

Shapes of molecules and VSEPR: AS Chemistry notes with practice

These notes cover shapes of molecules and ions for Cambridge International AS Chemistry (9701). You need to be able to state the shapes and bond angles of a set of standard molecules, explain them using electron-pair repulsion, and then predict the shape of any unfamiliar molecule or ion in the exam. The topic also links to polarity, intermolecular forces and to sigma and pi bonds, which are covered at the end.

1. Electron-pair repulsion theory

1.1 The key idea

The electrons around a central atom in a molecule exist in pairs. Each pair occupies a region of negative charge. Because these regions all carry negative charge, they repel one another and arrange themselves in space so that they are as far apart as possible. This arrangement, and therefore the positions of the atoms bonded to the central atom, decides the shape of the molecule.

Learn word for word: valence shell electron pair repulsion (VSEPR) theory

Electron pairs in the outer shell of the central atom repel each other and move as far apart as possible to minimise repulsion. The shape of the molecule is decided by the number of bonding pairs and lone pairs around the central atom.

1.2 Bonding pairs and lone pairs

A **bonding pair** is a pair of electrons shared between the central atom and another atom in a covalent bond. A **lone pair** (non-bonding pair) is a pair of outer-shell electrons on the central atom that is not involved in bonding.

Lone pairs are held closer to the central atom than bonding pairs, because they are attracted by only one nucleus. As a result, a lone pair occupies more space near the central atom and repels other electron pairs more strongly than a bonding pair does.

Learn: the order of repulsion

lone pair-lone pair repulsion > lone pair-bonding pair repulsion > bonding pair-bonding pair repulsion

The consequence is that each lone pair pushes the bonding pairs slightly closer together, reducing the bond angle. A useful rule of thumb for molecules based on four electron pairs is that each lone pair reduces the bond angle by about 2.5° . This is why the bond angle drops from 109.5° in CH_4 to 107° in NH_3 and 104.5° in H_2O .

1.3 Multiple bonds count as one region

A double or triple bond points in one direction from the central atom, so for working out the shape it counts as a single region of electron density, just like a single bond. For example, in CO_2 ($\text{O}=\text{C}=\text{O}$) the carbon has two regions of electron density, so the molecule is linear.



Some textbooks talk about "regions of electron density" or "electron domains" rather than "electron pairs" so that multiple bonds fit the rules neatly. Both language styles are accepted; just be consistent.

2. The shapes and bond angles you must know

The table lists the seven standard shapes. Learn the name, the bond angle and at least one example of each.

Bonding pairs	Lone pairs	Shape	Bond angle	Example
2	0	linear	180°	CO ₂ , BeCl ₂
3	0	trigonal planar	120°	BF ₃
4	0	tetrahedral	109.5°	CH ₄
3	1	(trigonal) pyramidal	107°	NH ₃
2	2	non-linear (bent, V-shaped)	104.5°	H ₂ O
5	0	trigonal bipyramidal	120° and 90°	PF ₅ , PCl ₅ (gas)
6	0	octahedral	90°	SF ₆

2.1 Linear: CO₂ and BeCl₂

Beryllium has two outer electrons. In BeCl₂ (as a gas molecule) each is shared with a chlorine atom, giving two bonding pairs and no lone pairs around Be. Two regions are furthest apart at 180°, on opposite sides of the central atom. Note that Be has only four electrons in its outer shell here: it does not obey the octet rule.

In CO₂ carbon forms two double bonds. Each double bond counts as one region, so there are two regions and the molecule is linear with an O=C=O angle of 180°.

2.2 Trigonal planar: BF₃

Boron has three outer electrons, each shared with a fluorine atom. There are three bonding pairs and no lone pairs. Three regions are furthest apart when they lie in one plane at 120° to each other. Boron has only six electrons in its outer shell, which is why BF₃ can accept a lone pair from another molecule to form a dative bond.

2.3 Tetrahedral: CH₄

Carbon has four outer electrons, each paired with an electron from a hydrogen atom: four bonding pairs, no lone pairs. Four regions are furthest apart in three dimensions when they point to the corners of a regular tetrahedron, with all H-C-H angles 109.5°. A common mistake is to draw methane as a flat cross with 90° angles; a flat arrangement would put the pairs closer together than a tetrahedron does.

2.4 Pyramidal: NH₃

Nitrogen has five outer electrons. Three are shared with hydrogen atoms and the remaining two form a lone pair. The four electron pairs are arranged roughly tetrahedrally, but the shape names only the positions of the atoms, so the molecule is described as (trigonal) pyramidal: the nitrogen sits at the top of a pyramid with three hydrogens forming the base. The lone pair repels the bonding pairs more

strongly than they repel each other, squeezing the H-N-H angle from 109.5° to 107° .

