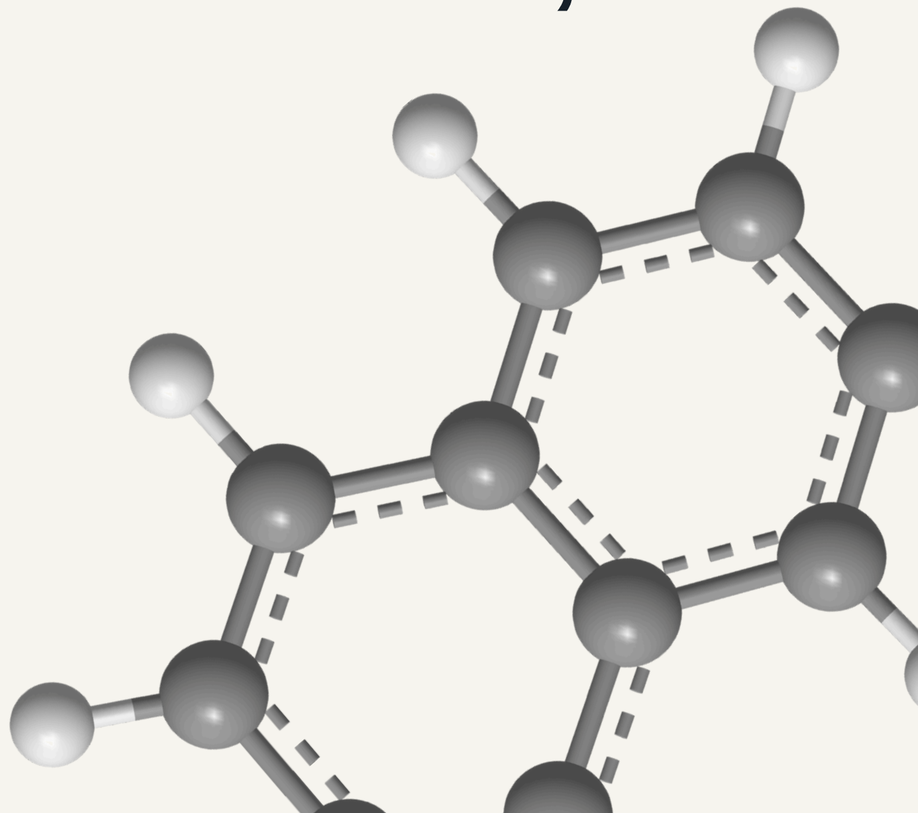
Lecture 5

Types of hybridization. Asymmetric carbon atom. Chirality. Conformation, conformers.



Lecture: PhD, acc. professor: Kudaibergenova B.M

Aim and Objectives

Aim: to study carbon hybridization types, asymmetric carbon atoms and chirality, and molecular conformations and conformers.

1. Define hybridization and its importance in molecular structure
2. Describe sp^3, sp^2 and sp hybridization
3. Compare bond angles and molecular geometries
4. Identify asymmetric carbon atoms
5. Explain chirality, enantiomers and optical activity
6. Investigate conformational isomerism
7. Compare staggered and eclipsed conformations

Introduction to Molecular Structure

The three-dimensional shape of an organic molecule affects its physical properties, reactivity and biological activity.

- **Hybridization:** mixing of atomic orbitals to form hybrid orbitals
- **Asymmetric carbon:** tetrahedral carbon bonded to four different substituents
- **Chirality:** a molecule not superimposable on its mirror image
- **Conformation:** spatial arrangement from rotation around single bonds
- **Conformers:** different conformations of the same molecule

Concept of Hybridization

A theoretical model in which atomic orbitals of one atom combine into new hybrid orbitals with specific orientations. Carbon ($1s^2\ 2s^2\ 2p^2$) can form four covalent bonds.

