

Taste

- The taste of a food depends on the interaction between the food molecules and taste cells on your tongue.
- The main factors that affect this interaction are the molecule's shape and charge distribution.
- The food molecule must fit snugly into the active site of specialized proteins on the surface of taste cells.
- When this happens, changes in the protein structure cause a nerve signal to transmit.

Sugar and Artificial Sweeteners

- Sugar molecules fit into the active site of taste cell receptors called T1r3 receptor proteins.
- When the sugar molecule (the key) enters the active site (the lock), the different subunits of the T1r3 protein split apart.
- This split causes ion channels in the cell membrane to open, resulting in nerve signal transmission.
- Artificial sweeteners also fit into the T1r3 receptor, sometimes binding to it even stronger than sugar, making them "sweeter" than sugar.

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Valence Shell Electron Pair Repulsion Theory

- Properties of molecular substances depend on the structure of the molecule.
- Valence shell electron pair repulsion (VSEPR) theory is a simple model that allows us to account for molecular shape.
- Electron groups are defined as lone pairs, single bonds, double bonds, and triple bonds.
- VSEPR is based on the idea that electron groups repel one another through coulombic forces.

VSEPR Theory

- Electron groups around the central atom will be most stable when they are as far apart as possible. We call this VSEPR theory.
 - Because electrons are negatively charged, they should be most stable when they are separated as much as possible.
- The resulting geometric arrangement will allow us to predict the shapes and bond angles in the molecule.































The Effect of Lone Pairs

- The actual geometry of the molecule may be different from the electron geometry.
- Lone pair electrons typically exert slightly greater repulsion than bonding electrons, affecting the bond angles.
- A lone electron pair is more spread out in space than a bonding electron pair because a lone pair is attracted to only one nucleus while a bonding pair is attracted to two nuclei.
- In general, electron group repulsions vary as follows:
- Lone pair–lone pair > lone pair–bonding pair > bonding pair–bonding pair
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Pyramidal and Bent Molecular Geometries: Derivatives of Tetrahedral Electron Geometry

- When there are four electron groups around the central atom, and one is a lone pair, the result is called a **pyramidal shape**, because it is a triangular-base pyramid with the central atom at the apex.
- When there are four electron groups around the central atom, and two are lone pairs, the result is called a **tetrahedral-bent shape**.











Derivatives of the Trigonal Bipyramidal Electron Geometry

- Lone pairs on central atoms with five electron groups will occupy the equatorial positions because there is more room.
- The result is called the **seesaw shape** (aka **distorted tetrahedron**).
- When there are two lone pairs around the central atom, the result is **T-shaped**.
- When there are three lone pairs around the central atom, the result is a **linear shape**.
- The bond angles between equatorial positions are less than 120°.
- The bond angles between axial and equatorial positions are less than 90°.

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- Linear = 180^{\circ} axial to axial.
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| Electron Groups* | Bonding Groups | Lone Pairs | Electron Geometry | Molecular Geometry | Approximate Bond Angles | | Example |
|---------------------|-------------------|---------------|----------------------|-----------------------|----------------------------|------------------|------------|
| 2 | 2 | 0 | Linear | Linear | 180° | :ö=c=ö: | • • • |
| 3 | 3 | 0 | Trigonal planar | Trigonal planar | 120° | :F: :F.—B.—F: | |
| 3 | 2 | 1 | Trigonal planar | Bent | <120° | :ö=š-ö: | _ _ |
| 4 | 4 | 0 | Tetrahedral | Tetrahedral | 109.5° | н—с—н н | |
| 4 | 3 | 1 | Tetrahedral | Trigonal pyramidal | <109.5° | н—й—н н | |
| 4 | 2 | 2 | Tetrahedral | Bent | <109.5° | н—ё—н | ° |
| | | | | | | | |
| | | | | | | | |



Predicting Molecular Geometry

- 1. Draw the Lewis structure.
- 2. Determine the number of electron groups around the central atom.
- 3. Classify each electron group as a bonding or lone pair, and then count each type.
 Remember, multiple bonds count as one group.
- 4. Use Table 10.1 to determine the shape and bond angles.

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Representing Three-Dimensional Shapes on Paper

- One of the problems with drawing molecules is trying to show their dimensionality.
- By convention, the central atom is put in the plane of the paper.
- Put as many other atoms as possible in the same plane and indicate with a **straight line**.
- For atoms in front of the plane, use a **solid wedge**.
- For atoms behind the plane, use a hashed wedge.



















