Alkanes

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

Hydrocarbons

- **Aliphatic** (Αλειφαρ = Ointment).
  - 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.

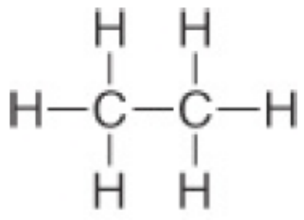
- **Aromatic**

Alkanes

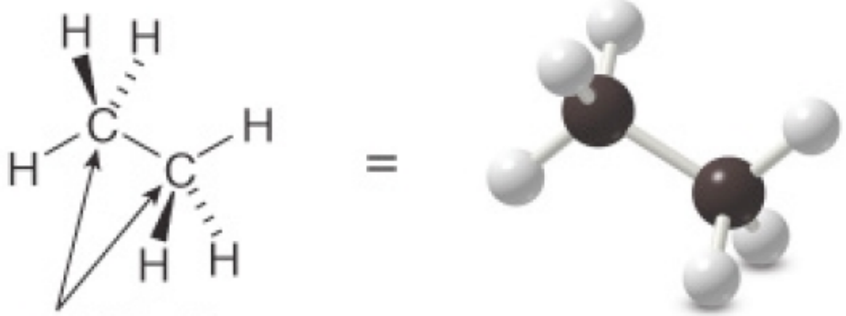
Numberof C-atoms	**Molecular formula**	**Name (*n*-alkane)**
1	CH_4	methane
2	C_2H_6	ethane
3	C_3H_8	propane
4	C_4H_{10}	butane
5	C_5H_{12}	pentane
6	C_6H_{14}	hexane
7	C_7H_{16}	heptane
8	C_8H_{18}	octane
9	C_9H_{20}	nonane
10	$C_{10}H_{22}$	decane
20	$C_{20}H_{42}$	eicosane

Empirical formula: C_nH2_{n+2}

Ethane

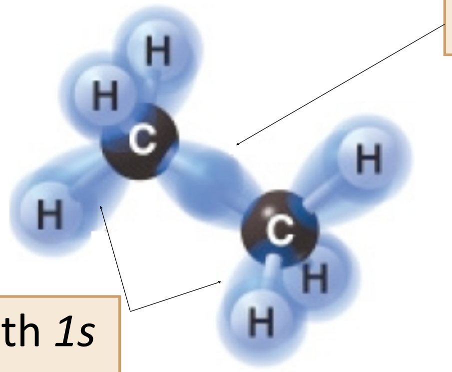


ethane

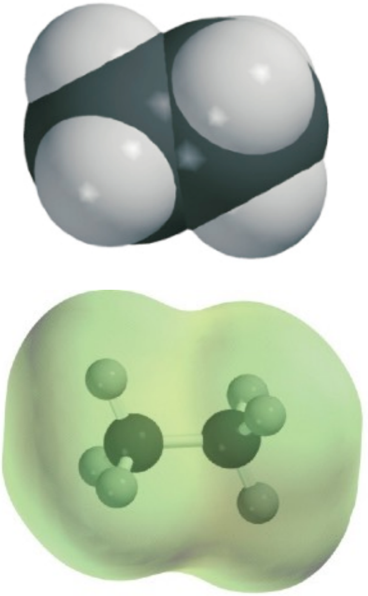


tetrahedral sp^3 C

Two sp^3 hybrids overlap giving the C–C σ bond

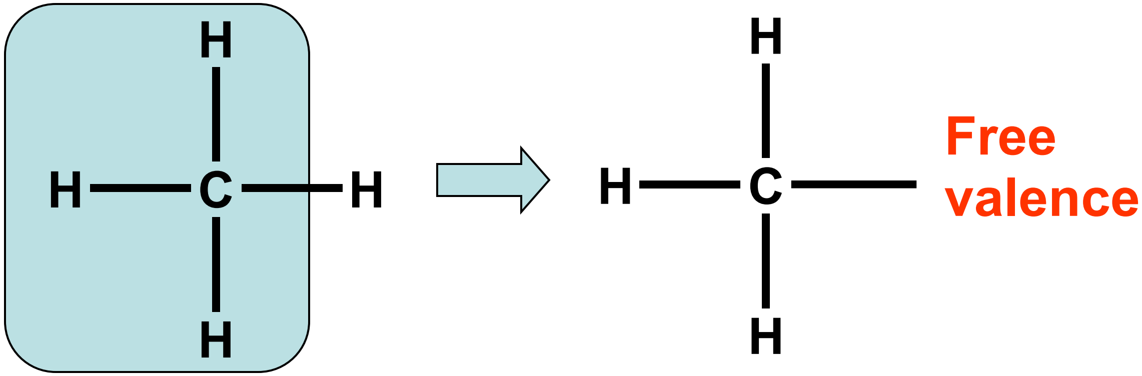


sp^3 hybrids on C overlap with *1s* orbitals on H giving the C-H σ bonds.



Alkyl Groups

Root-Suffix (= yl)



$= CH_3-$ **methyl**

$CH_3-CH_2- = C_2H_5-$ **ethyl**

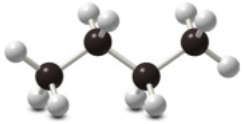
$CH_3-CH_2-CH_2- = C_3H_7-$ **propyl**

Alkanes – Structural Isomerism

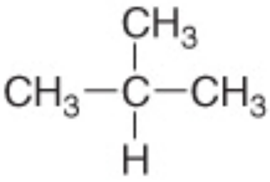
- There are two hydrocarbons with empirical formula C_4H_{10}: butane and isobutane.
- Butane and isobutane are structural isomers: they have the same composition but different physico-chemical properties.

$CH_3CH_2CH_2CH_3$

butane

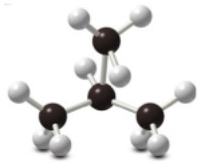


Linear Alkane



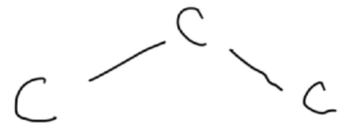
$$CH_3-\overset{\overset{\displaystyle CH_3}{|}}{\underset{\underset{\displaystyle H}{|}}{C}}-CH_3$$

isobutane

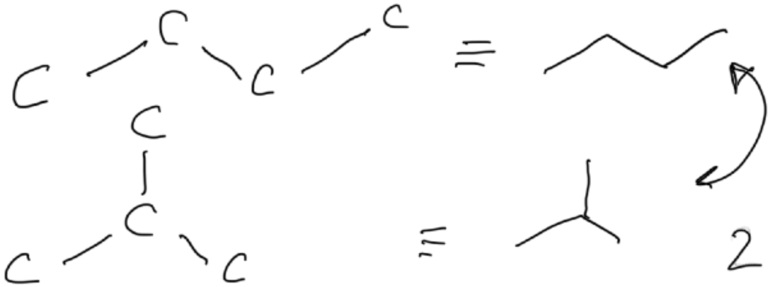


Branched Alkane

Alkanes – Structural Isomerism

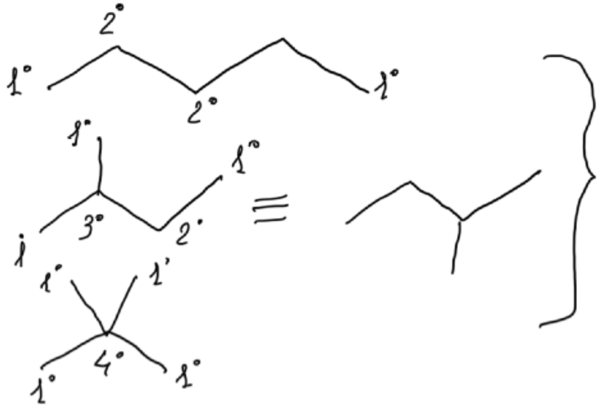


NO ISOMERS



C_4H_{10}

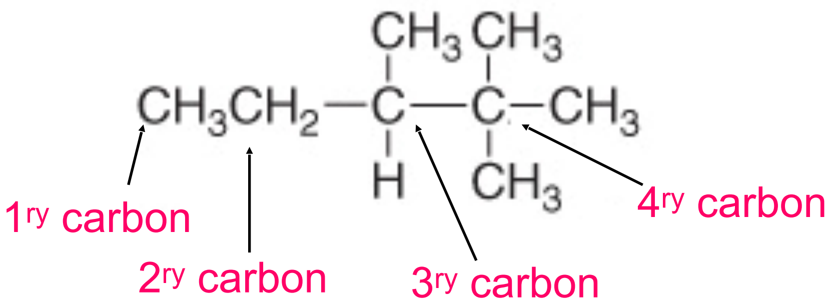
2 ISOMERS



C_5H_{12}

3 ISOMERS

Examples



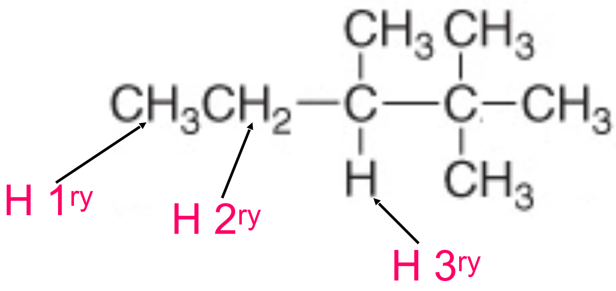
$CH_3CH_2-\overset{CH_3}{\underset{H}{C}}-\overset{CH_3}{\underset{CH_3}{C}}-CH_3$

