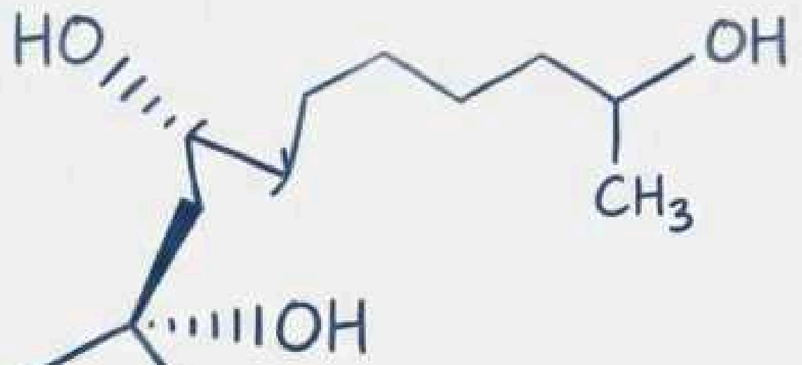
¶ 3.1



CHEM 210 B Lecture 3

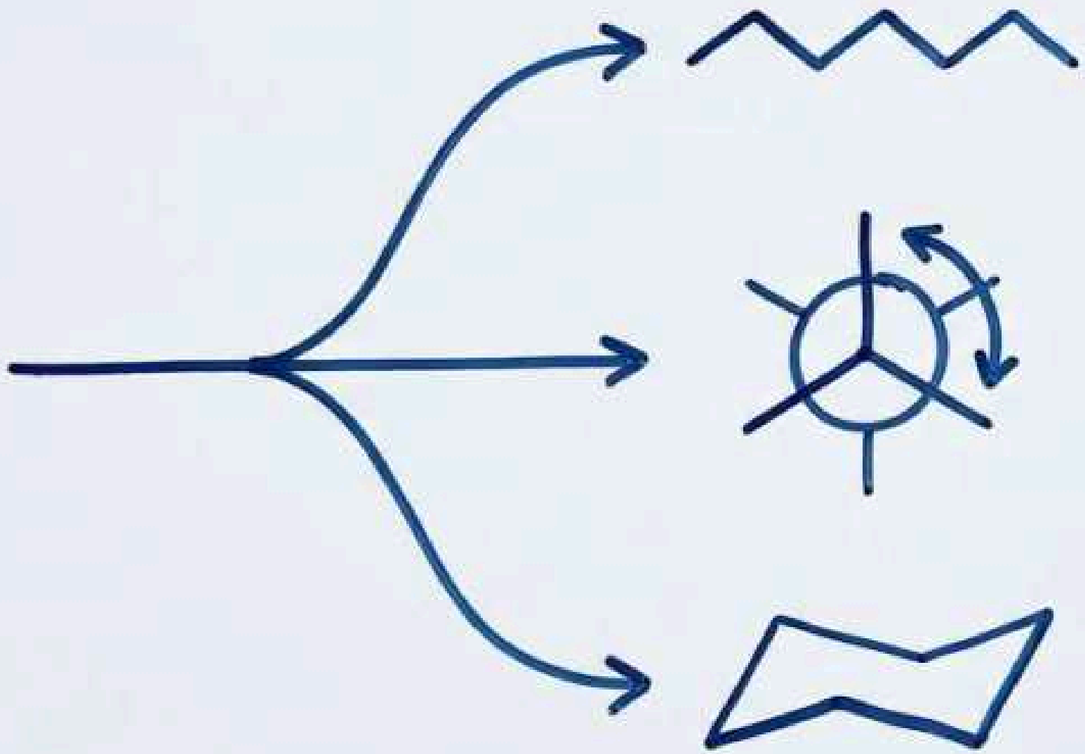
Alkanes, Cycloalkanes, and Molecular Shape

At a glance: Alkane naming, functional groups, combustion, radical halogenation, Newman projections, ring strain, and the cyclohexane chair.



Three Organizing Questions

¶ 3.1



1. How are alkanes named and classified, and what do functional groups add?

2. How does rotation around a single bond give a molecule many shapes?

3. Why does a six-membered ring adopt a puckered form with positions that are not all alike?

These answers prepare us for stereochemistry and reactions.

Alkane Foundations and Saturated Hydrocarbons

Saturated: Holding maximum possible hydrogen atoms.

$$C_nH_{2n+2}$$

Definition: Hydrocarbons with only single bonds. Main sources are natural gas and petroleum, separated by boiling point via fractional distillation.

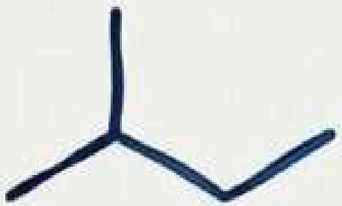
Historical Names (n = 1-4)	Greek Prefixes (n = 5-10)
n=1: Methane	n=5: Pentane
n=2: Ethane	n=6: Hexane
n=3: Propane	n=7: Heptane
n=4: Butane	n=8: Octane
	n=9: Nonane
	n=10: Decane

The Exponential Growth of Constitutional Isomers

Definition: Molecules with the same formula but different connections.