2.5 Non-linear: H₂O

Oxygen has six outer electrons. Two are shared with hydrogen atoms and four form two lone pairs. Again four pairs are arranged roughly tetrahedrally, but two of the positions are lone pairs, so the atoms form a bent shape. With two lone pairs, the extra repulsion closes the H-O-H angle further, to 104.5° .

Exam tip: Electron-pair arrangement and molecular shape are not the same thing. In NH₃ and H₂O the four electron pairs are arranged tetrahedrally, but the shapes are pyramidal and non-linear, because a shape describes where the **atoms** are. Never call water "tetrahedral".

2.6 Trigonal bipyramidal: PF₅

Phosphorus has five outer electrons, all used to bond to five fluorine atoms: five bonding pairs, no lone pairs. Three fluorine atoms lie in a plane around the phosphorus at 120° to each other (the **equatorial** positions). The other two lie above and below this plane, at 90° to it (the **axial** positions). There are therefore two different bond angles: 120° between equatorial bonds and 90° between an axial bond and an equatorial bond. The angle between the two axial bonds is 180° .

Here phosphorus has ten electrons in its outer shell. Elements in Period 3 and below can do this because they have a third shell that can hold more than eight electrons. This is called an expanded octet.

2.7 Octahedral: SF₆

Sulfur has six outer electrons, all used to bond to six fluorine atoms: six bonding pairs, no lone pairs, and twelve electrons in sulfur's outer shell. The six bonds point to the corners of an octahedron: four in a square plane and one above and one below. Every adjacent F-S-F angle is 90° (opposite bonds are at 180°).

2.8 Examples including ions

Ions follow exactly the same rules. The only difference is that you must adjust the electron count for the charge: add one electron for each negative charge and remove one for each positive charge.

Ion	Bonding pairs	Lone pairs	Shape	Bond angle
NH ₄ ⁺	4	0	tetrahedral	109.5°
BF ₄ ⁻	4	0	tetrahedral	109.5°
H ₃ O ⁺	3	1	pyramidal	107°
NH ₂ ⁻	2	2	non-linear	about 104.5°
CO ₃ ²⁻	3 regions	0	trigonal planar	120°
NO ₃ ⁻	3 regions	0	trigonal planar	120°
PCl ₄ ⁺	4	0	tetrahedral	109.5°

PCl_6^-	6	0	octahedral	90°
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Ion	Same shape as
NH_4^+	CH_4
BF_4^-	CH_4
H_3O^+	NH_3
NH_2^-	H_2O
CO_3^{2-}	BF_3
NO_3^-	BF_3
PCl_4^+	CH_4
PCl_6^-	SF_6

Ions or molecules with the same number of electrons and the same number of atoms often have the same shape. For example, NH_4^+ , CH_4 and BH_4^- are all tetrahedral, and H_3O^+ has the same shape as NH_3 . Species like this are called isoelectronic, and spotting them is a quick check on your answer.

For the bond angles in ions, quote the same value as the matching molecule. Exact experimental values in ions can differ slightly from the neutral molecule (for example, NH_2^- is often quoted as about 104° to 105°), and the mark scheme normally accepts the standard angle for that shape.

2.9 Beyond the core list (useful for stretch questions)

When five or six electron pairs include lone pairs, the lone pairs take the positions that keep them furthest from other pairs. The shapes below are not on the list of shapes you must name, but the method in Section 3 lets you work them out and some questions reward it.

Species	Bonding pairs	Lone pairs	Shape
SF_4	4	1	see-saw (lone pair in an equatorial position)
ClF_3	3	2	T-shaped
XeF_2	2	3	linear
XeF_4	4	2	square planar (lone pairs opposite each other)

3. Step-by-step method to predict a shape

The method (learn the steps)

1. Identify the central atom and write down the number of electrons in its outer shell (its group number for groups 1 and 2, or group number minus 10 for groups 13 to 18).
2. Add one electron for each atom joined to it by a single bond (each H or halogen atom supplies one electron to the bond).
3. Adjust for charge: add one electron for each negative charge, take one away for each positive charge.
4. Divide the total by 2 to get the number of electron pairs around the central atom.

5. The number of bonding pairs equals the number of atoms bonded to the central atom; the rest are lone pairs.
6. Use the total number of pairs to decide the arrangement, then use the positions of the atoms only to name the shape. Reduce the angle by about 2.5° for each lone pair in a four-pair arrangement.