1^{ry} carbon

2^{ry} carbon

3^{ry} carbon

4^{ry} carbon

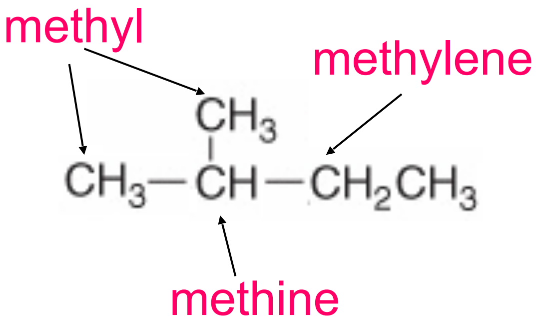


$CH_3CH_2-\overset{CH_3}{\underset{H}{C}}-\overset{CH_3}{\underset{CH_3}{C}}-CH_3$

H 1^{ry}

H 2^{ry}

H 3^{ry}



$CH_3-\overset{CH_3}{CH}-CH_2CH_3$

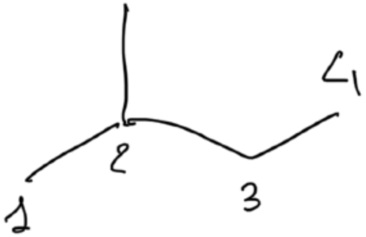
methyl

methylene

methine

Nomenclature

IUPAC = International Union for Pure and Applied Chemistry

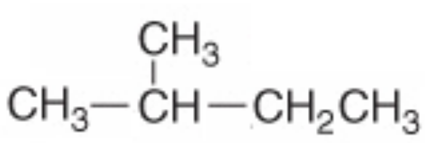


2-metil butano

2,2-dimetil propano

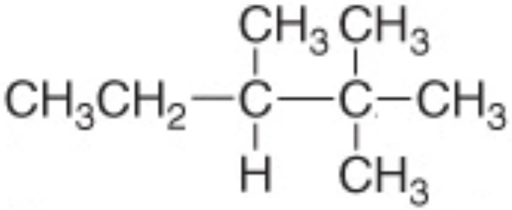
1) Individuare la catena + lunga
2) Identificare i sostituenti (in ordine alfabetico)
3) Assegnare la posizione a ciascun sostituente in modo che l'indice sia + basso possibile

Nomenclature



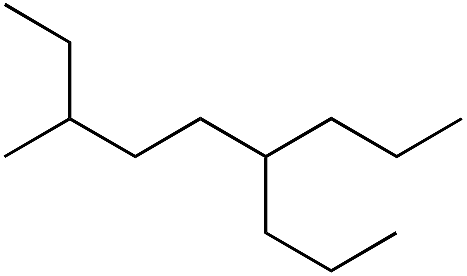
$CH_3-\overset{\overset{\displaystyle CH_3}{|}}{C}H-CH_2CH_3$

2-metylbutane

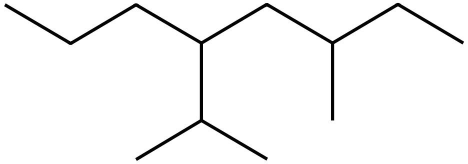


$CH_3CH_2-\underset{\underset{\displaystyle H}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{C}}-\underset{\underset{\displaystyle CH_3}{|}}{\overset{\overset{\displaystyle CH_3}{|}}{C}}-CH_3$

2,2,3-trimethylpentane

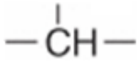
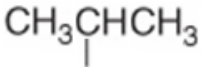
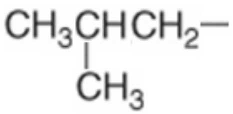
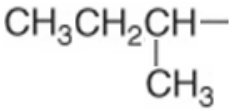
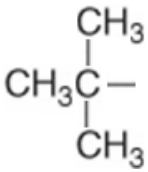
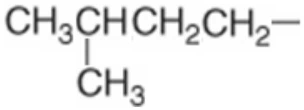
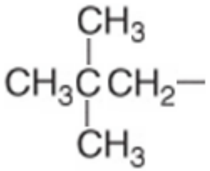
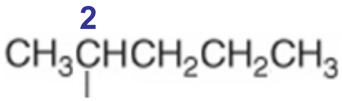
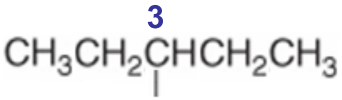


