

Lewis structures, shapes and hybridization of molecules

AP Chemistry · Lesson

Quick answer: A Lewis structure shows how valence electrons are shared as bonds and lone pairs, and formal charges help choose the best one. VSEPR predicts shape by counting electron domains around the central atom, and hybridization (sp , sp^2 , sp^3) describes the orbitals that match that count.

Level: AP Chemistry · **Curriculum:** AP Chem Unit 2

How are chemical bonds classified?

Definition

A bond forms when atoms lower their energy by sharing or transferring valence electrons. Ionic bonds transfer electrons between a metal and a non-metal. Covalent bonds share electron pairs. Metallic bonds hold a lattice of cations in a sea of delocalised electrons.

Electronegativity differences guide the classification. A difference above about 1.7 usually means ionic. A difference between about 0.4 and 1.7 gives a polar covalent bond, with partial charges δ^+ and δ^- . Below 0.4 the bond is nonpolar covalent.

How do you draw a Lewis structure?

Key law

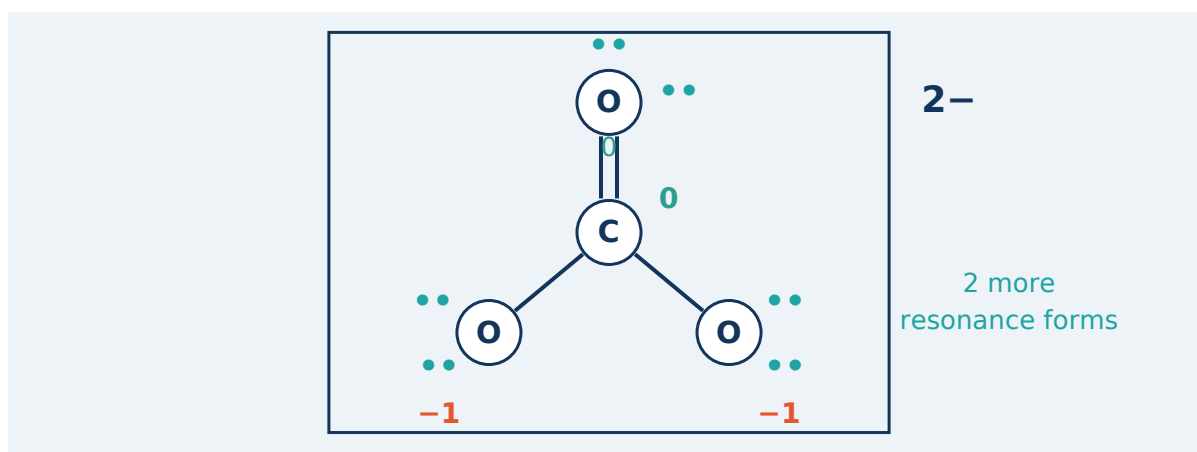
Count all valence electrons (adjust for charge). Join the atoms with single bonds, complete the octets of the outer atoms, put remaining electrons on the central atom, and form double or triple bonds if the central atom lacks an octet. Elements from period 3 down may hold more than eight electrons.

Formula

Formal charge = (valence electrons in the free atom) – (non-bonding electrons) – $\frac{1}{2}$ (bonding electrons). The charges add up to the charge of the species.

Worked example

Carbonate, CO_3^{2-} : valence electrons = $4 + 3(6) + 2 = 24$. One structure has $\text{C}=\text{O}$ and two $\text{C}-\text{O}^-$. Formal charges: $\text{C} = 4 - 0 - 4 = 0$; double-bonded $\text{O} = 6 - 4 - 2 = 0$; single-bonded $\text{O} = 6 - 6 - 1 = -1$ each. The total is -2 . The double bond can sit on any oxygen, so there are **three resonance forms** and an average bond order of $4/3$.