sp^3

109.5°

Four sp^3 orbitals · tetrahedral

sp^2

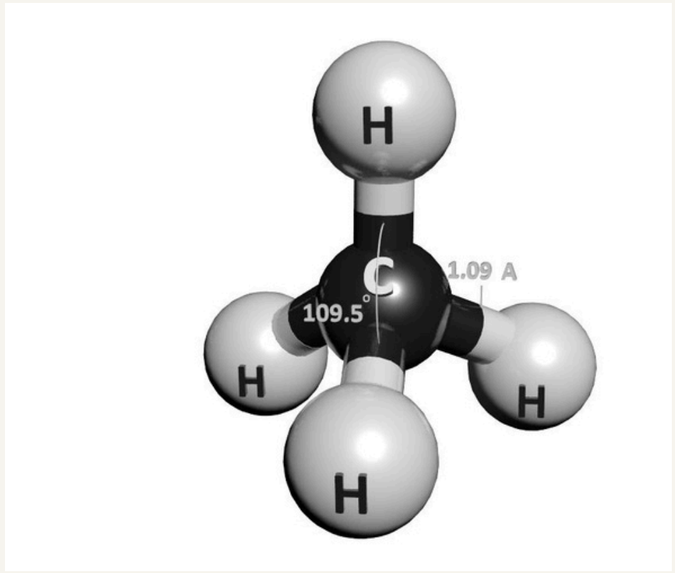
120°

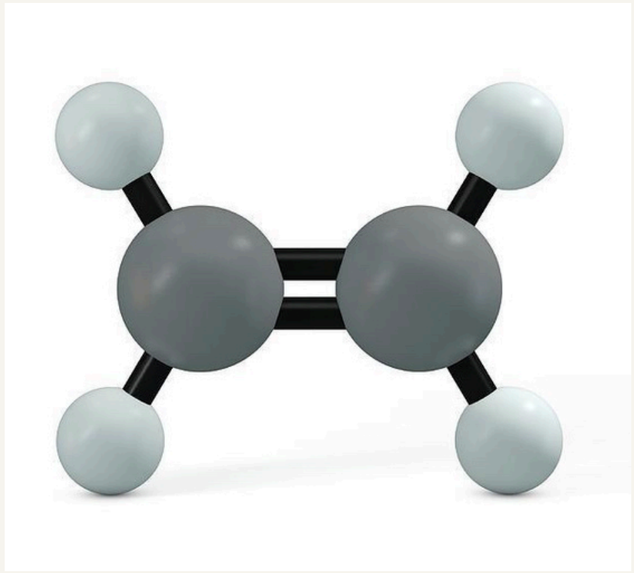
Three sp^2 orbitals · trigonal planar

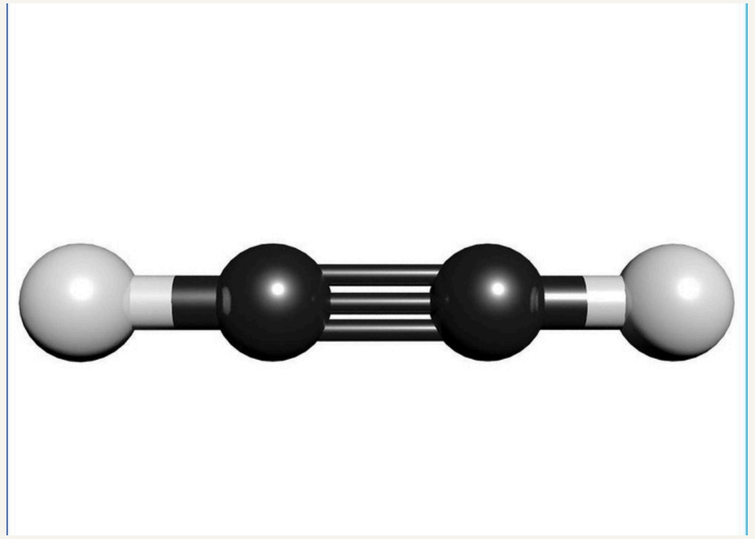
sp

180°

Two sp orbitals · linear







sp³ Hybridization

One s orbital and three p orbitals combine into four equivalent sp³ orbitals.