3-methyl-6-propylnonane

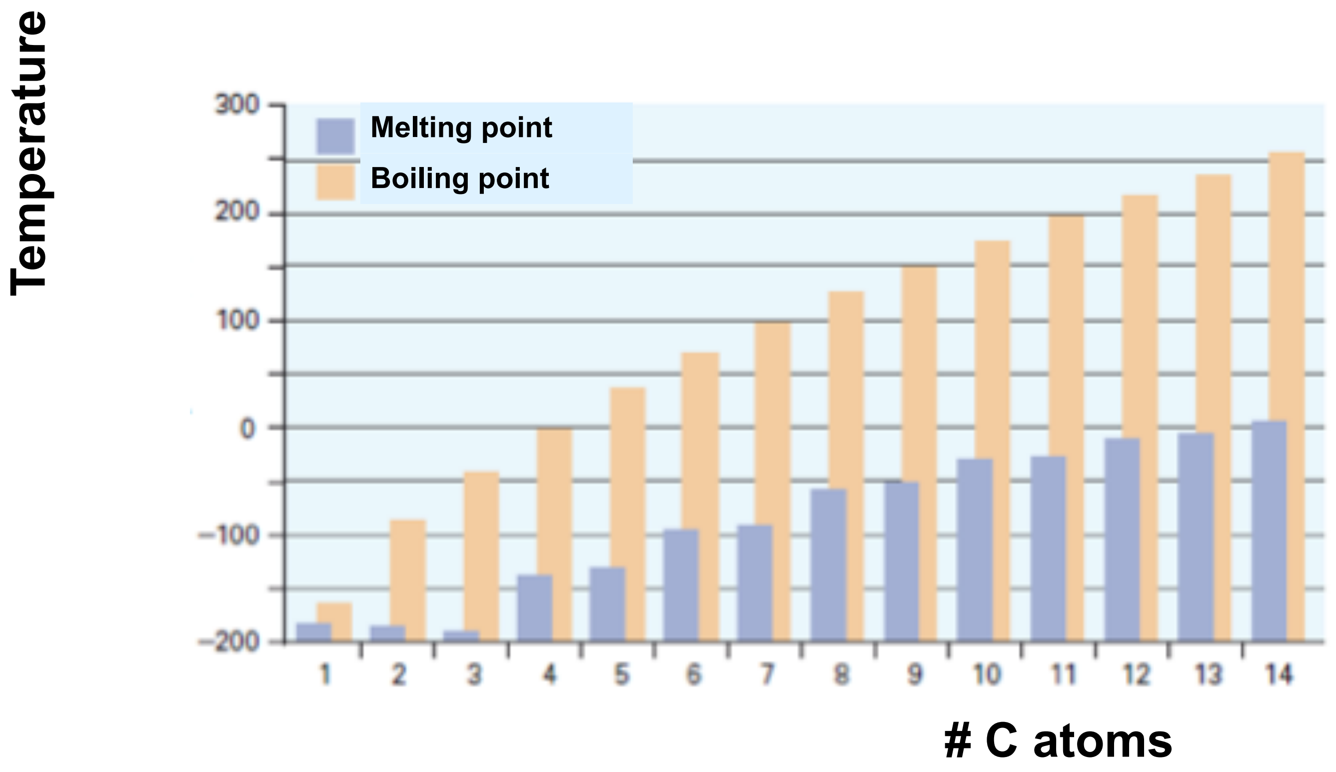


5-(1-methylethyl)-3-methyloctane

Alkyl Groups

C-Atoms	Structure	Name
1	CH_3-	**methyl**
	$-CH_2-$	**methylene**
	 $-\overset{\mid}{C}H-$	**methine**
2	CH_3CH_2-	**ethyl**
3	$CH_3CH_2CH_2-$	***n*-propyl**
	 $CH_3\underset{\mid}{C}HCH_3$	**isopropyl**
4	$CH_3CH_2CH_2CH_2-$	***n*-butyl**
	 $CH_3\underset{\underset{CH_3}{\mid}}{C}HCH_2-$	**isobutyl**
	 $CH_3CH_2\underset{\underset{CH_3}{\mid}}{C}H-$	***sec*-butyl**
	 $CH_3\overset{\overset{CH_3}{\mid}}{\underset{\underset{CH_3}{\mid}}{C}}-$	***tert*-butyl**
5	$CH_3CH_2CH_2CH_2CH_2-$	***n*-pentyl**
	 $CH_3\underset{\underset{CH_3}{\mid}}{C}HCH_2CH_2-$	**isopentyl**
	 $CH_3\overset{\overset{CH_3}{\mid}}{\underset{\underset{CH_3}{\mid}}{C}}CH_2-$	**neopentyl**
	 $CH_3\overset{2}{\underset{\mid}{C}}HCH_2CH_2CH_3$	***sec*-pentyl**
	 $CH_3CH_2\overset{3}{\underset{\mid}{C}}HCH_2CH_3$	

Physical Properties



Physical Properties

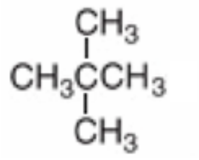
b.p.

$CH_3CH_2CH_2CH_3$
0 °C

$CH_3CH_2CH_2CH_2CH_3$
36 °C

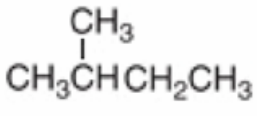
$CH_3CH_2CH_2CH_2CH_2CH_3$
69 °C

Surface area increases with C-atoms



$CH_3\overset{CH_3}{\underset{CH_3}{C}}CH_3$

10 °C



$CH_3\overset{CH_3}{C}HCH_2CH_3$

30 °C

$CH_3CH_2CH_2CH_2CH_3$

36 °C

Surface area decreases with branching

m.p.

$CH_3CH_2CH_2CH_3$
–138 °C

$CH_3CH_2CH_2CH_2CH_2CH_3$
–95 °C

Surface area increases with C-atoms

$CH_3CH_2CH(CH_3)_2$
–160°C

$(CH_3)_4C$
–17 °C

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

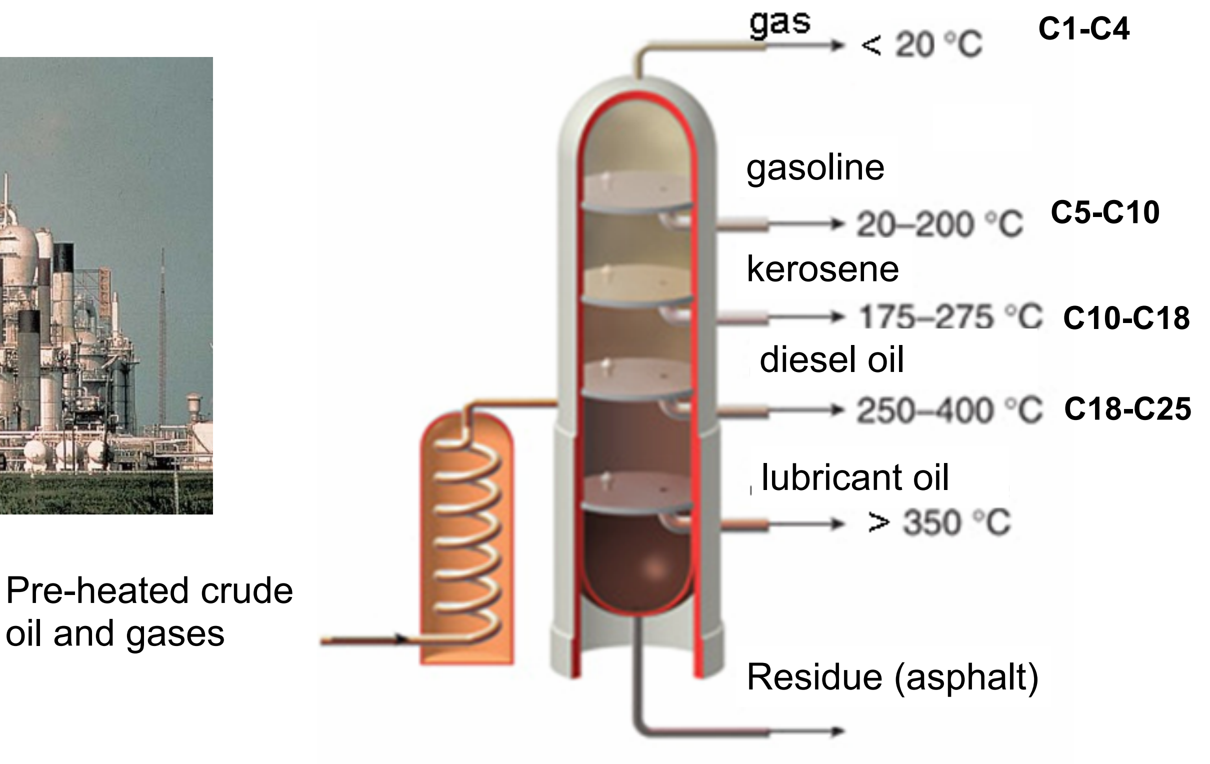
Natural sources of alkanes are natural gas and oil.

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

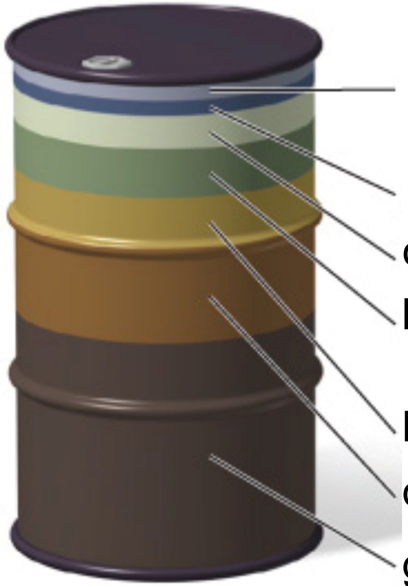
Oil is a complex mixture of, mainly, C_1-C_{40} hydrocarbons.
Distillation of crude oil (refining) separates oil in fractions with different boiling point. The main fractions are:
gasoline: $C_5H_{12} – C_{12}H_{26}$
kerosene: $C_{12}H_{26} – C_{16}H_{34}$
diesel oil: $C_{15}H_{32} – C_{18}H_{38}$

Refining

- In the refining process, crude oil is heated and the volatile fractions distill first, followed by fractions with higher boiling points.



Crude Oil



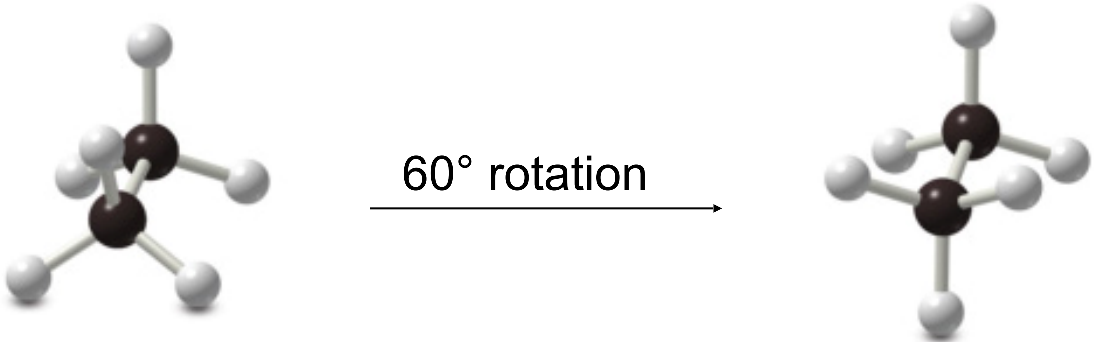
fine chemicals and plastics	1.25 gal	3%
asphalt	1,3 gal	3%
coolants	2,9 gal	7%
lubrificants, waxes, solvents	4,2 gal	10%
kerosene (aeroplanes)	4,2 gal	10%
diesel and fuel oil	8,4 gal	20%
gasoline	19,7 gal	47%

