Essential Question

How do electrons determine the shape of a molecule?

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What Is VSEPR?

- Electrons are negative, so groups of electrons around a central atom repel each other (Coulomb's law).
- The groups spread out as far apart as possible to minimize repulsion.

VSEPR stands for **V**alence **S**hell **E**lectron **P**air **R**epulsion.

Counting Electron Domains

- Each bond = 1 domain, whether it’s single, double, or triple.
- Each lone pair on the central atom = 1 domain.
- Count only around the central atom.

An **electron domain** is a region around the central atom where electrons are found.

Electron vs. Molecular Geometry

- **Electron geometry:** where all of the domains point, bonds and lone pairs.
- **Molecular geometry:** where the atoms are. This is the molecule's actual shape, and it's what the AP exam usually means by "shape."

Ammonia's 4 domains spread out into a tetrahedral electron geometry.

Two and Three Electron Domains

- **2 domains:** linear, 180° (example: CO_2)
- **3 domains, 0 lone pairs:** trigonal planar, 120° (example: BF_3)
- **3 domains, 1 lone pair:** bent, a little less than 120° (example: SO_2)

A bent molecule with 3 domains still has a trigonal planar electron geometry.

Four Electron Domains

- **0 lone pairs:** tetrahedral, 109.5° (example: CH_4)
- **1 lone pair:** trigonal pyramidal, less than 109.5° (example: NH_3)
- **2 lone pairs:** bent, less than 109.5° (example: H_2O)

If four domains lay flat in a square, they would only be 90° apart. In 3D they can do better: they point to the corners of a tetrahedron, 109.5° apart.

Lone Pairs Take Up More Space

- A bonding pair is shared by 2 nuclei, so it's held in a narrow region between the atoms.
- A lone pair is held by only 1 nucleus, so it spreads out and takes up more space.
- Lone pairs repel more strongly and push the bonds closer together.

More lone pairs means a smaller bond angle: 109.5° for CH_4, about 107° for NH_3, and about 104.5° for H_2O.

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Five Electron Domains

- Electron geometry: trigonal bipyramidal.
- The two **axial** positions point straight up and down. The three **equatorial** positions form a triangle around the middle.

Examples: PCl_5 is trigonal bipyramidal, $TeCl_4$ is seesaw, ClF_3 is T-shaped, and XeF_2 is linear.

Five Electron Domains

- Axial to equatorial is 90°, and equatorial to equatorial is 120°.
- Lone pairs go in the equatorial positions, where there’s more room.

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Six Electron Domains

- **0 lone pairs:** octahedral, all 90° (example: SF_6)
- **1 lone pair:** square pyramidal, slightly less than 90° (example: BrF_5)
- **2 lone pairs:** square planar, 90° (example: XeF_4)

A second lone pair goes directly opposite the first one, 180° away, so the two lone pairs are as far apart as possible.

Molecular Polarity

- A bond dipole arrow points toward the more electronegative atom, with a plus sign at the positive end.
- Polar bonds + asymmetric shape → polar molecule.
- Symmetric shape with identical outer atoms → bond dipoles cancel → nonpolar molecule.

CO_2 has two polar C=O bonds, but it's linear, so the two dipoles are equal and opposite and cancel.

Hybridization

- The s and p orbitals on the central atom mix to form new, identical **hybrid orbitals**.
- Hybrid orbitals point in exactly the directions VSEPR predicts.
- Number of domains = number of hybrid orbitals.

Lone pairs count as domains, so the nitrogen in NH_3 is sp^3.

Sigma and Pi Bonds

- **σ (sigma) bond:** orbitals overlap head-on, along the line between the two nuclei.
- **π (pi) bond:** two p orbitals overlap side by side, above and below the line between the nuclei.
- σ overlap is greater, so a σ bond is stronger than a π bond.

Counting σ and π Bonds

- Single bond = 1σ
- Double bond = 1σ + 1π
- Triple bond = 1σ + 2π

Every bond between two atoms has exactly one σ bond, and any extra lines are π bonds.

Bond Order, Length, and Energy

- Higher bond order → shorter, stronger bond.
- Larger atoms → longer bonds. For example, H-F < H-Cl < H-Br in bond length.

Bond order is the number of shared electron pairs between two atoms: 1 for a single bond, 2 for a double bond, and 3 for a triple bond.

Pi Bonds Block Rotation

- Atoms joined by only a σ bond can rotate freely around it.
- Twisting a double bond breaks the π overlap, so a double bond is locked in place.
- Locked double bonds → **cis** and **trans** isomers (geometric isomers).

In the cis isomer, the chlorines are on the same side of the double bond.

Example: Shape of Formaldehyde

Try it first!

Formaldehyde, CH_2O, has carbon as its central atom. Determine the electron geometry, molecular geometry, and bond angle around carbon.

Example: Sulfur Tetrafluoride

Try it first!

Determine the molecular geometry of SF_4. Is SF_4 polar or nonpolar? Justify your answer.

Example: Comparing Polarity

Try it first!

BF_3 is nonpolar, but NF_3 is polar. Explain this difference using electron domains and molecular geometry.

Example: Hybridization and Bonds

Try it first!

The Lewis structure of acetonitrile, CH_3CN, is shown. Identify the hybridization of carbon 1 and carbon 2, then count the σ and π bonds.

Diagram: Lewis structure of acetonitrile: a carbon labeled 1 bonded to three H atoms and to a carbon labeled 2, which has a triple bond to N. N has one lone pair.

Example: Ranking Bond Lengths

Try it first!

Rank the carbon-oxygen bonds in CO, CO_2, and CH_3OH from shortest to longest. Justify your ranking.

Big Ideas

- Electron domains spread out to reduce repulsion.
- Lone pairs change the shape and shrink bond angles.
- Domains → sp, sp^2, sp^3.
- More bonds → shorter, stronger bonds.