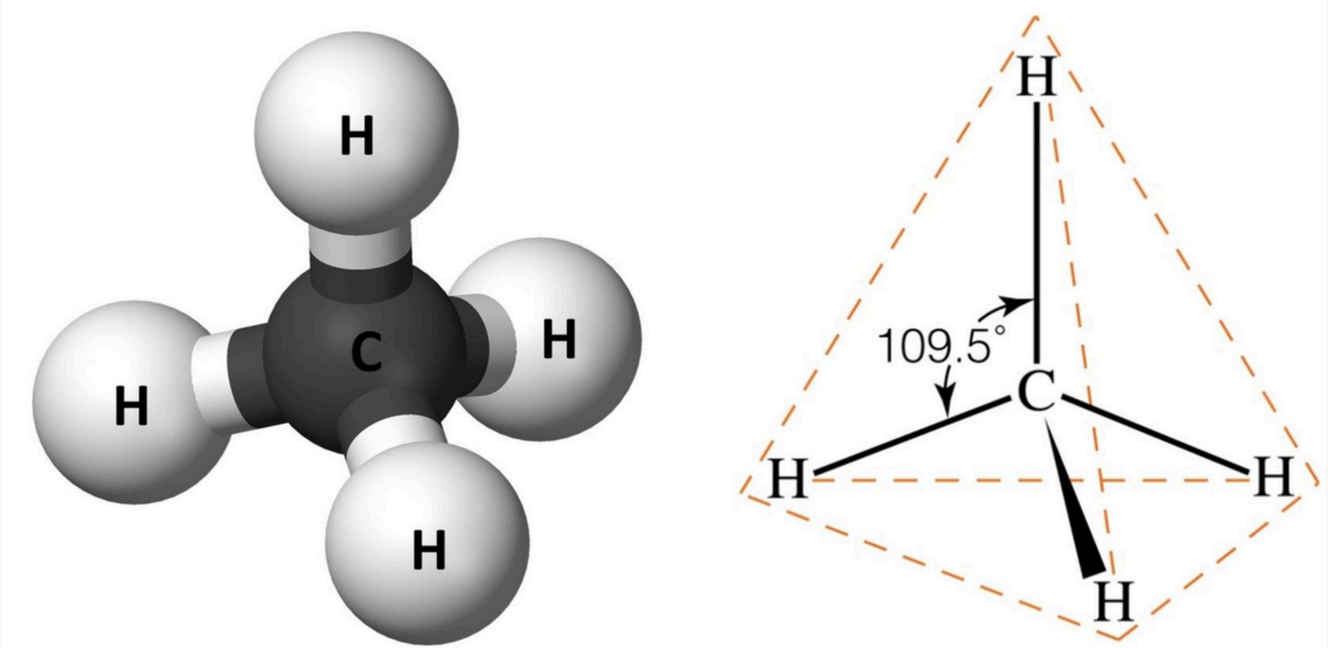
Main characteristics

- Four sp³ hybrid orbitals
- Tetrahedral geometry
- Ideal bond angle 109.5°
- Four σ bonds in methane
- Common in saturated compounds

Example: methane

CH_4

Found in alkanes such as methane, ethane and propane.

