

Molecular Shapes (VSEPR)

How do you predict the shape of a molecule using VSEPR theory?

●●○ Intermediate

Bonding & Molecular Structure

Last reviewed 3 October 2026

Before you start: it helps to understand [Lewis Structures](#).

What is it?

VSEPR stands for **valence-shell electron-pair repulsion**. It predicts the 3D shape of a molecule from one simple idea: the regions of electrons around a central atom **repel each other** and spread out to be **as far apart as possible**.

Each region of electrons around the central atom is called an **electron domain**. A domain is:

- a **lone pair**, or
- a **bond** to another atom: single, double or triple (a multiple bond counts as **one** domain).

KEY IDEA

Count the electron domains around the central atom to get the **electron-domain geometry**. Then look only at where the **atoms** are to name the **molecular shape**. Lone pairs affect the shape but are not part of its name.

Why does it matter?

- **Shape controls properties.** Whether a molecule is polar, and so how it dissolves and how high it boils, depends on its shape.
- **Shape controls biology.** Enzymes, drugs and smell receptors work because molecules have particular shapes that fit together.
- **It's quick.** With a Lewis structure, you can predict shapes and bond angles in seconds.

How does it work?

1. Steps

1. Draw the **Lewis structure**.
2. Count the **electron domains** on the central atom (bonds + lone pairs; multiple bonds count once).
3. Find the **electron-domain geometry** from the number of domains.

4. Name the **molecular shape** from the positions of the atoms.

2. The shapes

Domains	Lone pairs	Molecular shape	Bond angle	Example
2	0	linear	180°	CO ₂
3	0	trigonal planar	120°	BF ₃
3	1	bent	slightly less than 120°	SO ₂
4	0	tetrahedral	109.5°	CH ₄
4	1	trigonal pyramidal	about 107°	NH ₃
4	2	bent	about 104.5°	H ₂ O
5	0	trigonal bipyramidal	90° and 120°	PCl ₅
6	0	octahedral	90°	SF ₆

3. Why lone pairs squeeze bond angles

A lone pair is held by only one nucleus, so it sits closer to the central atom, takes up more space and **repels more strongly** than a bonding pair. The order of repulsion is:

lone pair–lone pair > lone pair–bond pair > bond pair–bond pair

That's why the angle drops from 109.5° in CH₄ to about 107° in NH₃ (one lone pair) and about 104.5° in H₂O (two lone pairs).

4. Shape and polarity

A molecule is **polar** if its bond polarities do **not** cancel out.

- CO₂ has two polar C=O bonds, but they point in opposite directions (linear), so they cancel: **nonpolar**.
- H₂O has two polar O–H bonds in a bent shape, so they don't cancel: **polar**.
- CCl₄ (tetrahedral, four identical bonds): **nonpolar**. CHCl₃ (one bond different): **polar**.

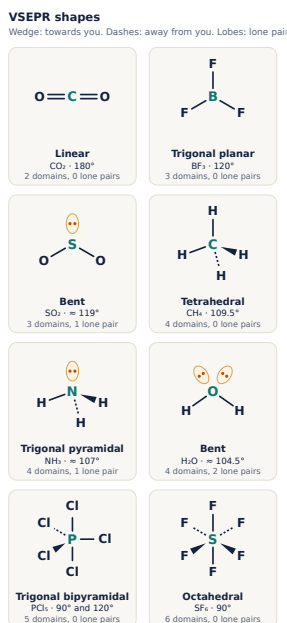
∞ THINK OF IT LIKE THIS

Tie four balloons together at their knots. They automatically point to the corners of a tetrahedron, because each balloon pushes the others away. Two balloons sit in a line; three spread out flat in a triangle.

Q MORE PRECISELY

With 5 or 6 domains, lone pairs give further shapes. With 5 domains, lone pairs go in the flat “equator” positions, giving **seesaw** (SF_4 , 1 lone pair), **T-shaped** (ClF_3 , 2) and **linear** (XeF_2 , 3). With 6 domains, you get **square pyramidal** (BrF_5 , 1) and **square planar** (XeF_4 , 2).

Visualise it



Common VSEPR shapes. Multiple bonds count as one domain; outer-atom lone pairs are not shown.

Worked example

WORKED EXAMPLE: Ammonia, NH_3

- Step 1** Lewis structure: N bonded to three H, with one lone pair on N.
- Step 2** Domains on N: 3 bonds + 1 lone pair = 4, so the electron-domain geometry is tetrahedral.
- Step 3** Atoms occupy only three corners, so the shape is **trigonal pyramidal**, with H–N–H about **107°** .
- Step 4** The N–H bond polarities don't cancel in this shape, so NH_3 is **polar**.

 WORKED EXAMPLE: Formaldehyde, CH₂O

- Step 1** Lewis structure: C in the centre, single bonds to two H and a double bond to O; no lone pairs on C.
- Step 2** Domains on C: **3** (the C=O double bond counts once).
- Step 3** Shape: **trigonal planar**, angles about 120°.

Common mistake

 COMMON MISTAKE: Counting a double bond as two domains

A double or triple bond points in one direction, so it counts as **one** electron domain. CO₂ has 2 domains on carbon, not 4.

 COMMON MISTAKE: Naming the shape from the electron domains

Water has 4 domains (tetrahedral electron geometry) but its **molecular shape** is **bent**, because only the atoms are counted when naming the shape.

 COMMON MISTAKE: Assuming polar bonds mean a polar molecule

CO₂ and CCl₄ have polar bonds but are nonpolar molecules, because their symmetry makes the bond polarities cancel.

 NOTATION NOTE

- In 3D drawings, a solid **wedge** points towards you and a **dashed** bond points away; ordinary lines lie in the plane of the page.
- Some books write “AX_mE_n” notation: A = central atom, X = bonded atoms, E = lone pairs. For example, water is AX₂E₂.

Remember this

REMEMBER THIS

- Electron domains (bonds + lone pairs, multiple bonds count once) spread out as far as possible.
- 2 linear 180° ; 3 trigonal planar 120° ; 4 tetrahedral 109.5° ; 5 trigonal bipyramidal; 6 octahedral.
- Lone pairs repel more and squeeze bond angles: CH_4 109.5° , NH_3 about 107° , H_2O about 104.5° .
- Polar molecule = polar bonds that do not cancel by symmetry.

References

1. Brown, T. L.; LeMay, H. E., Jr.; Bursten, B. E.; Murphy, C. J.; Woodward, P. M.; Stoltzfus, M. W. Chemistry: The Central Science, 15th ed.; Pearson, 2022.

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