Barrel
42 gal
159 l

1 US gal = 3.78 l

Conformational Isomerism

Ethane



eclipsed **staggered**

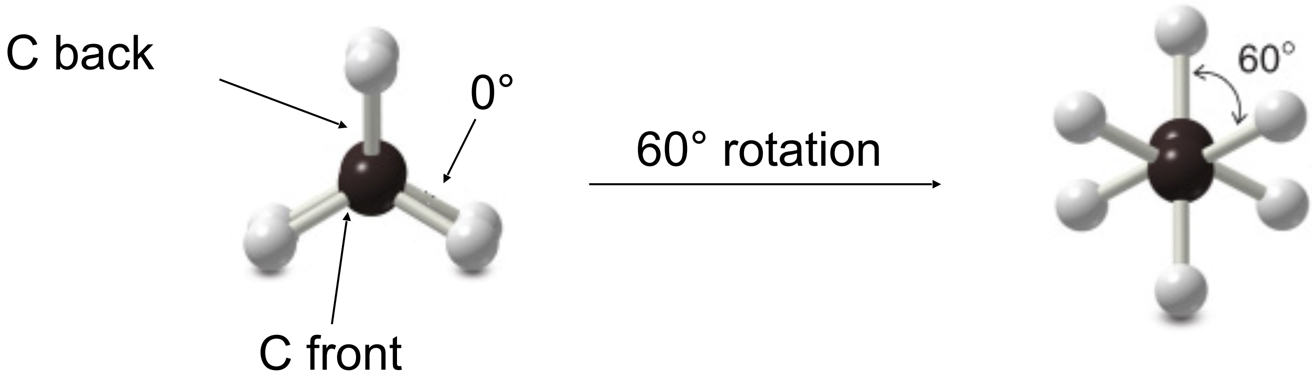
- In the eclipsed conformation, all C−H bonds are alligned.
- In the staggered conformation, C−H bonds on each carbon bisect the H−C−H angles on the other carbon.

https://moodle2.units.it/pluginfile.php/242148/mod_resource/content/2/Ethane%20Rotation%20About%20the%20Carbon-Carbon%20Single%20Bond.mp4