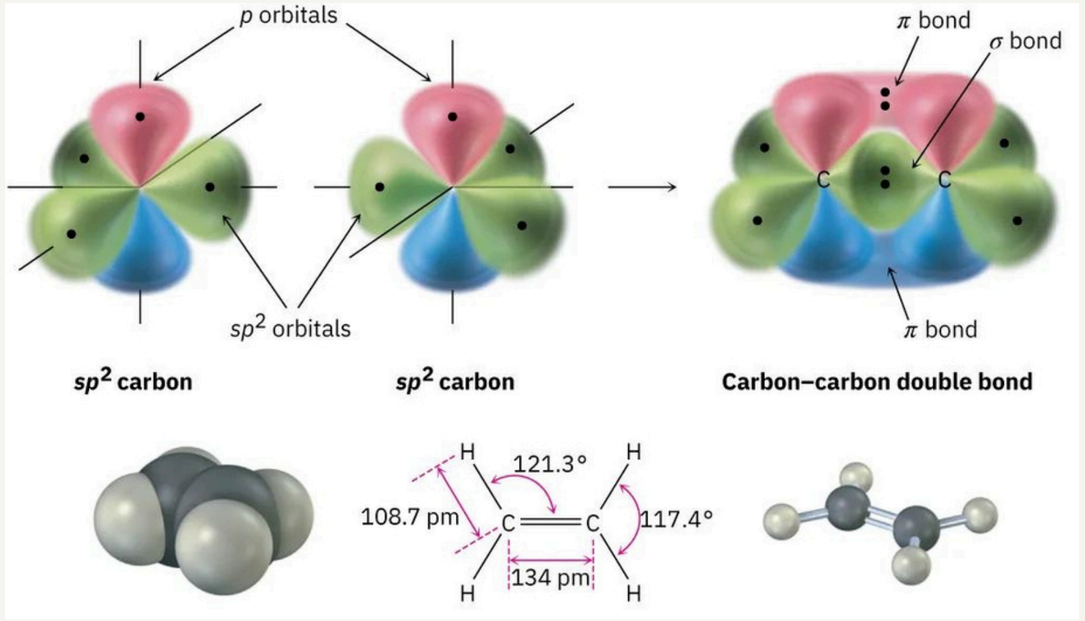


sp² Hybridization

One s and two p orbitals give three sp² orbitals; one unhybridized p orbital stays perpendicular to their plane.

Main characteristics

- Three sp² hybrid orbitals
- Trigonal planar arrangement
- Bond angle about 120°
- Forms σ and π bonds
- Common in alkenes and carbonyl compounds



Example: ethene

$$CH_2=CH_2$$

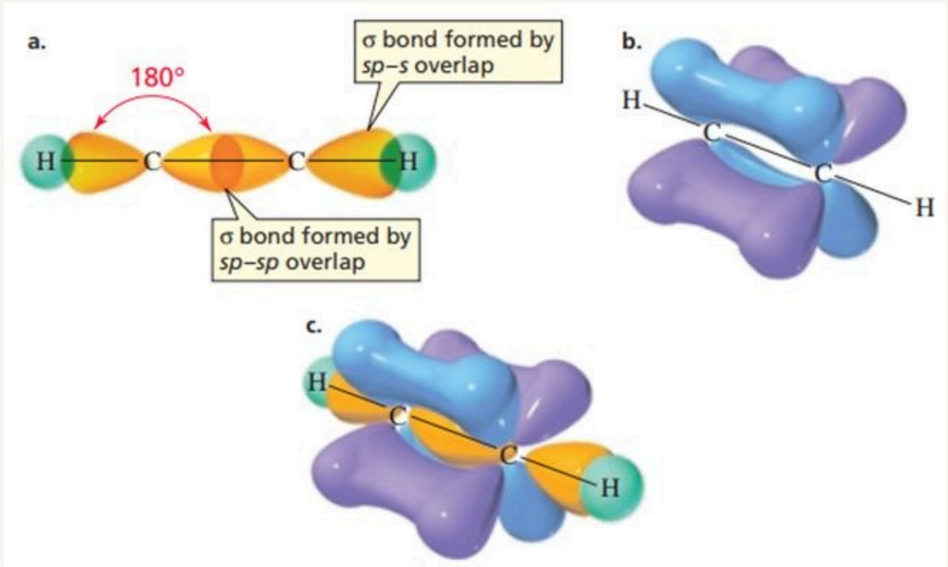
C=C is 1σ + 1π: a double bond has one sigma and one pi bond.

sp Hybridization

One s and one p orbital give two sp orbitals; two unhybridized p orbitals remain for π bonding.

Main characteristics

- Two sp hybrid orbitals
- Linear geometry
- Bond angle 180°
- Common in alkynes and nitriles
- Carbon can form two π bonds



Example: ethyne

HC≡CH

C≡C is 1σ + 2π: a triple bond has one sigma and two pi bonds.

Comparison of Hybridization Types

Characteristic	sp^3	sp^2	sp
Geometry	Tetrahedral	Trigonal planar	Linear
Ideal angle	109.5°	120°	180°
Hybrid orbitals	4	3	2
Unhybridized p orbitals	0	1	2
s-character	25%	33.3%	50%
Example	Methane	Ethene	Ethyne

Hybridization sets the arrangement of bonding orbitals and helps predict molecular geometry.

Asymmetric Carbon Atom

A tetrahedral carbon bonded to four different atoms or groups, also called a chiral carbon or stereogenic center.