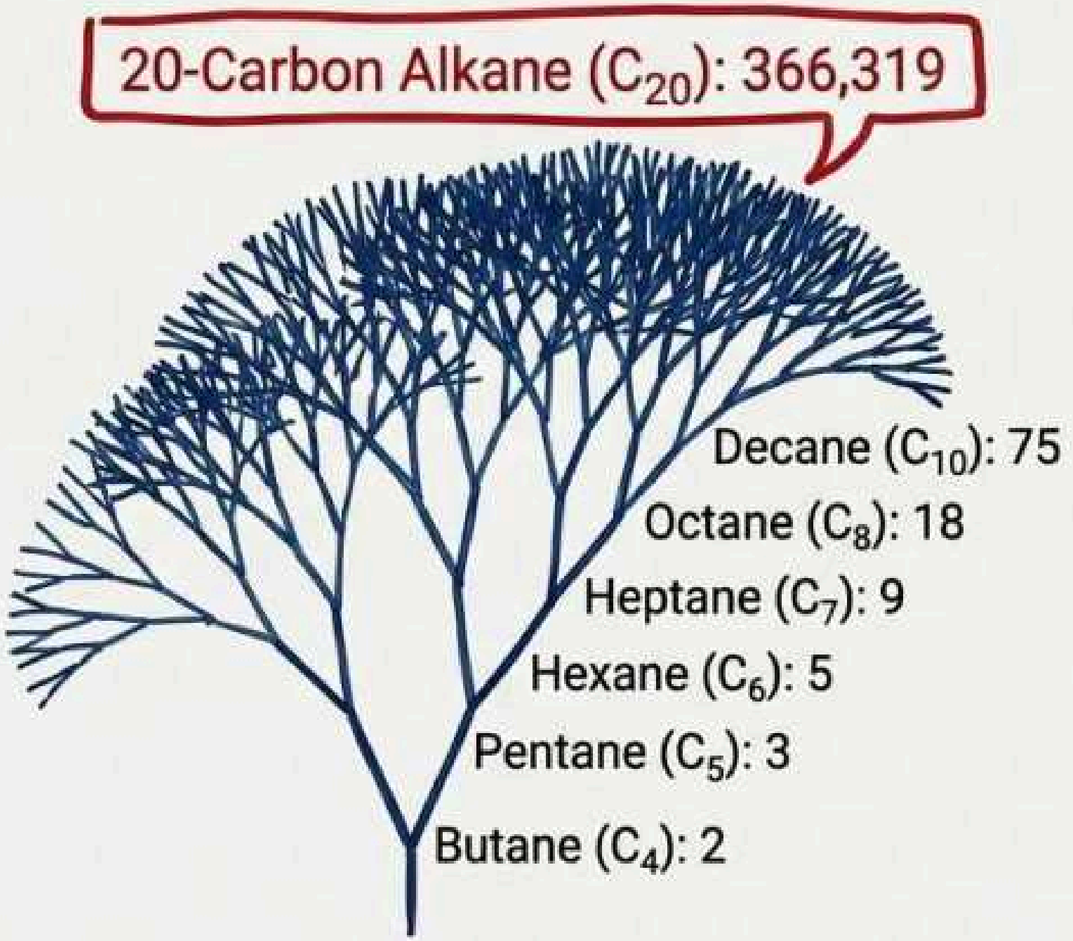


Butane
(Straight chain)



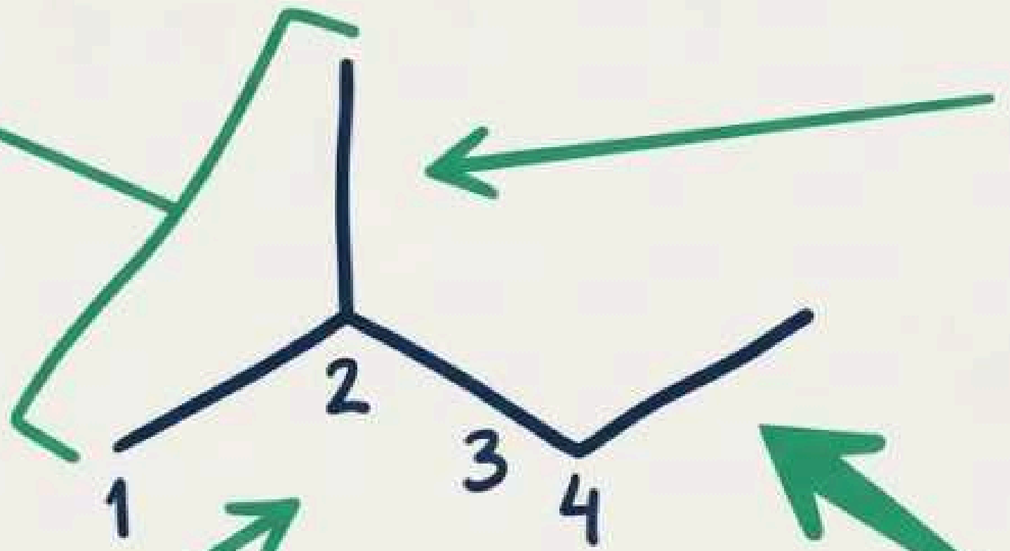
Isobutane
(Branched)

C_4H_{10}



Applying IUPAC Naming Rules

1. Find the base:
Identify the longest continuous chain (4 carbons = butane).



3. Identify branches:
Name each substituent (methyl group on carbon 2).

2. Number the chain:
Start from the end giving the lowest numbers to substituents.

4. Assemble:
List alphabetically with numbers, and join to the base.

Resulting Name: 2-methylbutane

Alkyl Branches and Carbon Classification

Common Alkyl Groups: Methyl, ethyl, propyl, isopropyl, tert-butyl.

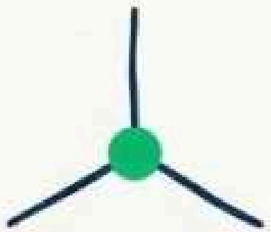
Primary (1°): One neighbor.



