

Alkanes

Chapters 3, 4, 10.2, 10.4
Organic Chemistry, 8th Edition
John E. McMurry

Hydrocarbons

- **Aliphatic** (*áleiphar* = Ointment (unguento)).
 - **Alkanes** (saturated hydrocarbons): hydrocarbons having only single C–C and C–H bonds.
 - Linear (*normal* alkanes, *n*-alkanes)
 - Branched
 - Cyclic
 - **Alkenes** (olefins): hydrocarbons having double bonds.
 - **Alkynes**: hydrocarbons having triple bonds.

- **Aromatic**

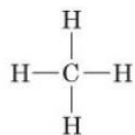
Alkanes

Number of C-atoms	Molecular formula	Name (<i>n</i> -alkane)
1	CH ₄	methane
2	C ₂ H ₆	ethane
3	C ₃ H ₈	propane
4	C ₄ H ₁₀	butane
5	C ₅ H ₁₂	pentane
6	C ₆ H ₁₄	hexane
7	C ₇ H ₁₆	heptane
8	C ₈ H ₁₈	octane
9	C ₉ H ₂₀	nonane
10	C ₁₀ H ₂₂	decane
20	C ₂₀ H ₄₂	eicosane

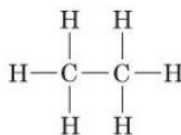
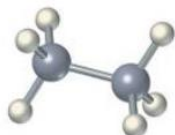
Empirical formula: C_nH_{2n+2}

Alkanes

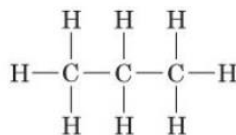
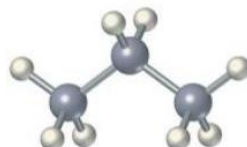
Carbon in alkanes always has a sp^3 hybridization and only single bonds are present, so the carbon geometry is tetrahedral.



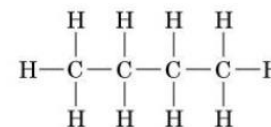
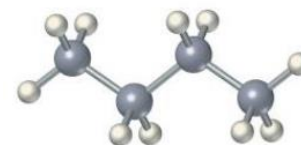
Metano, CH_4



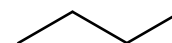
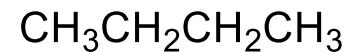
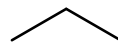
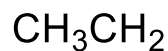
Etano, C_2H_6



Propano, C_3H_8

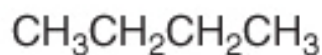


Butano

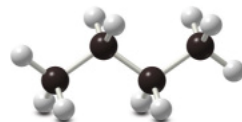


Alkanes – Structural Isomerism

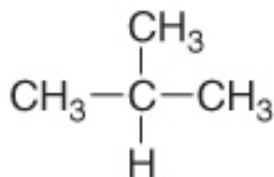
- There are two hydrocarbons with empirical formula C_4H_{10} : butane and isobutane.
- Butane and isobutane are structural isomers: they have the same composition but different physico-chemical properties.



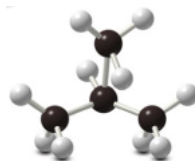
butane



Linear Alkane



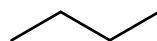
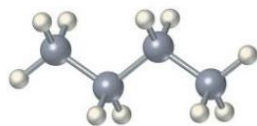
isobutane



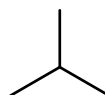
Branched Alkane

Alkanes – Structural Isomerism

C₄H₁₀

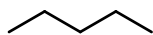
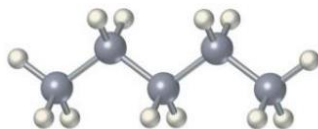


n-butane
linear alkane

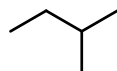
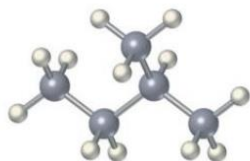


iso-butane
2-Methylpropano
branched alkane

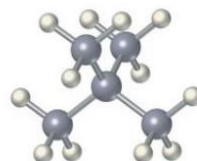
C₅H₁₂



pentano
linear alkane



2-metilbutano



2,2-dimetilpropano

branched alkane

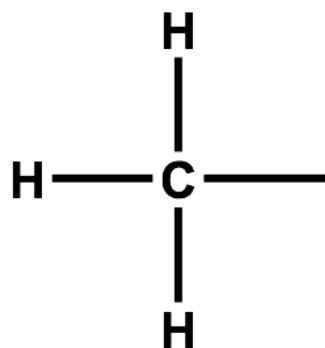
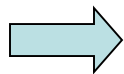
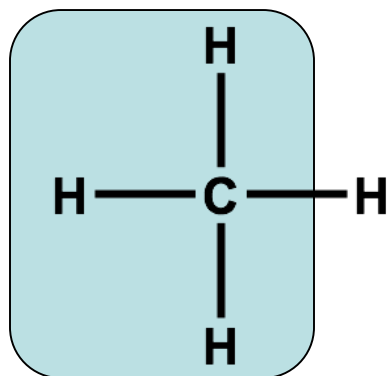
Nomi	Formule	Numero possibili isomeri
metano	CH ₄	1
etano	C ₂ H ₆	1
propano	C ₃ H ₈	1
butano	C ₄ H ₁₀	2
pentano	C ₅ H ₁₂	3
esano	C ₆ H ₁₄	5
eptano	C ₇ H ₁₆	9
ottano	C ₈ H ₁₈	18
nonano	C ₉ H ₂₀	35
decano	C ₁₀ H ₂₂	75

Alkyl Groups

In branched alkanes a main chain (the longest) is identified; the groups attached to the main chain are considered substitutes for the main chain and are called **alkyl groups**.

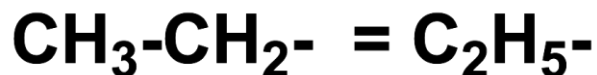
In general terms the alkyl substitute is referred to as **-R**.

Root-Suffix (= yl)



Free
valence = $\text{CH}_3\text{-}$

methyl



ethyl



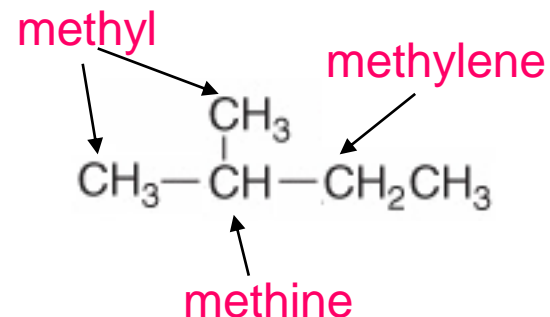
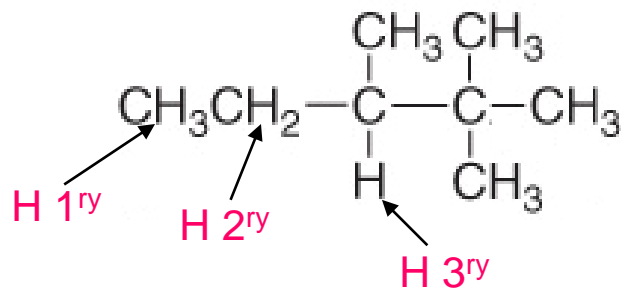
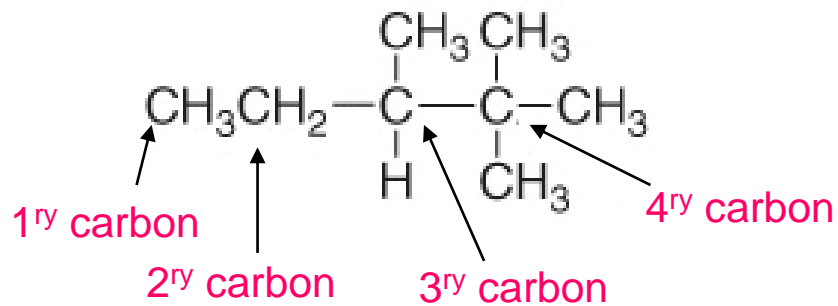
propyl

Alkyl Groups

C-Atoms	Structure	Name	C-Atoms	Structure	Name
1	CH_3-	methyl	5	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2-$	<i>n</i> -pentyl
	$-\text{CH}_2-$	methylene		$\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2\text{CH}_2-$	isopentyl
	$-\overset{ }{\text{C}}\text{H}-$	methine		$\text{CH}_3\text{C}(\text{CH}_3)_2\text{CH}_2-$	neopentyl
2	CH_3CH_2-	ethyl		$\text{CH}_3\overset{2}{\text{C}}\text{H}(\text{CH}_3)\text{CH}_2\text{CH}_2\text{CH}_3$	sec-pentyl
	$\text{CH}_3\text{CH}_2\text{CH}_2-$	<i>n</i> -propyl		$\text{CH}_3\text{CH}_2\overset{3}{\text{C}}\text{H}(\text{CH}_3)\text{CH}_2\text{CH}_3$	
3	$\text{CH}_3\text{CH}(\text{CH}_3)$	isopropyl			
	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2-$	<i>n</i> -butyl			
4	$\text{CH}_3\text{CH}(\text{CH}_3)\text{CH}_2-$	isobutyl			
	$\text{CH}_3\text{CH}_2\text{CH}(\text{CH}_3)-$	sec-butyl			
	$\text{CH}_3\text{C}(\text{CH}_3)_2-$	tert-butyl			

Classification of carbon atoms

Carbon atoms are classified according to the number of carbon atoms to which they are bound. Hydrogen atoms are also classified in analogy.



Nomenclatura IUPAC

Costruzione del nome

prefisso + infisso + suffisso

- numero di carboni (but-, pent- ecc.)
- presenza di doppi o tripli legami (an-, en-, in-)
- classe chimica (-o, -e, -olo, -ale, -one, ecc.)

et-an-o

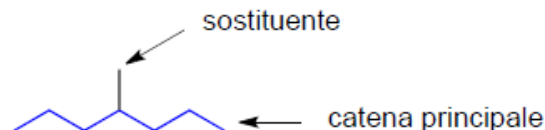
et-en-e

et-in-o

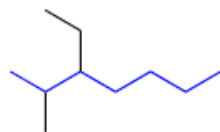
1. Agli alcani lineari il nome è assegnato in base al numero degli atomi di carbonio presenti:

Metano, etano, propano, butano, pentano, esano, eptano, ottano, nonano, decano, undecano, dodecano, ...

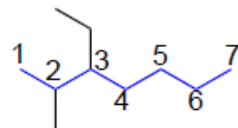
2. Per alcani contenenti catene di carbonio ramificate, si individua la catena principale:



3. Se due o più catene, nell'ambito della struttura, hanno la stessa lunghezza, si deve scegliere, come catena principale, quella con il numero maggiore di ramificazioni:

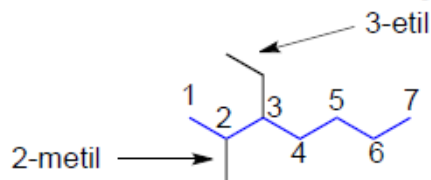


4. Si numerano consecutivamente i carboni della catena principale da una parte all'altra, nella direzione che attribuisce il numero più basso al primo punto di ramificazione:



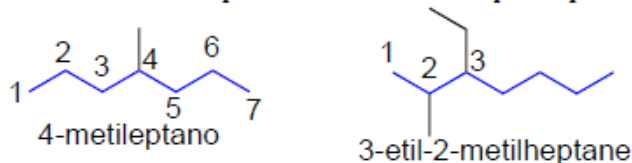
Nomenclatura IUPAC

5. Si assegna il nome a ciascuna ramificazione e si identifica il numero del carbonio della catena principale sul quale essa si trova. (ricorda: isopropile, isobutile, sec-butile, t-butile, neopentile):

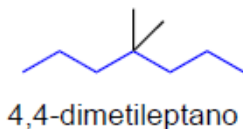


6. Costruisci il nome scrivendo il numero del carbonio della catena principale cui è legato il sostituente. un trattino. il nome del sostituente e il nome

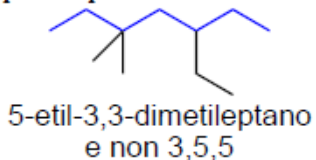
dell'alcano corrispondente alla catena principale:



7. Se la catena principale contiene più sostituenti dello stesso tipo, ognuno di essi riceve il proprio numero. Si utilizzano i prefissi di, tri, tetra e così via, per indicare il numero dei sostituenti uguali:



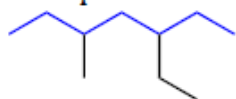
8. Se i gruppi sostituenti sono legati a carboni diversi della catena principale, si confrontano, posizione per posizione, i possibili schemi di numerazione alternative e viene scelto quello che attribuisce il numero più piccolo al primo punto di differenza:



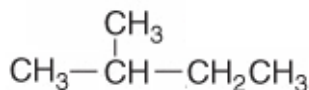
Nomenclatura IUPAC

9. I gruppi sostituenti sono citati nel nome in ordine alfabetico, senza tener conto della loro posizione nella catena principale. Nello stabilire quest'ordine alfabetico, i prefissi numerici di, tri, tetra e così via, così come i prefissi uniti con un trattino t- e sec- sono ignorati, a differenza dei prefissi iso, neo e ciclo che vanno invece considerati.