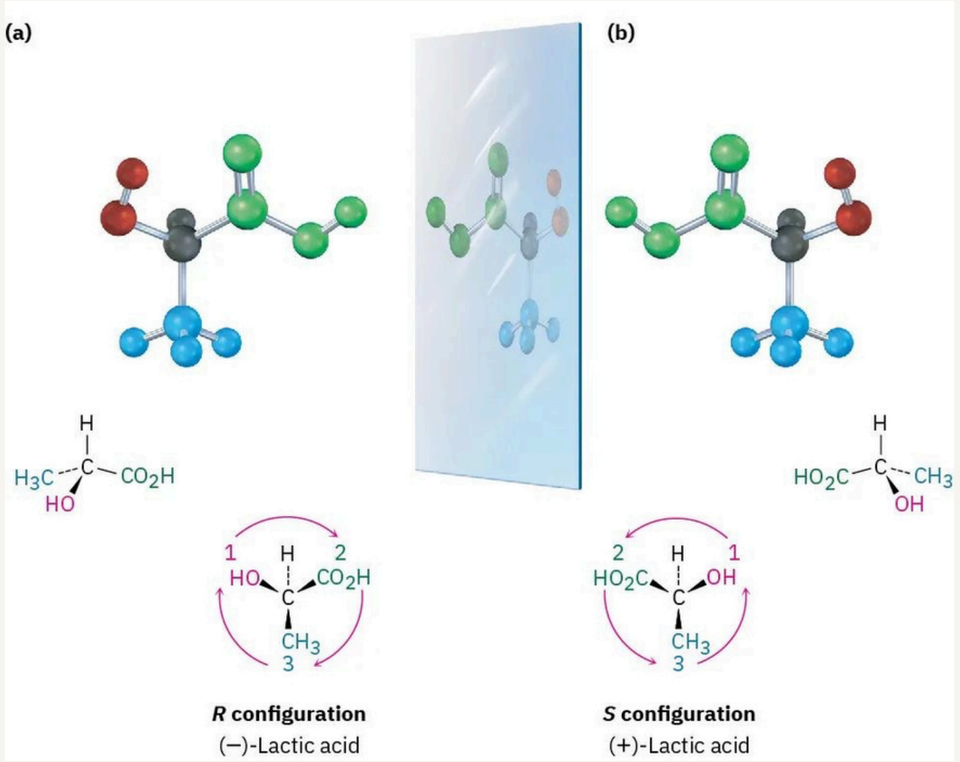
C*(A)(B)(D)(E)

Lactic acid: $CH_3–CH(OH)–COOH$

- The middle carbon bears H, OH, CH_3 and COOH
- All four groups are different

Important

A molecule with an asymmetric carbon is generally chiral, but with several stereocenters it can sometimes be achiral.



Chirality in Organic Chemistry

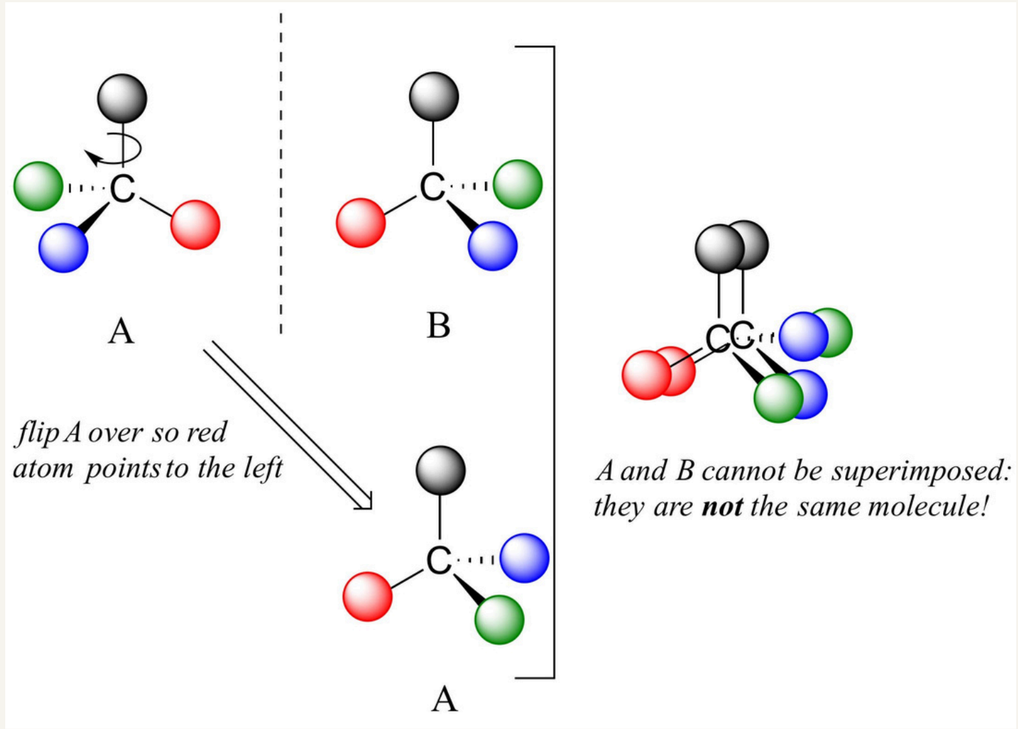
A chiral molecule has a mirror image that cannot be superimposed on it. The two forms are stereoisomers called enantiomers.