Secondary (2°): Two neighbors.



Tertiary (3°): Three neighbors.



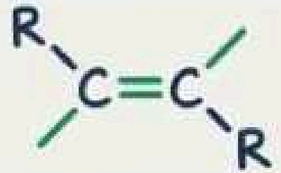
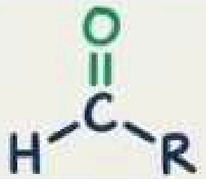
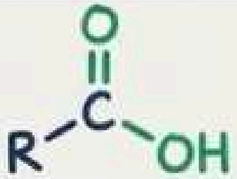
Quaternary (4°): Four neighbors.



Labels matter because these positions react differently (Lecture 5).

Functional Groups Determine Molecular Behavior

Small clusters of atoms that give a molecule its characteristic behavior.

Group Name	Characteristic Structure	Key Feature
Alkenes		Carbon–carbon double bond
Alcohols		Hydroxyl group
Aldehydes & Ketones		Carbonyl group
Carboxylic Acids		Carboxyl group
Amines		Amino group

Alkane Properties and Combustion Energy

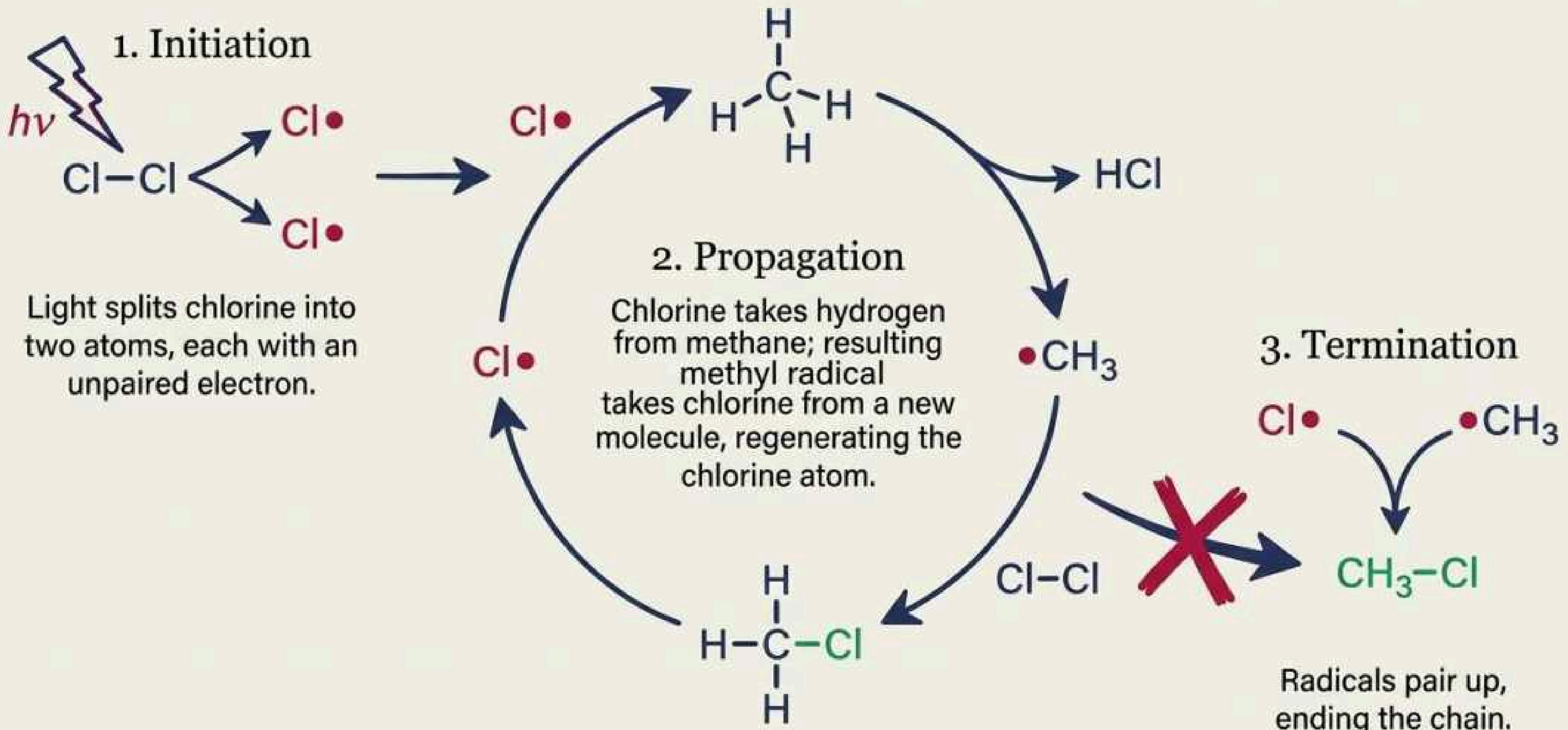
- Properties: Nonpolar and relatively unreactive. Historically named "paraffins" (Latin: little affinity).
- The Exception - Combustion: Burning one mole of methane releases massive energy.

