

Shapes of molecules and ions

Student worksheet

Chemistry for the gifted and talented

Shapes of molecules and ions

1. Complete the table below by drawing the shape of the molecule or ion. The shape is given in the table below. The shape is given in the table below. The shape is given in the table below.

Chemical formula	Geometry	Shape
CH_4	tetrahedral	
NH_3	trigonal pyramidal	
H_2O	bent	
CO_2	linear	
BF_3	trigonal planar	
XeF_4	square planar	
XeF_6	octahedral	

2. Complete the table below by drawing the shape of the molecule or ion. The shape is given in the table below. The shape is given in the table below. The shape is given in the table below.

Chemical formula	Geometry	Shape
CH_3^+	trigonal planar	
NH_4^+	tetrahedral	
NO_2	bent	
NO_2^+	linear	
NO_2^-	bent	
CO_3^{2-}	trigonal planar	
SO_4^{2-}	tetrahedral	
PO_4^{3-}	tetrahedral	

3. Complete the table below by drawing the shape of the molecule or ion. The shape is given in the table below. The shape is given in the table below. The shape is given in the table below.

Chemical formula	Geometry	Shape
CH_3^-	tetrahedral	
NH_2^-	tetrahedral	
OH^-	tetrahedral	
ClO_2	bent	
ClO_2^-	bent	
ClO_3^-	trigonal pyramidal	
ClO_4^-	tetrahedral	

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NH_2	tetrahedral	
OH	tetrahedral	
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Student worksheet: CDROM index 33SW

Discussion of answers

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Discussion of answers: CDROM index 33DA

Topics

Valence shell electron pair repulsion (VSEPR) theory application.

Level

Very able post-16 students.

Prior knowledge

Valence shell electron pair repulsion (VSEPR) theory.

(An explanation of the VSEPR theory is given but this activity is best done after some discussion of the theory in class.)

Resolving forces (questions 3 and 4).

Rationale

This activity draws some extra concepts and mathematical skills into the discussion of molecular shape. A distinction between geometry around the central atom and the shape of the molecule is made. Students are asked to apply the VSEPR theory to some challenging examples, including species with unpaired electrons. Students are introduced to the alternative model of hybridised atomic orbitals.

Use

This can be used as a follow up to a theory lesson on VSEPR theory for very able students. It can also be used as a differentiated activity for the most able students in a mixed ability group. If the students do not know how to resolve forces, they should leave out questions 3 and 4.



This symbol means those questions are best tackled as a discussion if a group of students is doing this activity.

Shapes of molecules and ions

An important theory used to explain and predict the shapes of molecules and ions is the Valence Shell Electron Pair Repulsion (VSEPR) theory. This model is based on the idea that the pairs of electrons in the valence, or outer, shell of the central atom repel each other. The species therefore adopts a geometry that minimises the electron pair repulsion. The geometry around the central atom depends on the effective number of electron pairs (double bonds count as one pair because both pairs in a double bond are constrained to point in the same direction). The table below summarises the relationship between the number of electron pairs and geometry.

Effective number of electron pairs	Geometry	Structure
2	Linear	$B-A-B$
3	Trigonal planar	
4	Tetrahedral	
5	Trigonal bipyramidal	
6	Octahedral	
7	Several – including pentagonal bipyramidal	

If the electron pairs are not all the same, some distortion of the geometry can occur. Lone pairs are thought to take up more space around the central atom than double bonds, which in turn take up more space than single bonds. The amount of space taken up by a bonding pair may be affected by the bond polarity.

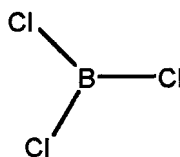
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Questions

1. By drawing dot and cross diagrams and carefully counting the electrons or otherwise, suggest the geometry and draw the shapes of the molecules and ions a)–e). Put your answers in a table like the one below:

Molecule or ion	Effective number of electron pairs in valence shell of central atom	Geometry around central atom	Shape

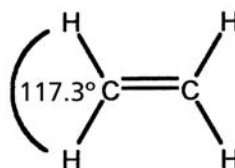
- a) SO_2 (**Hint:** it is not linear)
 b) O_3
 c) IF_7
 d) SF_4 (There are five pairs of electrons around the sulfur. You need to think carefully about the position of the lone pair.)
 e) NO_3^-
2. Phosphorus(V) chloride in the solid state is thought to consist of the ions PCl_4^+ and PCl_6^- . Work out the shape of these ions.
3. By considering each pair of electrons as an equal outward pull on the central nucleus and resolving forces along one of the bonds, show that the bond angle in a symmetric trigonal planar molecule, like BCl_3 , is 120° .