Everyday analogy

Left and right hands are mirror images, yet they cannot be superimposed perfectly.

Main characteristics

- Enantiomers are non-superimposable mirror images
- Same molecular formula and connectivity
- Identical physical properties in achiral environments, except for effects on polarized light
- May behave differently in biological systems



Enantiomers and Optical Activity

Many chiral compounds rotate the plane of polarized light.

Optical rotation

- Dextrorotatory (+): clockwise
- Levorotatory (−): counterclockwise
- Lactic acid has two enantiomers, (R) and (S)
- R/S does not by itself decide (+) or (−)

Specific rotation

$$[\alpha] = \alpha / (l \cdot c)$$

α: observed rotation (°) · l: path length (dm) · c: concentration (g/mL) · T: temperature · λ: wavelength

R and S Configuration

These rules hold when substituent 4 points away from the viewer.

The Cahn–Ingold–Prelog system assigns the absolute configuration of a stereogenic center.

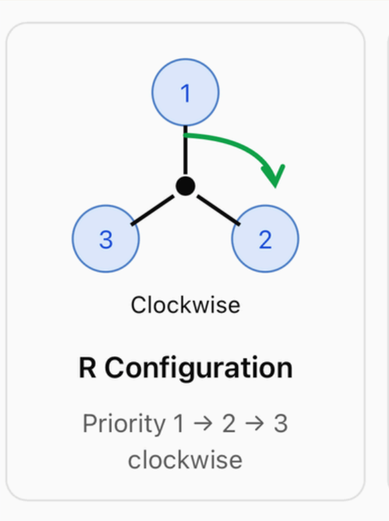
1. Identify the stereogenic center
2. Rank the four substituents by atomic number and CIP rules
3. Point the lowest-priority group away from the viewer
4. Follow priority 1 → 2 → 3

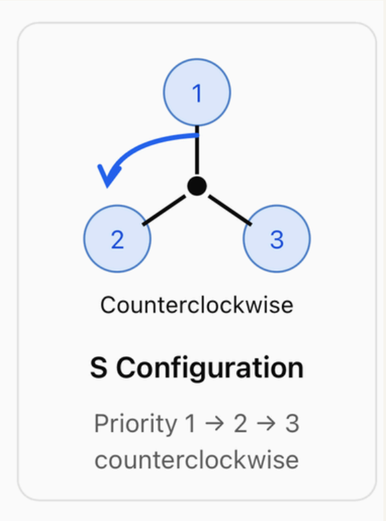
R configuration

Priority 1 → 2 → 3 runs clockwise

S configuration

Priority 1 → 2 → 3 runs counterclockwise





Conformation of Organic Molecules

The three-dimensional arrangement of atoms that changes through rotation around single bonds. Each arrangement is a conformer.