$$CH_4 + 2O_2 \longrightarrow CO_2 + 2H_2O$$

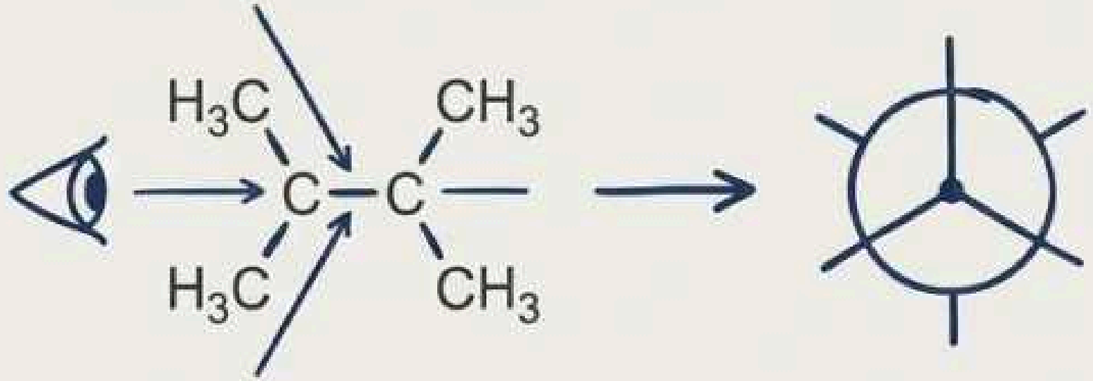
Output:

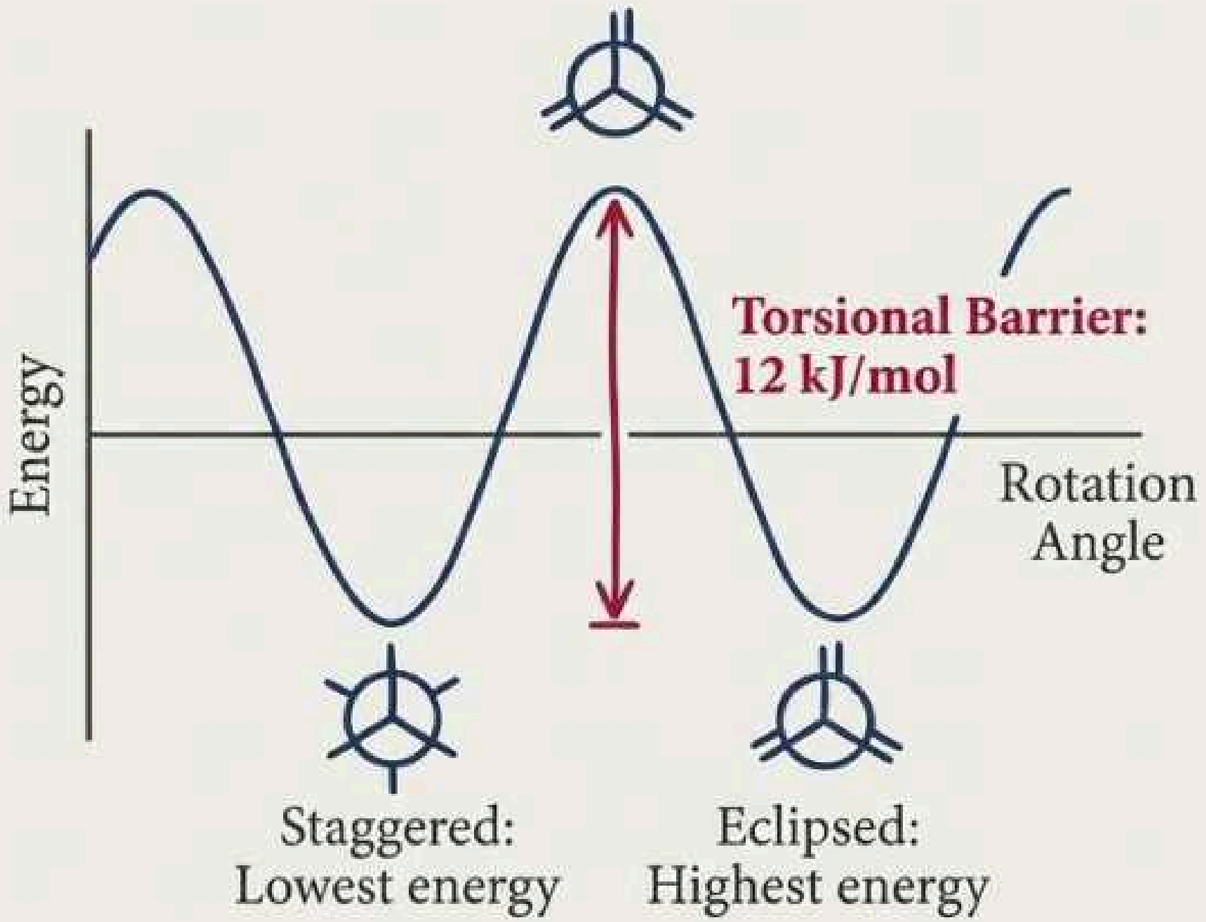
ΔH = -890 kJ/mol

The Radical Halogenation Cycle



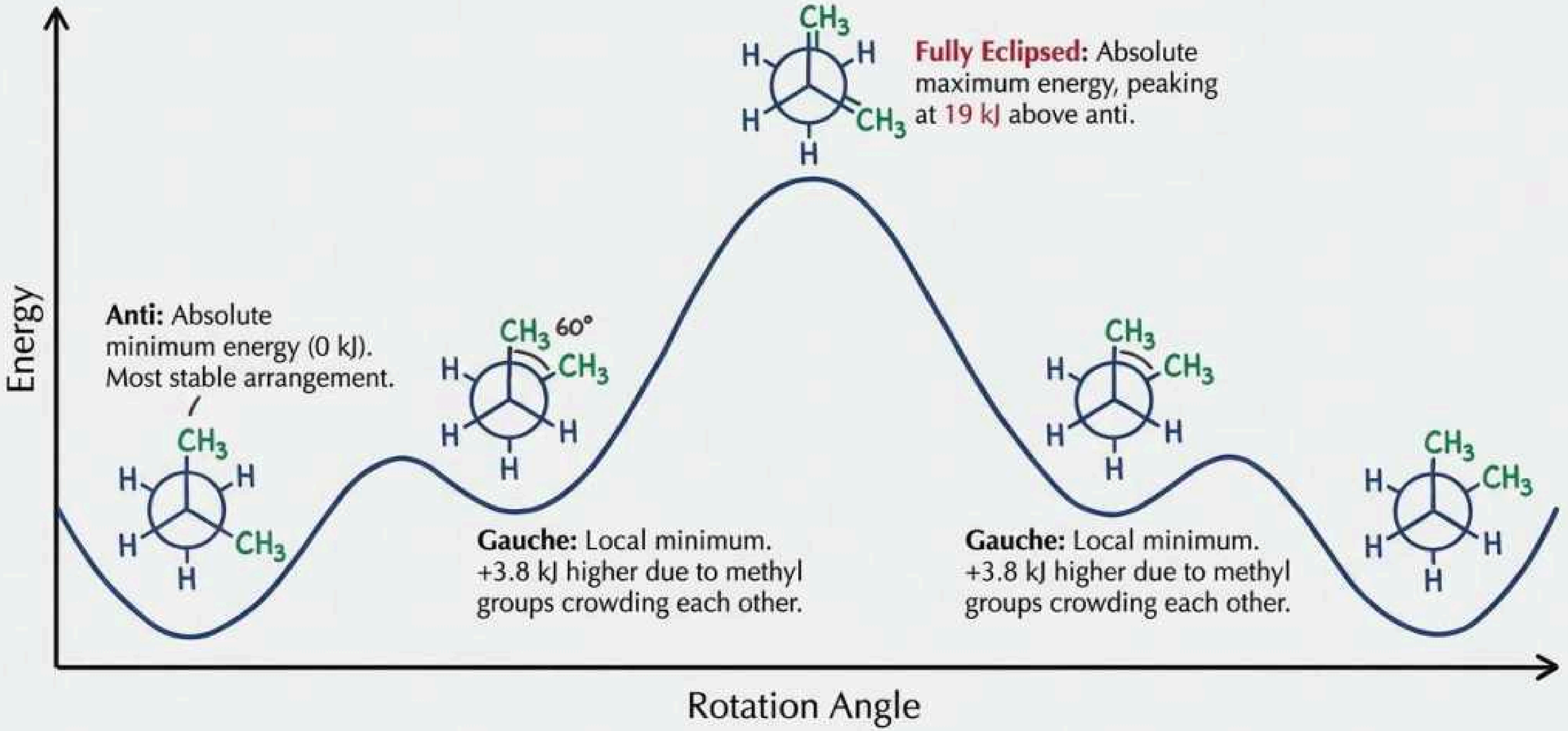
Ethane Rotation and the Torsional Barrier





Small enough that rotation is rapid at room temperature.

Butane Conformations: Navigating Crowded Space

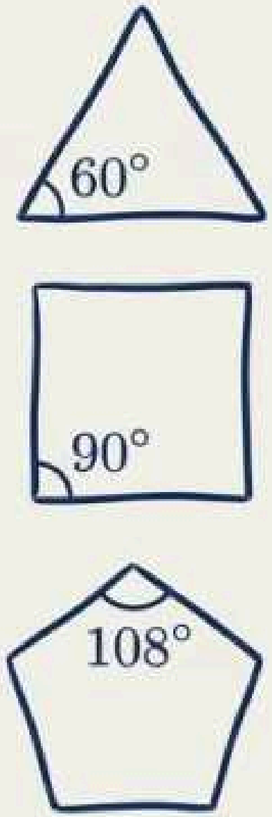


Bulky groups prefer to stay apart.

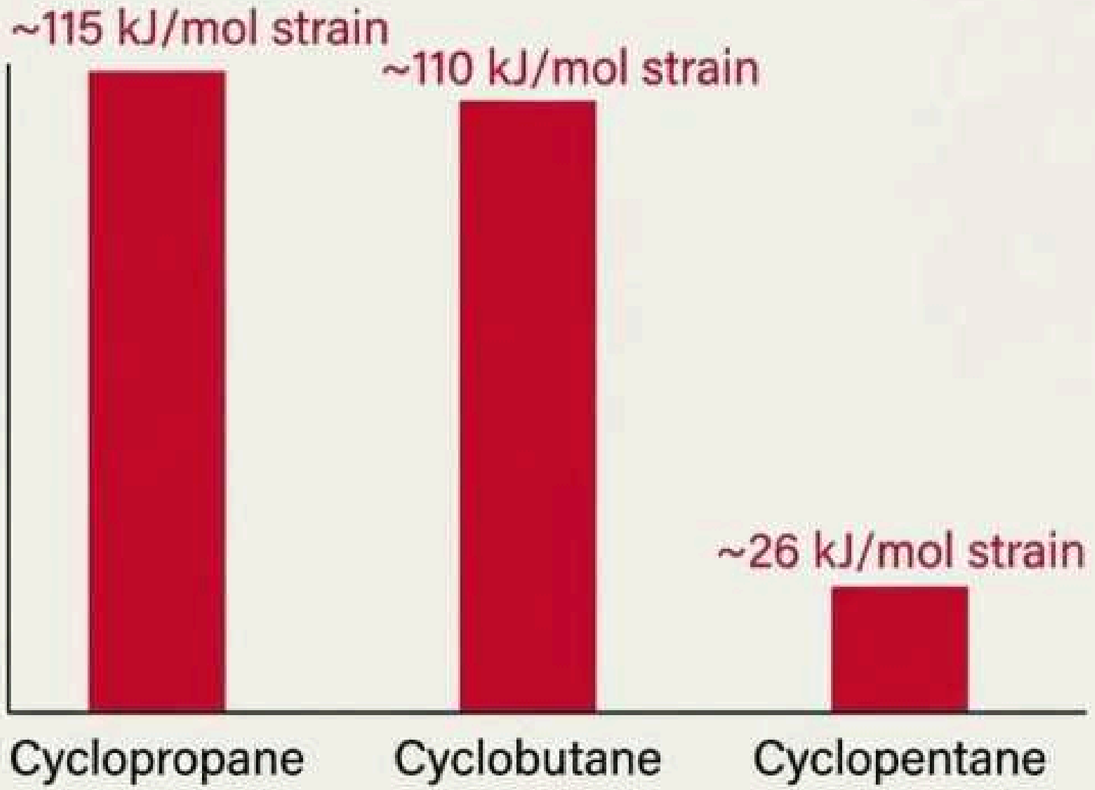
Ring Strain and the Failure of Flat Theory