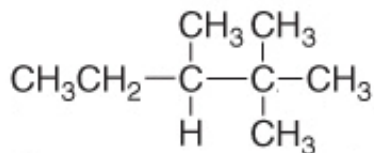
10. Se la scelta della numerazione dei gruppi differenti non può essere effettuata sulla base delle regole precedenti, al gruppo citato per primo viene attribuito il numero più basso:



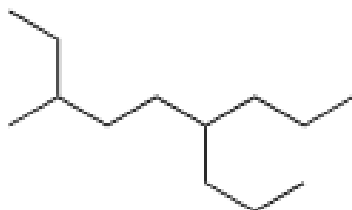
3-etil-5-metileptano
e non 5-etil-3-metileptano



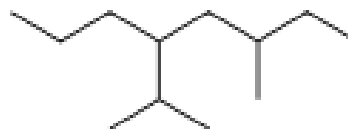
2-metilbutano



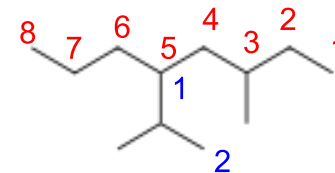
2,2,3-trimetilpentano



3-metil-6-propilnonano



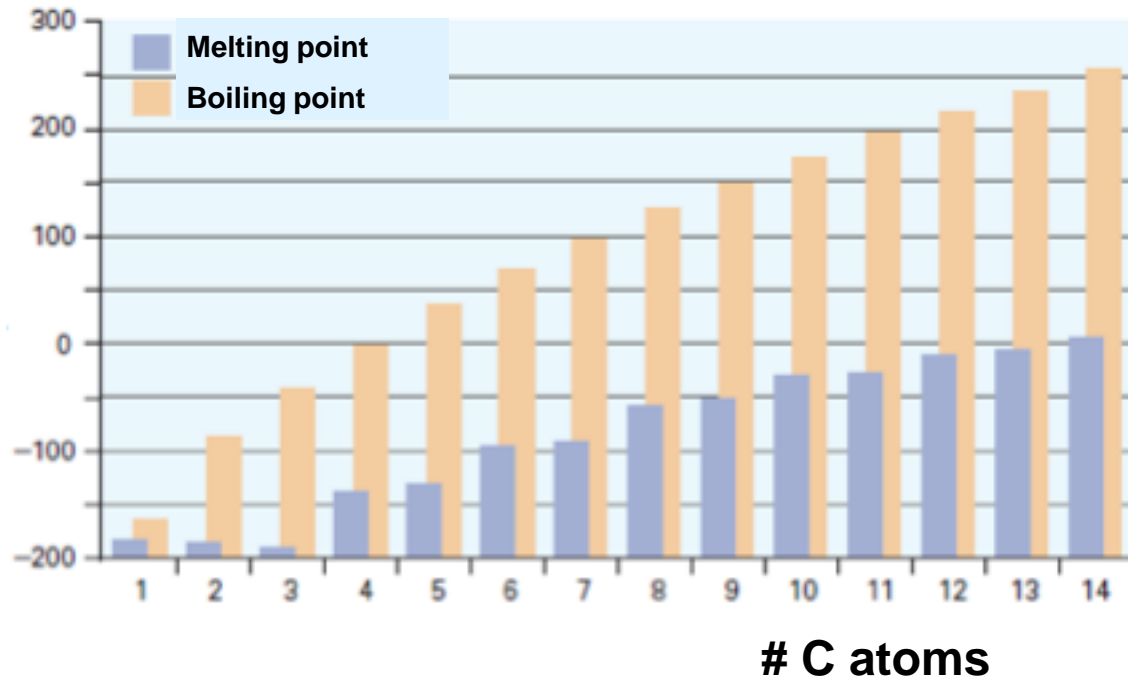
5-isopropil-3-metilottano



5-(1-metiletil)-3-metilottano

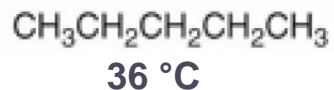
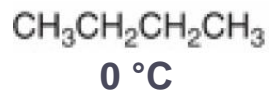
Physical Properties

Temperature

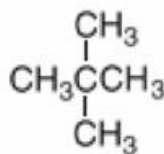


Physical Properties

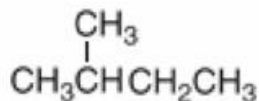
b.p.



Surface area increases with C-atoms 



10 °C



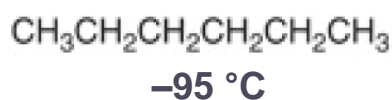
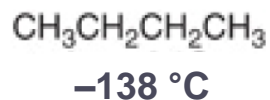
30 °C



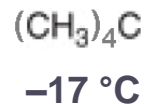
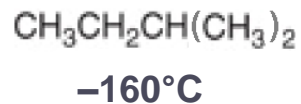
36 °C

Surface area decreases with branching 

m.p.



Surface area increases with C-atoms 



Increases with symmetry 

Physical Properties

Physical state: C1-C4 gas /b.p. -160° - 0°
 C5-C17 liq./m.p. -130° - 20°
 >C17 solid

Solubility: soluble in organic solvents (apolar)
 insoluble in water

Natural Sources

Natural sources of alkanes are natural gas and oil.

Natural gas contains mainly methane: minor components are ethane, propane and butane.

Oil is a complex mixture of, mainly, C_1 - C_{40} hydrocarbons.

Distillation of crude oil (refining) separates oil in fractions with different boiling point. The main fractions are:

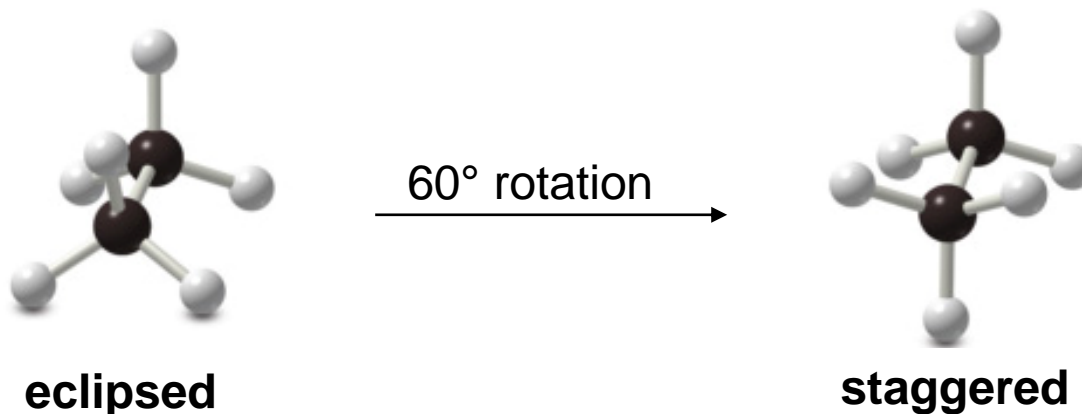
gasoline: C_5H_{12} – $C_{12}H_{26}$

kerosene: $C_{12}H_{26}$ – $C_{16}H_{34}$

diesel oil: $C_{15}H_{32}$ – $C_{18}H_{38}$

Conformational Isomerism

Ethane

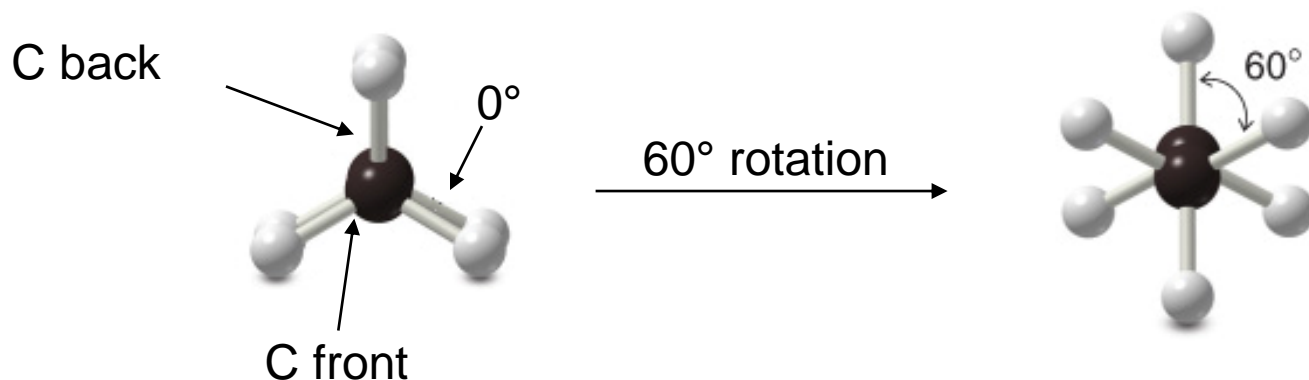


- In the **eclipsed** conformation, all C–H bonds are aligned.
- In the **staggered** conformation, C–H bonds on each carbon bisect the H–C–H angles on the other carbon.

Ethane Conformations

- The H-C-C-H angle is called dihedral angle (0° in the eclipsed and 60° in the staggered conformation).

View along the C-C bond



Eclipsed conformation

Staggered conformation

The front C-H bonds bisect the H-C-H angles on the carbon atom at the back

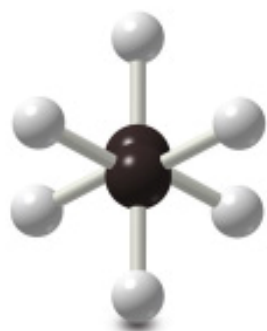
Newman Projection

➤ How to draw a Newman projection

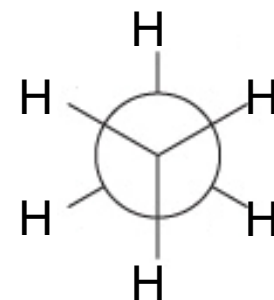
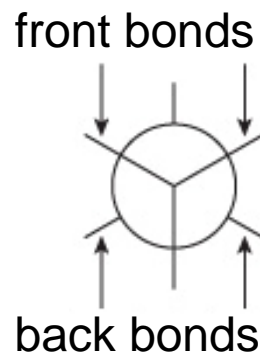
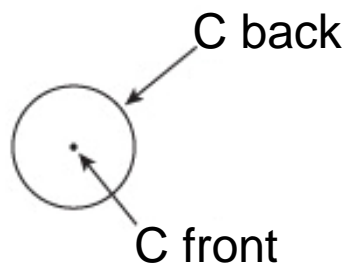
[1] Look along the C-C bond and draw a circle (the back C atom) with a dot in the centre (the front C atom).

[2] Draw the bonds

[3] Add the atoms



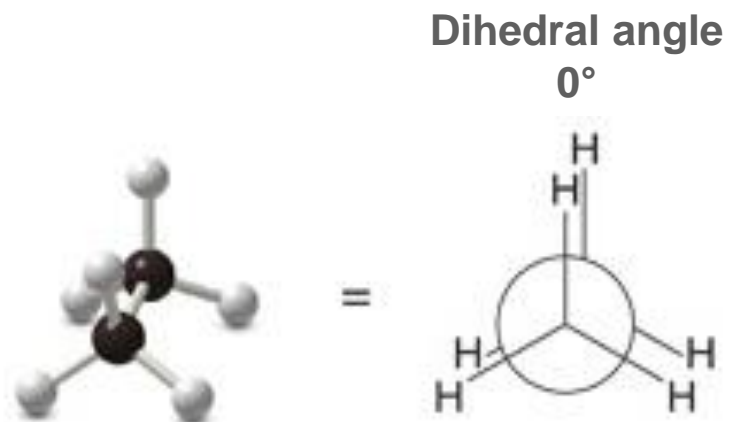
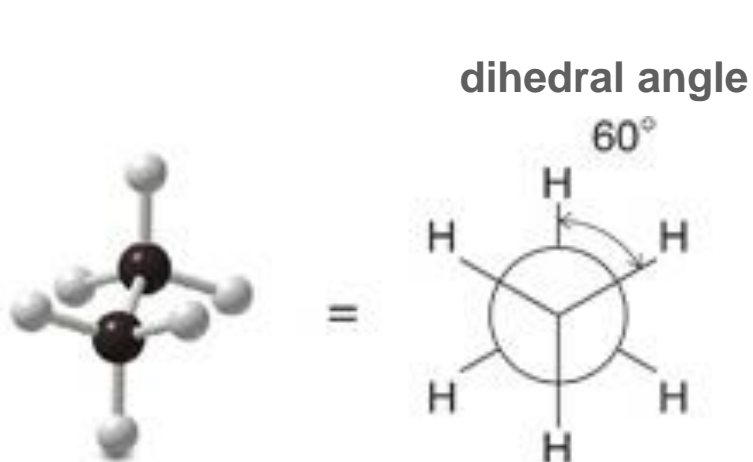
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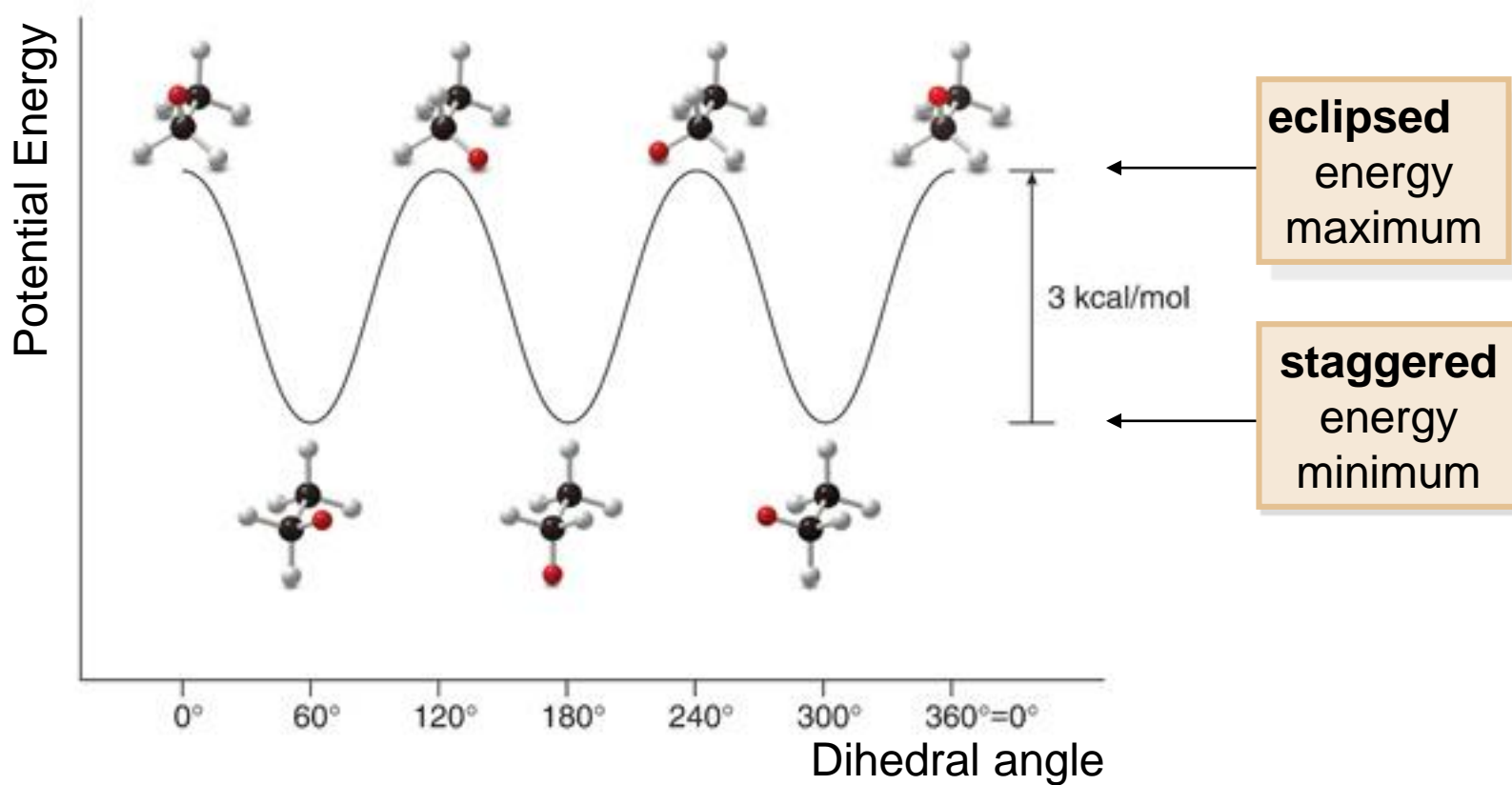
Newman Projections of Ethane

staggered conformation

eclipsed conformation

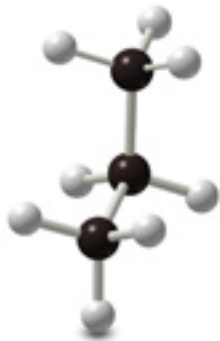
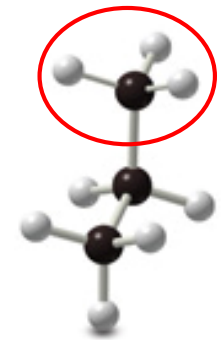
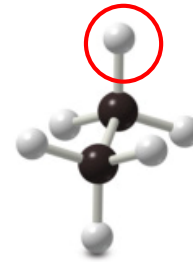
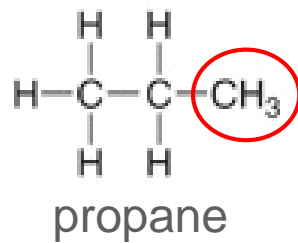
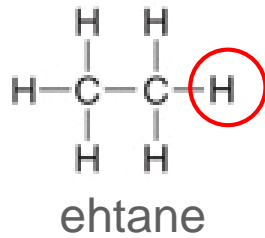