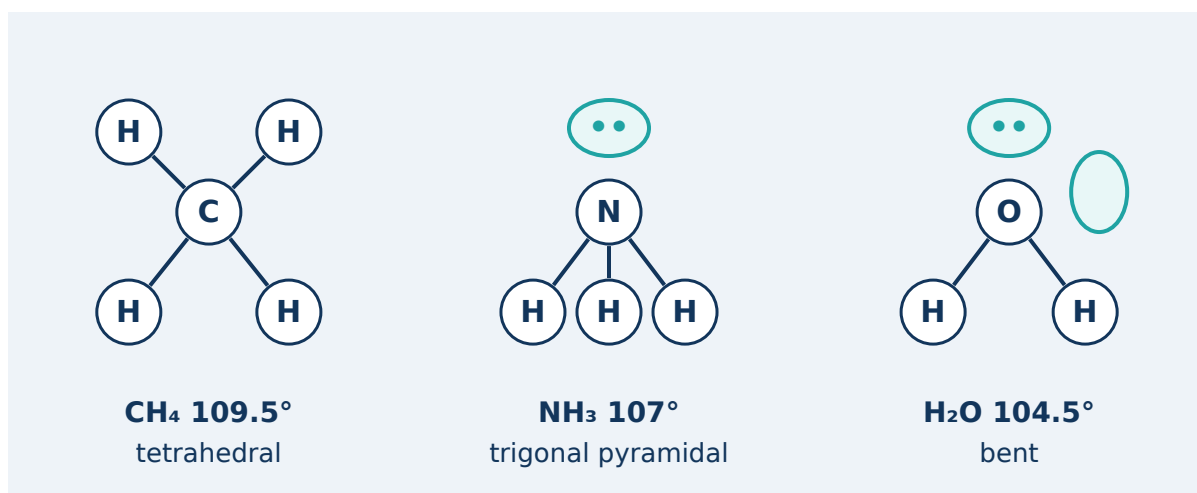
CO_3^{2-} has 24 valence electrons. The double bond can be on any of the three oxygens, so each C-O bond has order 4/3.

When several structures are possible, the best has formal charges closest to zero, with any negative charge on the most electronegative atom. Resonance means the real structure is a hybrid, not a switch between the drawings.

How does VSEPR predict molecular shape?

Electron domains (bonds of any order and lone pairs) repel each other and spread as far apart as possible. The number of domains gives the electron geometry. Lone pairs are not included in the name of the molecular shape, but they squeeze the bond angles.

Domains	Electron geometry	Examples (molecular shape)	Hybridization
2	linear, 180°	CO_2 (linear)	sp
3	trigonal planar, 120°	BF_3 (trigonal planar), SO_2 (bent)	sp^2
4	tetrahedral, 109.5°	CH_4 , NH_3 (pyramidal), H_2O (bent)	sp^3
5	trigonal bipyramidal	PCl_5 , SF_4 (seesaw), ClF_3 (T-shaped)	sp^3d
6	octahedral, 90°	SF_6 , XeF_4 (square planar)	sp^3d^2



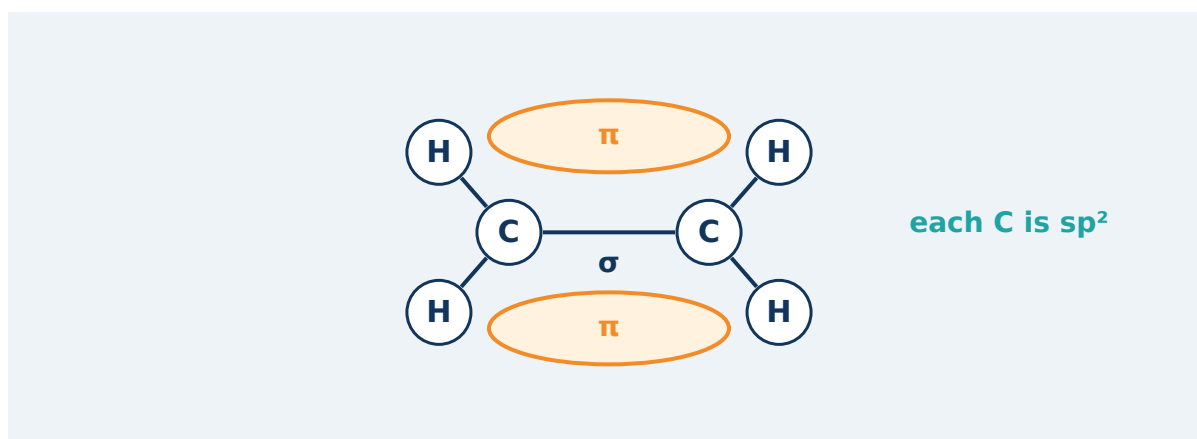
Lone pairs repel more than bonding pairs, so the angle closes from 109.5° to 107° to 104.5° .