For molecules or ions where the central atom forms double bonds to oxygen (CO_2 , SO_2 , CO_3^{2-} , SO_4^{2-}), it is safer to draw a dot-and-cross diagram first and then count regions of electron density, remembering that each double bond counts as one region.

Worked example 1: PCl_3

1. Central atom P: 5 outer electrons.
2. Three Cl atoms: +3 electrons. Total = 8.
3. No charge.
4. $8 \div 2 = 4$ electron pairs.
5. Three atoms bonded, so 3 bonding pairs and 1 lone pair.
6. Four pairs arranged tetrahedrally; with one lone pair the shape is pyramidal, bond angle about 107° .

Worked example 2: H_3O^+

1. Central atom O: 6 outer electrons.
2. Three H atoms: +3. Total = 9.
3. Positive charge: subtract 1. Total = 8.
4. $8 \div 2 = 4$ pairs.
5. 3 bonding pairs, 1 lone pair.
6. Pyramidal, about 107° .

Worked example 3: PCl_6^-

1. Central atom P: 5.
2. Six Cl atoms: +6. Total = 11.
3. Negative charge: add 1. Total = 12.
4. $12 \div 2 = 6$ pairs.
5. 6 bonding pairs, 0 lone pairs.
6. Octahedral, 90° .

Worked example 4: SO_2 (double bonds)

A dot-and-cross diagram shows sulfur forming a double bond to each oxygen and keeping one lone pair. There are three regions of electron density around sulfur (two double bonds and one lone pair), arranged trigonal planar. Only two positions hold atoms, so the shape is non-linear. The lone pair repels the bonding regions more strongly, so the O-S-O angle is slightly less than 120° (commonly quoted as about 119°).

Worked example 5: SO_4^{2-}

Sulfur is bonded to four oxygen atoms and has no lone pairs (all six of its outer electrons, plus the two from the charge, are used in bonding). Four regions of electron density with no lone pairs give

a tetrahedral shape, bond angle 109.5° .

3.1 How to draw shapes in the exam

- Use a solid line for a bond in the plane of the paper, a wedge for a bond coming towards you and a dashed (hashed) wedge for a bond going away from you. A tetrahedral molecule needs two plain lines, one wedge and one dashed wedge.
- Show lone pairs on the central atom as a pair of dots or a lobe, especially when they explain the shape.
- Label at least one bond angle with its value.
- Write the name of the shape as well as drawing it, because many mark schemes give a separate mark for the name.

4. Polarity of molecules

4.1 Polar bonds

When two atoms with different electronegativities share electrons, the more electronegative atom pulls the bonding pair towards itself. It gains a small negative charge (δ^-) and the other atom a small positive charge (δ^+). The bond is polar and has a dipole.

Learn: electronegativity

Electronegativity is the power of an atom to attract the electrons in a covalent bond towards itself.

4.2 Polar and non-polar molecules

Whether a whole molecule is polar depends on two things: whether it has polar bonds, and whether its shape lets the bond dipoles cancel.

Learn: A molecule is polar if it has polar bonds and its shape is not symmetrical, so that the bond dipoles do not cancel and the molecule has an overall dipole. If the molecule is symmetrical and all the outer atoms are the same, the dipoles cancel and the molecule is non-polar even though its bonds are polar.

Molecule	Shape	Polar bonds?	Dipoles cancel?	Molecule polar?
CO ₂	linear	yes (C=O)	yes, they point in opposite directions	no
BF ₃	trigonal planar	yes	yes	no
CCl ₄	tetrahedral	yes	yes	no
SF ₆	octahedral	yes	yes	no
CHCl ₃	tetrahedral (distorted)	yes	no, one outer atom is different	yes
NH ₃	pyramidal	yes	no	yes

H ₂ O	non-linear	yes	no	yes
SO ₂	non-linear	yes	no	yes

Worked example: explaining polarity

Question: Both CO₂ and H₂O contain polar bonds. Explain why H₂O is a polar molecule but CO₂ is not.

Answer: Oxygen is more electronegative than both carbon and hydrogen, so all the bonds are polar. CO₂ is linear, so the two C=O dipoles are equal and act in opposite directions; they cancel and there is no overall dipole. H₂O is non-linear because oxygen has two lone pairs, so the two O-H dipoles do not point in opposite directions and do not cancel. The molecule has an overall dipole, with the oxygen end δ⁻ and the hydrogen end δ⁺.

Polarity matters because it decides which intermolecular forces act between molecules: polar molecules have permanent dipole-permanent dipole forces in addition to instantaneous dipole-induced dipole forces, which raises their boiling points compared with non-polar molecules of similar size.