Conformations of Ethane

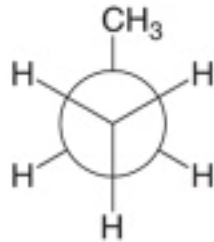


Torsional Strain 3.0 kcal/mole

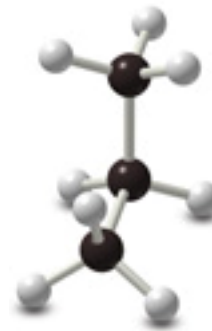
Conformations of Propane



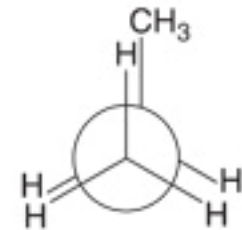
=



staggered conformation

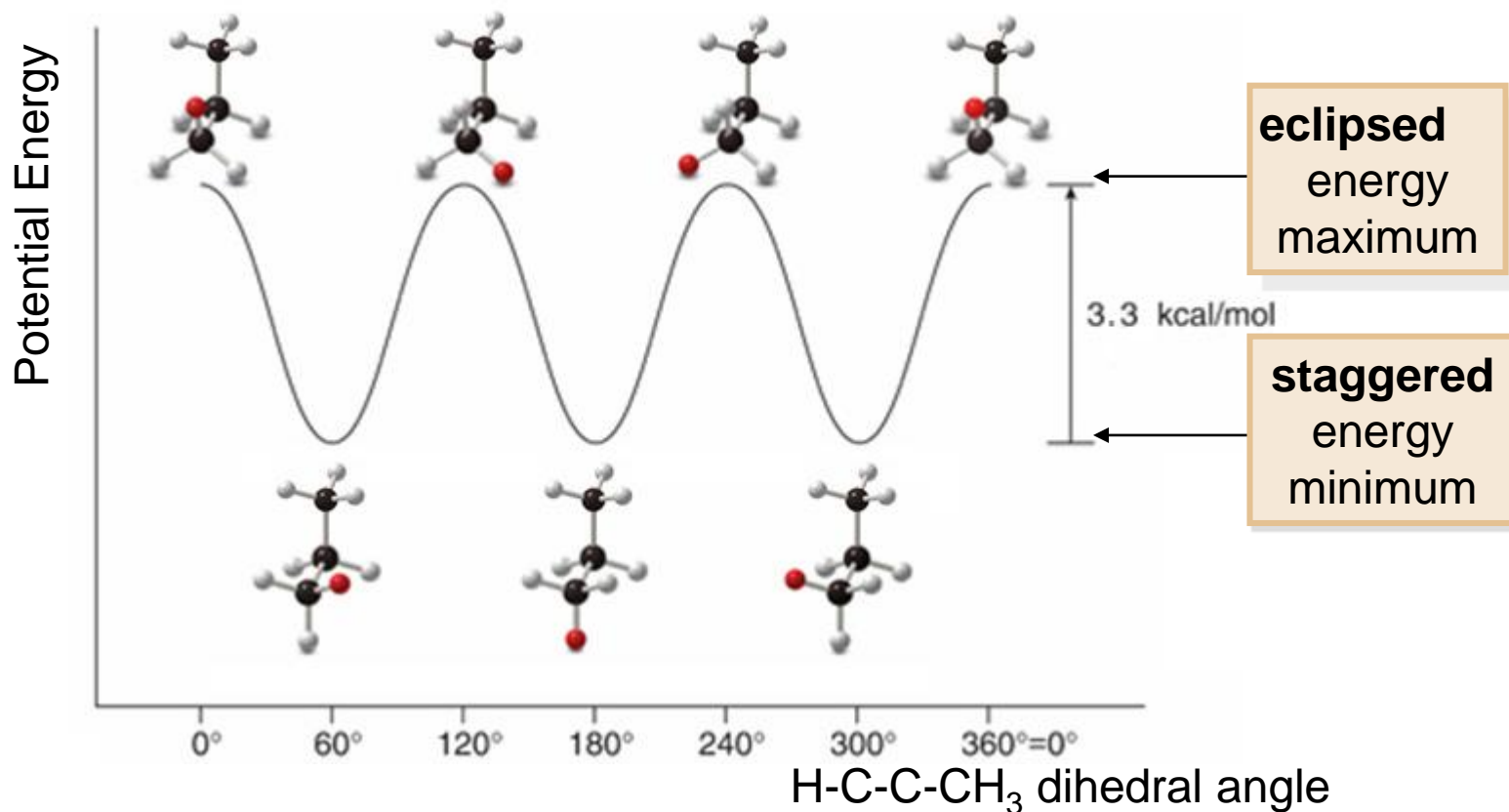


=



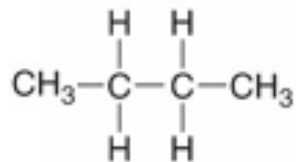
eclipsed conformation

Conformations of Propane

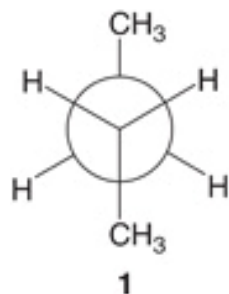


Torsional Strain (3.3 kcal/mole) is higher than in ethane. The methyl group is bulkier than a hydrogen atom

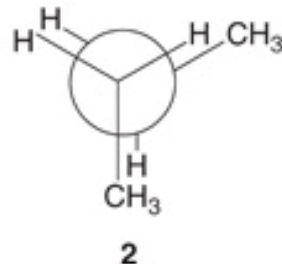
Conformations of Butane



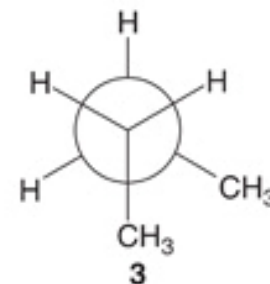
6 different conformations



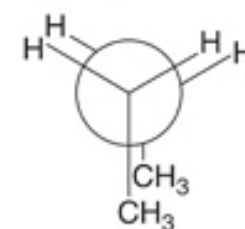
staggered, anti



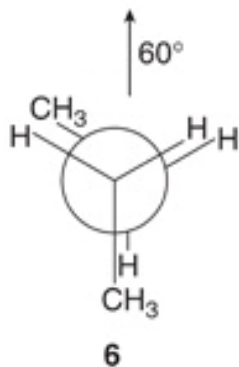
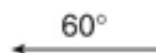
eclipsed



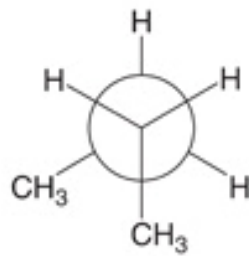
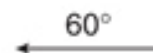
staggered, gauche



eclipsed



staggered, gauche

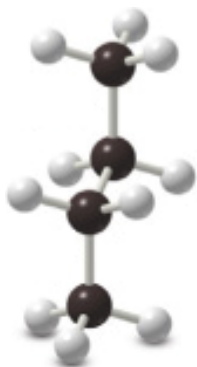


eclipsed

Conformations of Butane

A staggered conformation with two large groups at 180° is called *anti*

anti conformation



The CH_3 are at 180°

1

A staggered conformation with two large groups at 60° is called *gauche*.

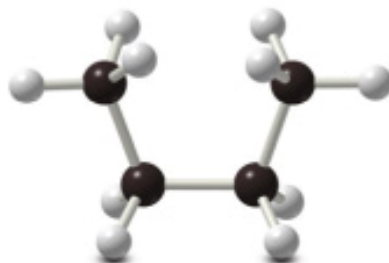
conformazione *gauche*



The CH_3 are at 60°
steric strain

3

Eclipsed conformation



The CH_3 are at 0°
steric strain

4

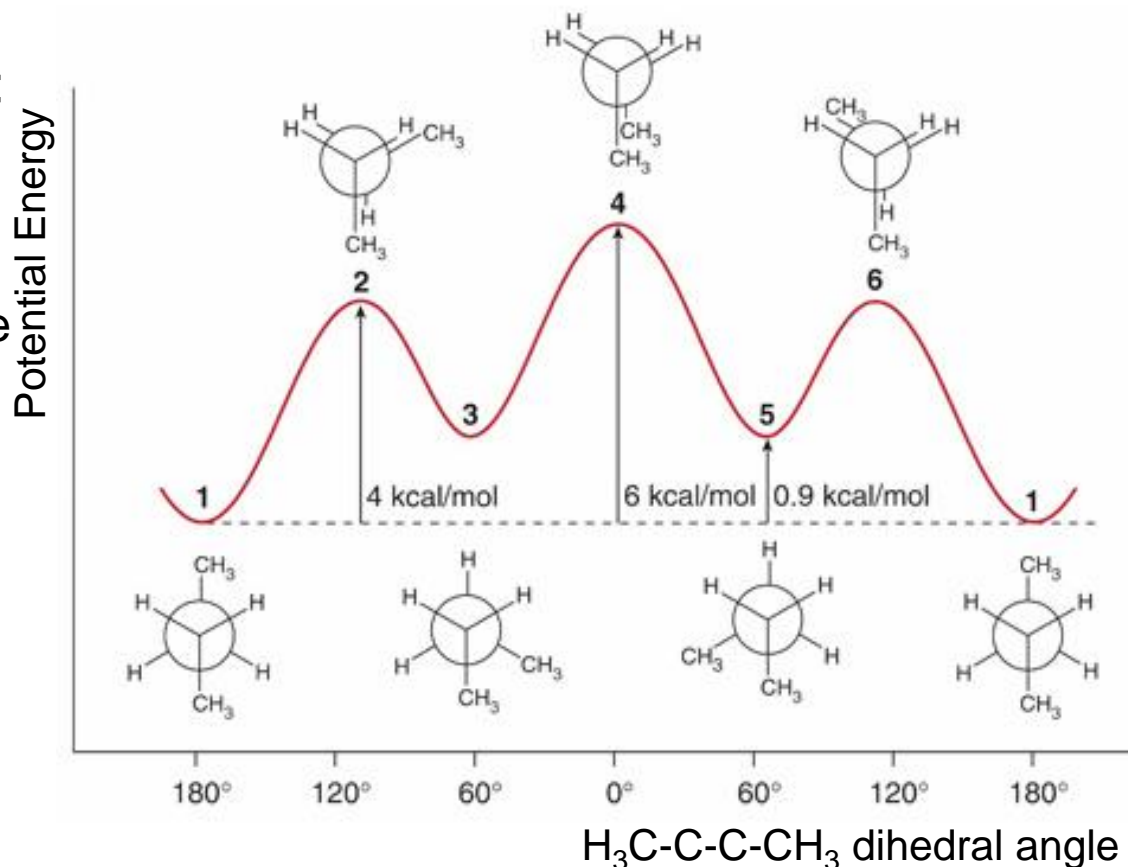
Conformations of Butane

➤ *Staggered conformations:*

- **1** (anti) is the absolute minimum
- **3,5** (gauche) are relative minima

➤ *Eclipsed conformations:*

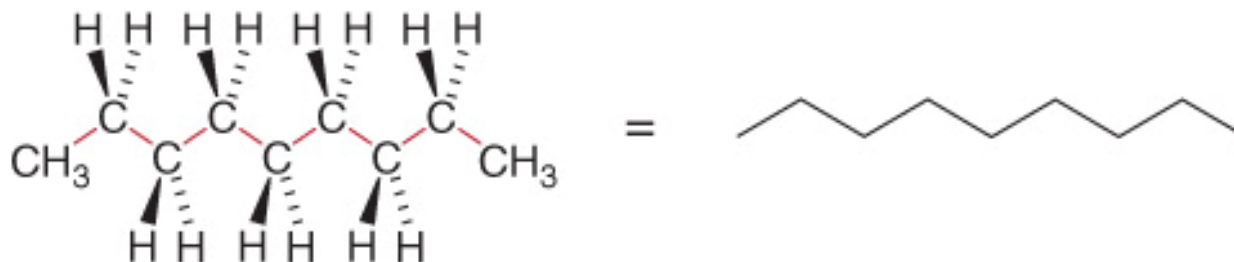
- **4** is the absolute maximum (CH₃ eclipsed)
- **2,6** are relative maxima



Torsional Strain in Linear Alkanes

Interaction	Energy (kcal/mole)
Eclipsing H,H	1
Eclipsing H,CH ₃	1.5
Eclipsing CH ₃ ,CH ₃	4
Gauche CH ₃ ,CH ₃	0.9

- A **rotational barrier** is the energy difference between two minima.
- The most stable conformation of linear hydrocarbons is staggered with the bulky groups in anti. Thus long chains are usually drawn with a zigzag.