Baeyer's 1885 Proposal: Rings are flat; deviation from the ideal tetrahedral angle creates strain.

The Flawed Theory



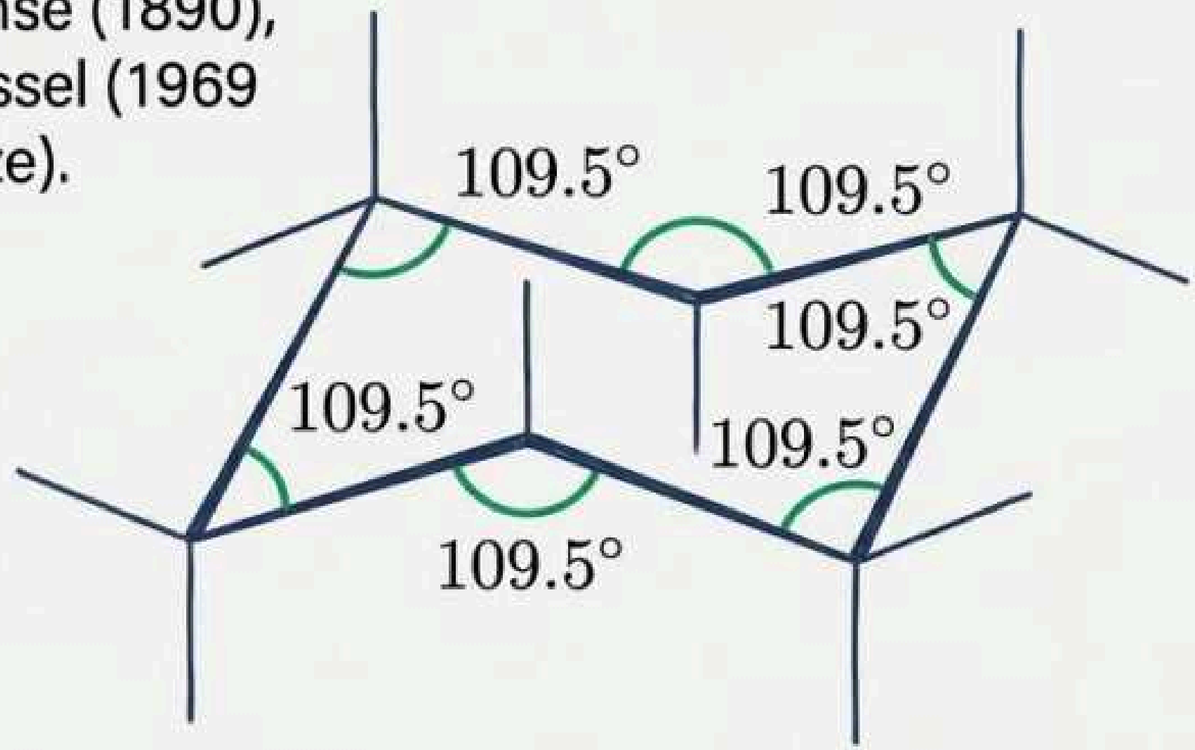
The Reality



The Flaw: For larger rings, the flat assumption fails completely because real rings pucker to relieve strain.

Cyclohexane: The Perfect Chair Conformation

Proposed by Sachse (1890), confirmed by Hassel (1969 Nobel Prize).