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



C back

0°

C front

60° rotation

Eclipsed conformation

Staggered conformation

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

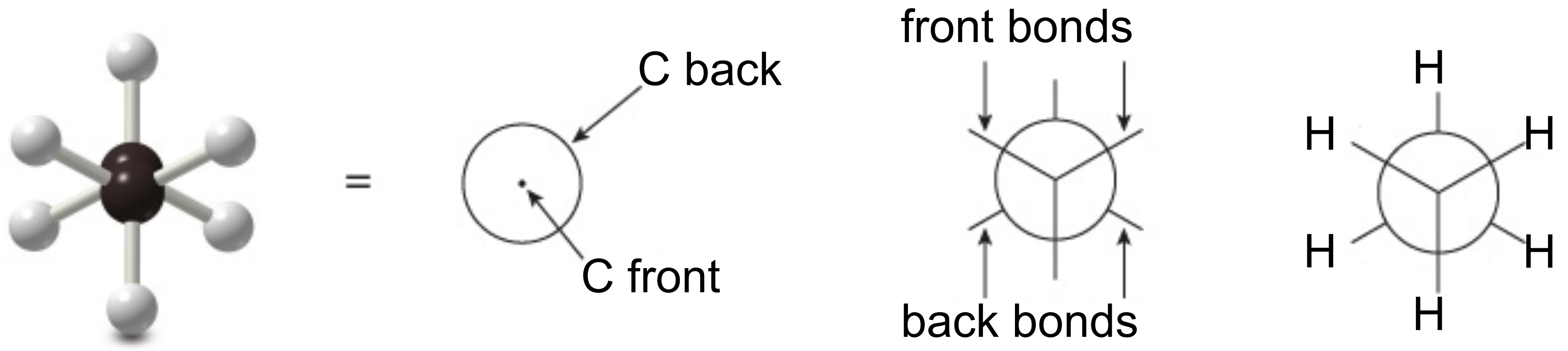
Newman Projection

- 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

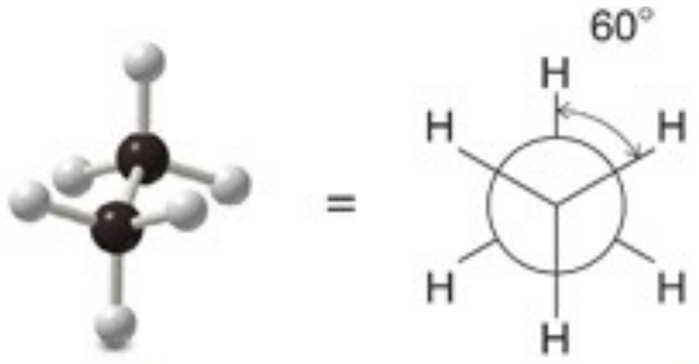
[3] Add the atoms



Newman Projections of Ethane

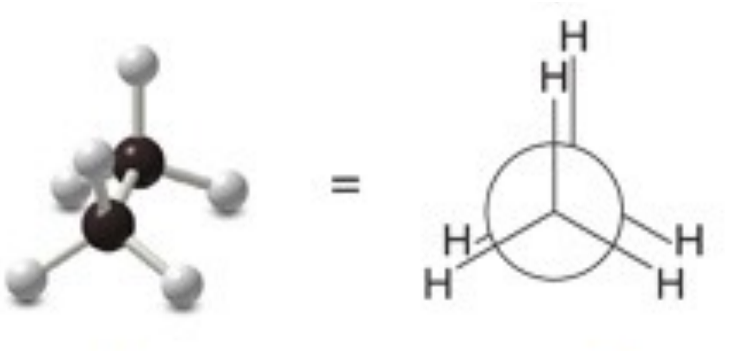
staggered conformation

dihedral angle

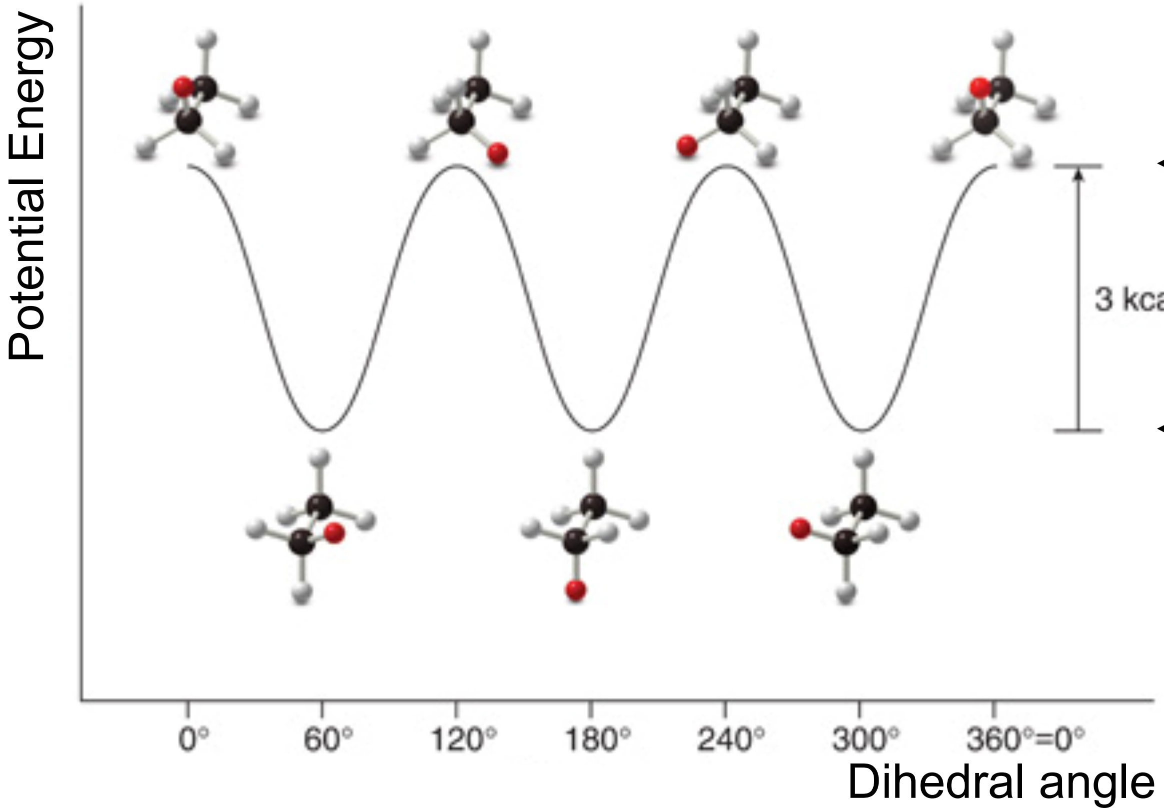


eclipsed conformation

Dihedral angle
0°



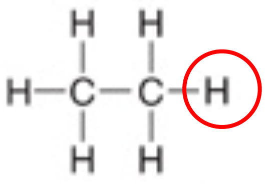
Conformations of Ethane



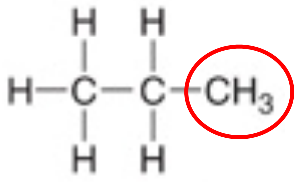
eclipsed
energy
maximum

staggered
energy
minimum

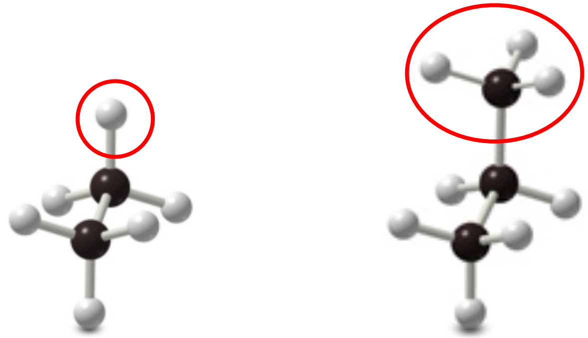
Conformations of Propane

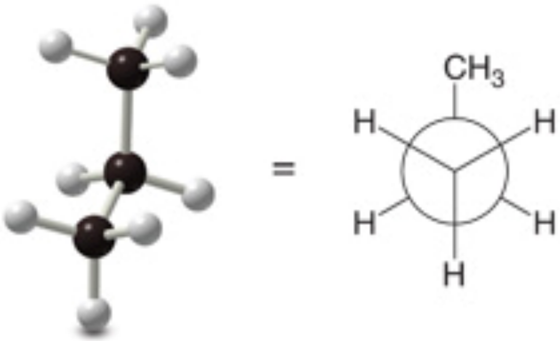


ehtane

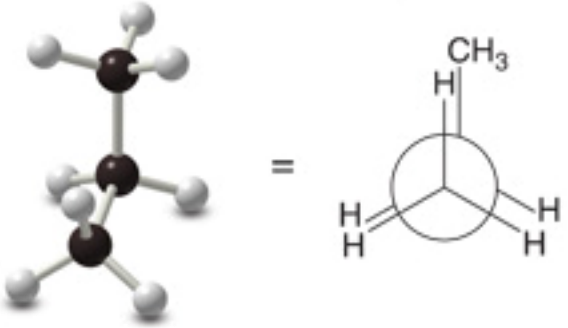


propane



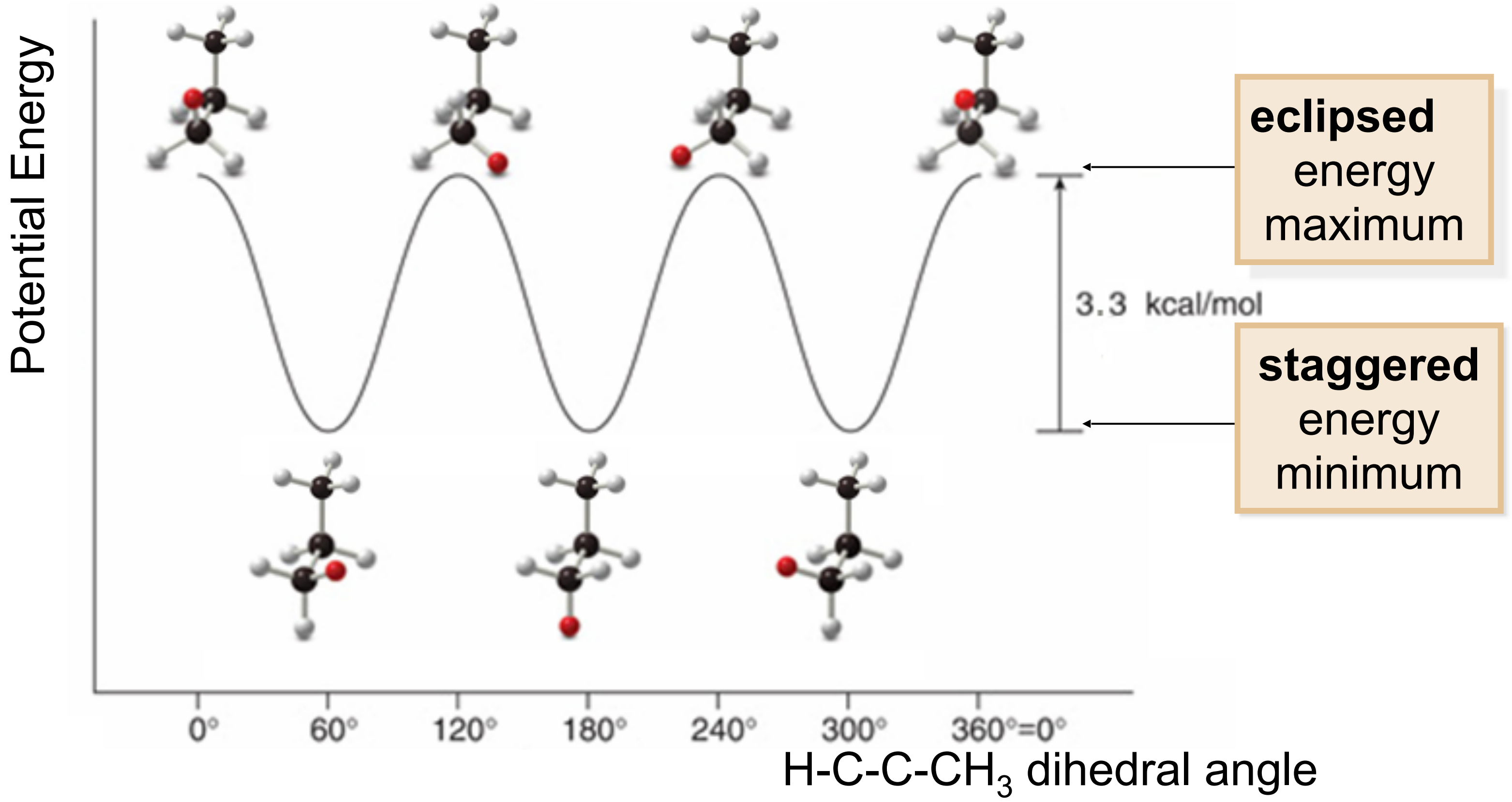


staggered conformation



eclipsed conformation

Conformations of Propane

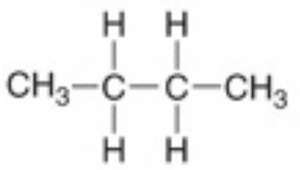


eclipsed energy maximum

staggered energy minimum

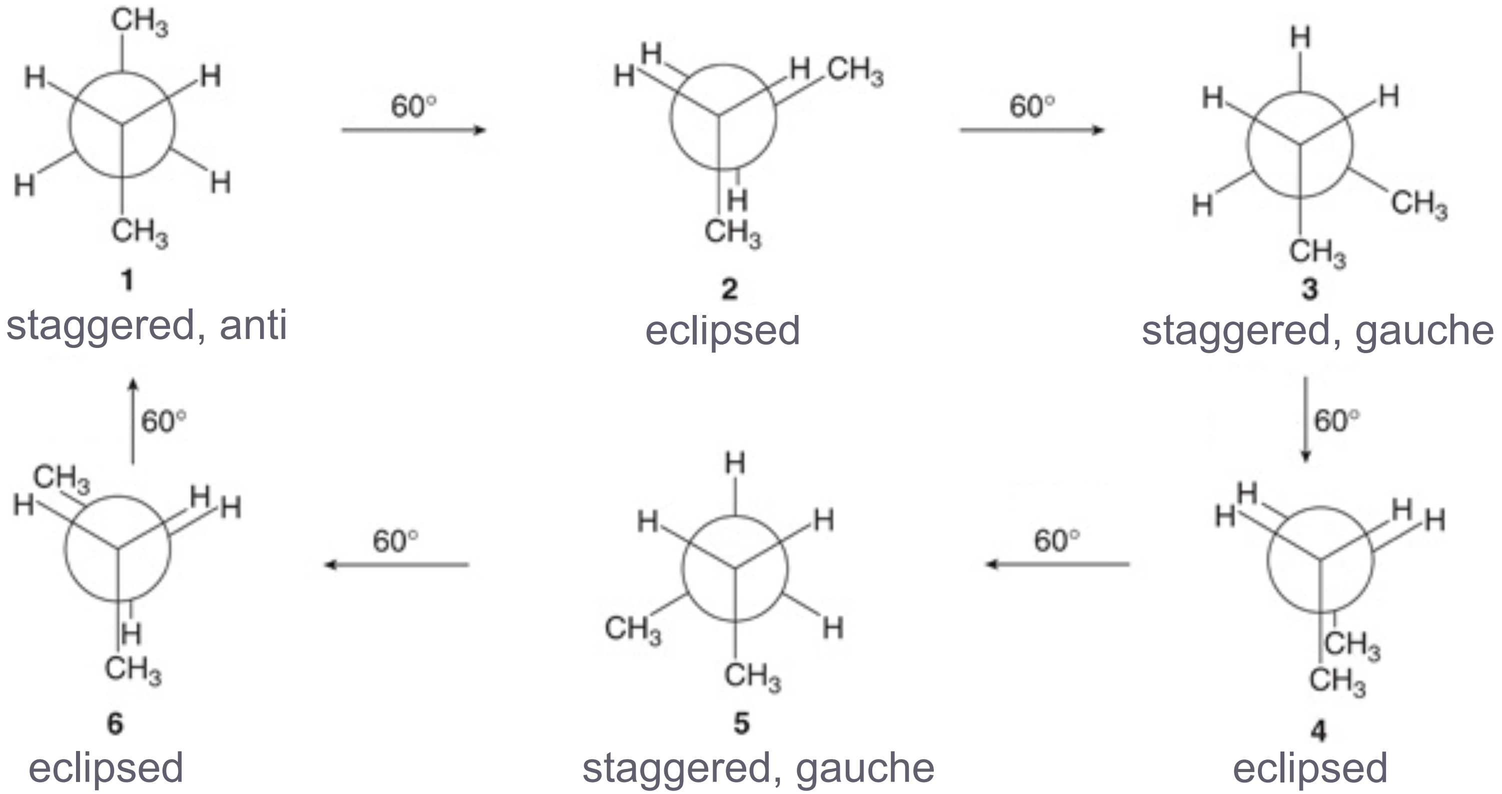