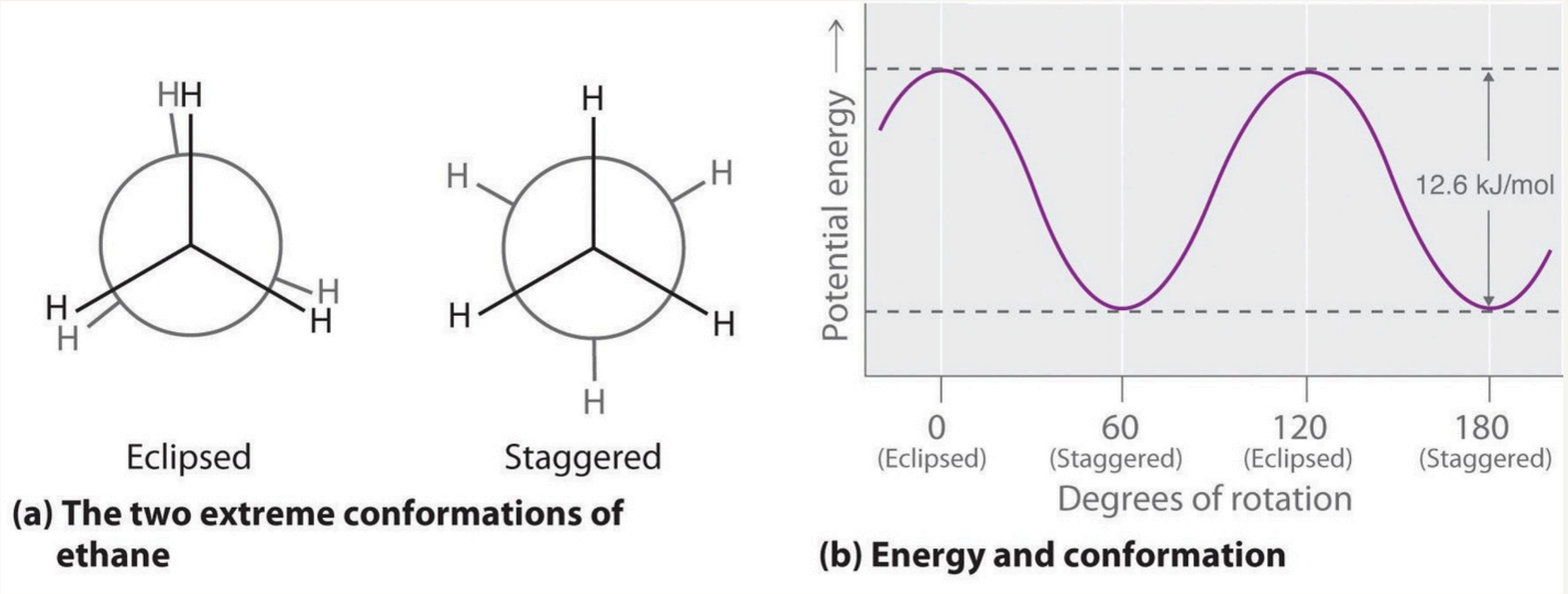
Main characteristics

- Rotation around σ bonds creates conformations
- Conformers interconvert without breaking bonds
- Conformations differ in potential energy
- Steric repulsion and torsional strain affect stability

Example: ethane

C_2H_6

Rotation about the C–C single bond gives staggered and eclipsed conformations.



Staggered and Eclipsed Conformations

Staggered

- Dihedral angle 60°
- Lower torsional strain
- More stable
- Hydrogens are offset

Eclipsed

- Dihedral angle 0°
- Higher torsional strain
- Less stable
- Hydrogens align

E(staggered) < E(eclipsed)

The rotational energy barrier of ethane is about 12 kJ/mol.

Conformational Analysis of Butane

Rotation about the central C2–C3 bond of butane (C_4H_{10}) gives four main conformations.

Anti
Methyl groups 180° apart (staggered)

Gauche
Methyl groups 60° apart (staggered)

Eclipsed
Methyl and hydrogen groups overlap in projection

Fully eclipsed
Two methyl groups aligned at 0°

Anti > Gauche > Eclipsed > Fully eclipsed

Greater stability means lower potential energy.

Conclusion

1. Hybridization explains orbital arrangement and geometry
2. sp^3, sp^2, sp: ideal angles of 109.5°, 120° and 180°
3. Asymmetric carbons are key stereogenic centers
4. Chirality explains enantiomers
5. Conformers arise from rotation around single bonds and differ in energy
6. Conformational analysis helps predict stability, behavior and biological interactions

Understanding geometry and stereochemistry is essential for reaction mechanisms, drug molecules and structure–property relationships.

References: Clayden, Greeves & Warren; McMurry; Smith (March’s); Eliel, Wilen & Mander