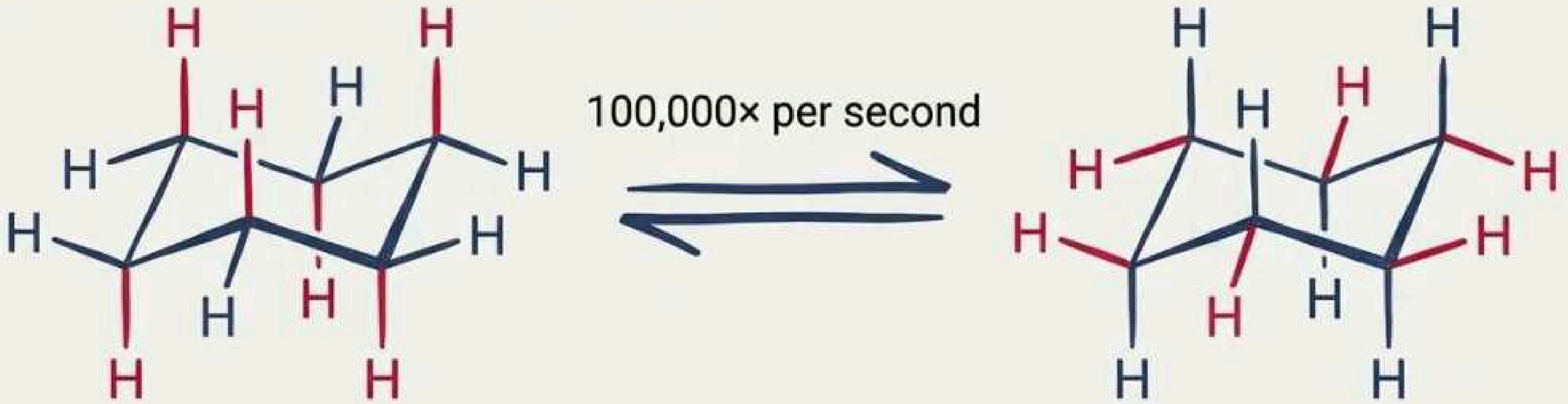


Strain = 0

Result: This makes cyclohexane the most common ring structure in nature.

The Architecture of Stability: All angles are close to tetrahedral, and all bonds are perfectly staggered.

The Dynamics of Ring Flipping

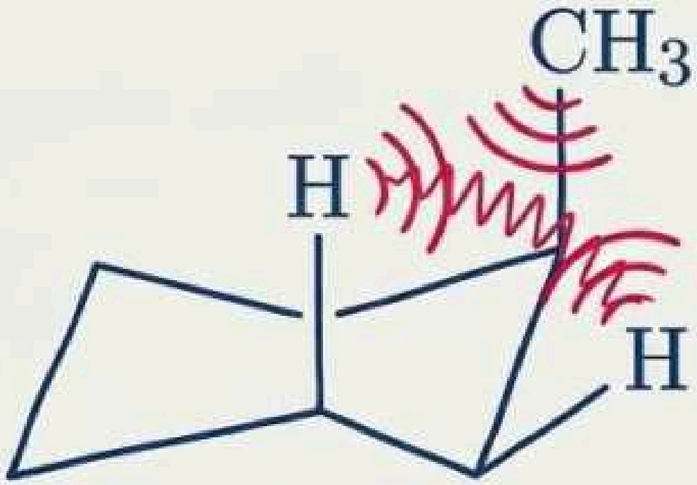


Axial positions: Point straight up or down, alternating around the ring.

Equatorial positions: Point outward, roughly in the plane of the ring.

At room temperature, rapid flipping means axial positions become equatorial and vice versa.

1,3-Diaxial Interactions: The Cost of Crowding



An axial group crowds the hydrogens on the same face, causing repulsion.

Energy Costs Methyl group: costs 7 kJ in axial.

Result: 95% of molecules sit **equatorial** at room temperature.

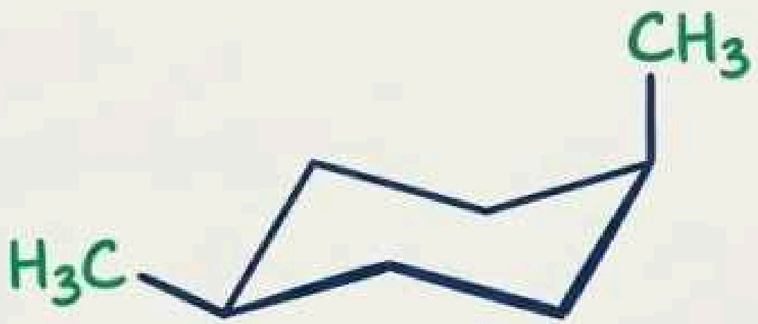
Tert-butyl group: costs 20 kJ.

Result: Effectively locked in the equatorial position.

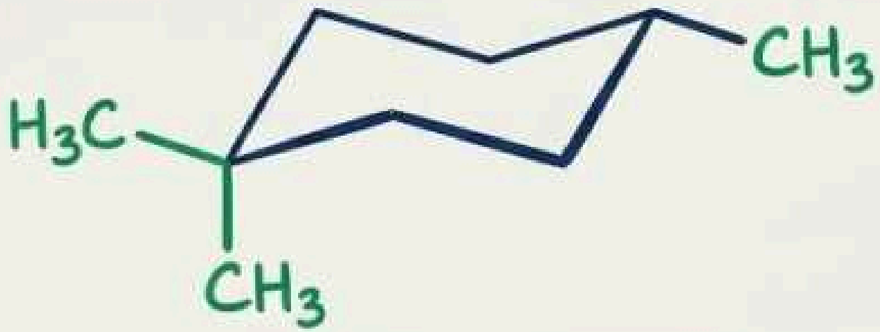
Stereoisomers: Cis vs. Trans Geometry

Definition: Not constitutional isomers (atoms connect identically). They are stereoisomers, differing only in their arrangement in space.

Cis: Both groups lie on the same face of the ring.



Trans: Groups lie on opposite faces.