Molecular Polarity Affects Solubility in Water

- Polar molecules are attracted to other polar molecules.
- Because water is a polar molecule, other polar molecules dissolve well in water.
 - And ionic compounds as well
- Some molecules have both polar and nonpolar parts.







Valence Bond Theory

- Valence Bond theory (VB) approaches chemical bonding based on an extension of the quantum-mechanical model.
- When orbitals on atoms interact, they make a bond.
- These orbitals are **hybridized atomic orbitals**, a kind of blend or combination of two or more standard atomic orbitals.

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Valence Bond Theory

- When two atoms approach each other, the electrons and nucleus of one atom interact with the electrons and nucleus of the other atom.
- If the energy of the system is lowered because of the interactions, a chemical bond forms.
- A chemical bond results from the overlap of two half-filled orbitals with spin-pairing of the two valence electrons (or less commonly the overlap of a completely filled orbital with an empty orbital).
- The geometry of the overlapping orbitals determines the shape of the molecule.



Orbital Interaction

- As two atoms approach each other, the half-filled valence atomic orbitals on each atom would interact to form molecular orbitals.
 - Molecular orbitals are regions of high probability of finding the shared electrons in the molecule.
- The molecular orbitals would be more stable than the separate atomic orbitals because they would contain paired electrons shared by both atoms.
 - The potential energy is lowered when the molecular orbitals contain a total of two paired electrons compared to separate, one-electron atomic orbitals.







Valence Bond Theory: Main Concepts 1. The valence electrons of the atoms in a molecule reside in quantum-mechanical atomic orbitals. The orbitals can be the standard *s*, *p*, *d*, and *f* orbitals, *or* they may be hybrid combinations of these. 2. A chemical bond results when these atomic orbitals interact and there is a total of two electrons in the new molecular orbital. The electrons must be spin paired. 3. The shape of the molecule is determined by the geometry of the interacting orbitals.



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Hybrid Orbitals

- The number of standard atomic orbitals combined = the number of hybrid orbitals formed.
 - Combining a 2s with a 2p gives two 2sp hybrid orbitals.
 - H cannot hybridize!
 - Its valence shell has only one orbital.
- The number and type of standard atomic orbitals combined determines the shape of the hybrid orbitals.
- The particular kind of hybridization that occurs is the one that yields the lowest overall energy for the molecule.







Bonding with Valence Bond Theory According to valence bond theory, bonding takes place between atoms when their atomic or hybrid orbitals interact. "Overlap" To interact, the orbitals must either be aligned along the axis between the atoms, or be parallel to each other and perpendicular to the interatomic axis.









Types of Bonds

- A **sigma** (*o*) **bond** results when the interacting atomic orbitals point along the axis connecting the two bonding nuclei.
 - Either standard atomic orbitals or hybrids
 - *s* to *s*, *p* to *p*, hybrid to hybrid, *s* to hybrid, etc.
- A pi (π) bond results when the bonding atomic orbitals are parallel to each other and perpendicular to the axis connecting the two bonding nuclei.
 - Between unhybridized parallel p orbitals
- The interaction between parallel orbitals is not as strong as between orbitals that point at each other; therefore, σ bonds are stronger than π bonds.





























Predicting Hybridization and Bonding Scheme

- 1. Start by drawing the Lewis structure.
- 2. Use VSEPR theory to predict the electron group geometry around each central atom.
- 3. Use Table 10.3 to select the hybridization scheme that matches the electron group geometry.
- 4. Sketch the atomic and hybrid orbitals on the atoms in the molecule, showing overlap of the appropriate orbitals.
- 5. Label the bonds as σ or π .







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• When the wave functions combine constructively, the resulting molecular orbital has less energy than the original atomic orbitals; it is called a **bonding molecular orbital**.

σ, π

- Most of the electron density between the nuclei
- When the wave functions combine destructively, the resulting molecular orbital has more energy than the original atomic orbitals; it is called an antibonding molecular orbital.

 σ^*, π^*

- Most of the electron density outside the nuclei
- Nodes between nuclei





















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- Dioxygen is paramagnetic.
- Paramagnetic material has unpaired electrons.
- Neither Lewis theory nor valence bond theory predict this result.

