5. Sigma and pi bonds, and hybridisation

5.1 Sigma (σ) and pi (π) bonds

A covalent bond forms when atomic orbitals overlap and the shared electrons are attracted to both nuclei. The way the orbitals overlap gives two kinds of bond.

Learn:

A **sigma (σ) bond** is formed by the direct, end-on (head-on) overlap of orbitals, with the electron density concentrated between the two nuclei along the line joining them.

A **pi (π) bond** is formed by the sideways overlap of two p orbitals, with the electron density above and below the line joining the two nuclei.

- A σ bond can form from s-s overlap (H₂), s-p overlap (HCl), p-p end-on overlap (Cl₂) or overlap of hybrid orbitals (C-H in CH₄).
- Every single bond is one σ bond.
- A double bond is one σ bond plus one π bond.
- A triple bond is one σ bond plus two π bonds.

Properties of π bonds. Sideways overlap is less effective than end-on overlap, so a π bond is weaker than a σ bond. This is why the C=C bond energy is less than twice the C-C bond energy (use the data booklet values if asked to compare). The π electrons are also more exposed, above and below the bond, which makes alkenes reactive towards electrophiles. A π bond prevents rotation about the double bond, because rotating would break the sideways overlap; this is the origin of cis/trans (geometrical) isomerism.

5.2 Hybridisation

Carbon's ground-state configuration, 1s² 2s² 2p², has only two unpaired electrons, yet carbon forms four equal bonds in methane. The model of hybridisation explains this: the 2s and 2p orbitals mix to form a set of identical hybrid orbitals, which then overlap with orbitals on other atoms to form σ bonds.

Hybridisation	Orbitals mixed	Number of hybrid orbitals	Arrangement and angle	Unhybridised p orbitals left
sp^3	one s + three p	4	tetrahedral, 109.5°	0
sp^2	one s + two p	3	trigonal planar, 120°	1
sp	one s + one p	2	linear, 180°	2

Hybridisation	Example
sp^3	CH_4 , C_2H_6
sp^2	C_2H_4 , BF_3
sp	C_2H_2 , CO_2 (carbon)

Methane (sp^3). Carbon's four sp^3 orbitals each overlap end-on with a hydrogen 1s orbital, giving four σ bonds at 109.5° .

Ethene (sp^2). Each carbon uses its three sp^2 orbitals to form three σ bonds: two to hydrogen atoms and one to the other carbon. These lie in one plane at about 120° . The remaining p orbital on each carbon is at right angles to that plane; the two p orbitals overlap sideways to form a π bond above and below the plane. So the C=C double bond is one σ bond and one π bond, and the whole molecule is planar.

Ethyne (sp). Each carbon uses two sp orbitals to form two σ bonds (one to H, one to the other C) in a straight line. The two remaining p orbitals on each carbon, at right angles to each other, overlap sideways to form two π bonds. The C $\equiv$ C triple bond is one σ bond and two π bonds, and the molecule is linear.

Linking hybridisation to VSEPR. The number of regions of electron density around an atom tells you its hybridisation: four regions means sp^3 , three means sp^2 , two means sp. Lone pairs count as regions. So the nitrogen in NH_3 and the oxygen in H_2O are both described as sp^3 hybridised, with lone pairs in some of the hybrid orbitals.

Worked example: counting σ and π bonds

Question: How many σ bonds and π bonds are there in propene, $CH_3CH=CH_2$?

Answer: Count every bond. There are six C-H bonds, one C-C single bond and one C=C double bond. Every single bond is σ , so six C-H plus one C-C gives 7 σ bonds. The double bond adds 1 σ and 1 π . Total: 8 σ bonds and 1 π bond.

Hybridisation: the CH_3 carbon is sp^3 (four σ bonds); the two carbons of the double bond are sp^2 (three regions each).

Quick check

1. State the main idea of electron-pair repulsion theory. [2]
2. State the order of repulsion between bonding pairs and lone pairs. [1]