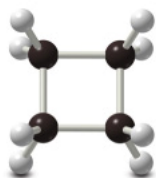
Cycloalkanes

Cycloalkanes

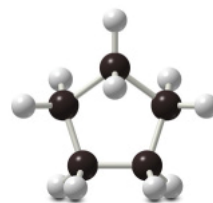
- Cycloalkanes have empirical formula C_nH_{2n} and contain carbon atoms arranged in a cyclic chain
- Nomenclature: cyclo + name of the corresponding alkane



cyclopropane



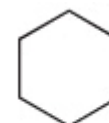
cyclobutane



cyclopentane

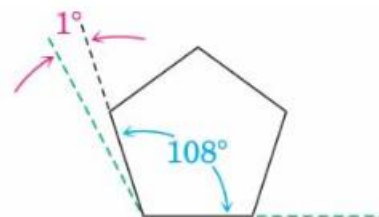
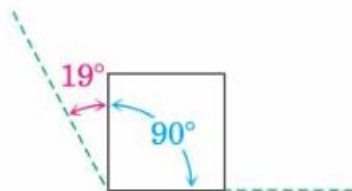
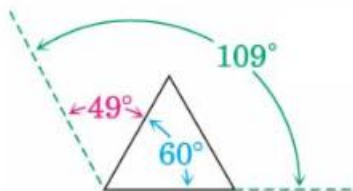


cyclohexane



Stability: Angular Strain (Baeyer's Strain)

- Baeyer (1885): as carbon prefers 109° bond angles, rings other than five or six membered may be too **strained** to exist.
- Cycloalkanes from C_3 to C_{30} do exist, but some of them are strained because of distorted bond angles and other interactions.



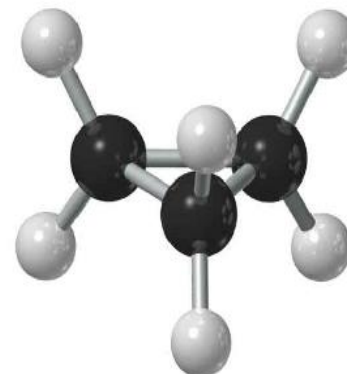
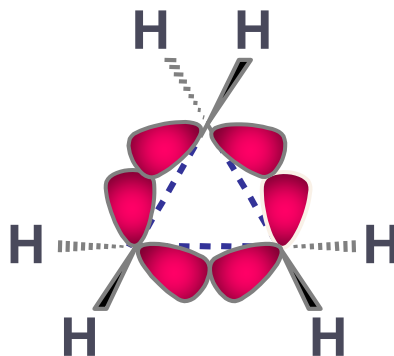
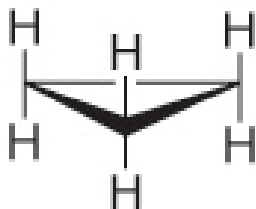
Ring Strain

Stability of cycloalkanes depend on **ring strain**:

- ✦ **angle strain**: distorted bond angles.
- ✦ **torsional strain**: eclipsing of C-H bonds.
- ✦ **VdW or steric strain**: repulsions between non bonded atoms.

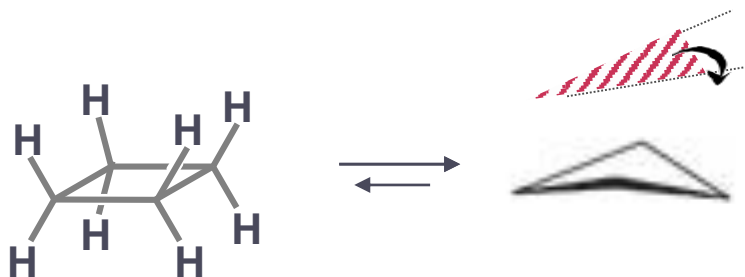
Cyclopropane C_3H_6

- Planar.
- Angle strain: 60° CCC angles.
- Torsional strain: all H are eclipsed.
- May be described as sp^3 hybridized with banana bonds.



Cyclobutane C₄H₈

- In planar cyclobutane all hydrogens would be eclipsed.
- To relieve torsional strain, cyclobutane is puckered by about 25°.
- In doing so the CCC bond angles decrease to 88° and hydrogens on opposite carbons become closer.



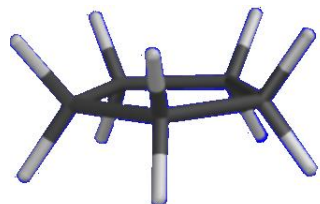
25°
puckering
angle



Planar
angle strain
torsional strain

Puckered
slightly higher angle strain
lower torsional strain
some VdW strain

Cyclopentane C_5H_{10}

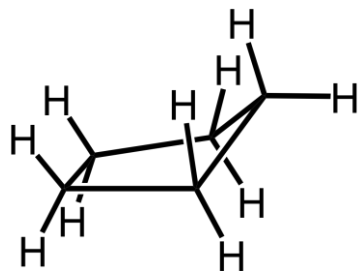
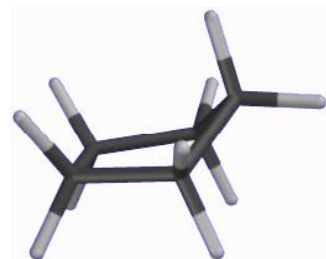


angle strain
torsional strain

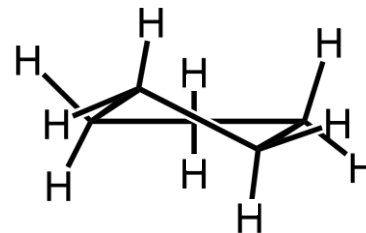


25°
puckering angle

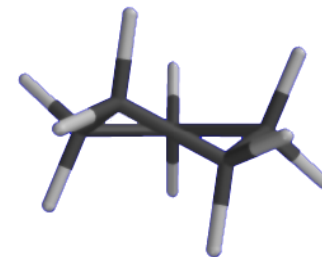
“envelope” conformation
eclipsing is partially relieved



envelope



half-chair

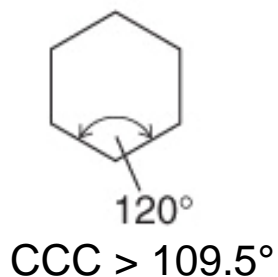


envelope and *half-chair* conformations have similar energies and rapidly interconvert into one another

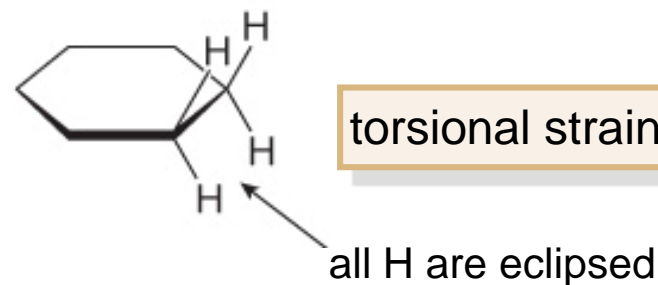
Cyclohexane C_6H_{12}

→ Planar cyclohexane.

angle strain

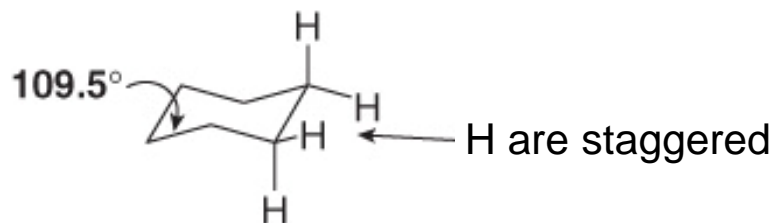


torsional strain

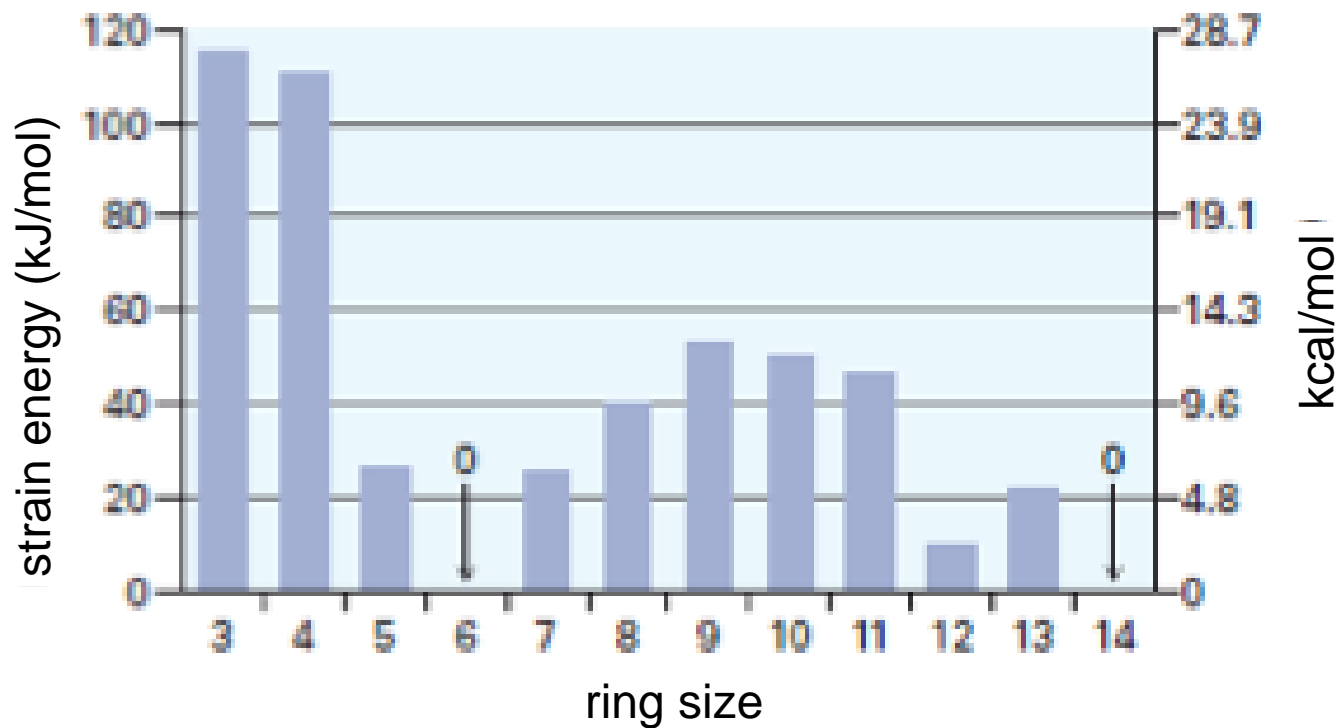


→ *Chair* conformation.

strainless

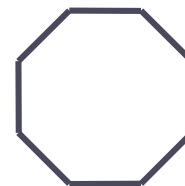
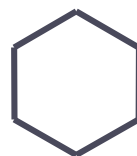





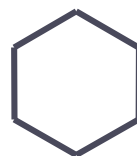

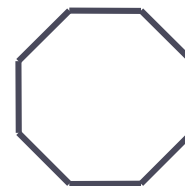
Strain Energies of Cycloalkanes



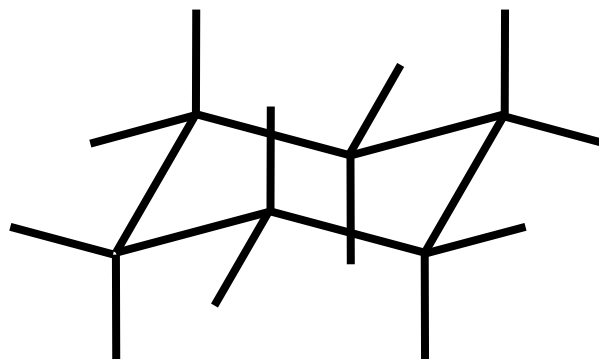
Strain Energies of Cycloalkanes

- Heats of combustion are used to calculate strain energies of cycloalkanes.
- Heats of combustion increase with the number of C atoms.
- Cyclohexane is taken as reference (Strain = 0).



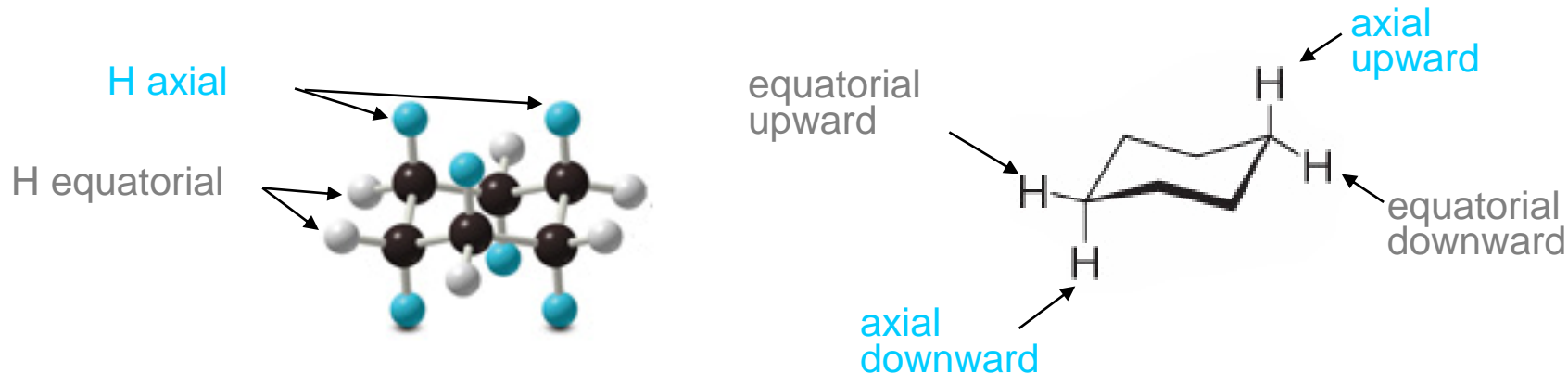
						
kJ/mol	2091	2724	3290	3910	4599	5264
Per CH ₂	697	681	658	653	657	658
Strain	132	112	25	0	28	40

How to Draw Chair Cyclohexane



Chair Conformation of Cyclohexane

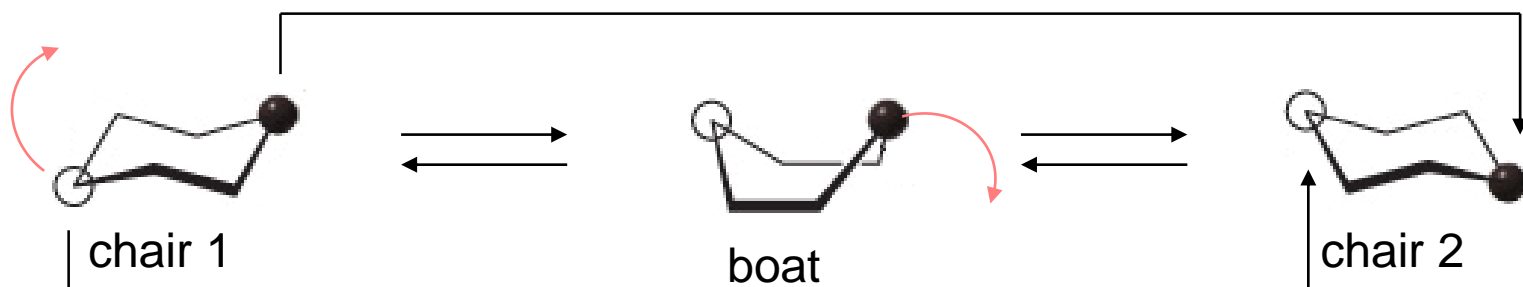
- There are two types of hydrogens:
 - ✦ **Axial**: perpendicular to the ring's mid-plane, above and below the ring.
 - ✦ **Equatorial**: in the ring's mid-plane, all around the ring.