Torsional Strain (3.3 kcal/mole) is higher than in ethane. The methyl group is bulkier than a hydrogen atom

Conformations of Butane



$$\mathrm{CH_3-\overset{H}{\underset{H}{C}}-\overset{H}{\underset{H}{C}}-CH_3}$$

6 different conformations



1 staggered, anti

2 eclipsed

3 staggered, gauche

4 eclipsed

5 staggered, gauche

6 eclipsed

Conformations of Butane

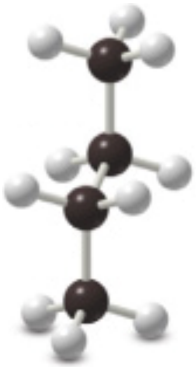
A staggered conformation with two large groups at 180° is called *anti*

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

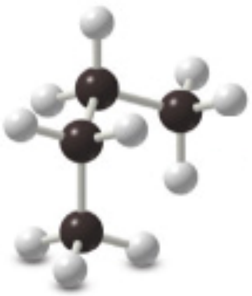
anti conformation

conformazione gauche

The CH_3 are at 180°



1

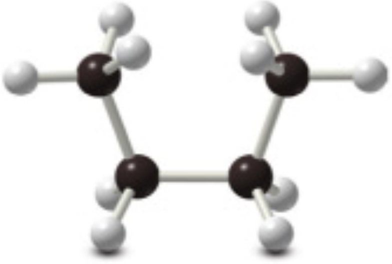


3

The CH_3 are at 60°

steric strain

Eclipsed conformation



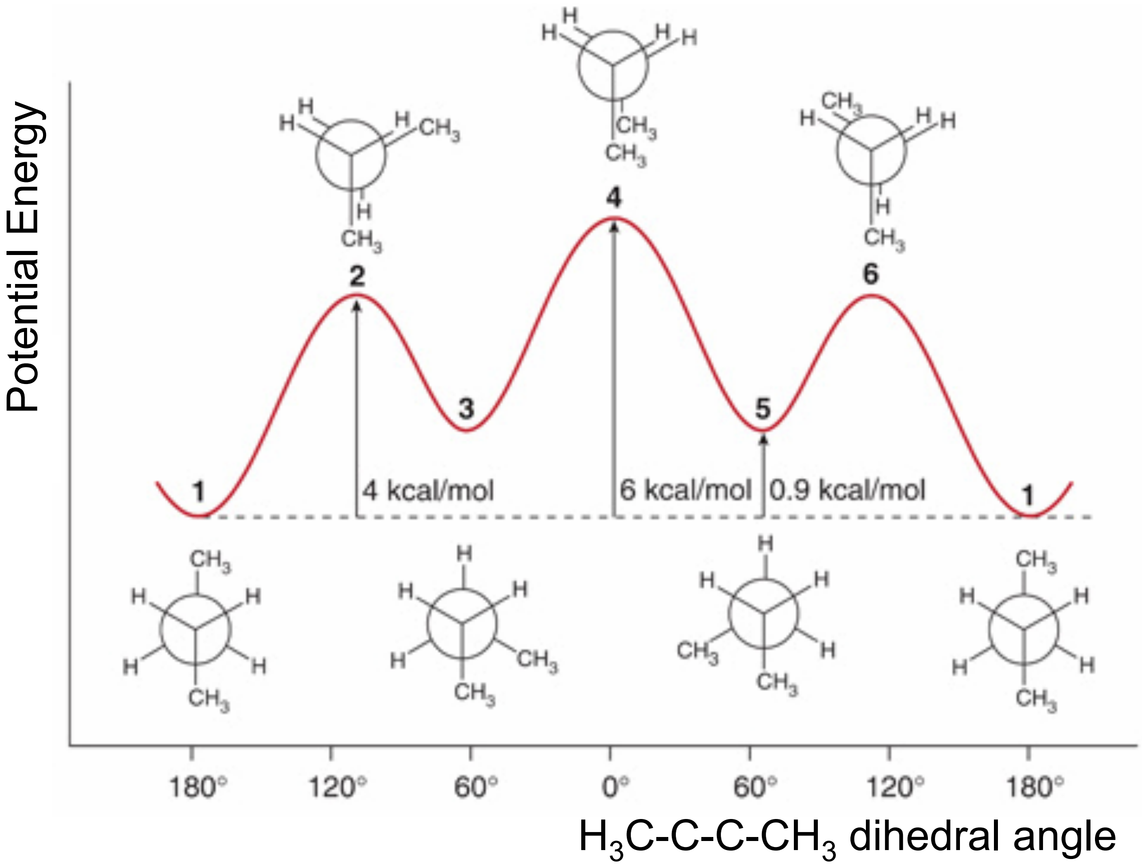
4

The CH_3 are at 0°

steric strain

Conformations of Butane

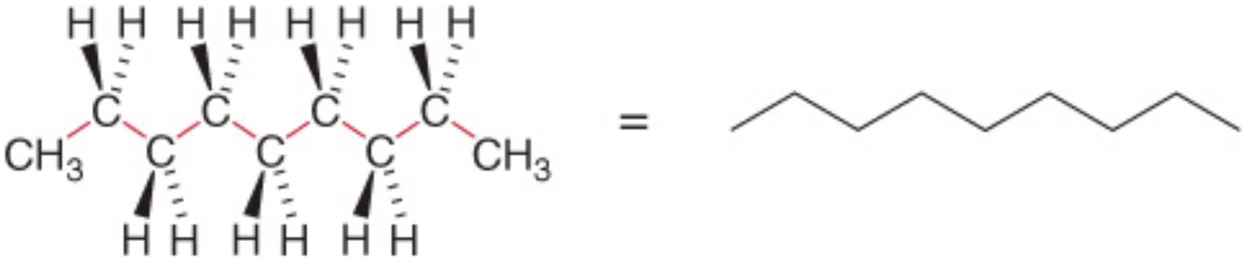
- *Staggered conformations*:
  - **1** (anti) is the absolute minimum
  - **3,5** (gauche) are relative minima
- *Eclipsed conformations:*
  - **4** is the absolute maximum (CH_3 eclipsed)
  - **2,6** are relative maxima



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.