Worked example

Ammonia, NH_3 : valence electrons = $5 + 3 = 8$. Three N-H bonds use 6 electrons, and the other 2 form a lone pair. Four domains give a tetrahedral electron geometry, so the molecular shape is **trigonal pyramidal**, the angle is about 107° and the nitrogen is sp^3 .

What is hybridization?

Hybridization mixes atomic orbitals on one atom to make equivalent orbitals pointing toward the electron domains. The number of hybrid orbitals equals the number of domains. A single bond is a sigma (σ) bond, formed by end-on overlap. A double bond is one σ and one pi (π) bond. A triple bond is one σ and two π bonds.



Ethene: five sigma bonds and one pi bond. The pi bond forms from p orbitals that overlap sideways.

Worked example

Ethyne, $\text{H}-\text{C}\equiv\text{C}-\text{H}$, has two domains on each carbon, so each carbon is **sp** hybridized and the molecule is linear. The bonds are 3 σ (two C-H and one C-C) and 2 π .

Common mistake

Students count lone pairs when naming the molecular shape. The shape names the atoms only, so NH_3 is trigonal pyramidal, not tetrahedral, even though its electron geometry is tetrahedral.

Lina's tip

Check your Lewis structure by counting: electrons drawn must equal electrons available. Then count domains around the central atom to get the shape.

Bond order also governs strength and length: triple bonds are shortest and strongest, single bonds longest and weakest. A polar molecule needs polar bonds and an asymmetric shape, so the bond dipoles do not cancel.

Key points to remember

- Formal charge = valence – nonbonding – $\frac{1}{2}$ bonding electrons
- Domains 2, 3, 4, 5, 6 give linear, trigonal planar, tetrahedral, trigonal bipyramidal,

octahedral

- Hybridization: sp , sp^2 , sp^3 , sp^3d , sp^3d^2 match 2 to 6 domains
- Double bond = $1 \sigma + 1 \pi$; triple bond = $1 \sigma + 2 \pi$
- Higher bond order means a shorter and stronger bond

Lewis structures, shapes and hybridization of molecules: frequently asked questions

How do you find the formal charge of an atom?

Subtract the non-bonding electrons and half the bonding electrons from the valence electrons of the free atom. For a good Lewis structure the formal charges are as small as possible.

What is resonance in chemistry?

Resonance describes a species whose electron distribution is better represented by several Lewis structures than by one. The true structure is an average, and the bond lengths are equal.

How does VSEPR predict shape?

Count the electron domains around the central atom. Domains spread to minimise repulsion, which gives the electron geometry, and the lone pairs are then ignored to name the molecular shape.

How do you find the hybridization of an atom?

Count its electron domains: 2 is sp , 3 is sp^2 , 4 is sp^3 , 5 is sp^3d and 6 is sp^3d^2 . Lone pairs count as domains.

Why is CO_2 nonpolar when its bonds are polar?

The molecule is linear, so the two bond dipoles are equal and opposite and cancel. Polar bonds only give a polar molecule when the shape is asymmetric.