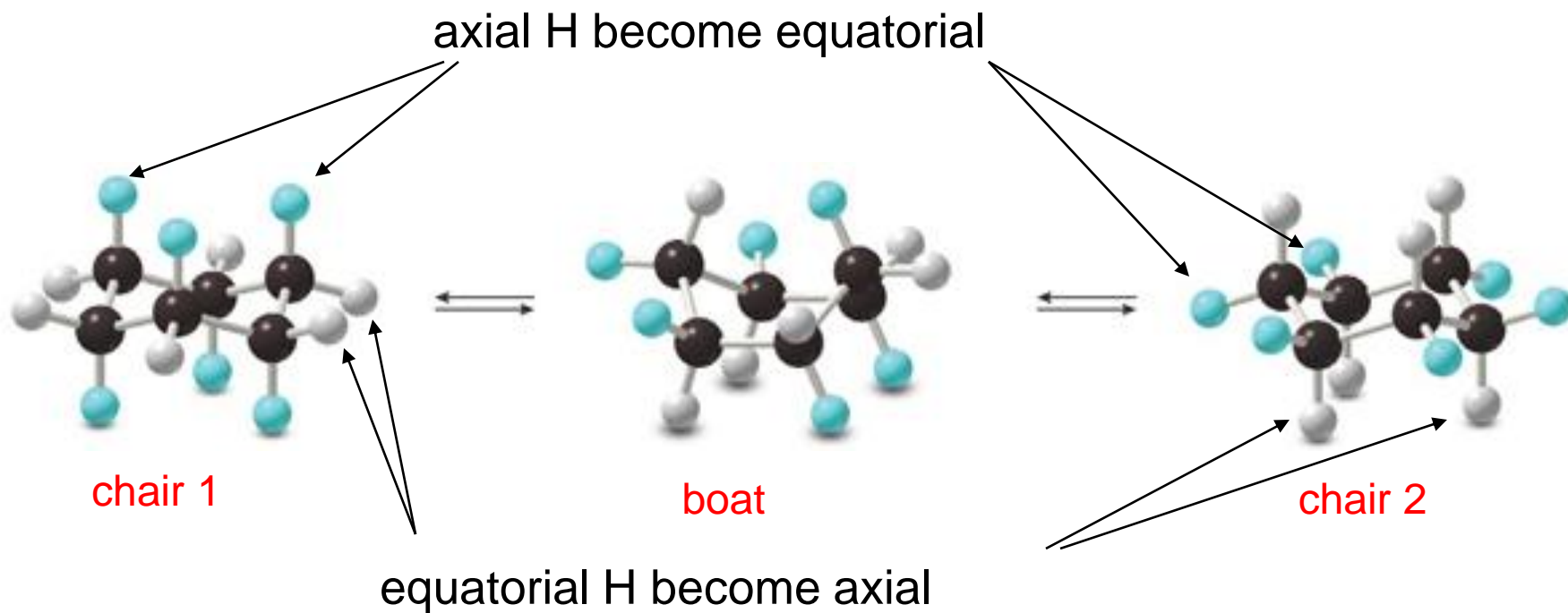
- There are 6 axial and 6 equatorial hydrogens in cyclohexane.

Ring Flipping

- **Ring flipping** is the interconversion between two chair conformations of cyclohexane.
- Upwards C become downwards and viceversa.
- Axial H become equatorial and viceversa.

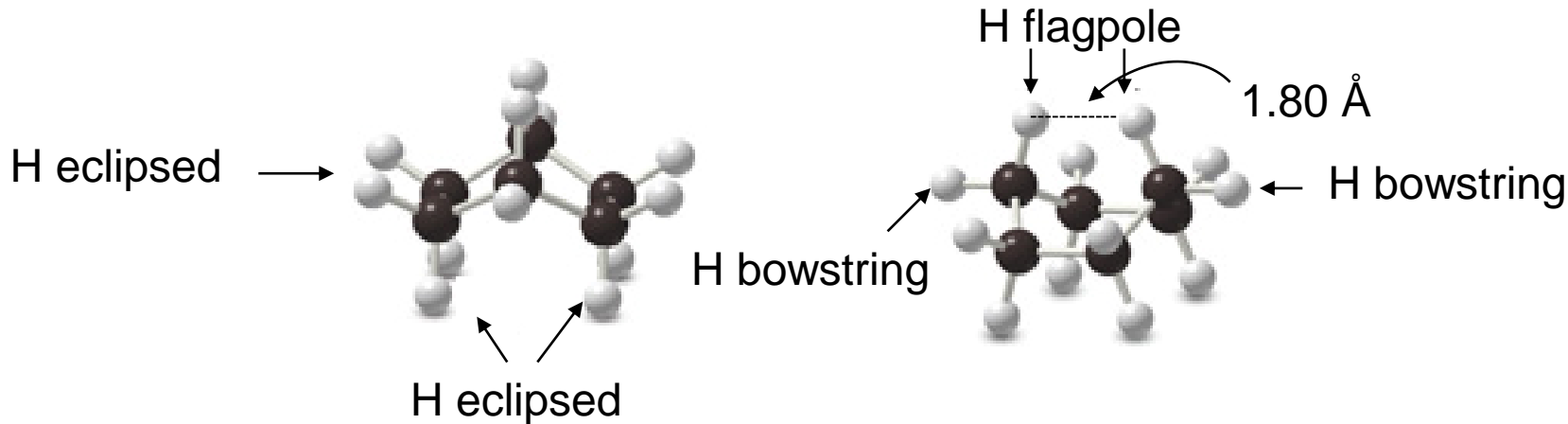


Ring Flipping

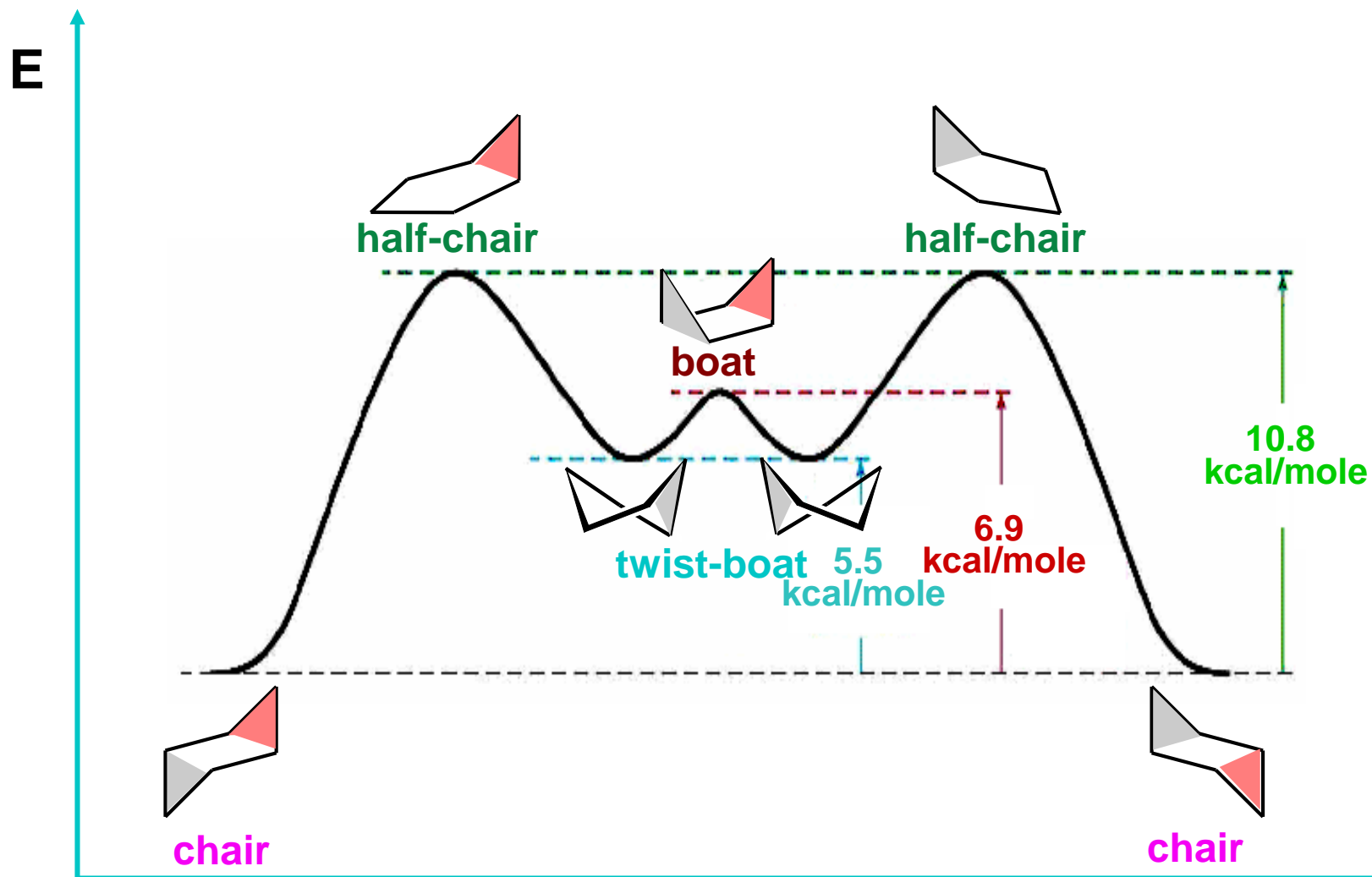


Conformations of Cyclohexane

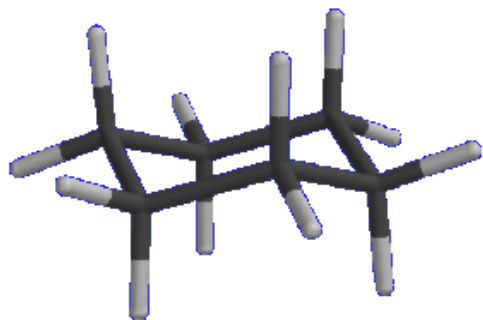
- Chair conformations are 7 kcal/mol more stable than boat conformations.
- **Torsional strain.** In the boat conformation the H on the base are eclipsed.
- **Steric strain.** Flag pole H are forced in close proximity.



Conformations of Cyclohexane

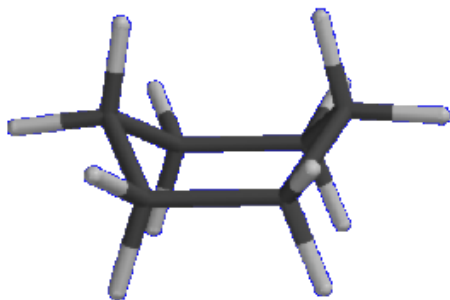


Conformations of Cyclohexane



chair

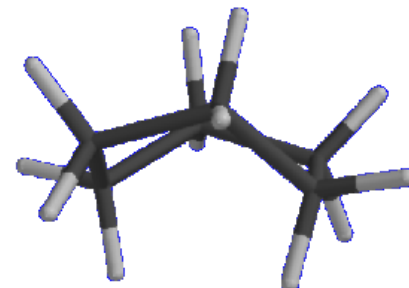
no ring strain
(99.99% at 25°C)



boat

- torsional strain
- steric strain

ring strain: ~ 7 kcal

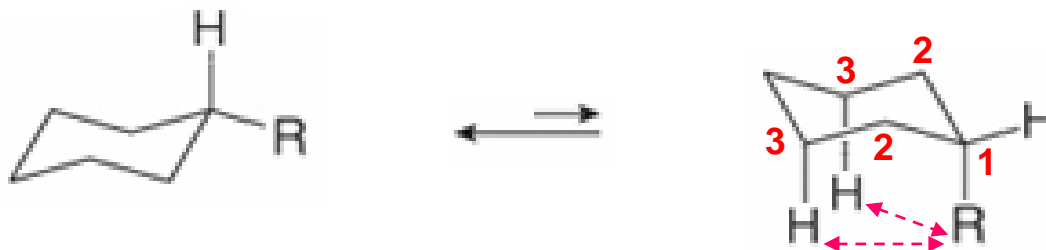


twist-boat

~ 1.5 kcal more stable
than the boat
(0.01% at 25°C)

Substituted Cyclohexanes

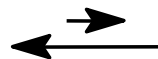
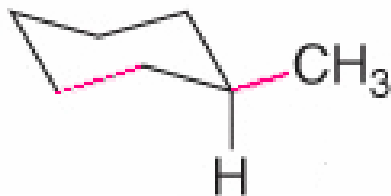
- The chair conformations are no longer equivalent: they have different energies.



- The axial conformer is destabilized by **1,3-diaxial interactions** (VdW interactions) between the substituent and axial hydrogens.
- The larger the substituent, the less stable the axial conformation.