4. Using a similar method, show that the pure tetrahedral angle is 109.5° .



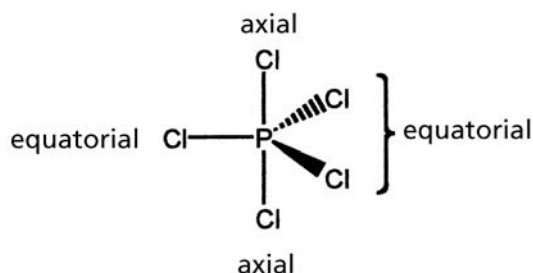
5. The HCH bond angle in ethene is 117.3° . Calculate how much greater the force of attraction from the double bond is, compared to the single bonds. Comment on your answer.



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6. Phosphorus(V) chloride decomposes on heating to give PCl_3 and Cl_2 . Explain whether it is from the axial or equatorial positions that the chlorines break away.



7. Account for the bond angles in the following molecules:

Molecule	Bond angle
NH_3	107°
NF_3	102°
CH_4	109.5°
CH_3Cl	110.5° (HCH)
H_2O	104.5°
H_2S	92.2°
NO_2	134°

An alternative model for explaining the shapes of molecules and ions uses **hybrid atomic orbitals** (see *further reading*). The suggested hybridisation for different geometries is shown below.

Geometry	Linear	Trigonal planar	Tetrahedral	Trigonal bipyramidal	Octahedral
Hybridisation	sp	sp ²	sp ³	sp ³ d	sp ³ d ²

Further reading

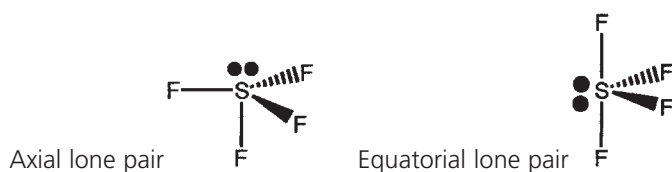
- To read more about hybridised atomic orbitals, J. Keeler and P. Wothers, *Why chemical reactions happen*, Oxford: Oxford University Press, 2003 (p82–93).
- A good website to visit is:
www.psigate.ac.uk/newsite/reference/plambeck/chem1/p02201.htm (accessed June 2007).

Shapes of molecules and ions

1. State the geometry and draw the shapes of the following molecules and ions.

Question	Molecule or ion	Effective number of electron pairs	Geometry around central atom	Shape
a)	SO ₂	3 (sulfur can 'expand' its octet)	Trigonal planar	
b)	O ₃	3 (double bonds count as 1 pair)	Trigonal planar	
c)	IF ₇	7	Pentagonal bipyramidal	
d)	SF ₄	5	Trigonal bipyramidal (distorted)	
e)	NO ₃ ⁻	3	Trigonal planar	

Note: In SF₄ the lone pair could potentially be in an axial position or an equatorial position. The configuration with the lone pair in the equatorial position allows more space for the bulky lone pair, as there are only two other pairs at 90° to it.



The lone pair takes up more room than bonding pairs of electrons, so the shape is slightly distorted with the bonding electrons pushed away from the lone pair.

The FSF bond angle (for axial fluorines) is 173.1°.

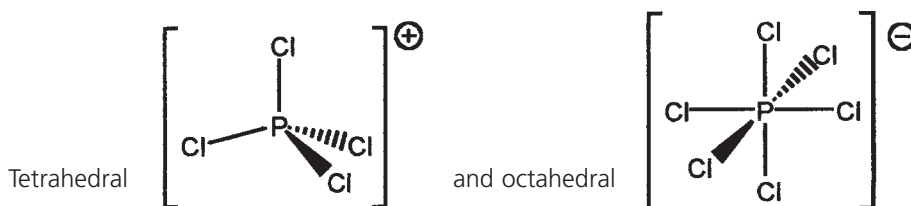


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SF_4 , SO_2 and IF_7 are all examples of where the central atom has 'expanded its octet' – i.e. contains more than eight electrons in its valence shell. This is easier in the third period of the Periodic Table than in the first or second periods because of the availability of d atomic orbitals.

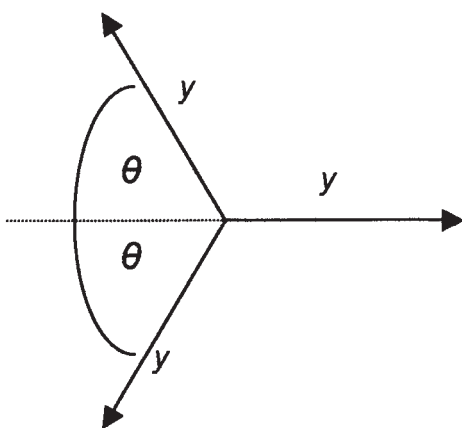
The nitrate ion is thought to have a conjugated structure (as shown in the second structure), in a similar way to carboxylate ions.