3. Name the shape and state the bond angle of (a) BF_3 , (b) SF_6 , (c) CO_2 . [3]
4. Explain why the bond angle in NH_3 is smaller than the bond angle in CH_4 . [3]
5. Explain why water has a bond angle of 104.5° . [3]
6. Describe the shape of PF_5 , including all the bond angles. [3]
7. Predict the shape and bond angle of the NH_4^+ ion. Show your working. [2]
8. Predict the shape and bond angle of PH_3 . [2]
9. Predict the shape and bond angle of the BF_4^- ion. [2]
10. Predict the shape and bond angle of the PCl_4^+ ion. [2]
11. Predict the shape of the NO_3^- ion and state its bond angle. [2]
12. Tetrachloromethane, CCl_4 , contains polar bonds. Explain why the molecule is non-polar. [2]
13. State and explain whether each of these molecules is polar: (a) NH_3 , (b) BF_3 . [4]
14. Describe the difference between a σ bond and a π bond. [2]
15. For ethene, C_2H_4 : (a) state the number of σ and π bonds, (b) state the hybridisation of each carbon atom, (c) explain why the molecule is planar. [4]

Answers

1. Pairs of electrons in the outer shell of the central atom repel each other, so they move as far apart as possible to minimise repulsion. The number of bonding pairs and lone pairs therefore decides the shape.
2. Lone pair-lone pair > lone pair-bonding pair > bonding pair-bonding pair.
3. (a) BF_3 : three bonding pairs, no lone pairs: trigonal planar, 120° .
(b) SF_6 : six bonding pairs, no lone pairs: octahedral, 90° .
(c) CO_2 : two double bonds, each counting as one region, no lone pairs on carbon: linear, 180° .
4. Both have four electron pairs around the central atom. CH_4 has four bonding pairs, which repel equally, giving 109.5° . NH_3 has three bonding pairs and one lone pair. The lone pair repels more strongly than a bonding pair, so it pushes the three N-H bonding pairs closer together, reducing the angle to 107° .
5. Oxygen has six outer electrons: two are used in bonds to H and four form two lone pairs, so there are four pairs in total, arranged roughly tetrahedrally. Lone pair repulsion is greater than bonding pair repulsion, and with two lone pairs the two bonding pairs are pushed closer together. Each lone pair reduces the angle by about 2.5° , from 109.5° to about 104.5° .
6. PF_5 is trigonal bipyramidal. Five bonding pairs, no lone pairs. Three F atoms lie in a plane (equatorial) at 120° to each other; two F atoms lie above and below the plane (axial) at 90° to the equatorial bonds. The two axial bonds are at 180° to each other.
7. N has 5 outer electrons, +4 from H atoms = 9, minus 1 for the positive charge = 8. $8 \div 2 = 4$ pairs, all bonding (four H atoms). Tetrahedral, 109.5° .
8. P has 5 outer electrons, +3 from H atoms = 8. 4 pairs: 3 bonding, 1 lone. Pyramidal, about 107° (the same shape as NH_3). Accept "pyramidal, angle less than 109.5° ". The measured angle in PH_3 is actually much smaller than 107° , but at AS level the VSEPR prediction of about 107° is what is expected unless the question gives data.

9. B has 3 outer electrons, +4 from F atoms = 7, +1 for the negative charge = 8. 4 pairs, all bonding. Tetrahedral, 109.5° .

10. P has 5 outer electrons, +4 from Cl atoms = 9, minus 1 for the positive charge = 8. 4 pairs, all bonding. Tetrahedral, 109.5° .

11. The nitrogen is bonded to three oxygen atoms and has no lone pairs, so there are three regions of electron density (one double bond and two single bonds in a dot-and-cross diagram, each counting as one region). Trigonal planar, 120° .

12. Each C-Cl bond is polar because chlorine is more electronegative than carbon. CCl_4 is tetrahedral and symmetrical with four identical outer atoms, so the four bond dipoles are equal and cancel out. There is no overall dipole.

13. (a) NH_3 is polar. N-H bonds are polar (N is more electronegative than H). The molecule is pyramidal (because of the lone pair on N), which is not symmetrical, so the dipoles do not cancel and there is an overall dipole.

(b) BF_3 is non-polar. B-F bonds are polar, but the molecule is trigonal planar and symmetrical with three identical outer atoms at 120° , so the three dipoles cancel.

14. A σ bond forms by direct, end-on overlap of orbitals, with electron density concentrated between the two nuclei on the line joining them. A π bond forms by sideways overlap of p orbitals, with electron density above and below the line joining the nuclei. (A π bond is weaker than a σ bond.)

15. (a) Four C-H σ bonds and the C=C double bond (1 σ + 1 π): 5 σ bonds and 1 π bond.

(b) Both carbon atoms are sp^2 hybridised (three regions of electron density each).

(c) The three sp^2 orbitals on each carbon form σ bonds in one plane at about 120° . The π bond forms by sideways overlap of the unhybridised p orbitals, which must be parallel; this only happens when both CH_2 groups lie in the same plane, so all six atoms are in one plane and rotation about the C=C bond is prevented.