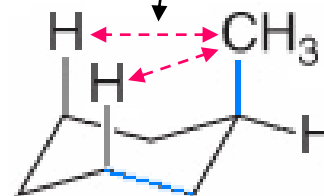
Methylcyclohexane

equatorial
(95%)
no steric strain



$\Delta G \sim 1.8 \text{ kcal}$

1,3-diaxial
interactions

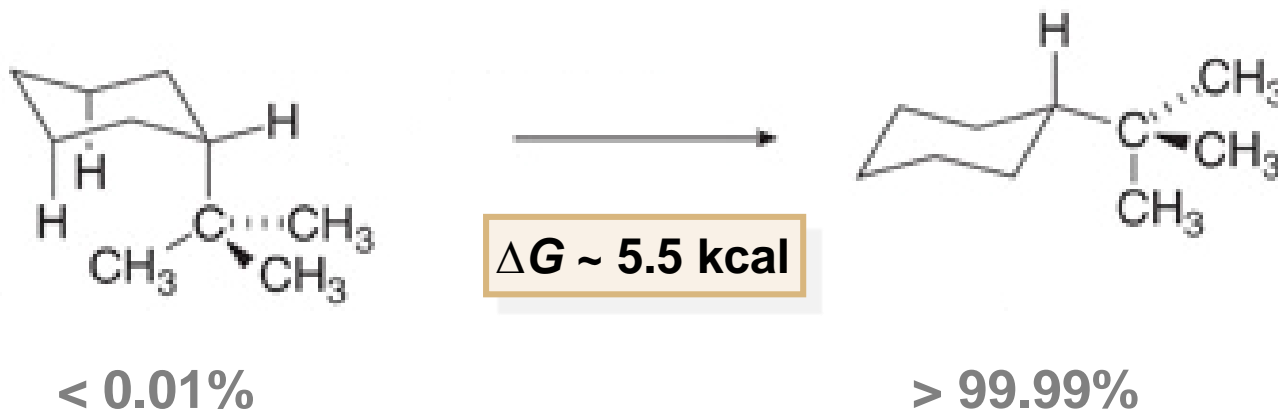


axial
(5%)
steric
repulsion

Each CH₃ / H interaction destabilizes the axial conformer by 0.9 kcal/mol

tert-Butylcyclohexane

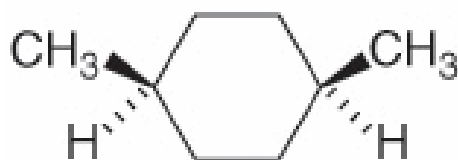
- The *tert*-butyl group is so bulky that there is no axial conformer at the equilibrium.



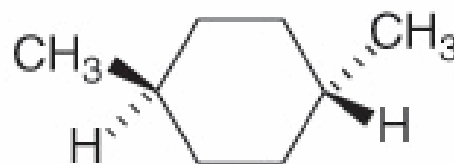
The *tert*-butyl group **freezes** the conformational equilibrium.

Disubstituted Cyclohexanes. Geometrical Stereoisomerism

- There are two isomers of 1,4-dimethylcyclohexane.



cis

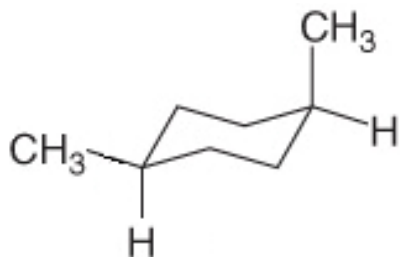


trans

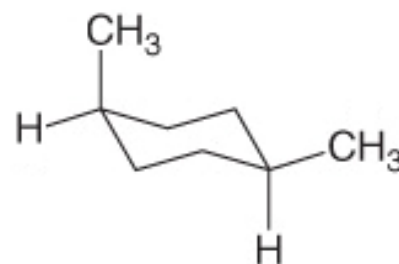
- Each geometrical isomer has two possible chair conformations.

1,4-Dimethylcyclohexane

cis



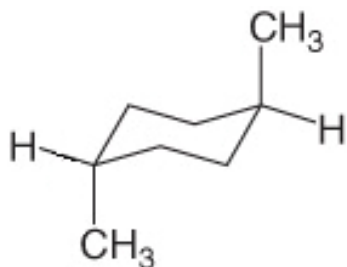
equatorial-axial
2 1,3-diaxial interactions
 $2 \times 0.9 = 1.8$ kcal



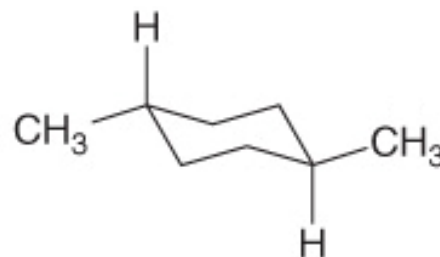
axial-equatorial
2 1,3-diaxial interactions
 $2 \times 0.9 = 1.8$ kcal

$\Delta G = 0$ kcal

trans



bisaxial
4 1,3-diaxial interactions
 $4 \times 0.9 = 3.6$ kcal

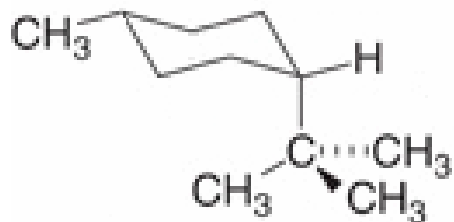
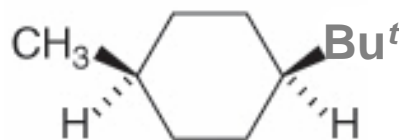


bisequatorial
no repulsions

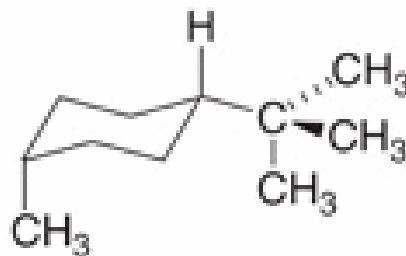
$\Delta G \sim 3.6$ kcal

cis-1-*t*-Butyl-4-methylcyclohexane

→ The conformational equilibrium is frozen by the bulky *t*-butyl group.



5.5 kcal/mol

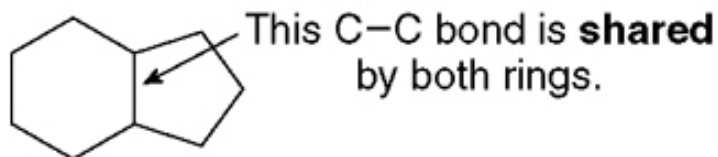


1.8 kcal/mole

$\Delta G \sim 3.7$ kcal

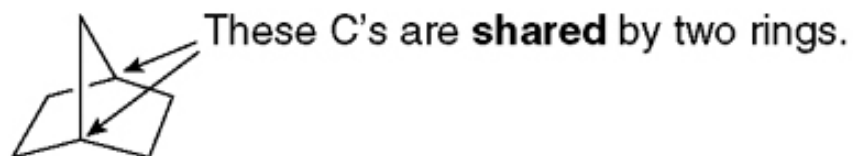
Polycyclic compounds

A fused bicyclic system



- One bond is shared by two rings.
- The shared C's are adjacent.

A bridged bicyclic system



- Two non-adjacent atoms are shared by both rings.

A spiro bicyclic system

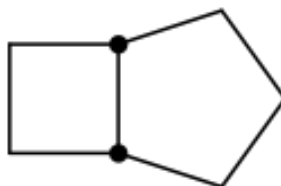


- One atom is shared by two rings

Polycyclic compounds



bicyclo[2.2.2]octane



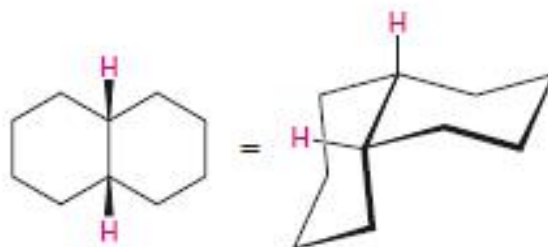
bicyclo[3.2.0]heptane



spiro[4,5]decane

Polycyclic Hydrocarbons

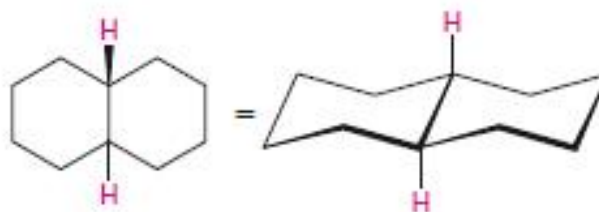
less stable
(1 axial substituent)



cis-decaline



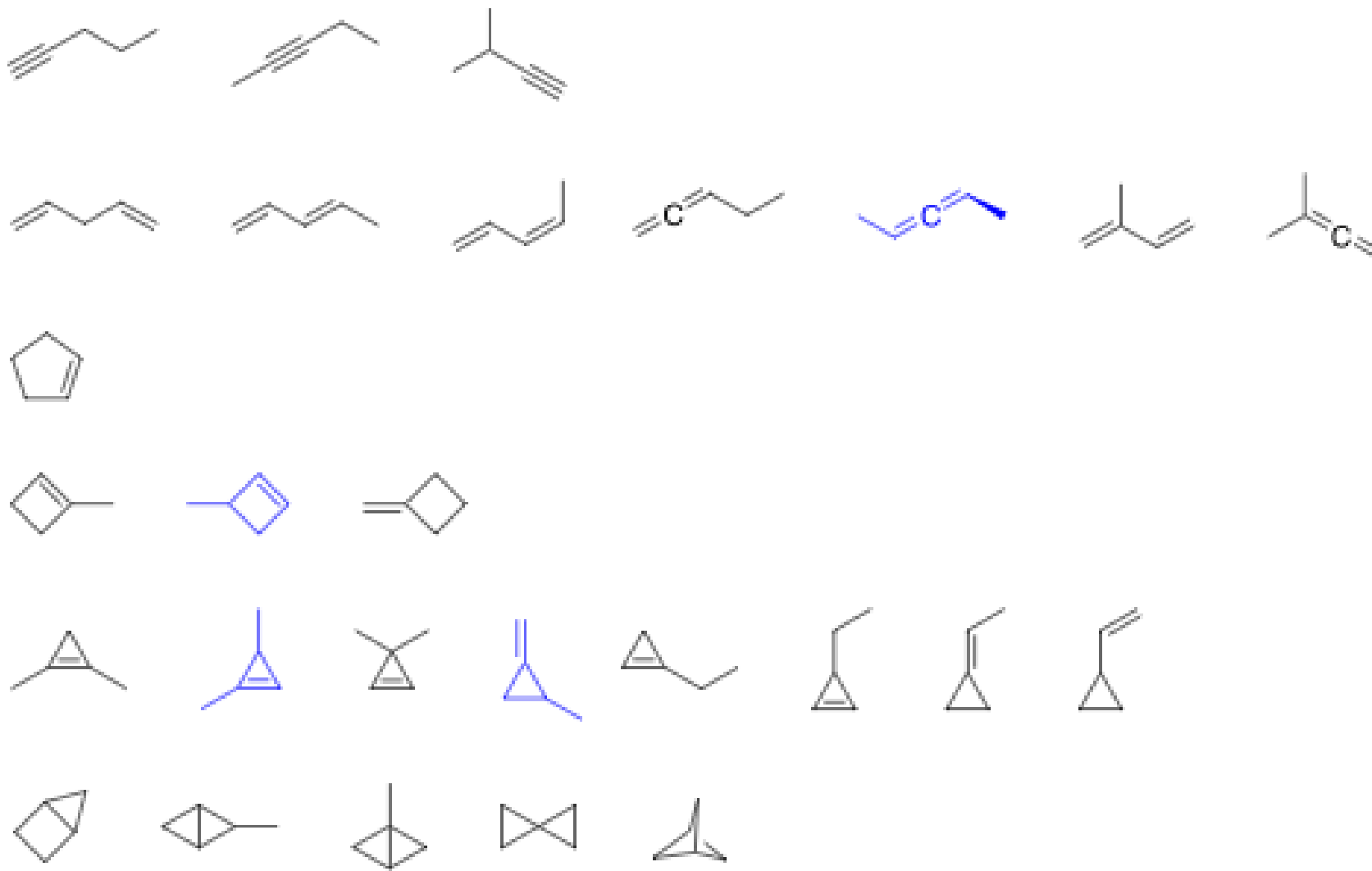
more stable
(equatorial substituents)



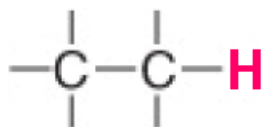
trans-decaline



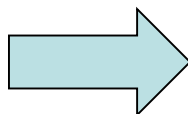
C5H8 Isomers



Reactions of Alkanes



- no lone pairs
- no π bonds
- no heteroatoms
- not nucleophilic
- not electrophilic
- strong, not polar C–C, C–H bonds



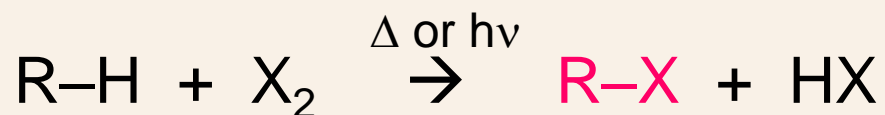
Alkanes react only at high temperatures, with radical mechanisms.

Halogenation of Alkanes

Chapt. 10 Organic Chemistry, 8th Edition
John E. McMurry

Halogenation of Alkanes

- In the presence of heat or light, alkanes react with halogens, with a radical mechanism, to give alkyl halides.



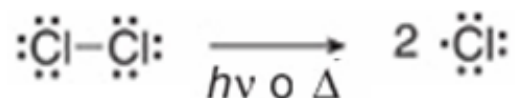
radical substitution

- Halogenation of alkanes is carried out with Cl_2 or Br_2 . The reaction with F_2 is too violent and the reaction with I_2 is too slow.