2. Phosphorus(V) chloride in the solid state is thought to consist of the ions PCl_4^+ and PCl_6^- . Work out the shape of these ions.



3. By considering each pair of electrons as an outward pull on the central nucleus and resolving forces along one of the bonds, show that the bond angle in a symmetrical trigonal planar molecule like BCl_3 is 120° .

Each arrow represents a force of y . Resolving forces in the horizontal direction, $2y\cos\theta = y$ because the forces on the nucleus must be balanced, $\cos\theta = \frac{1}{2}$ therefore $\theta = 60^\circ$.
 $180^\circ - 60^\circ = 120^\circ$, or bond angle = $2\theta = 120^\circ$.



4. Using a similar method, show that the pure tetrahedral angle is 109.5° .

The method is the same, but this time there are three arrows pointing to the left so $3y\cos\theta = y$
 $\cos\theta = \frac{1}{3}$ therefore $\theta = 70.5^\circ$
 Thus bond angles $180^\circ - 70.5^\circ = 109.5^\circ$.

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5. The HCH bond angle in ethene is 117.3° . Calculate how much greater the force of attraction from the double bond is, compared to the single bonds. Comment on your answer.

Let d be the pull from the double bond and let s be the pull from the single bond. Resolving forces along the double bond gives:

$$d = 2s \cos 58.65^\circ$$

$$d = 1.04s.$$

This is surprisingly small, given that there are four electrons in the double bond compared with only two in the single bond. The explanation for the surprisingly small attraction along the axis of the double bond must be that, because the electron density of the π electrons is largely above and below the plane of the molecule, most of the attraction of the π electrons is perpendicular to the attraction of the σ electrons.

6. Phosphorus(V) chloride decomposes on heating to give PCl_3 and Cl_2 . Explain whether it is from the axial or equatorial positions that the chlorines break away.

Chlorines break away from the axial positions since these are more crowded, with three neighbours at 90° rather than two neighbours at 90° and two at 120° for the equatorial chlorines.

7. Account for the bond angles in the following molecules:

Molecule	Bond angle
NH_3	107°
NF_3	102°
CH_4	109.5°
CH_3Cl	110.5° (HCH)
H_2O	104.5°
H_2S	92.2°
NO_2	134°

The NH_3 bond angle is 107° . This is distorted from the pure tetrahedral angle by the lone pair taking up more space than the single bonds.

The NF_3 bond angle is 102° . There is more distortion than for NH_3 because the single bonds are taking up less room, close to the nitrogen. Fluorine is more electronegative than hydrogen and the electron density in the N–F bond is skewed towards the fluorine.

The CH_4 bond angle is 109.5° . This is the undistorted tetrahedral angle.

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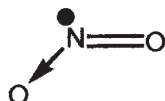
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The (HCH) bond angle in CH_3Cl is 110.5° . The HCH bond angle is wider than in CH_4 which suggests that the C–Cl single bond takes up less space close to the carbon. This is due to the C–Cl bonds polarity with δ^- on the chlorine, chlorine being more electronegative than carbon (and hydrogen). The C–H bond has more electron density around the carbon because the carbon is δ^- , carbon being more electronegative than hydrogen.

The H_2O bond angle is 104.5° . There is greater distortion than in NH_3 because there are *two* lone pairs on the oxygen.

The H_2S bond angle is 92.2° . There is a surprisingly large difference between this and the bond angle in H_2O . Sulfur is less electronegative than oxygen, so the S–H bond takes up **less** space around the central atom than the O–H bond. In terms of hybridisation, the reduced bond angle in H_2S implies the bonds that are formed are much closer to p atomic orbitals, rather than sp^3 hybrid atomic orbitals. A reason for this might be weaker bonds, therefore less return on the investment in energy to hybridise the atomic orbitals.

The NO_2 bond angle is 134° . This is a perhaps a surprising value. The first step towards explaining this is to propose a structure for NO_2 that is consistent with this bond angle.



Around the nitrogen there is a double bond, a single bond and an unpaired electron (remember that NO_2 dimerises to form N_2O_4). The geometry is trigonal planar but the unpaired electron repels the bonding pairs *less* than a *pair* of electrons so the bond angle is *greater* than 120° .

For more discussion on NO_2 visit:

<http://dbhs.wvusd.k12.ca.us/webdocs/VSEPR/Odd-Electron-Molecules.html>

(accessed May 2007).