

Predicting molecular shape, bond angles and polarity

Chemistry grades 11-12 (A Level · IB · Class 11-12) · Worksheet answers

Each answer states the number of domains, the shape and the reasoning. Where the question asks for an explanation, check that you named lone pairs, symmetry or electronegativity, since the marks are for the reasoning, not just the shape.

Level: Chemistry grades 11-12 (A Level · IB · Class 11-12) · **Curriculum:** IB S2.2

Problem 1 Counting electron domains

CH₄: **4 bonding, 0 lone pairs, 4 domains.**

NH₃: **3 bonding, 1 lone pair, 4 domains.**

H₂O: **2 bonding, 2 lone pairs, 4 domains.**

CO₂: two double bonds count as **2 domains, 0 lone pairs.**

Problem 2 Naming the shapes

1. **Linear.**
2. **Trigonal planar.**
3. **Tetrahedral.**
4. **Octahedral.**

Problem 3 Bond angles

1. **109.5°.**
2. **120°.**
3. **180°.**
4. **90°.**

Problem 4 Electronegativity trends

1. **Fluorine (4.0).**
2. N (3.0) < O (3.4) < F (4.0): **N, O, F.**
3. Across the period the nuclear charge increases while the electrons are added to the same shell with similar shielding, so the atom attracts the bonding pair more strongly.

Problem 5 Polar or non-polar bond?

1. H-H: difference 0, **non-polar.**
2. C-H: $2.6 - 2.2 = 0.4$, which is on the dividing line; it is classed as **non-polar (or very**

weakly polar).

3. H-Cl: $3.2 - 2.2 = 1.0$, so **polar**. Hydrogen is $\delta+$ and chlorine $\delta-$.

Problem 6 What is a lone pair?

1. A **lone pair** is a pair of valence electrons on an atom that is not used in bonding.
2. A lone pair is attracted by only one nucleus, so it is held closer and spreads out more, occupying more space. It therefore repels neighbouring pairs more strongly than a bonding pair, which is shared between two nuclei.

Problem 7 Shape of ammonia

1. **Trigonal pyramidal**.
2. About **107°** .
3. The lone pair repels the three bonding pairs more than they repel each other, so the bonds are pushed closer together than the tetrahedral 109.5° .

Problem 8 The ammonium ion

1. **4 bonding pairs and 0 lone pairs** (the fourth bond is dative).
2. **Tetrahedral, 109.5°** .
3. All four pairs are bonding and repel equally, whereas NH_3 has a lone pair that compresses the angle to about 107° .

Problem 9 Sulfur dioxide

1. 2 bonding domains (each double bond counts as one) + 1 lone pair = **3 domains**.
2. The arrangement is trigonal planar and the shape is **bent**, with an angle a little **less than 120°** (about 119°).
3. The molecule is **polar**: the S=O dipoles point toward oxygen and, because of the bent shape, they do not cancel.

Problem 10 Hydrogen sulfide

1. **Bent**.
2. Less than 109.5° ; the observed value is about 92° , because the two lone pairs repel the bonds.

Problem 11 Phosphorus pentachloride

1. **Trigonal bipyramidal**.
2. **120°** in the plane of three chlorines and **90°** between the axial and equatorial bonds.
3. The five identical P-Cl dipoles are arranged symmetrically and cancel, so the net dipole is zero.

Problem 12 Carbon tetrachloride and chloroform

1. C-Cl: $3.2 - 2.6 = 0.6$; C-H: $2.6 - 2.2 = 0.4$.
2. The four equal C-Cl dipoles in a tetrahedron cancel exactly, so A has no net dipole.
3. In B the C-H dipole is smaller and is in the opposite sense, so it cannot cancel the three C-Cl dipoles. B has a net dipole and is **polar**.

Problem 13 Boron trifluoride and ammonia

1. BF_3 is **trigonal planar**; NH_3 is **trigonal pyramidal**.
2. In BF_3 the three B-F dipoles lie at 120° in a plane and cancel. In NH_3 the molecule has a lone pair and a pyramidal shape, so the dipoles add and give a **net dipole**.

Problem 14 Partial charges

1. H-Cl: $3.2 - 2.2 = 1.0$; Na-Cl: $3.2 - 0.9 = 2.3$.
2. H-Cl is **polar covalent**; Na-Cl is **ionic** (above 1.8).
3. $\text{H}^{6+}\text{-Cl}^{6-}$.

Problem 15 Trend in bond angles

1. The bond angle **decreases** from 109.5° to 107° to 104.5° as the number of lone pairs goes from 0 to 1 to 2.
2. Lone pairs repel more than bonding pairs, so each extra lone pair squeezes the bonding pairs closer.
3. NH_2^- has two lone pairs, like water, so its angle is **smaller** than in NH_3 , about 104° .

Problem 16 Xenon tetrafluoride

1. Six domains arranged **octahedrally**.
2. Lone pair-lone pair repulsion is the largest, so placing them at 180° apart minimises it.
3. The four fluorines lie in one plane: **square planar**, $\text{F-Xe-F} = 90^\circ$.
4. The four Xe-F dipoles cancel by symmetry, so the molecule is non-polar.

Problem 17 Chlorine trifluoride

1. Five domains, arranged as a trigonal bipyramid.
2. In equatorial positions each lone pair has only two neighbours at 90° , whereas an axial position would give three. This reduces repulsion.
3. **T-shaped** (F-Cl-F about 87.5°).
4. The molecule is **polar**: the bond dipoles and the lone pairs are not symmetrical, so they do not cancel.

Problem 18 Ammonia against nitrogen trifluoride

1. Both bond dipoles point **toward the more electronegative atom**: toward N in N-H (3.0 against 2.2) and toward F in N-F (4.0 against 3.0).
2. In NH_3 the N-H dipoles point toward N, the same direction as the lone pair's dipole, so they reinforce each other. In NF_3 the N-F dipoles point away from N, opposing the lone pair's.
3. The opposing contributions largely cancel, so NF_3 has a **very small net dipole**.

Problem 19 Cis and trans isomers

1. Cis: both Cl on the same side, with C-Cl arrows both pointing to that side. Trans: arrows pointing in opposite directions.
2. The **cis isomer is polar**.
3. In the cis isomer the two C-Cl dipoles add to a net dipole. In the trans isomer they are equal and opposite, so they cancel.

Problem 20 Shapes of ions

1. NO_3^- : 3 domains, 0 lone pairs, **trigonal planar**. ClO_3^- : 4 domains, 1 lone pair, **trigonal pyramidal**. SO_4^{2-} : 4 domains, 0 lone pairs, **tetrahedral**.
2. The O-Cl-O angle is **less than 109.5°** (about 107°), because of the lone pair.
3. Nitrogen has no lone pair left in NO_3^- , but chlorine has one in ClO_3^- , so its four domains give a pyramid instead of a flat triangle.