Halogenation of Methane

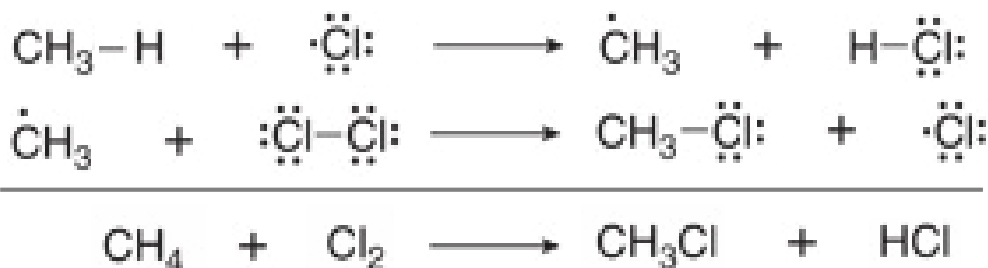
Initiation

Stage [1]: formation of $\text{Cl}\cdot$ radicals



Propagation

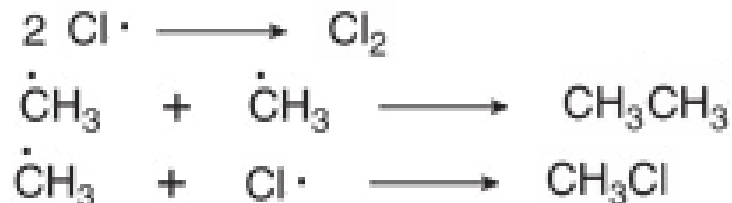
Stages [2] and [3]: A new radical is formed for each reacting radical



thousands of
cycles.
Chain reaction

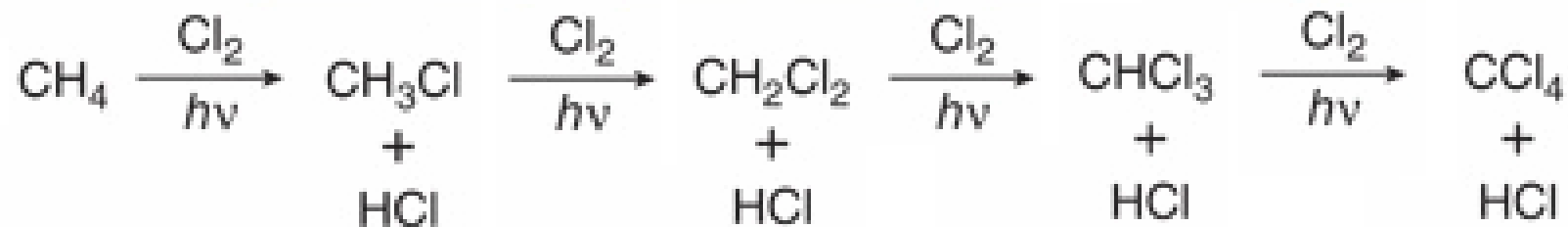
Termination

Stage [4]: Two radicals recombine forming a σ bond.



Halogenation of Alkanes

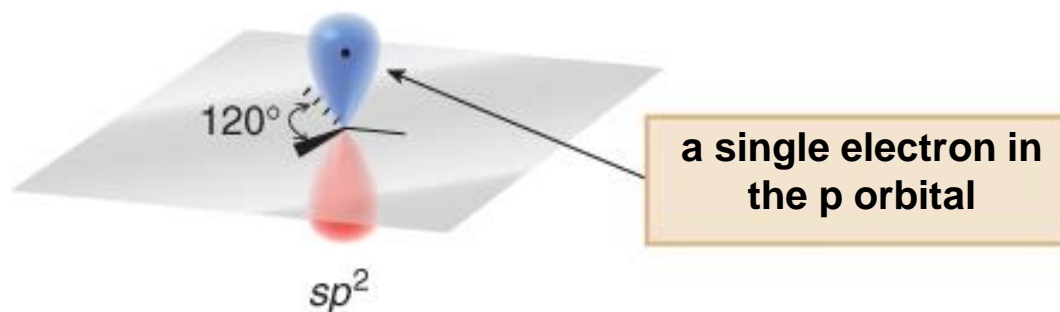
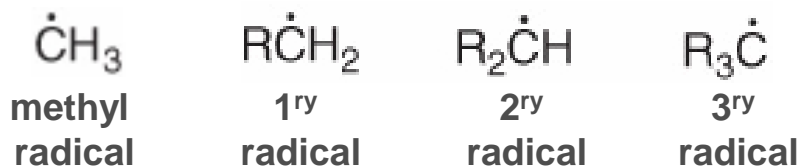
- Monohalogenation is only possible with an excess of substrate, otherwise polyhalogenation predominates.



- Problem: mixture of halogenated products.
- Solution: CH₄ in large excess and recycled.

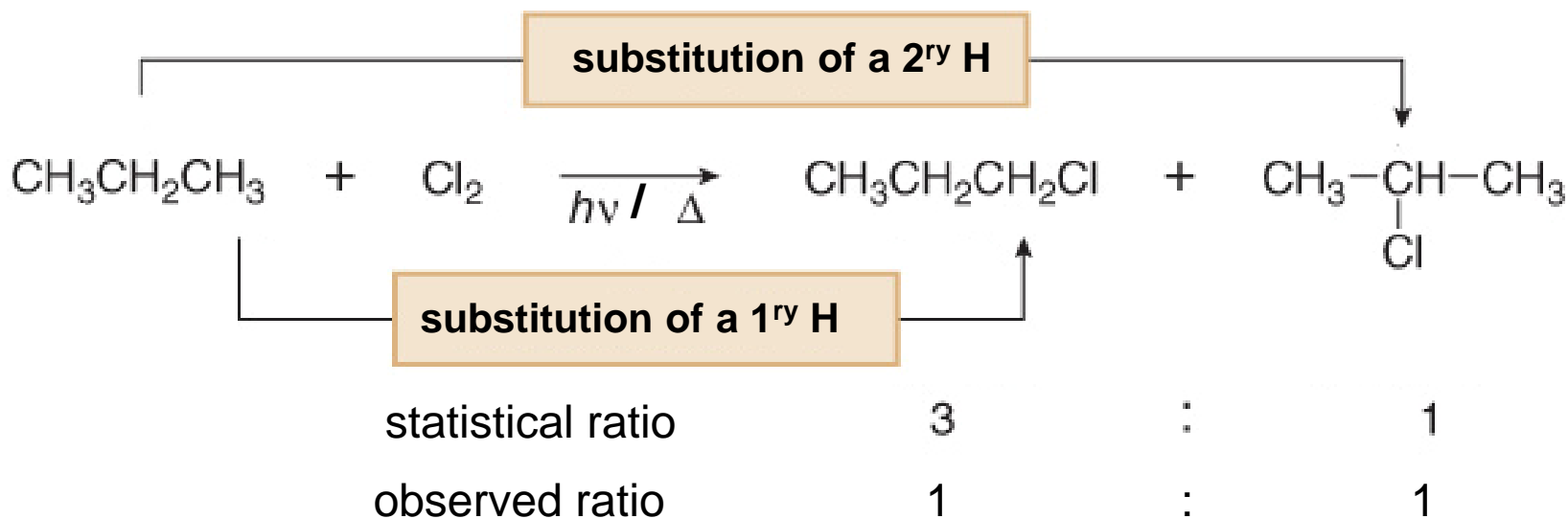
Structure of Radicals

- Alkyl radicals are sp^2 hybridized with a trigonal planar geometry.
- The p orbital contains an unpaired electron.

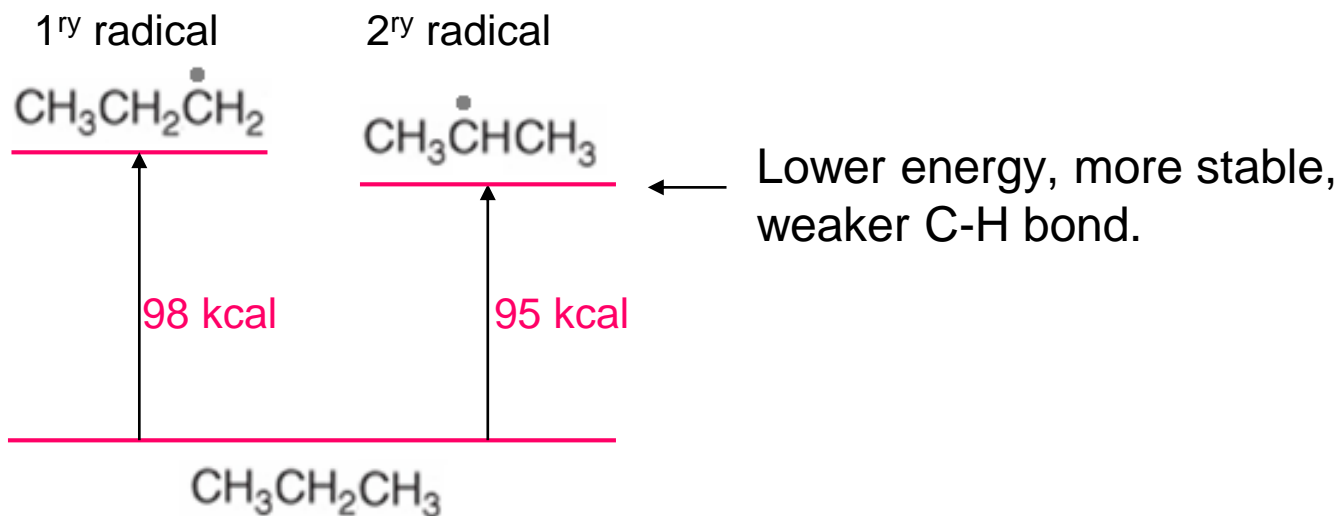


Regioselectivity

- Isomers are formed in the halogenation of propane and higher hydrocarbons:



Regioselectivity



- Radical stability: $3^\circ > 2^\circ > 1^\circ$.
- Strength of C-H bonds: $3^\circ < 2^\circ < 1^\circ$.

C-H Bond Dissociation Energies



$DH = \text{BDE}$ bond dissociation energy

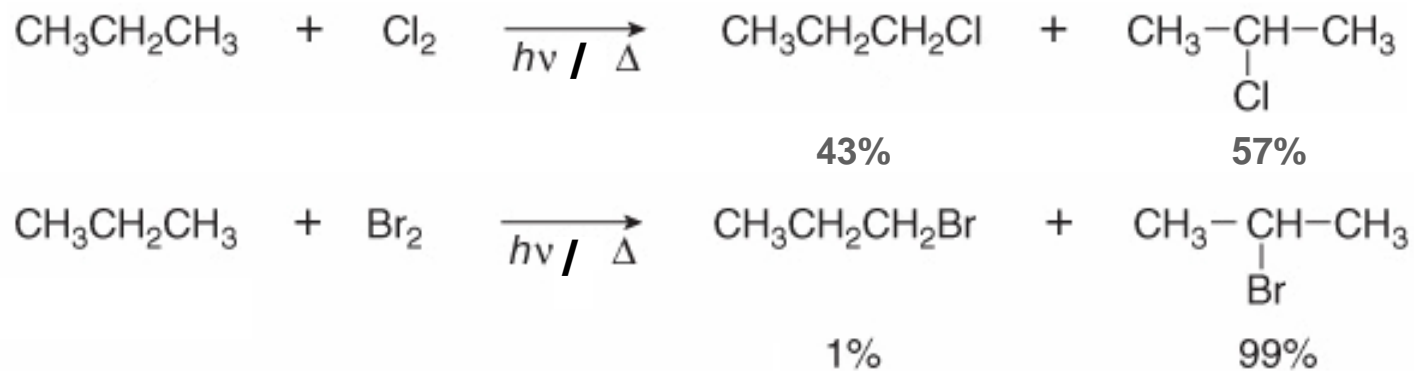
$\text{CH}_3\text{-H}$	104 kcal/mole	
$\text{CH}_3\text{CH}_2\text{-H}$	98 kcal/mole	
$\text{CH}_3\text{CH}_2\text{CH}_2\text{-H}$	98 kcal/mole	(1 ^{ry} C-H)
$\begin{array}{c} \text{CH}_3\text{CHCH}_3 \\ \\ \text{H} \end{array}$	95 kcal/mole	(2 ^{ry} C-H)
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3\text{C-H} \\ \\ \text{CH}_3 \end{array}$	91 kcal/mole	(3 ^{ry} C-H)

↑ BDE
↓ REACTIVITY

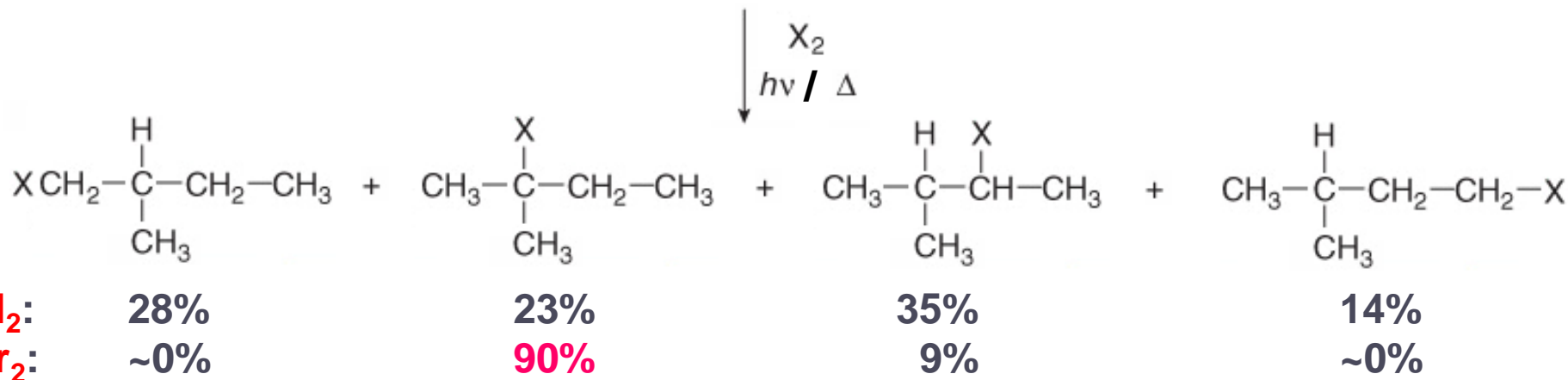
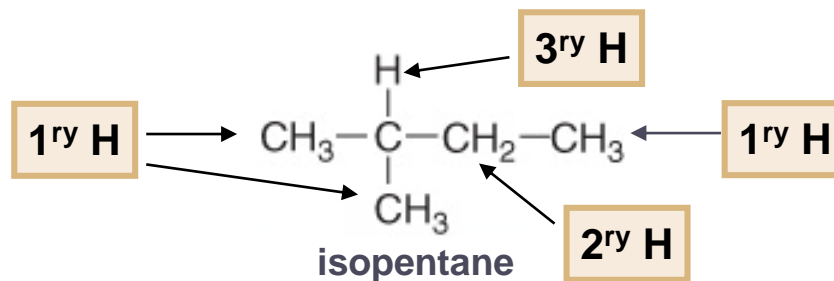
Reactivity of C-H bonds:
 $3^{\text{ry}} > 2^{\text{ry}} > 1^{\text{ry}} > \text{CH}_3\text{-H}$

Reactivity and Selectivity

- ✦ Chlorination of alkanes is faster than bromination.
- ✦ Bromination of alkanes is more selective.



