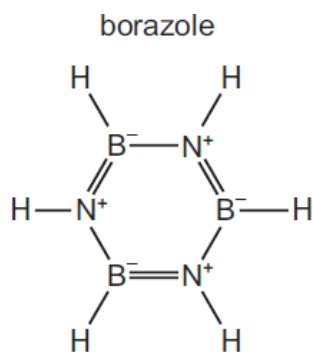
Complete Table 2.2 to identify the shapes of each of these species.

species	PCl ₅	PCl ₄ ⁺	PCl ₆ ⁻
shape		tetrahedral	

15. Tellurium is an element in Group 16. The most common isotope of tellurium is ¹³⁰Te. Its electronic configuration is [Kr] 4d¹⁰ 5s² 5p⁴.

Te reacts with F₂ at 150°C to form TeF_x. Molecules of TeF_x are octahedral with bond angles of 90° . Explain why TeF_x is octahedral with bond angles of 90° .

30. A structure for borazole, $\text{N}_3\text{B}_3\text{H}_6$, is shown.



Which shape is borazole and how many π electrons are there in the structure?

	shape	number of π electrons
A	non-planar	3
B	non-planar	6
C	planar	3
D	planar	6

31. Arsenic forms a compound with fluorine. In this compound, the arsenic atom has no lone pair of electrons and there are no dative bonds.
 Selenium also forms a compound with fluorine. In this compound, the selenium atom has no lone pair of electrons and there are no dative bonds.
 In which compounds are there two different bond angles?
 (In this question, 180° bond angles should be ignored.)
- A** both arsenic fluoride and selenium fluoride
B arsenic fluoride only
C selenium fluoride only
D neither arsenic fluoride nor selenium fluoride

32. Atom X is the central atom in a molecule.
 In this molecule, atom X has four pairs of valence electrons in its outer shell.
 The four pairs of valence electrons include at least one bond pair and at least one lone pair.
 What could be a possible shape for the molecule?
- A** linear
B non-linear
C trigonal bipyramidal
D trigonal planar

33. In which pair is the bond angle in the first species smaller than the smallest bond angle in the second species?
- A** CH_4 and SF_6
B CO_2 and BF_3
C H_2O and H_3O^+
D NH_4^+ and NH_3

34. Which row is correct?

	smallest bond angle	→	largest bond angle
A	H ₂ O	NH ₃	BF ₃
B	BF ₃	NH ₃	H ₂ O
C	NH ₃	H ₂ O	BF ₃
D	H ₂ O	BF ₃	NH ₃

*****This is not a complete note. It is to guide you. It is recommended to study the prescribed textbooks along with this material. *****