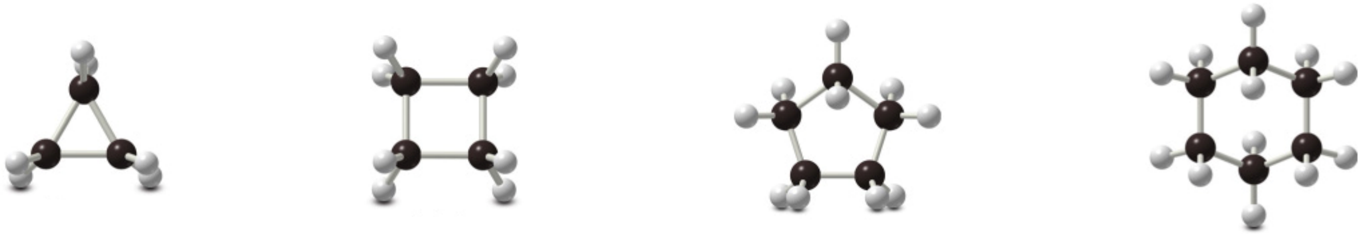


Cycloalkanes

Cycloalkanes

- Cycloalkanes have empirical formula $\mathbf{C_nH_{2n}}$ and contain carbon atoms arranged in a cyclic chain

- Nomenclature: cyclo + name of the corresponding alkane



cyclopropane C_3H_6

cyclobutane C_4H_8

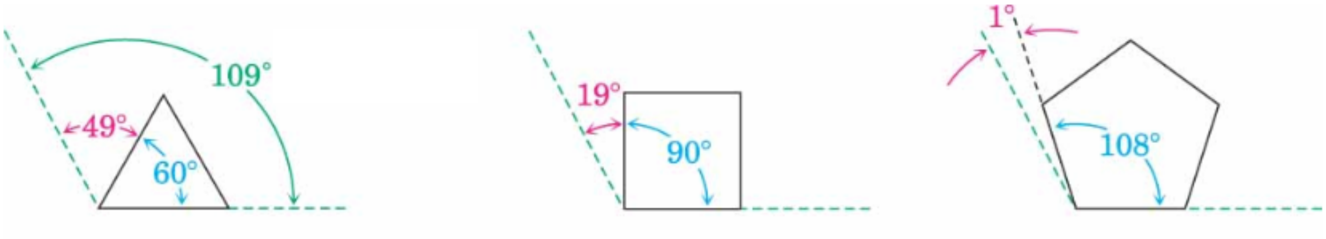
cyclopentane C_5H_{10}

cyclohexane C_6H_{12}

Stability: Angular Strain (Baeyer's Strain)

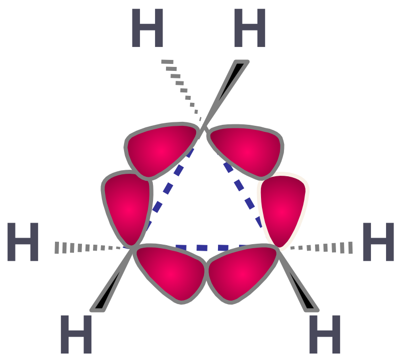
- Baeyer (1885): as carbon prefers 109° bond angles, rings other than five or six membered may be too strained to exist.

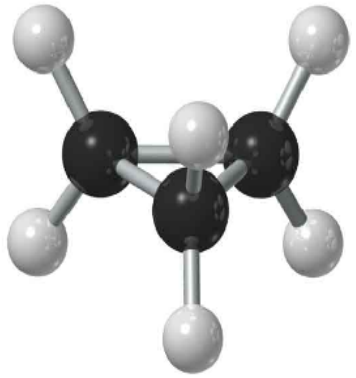
- Cycloalkanes from C_3 to C_{30} do exist, but some of them are strained because of distorted bond angles and other interactions.



Cyclopropane C_3H_6

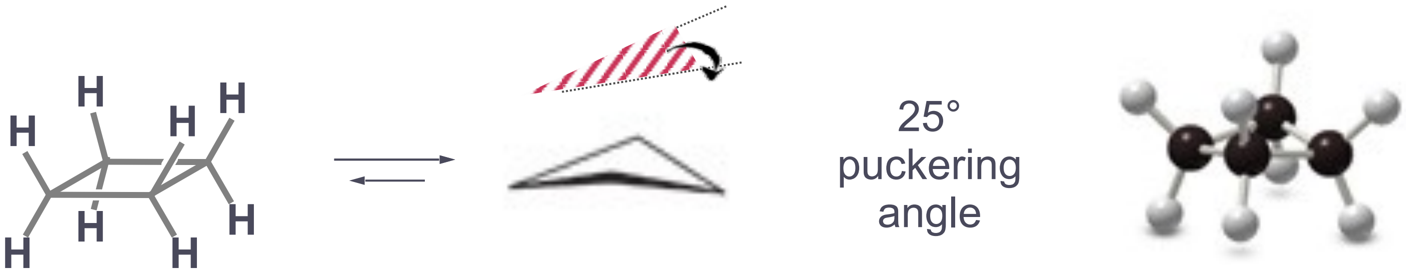
- Planar.
- Angle strain: 60° CCC angles.
- Torsional strain: all H are eclipsed.
- May be described as sp3 hybridized with banana bonds.





Cyclobutane C_4H_8

- 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.



Planar
angle strain
torsional strain

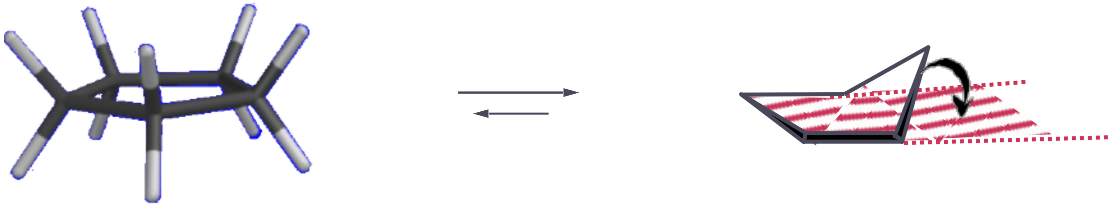
Puckered
slightly higher angle strain
lower torsional strain
some VdW strain

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.

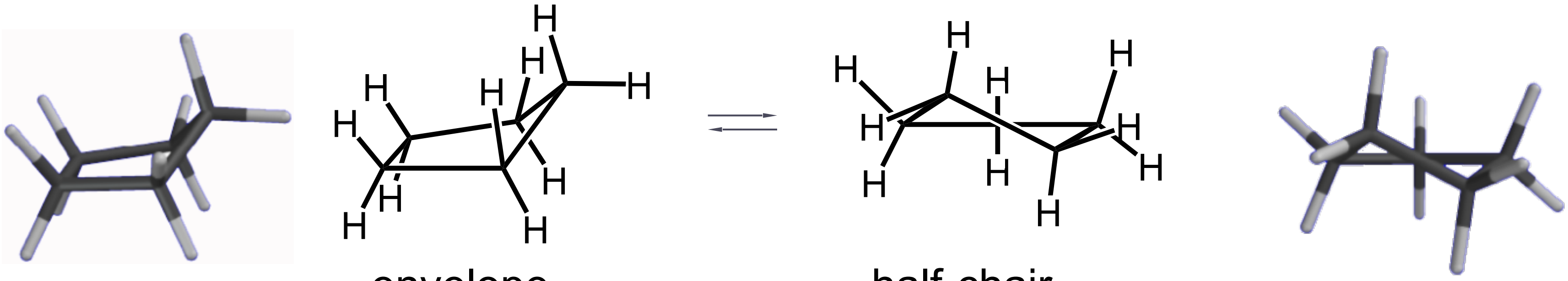
Cyclopentane C5H10



25°
puckering angle

angle strain
torsional strain

“envelope” conformation
eclipsing is partially relieved



envelope

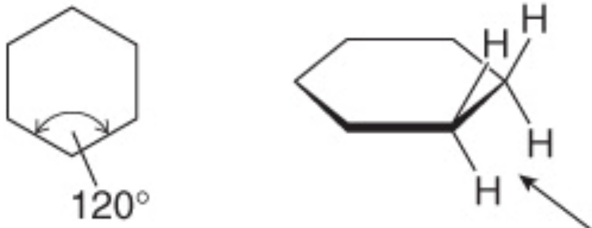
half-chair

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

Cyclohexane C6H12

- Planar cyclohexane.