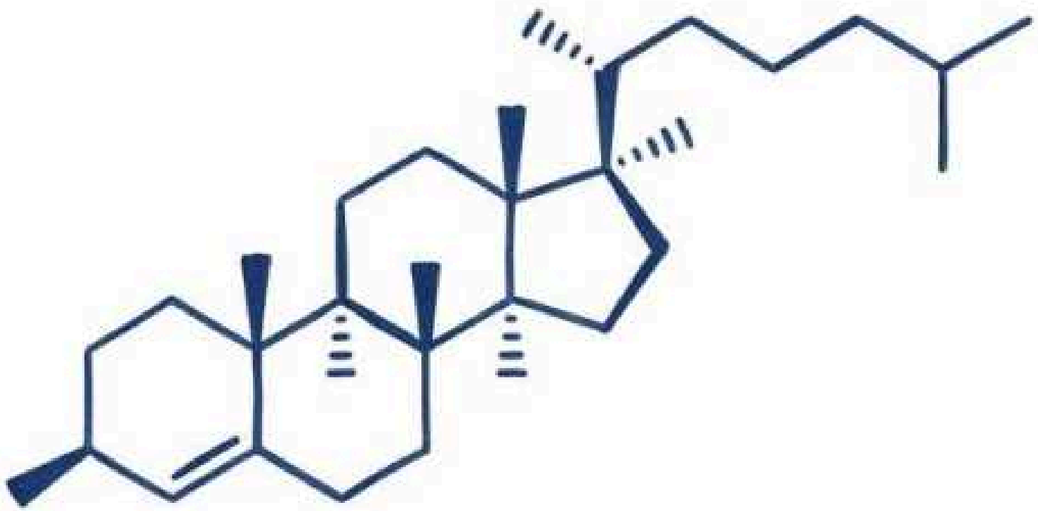


Key Insight: In *trans*-1,4-dimethylcyclohexane, both methyls can sit equatorial, making it the more stable isomer.

Fused Rings Build Biological Frameworks

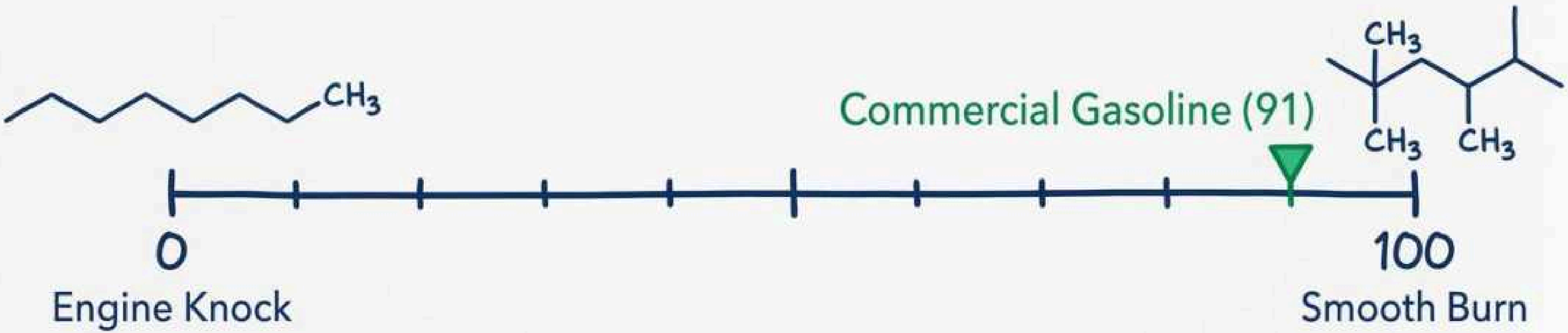


Decalin: Two cyclohexane rings sharing an edge.



Steroid Hormones & Cholesterol: Constructed entirely from a fused backbone of three six-membered rings and one five-membered ring joined together.

Real-World Application: The Octane Scale



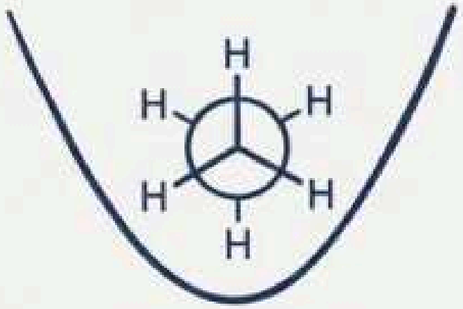
Why shape matters: Branched alkanes burn more smoothly in engines than straight chains.

Gasoline rated 91: Behaves identically to a mixture of 91% 2,2,4-trimethylpentane and 9% straight-chain heptane. Fewer knocks come from more branching.

Synthesis & Next Steps



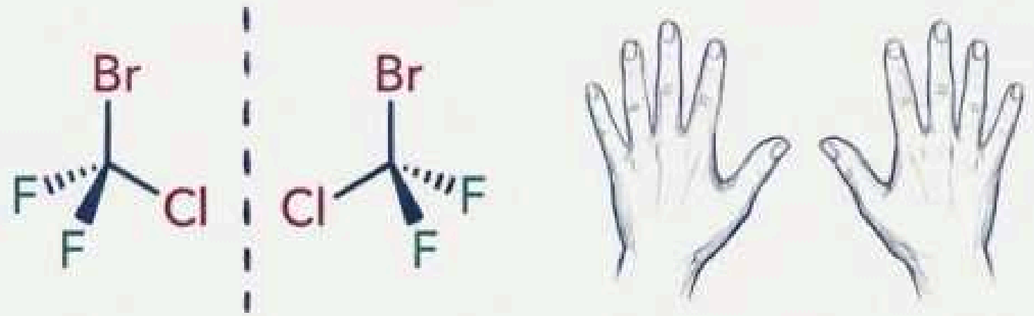
Alkanes are named by the longest chain and lowest numbers; functional groups dictate behavior.



Single bonds rotate; staggered conformations always beat eclipsed.



Cyclohexane adopts a strain-free chair where bulky groups strongly prefer equatorial positions.



Next: Lecture 4 examines molecules whose 3D shape makes them mirror images (Chirality).