

Predicting molecular shape, bond angles and polarity

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

Quick answer: Molecular shape follows VSEPR theory: electron domains around the central atom repel and spread as far apart as possible, with lone pairs repelling more than bonding pairs. This sets the shape and bond angle, and with electronegativity differences it decides whether a molecule is polar.

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

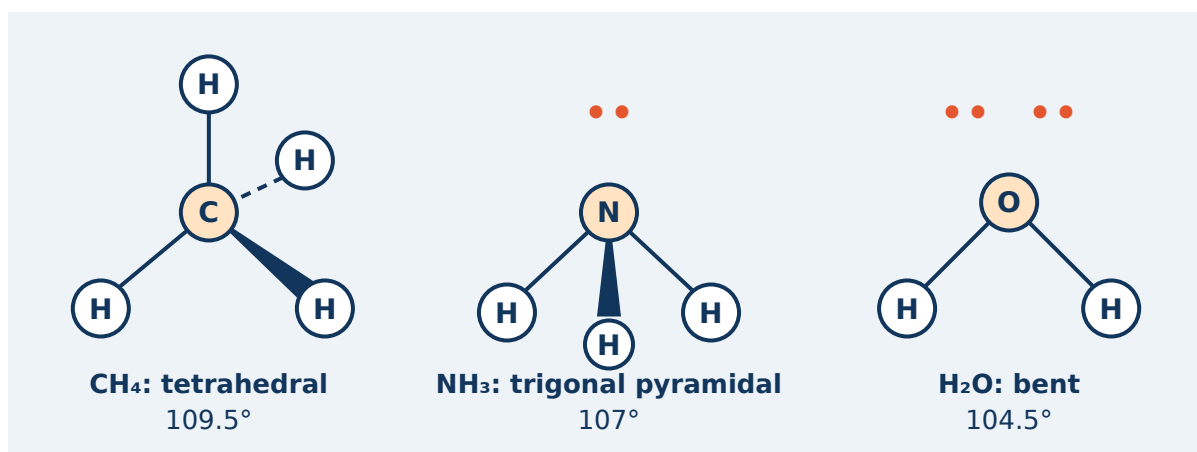
What decides the shape of a molecule?

Electrons repel one another. In the valence shell of the central atom, every region of electron density pushes the others as far away as possible, and that determines the shape.

Key law

VSEPR theory: electron domains (bonding pairs and lone pairs) around a central atom repel and take positions of minimum repulsion. A double or triple bond counts as **one** domain. Repulsion strength: lone pair-lone pair > lone pair-bonding pair > bonding pair-bonding pair.

Domains	Lone pairs	Shape	Angle	Example
2	0	linear	180°	CO ₂ , BeCl ₂
3	0	trigonal planar	120°	BF ₃
3	1	bent	slightly under 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



Four electron domains always point to the corners of a tetrahedron; lone pairs (red dots) squeeze the bond angle.

Methane has four bonding pairs and a perfect tetrahedral angle of 109.5°. In ammonia one of the four domains is a lone pair, which sits closer to the nucleus and pushes the three N-H bonds together to about 107°. Water has two lone pairs, so the angle shrinks to about 104.5°.

How do you predict a shape step by step?

1. Find the number of valence electrons of the central atom and adjust for any charge.
2. Count the bonding domains: each bonded atom is one domain, whatever the bond order.
3. Lone pairs = (valence electrons – electrons used in bonds) ÷ 2.
4. Add the domains, choose the arrangement, then name the shape from the bonding atoms only.

Worked example 1

Predict the shape and the H-N-H angle in ammonia, NH₃.

N has 5 valence electrons; 3 are shared with H, leaving 2 electrons = 1 lone pair.

Domains = 3 + 1 = 4, so the arrangement is tetrahedral. Only three domains are atoms.

Answer: **trigonal pyramidal, about 107°**, smaller than 109.5° because the lone pair repels more.

Common mistake

Do not name the shape from all the domains. Water has four domains in a tetrahedral arrangement, but its shape is bent, because the lone pairs are not atoms.

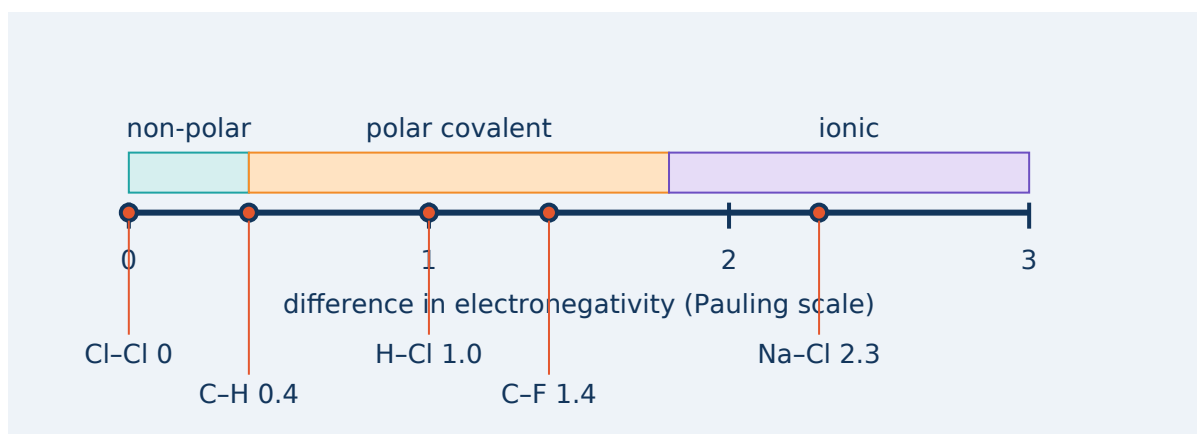
What is electronegativity?