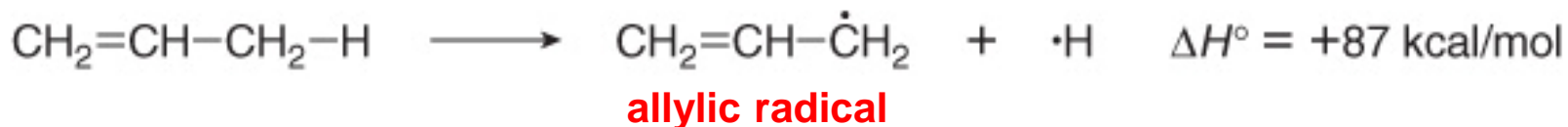
Regioselectivity



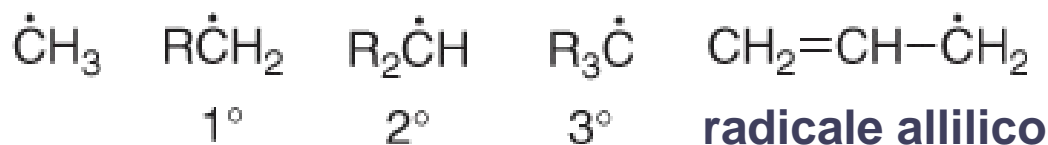
C-H relative reactivity	3ry	2ry	1ry
with Cl₂	5.2	3.9	1
with Br₂	1640	82	1

Halogenation of Allylic Carbons

- **Allylic** carbons are sp^3 carbons adjacent to a double bond.
- A resonance-stabilized **allylic radical** is obtained by homolysis of an allylic C–H bond.

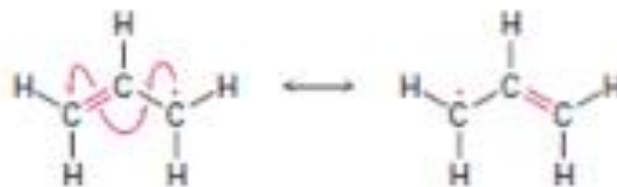
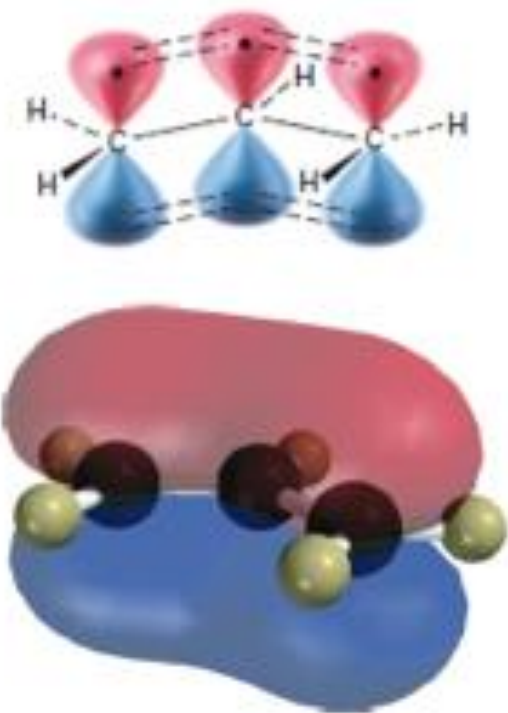


- BDEs of allylic C–H bonds are approximately 4 kcal/mol lower than BDE for 3^{ry} C–H bonds.
- The delocalized allylic radical is more stable than a 3^{ry} radical.



radical stability 

The Allylic Radical

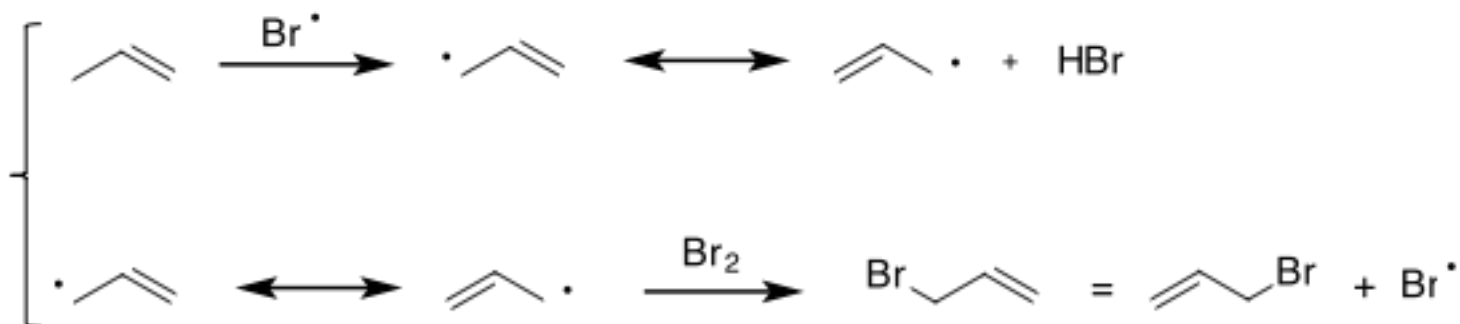


Halogenation of Allylic Carbons

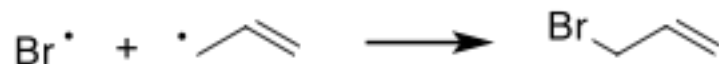
initiation



propagation

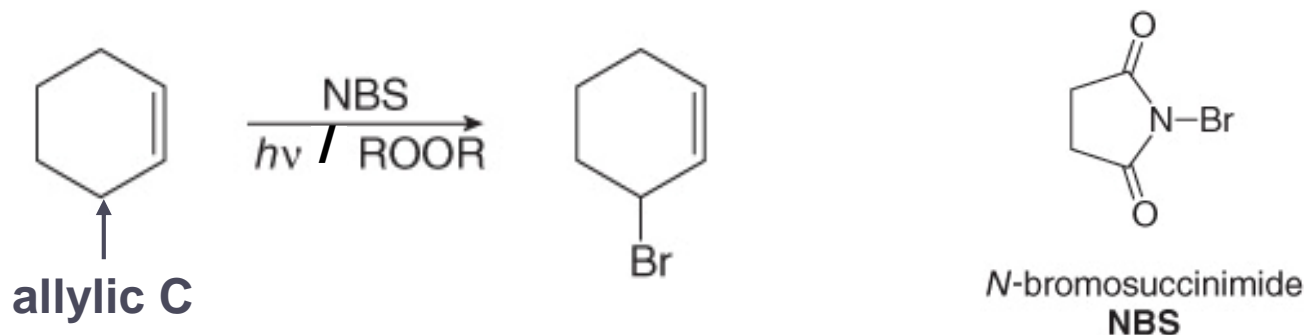


termination

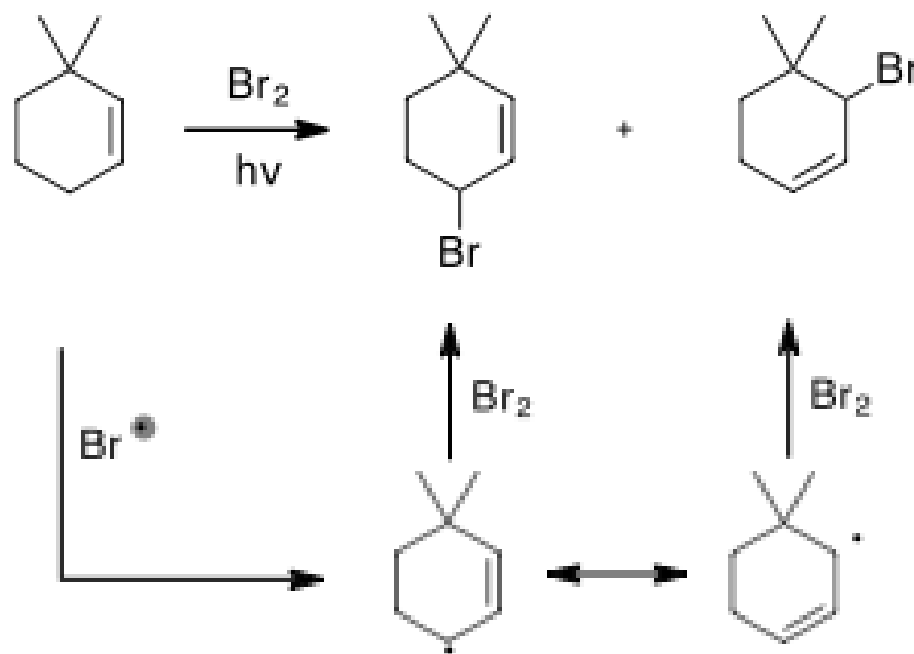


Halogenation of Allylic Carbons

- Allylic carbons can be selectively brominated with NBS and UV irradiation or a radical initiator.
- Breaking of the weak N-Br bond of NBS initiates the radical chain reaction.

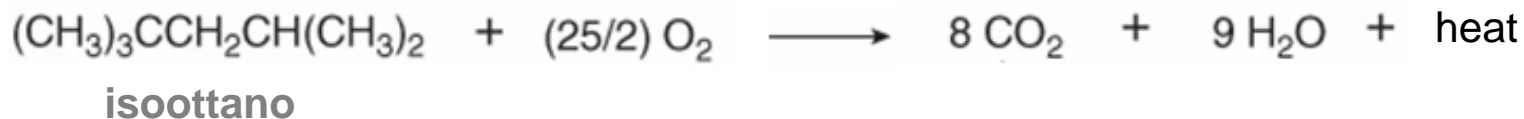


Halogenation of Allylic Carbons



Combustion

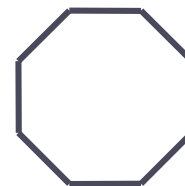
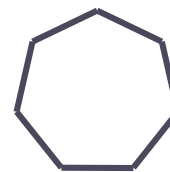
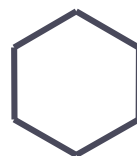
- Combustion is a redox reaction. C is oxidized and O is reduced.
- All hydrocarbons burn giving carbon dioxide, water and heat ($\Delta H < 0$).
- C-C e C-H bonds are converted into C-O and H-O bonds.




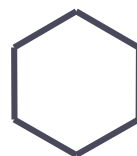
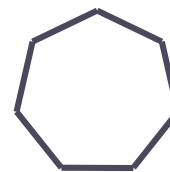
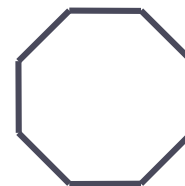


Every C atom is converted into CO_2

Strain Energies of Cycloalkanes

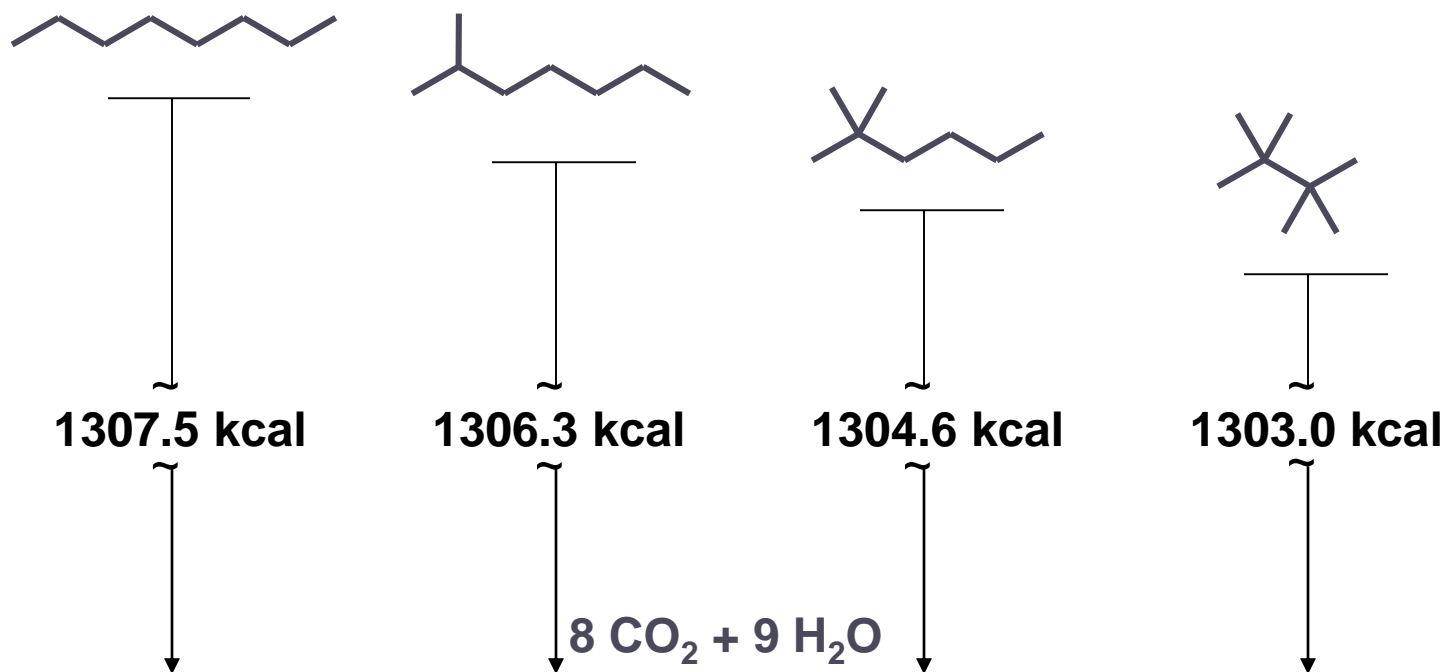
- Heats of combustion are used to calculate strain energies of cycloalkanes.
- Heats of combustion increase with the number of C atoms.
- Cyclohexane is taken as reference (Strain = 0).



						
kJ/mol	2091	2724	3290	3910	4599	5264
Per CH ₂	697	681	658	653	657	658
Strain	132	112	25	0	28	40

Stability of Isomers

- Heats of combustion are used to compare the stability of isomers. E.g.: C_8H_{18}



Branched isomers are more stable than linear ones.