Definition

Electronegativity is the ability of an atom in a covalent bond to attract the bonding pair of electrons towards itself. On the Pauling scale fluorine is highest (4.0).

Electronegativity rises across a period, because the nuclear charge increases at a similar

radius, and falls down a group, because of distance and shielding. Pauling values: H 2.2, C 2.6, N 3.0, O 3.4, F 4.0, Cl 3.2, S 2.6, P 2.2.

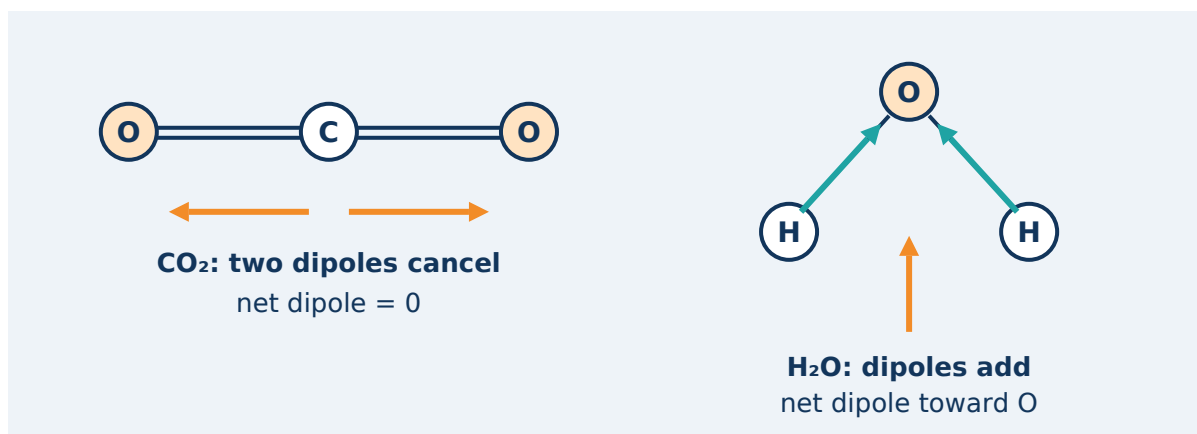


The bigger the electronegativity difference, the more polar the bond.

A bond is polar when the two atoms differ in electronegativity. The atom with the higher value carries a partial negative charge, written δ^- , and the other carries δ^+ .

Why can a molecule with polar bonds be non-polar?

Each polar bond has a dipole, which acts like a small arrow. The molecule is polar only if the arrows do not cancel. Symmetrical shapes such as linear CO_2 , trigonal planar BF_3 and tetrahedral CCl_4 have zero net dipole. Bent H_2O and pyramidal NH_3 do not cancel, so they are polar.



Molecular polarity depends on shape: the arrows point toward the more electronegative atom.

Worked example 2

Is chloromethane, CH_3Cl , polar?

The shape is tetrahedral. The C-Cl bond (difference 0.6) points toward Cl, and the three C-H bonds (0.4) are much weaker and are not balanced by a second chlorine.

The dipoles do not cancel, so CH_3Cl is **polar**, with δ^- on Cl.

Lina's tip

To test polarity, ask two questions in order: are the bonds polar? Does the shape cancel the arrows? If a molecule has lone pairs on the central atom, it is almost never

symmetrical enough to cancel.

Key points to remember

- Domains: 2 linear 180° , 3 trigonal planar 120° , 4 tetrahedral 109.5°
- Lone pairs repel more: NH_3 about 107° , H_2O about 104.5°
- A double bond counts as one electron domain
- Electronegativity rises across a period and falls down a group
- A molecule is polar only if its bond dipoles do not cancel

Predicting molecular shape, bond angles and polarity: frequently asked questions

Why is the water bond angle smaller than the tetrahedral angle?

Water has two lone pairs and two bonding pairs. Lone pairs are held nearer the central atom and repel more strongly than bonding pairs, so they squeeze the H-O-H angle to about 104.5° instead of 109.5° .

How is a double bond treated in VSEPR?

A double or triple bond counts as one electron domain, because all its electrons lie in the same region between the two nuclei. That is why carbon dioxide, with two double bonds, is linear.

What is the difference between a polar bond and a polar molecule?

A polar bond is a bond between atoms of different electronegativity. A polar molecule has a net dipole after adding all bond dipoles. CCl_4 has four polar bonds but is non-polar.

Which bond is more polar, C-F or C-O?

C-F is more polar. The difference in electronegativity is $4.0 - 2.6 = 1.4$ for C-F and $3.4 - 2.6 = 0.8$ for C-O. A larger difference means a greater partial charge.

How do you find the number of lone pairs on the central atom?

Take the valence electrons of the central atom, adjust for charge, subtract one electron for each bond it makes, and divide the remainder by two. In ammonia this is $(5 - 3) \div 2 = 1$.