angle strain



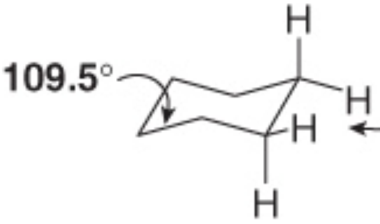
CCC > 109.5°

torsional strain

all H are eclipsed

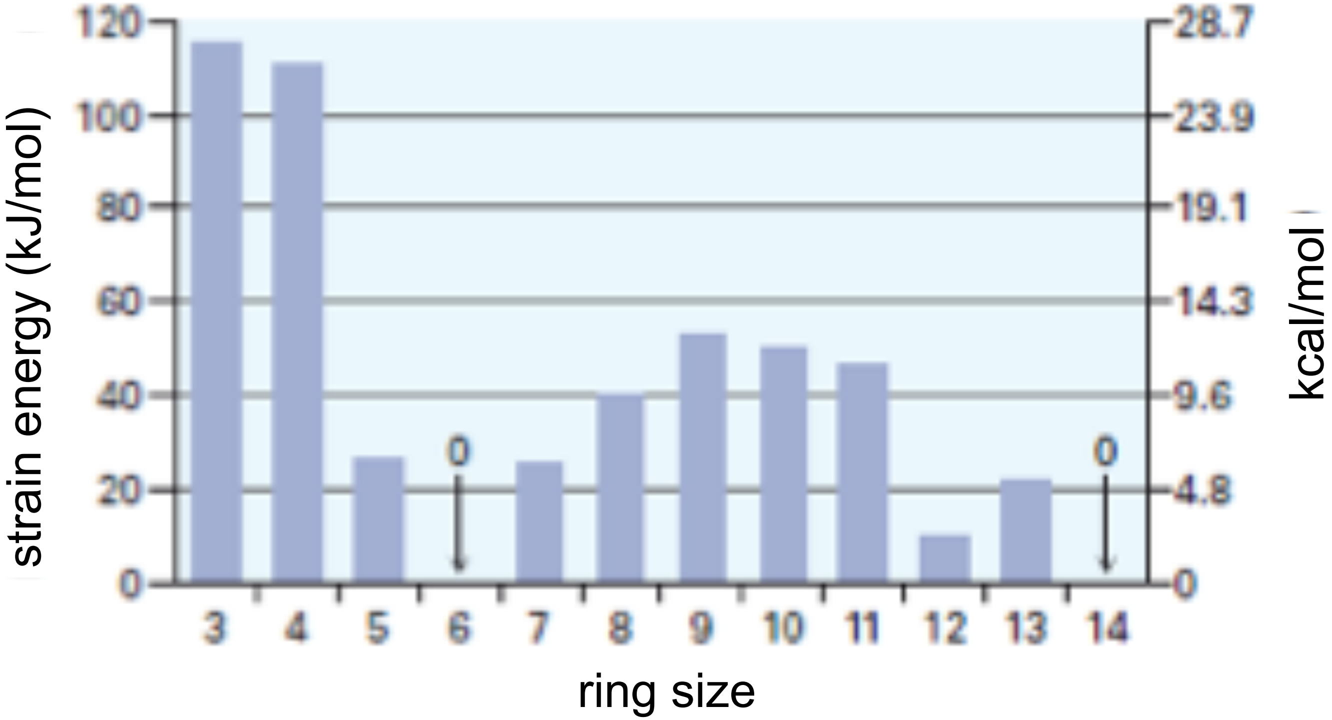
- *Chair* conformation.

strainless



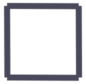
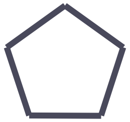
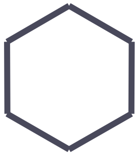
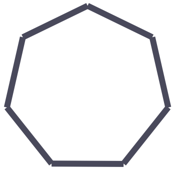
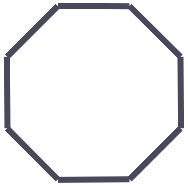
H are staggered

Strain Energies of Cycloalkanes

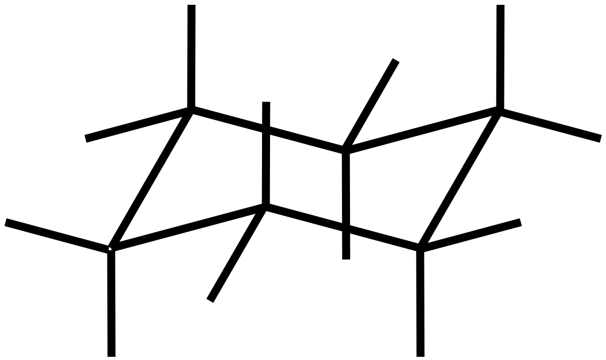


Strain Energies of Cycloalkanes

- 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).

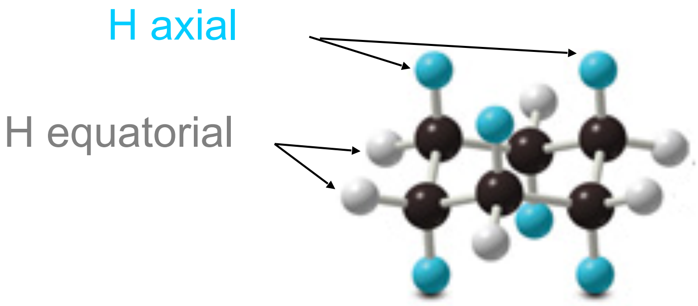
						
kJ/mol	2091	2724	3290	3910	4599	5264
Per CH_2	697	681	658	653	657	658
Strain	132	112	25	0	28	40

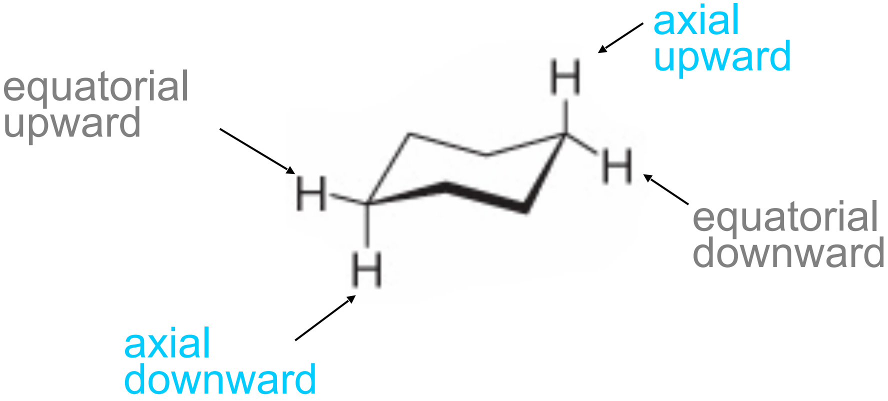
How to Draw Chair Cyclohexane



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.

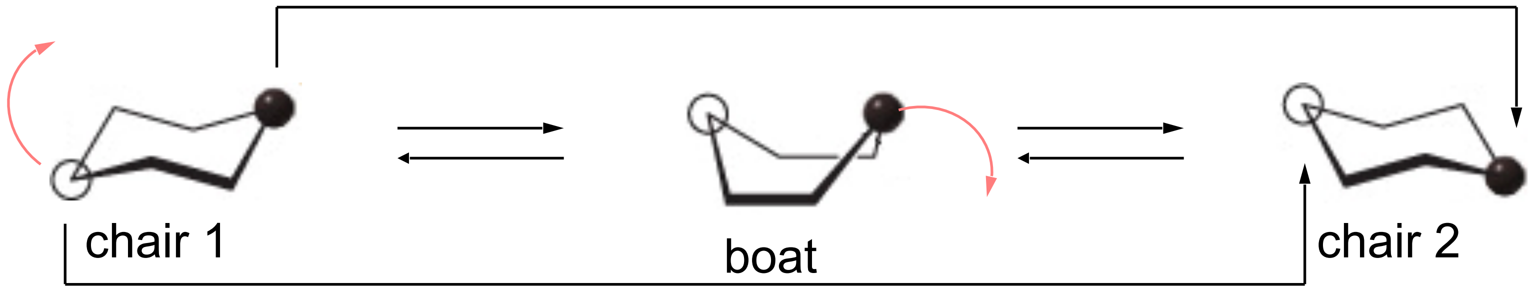




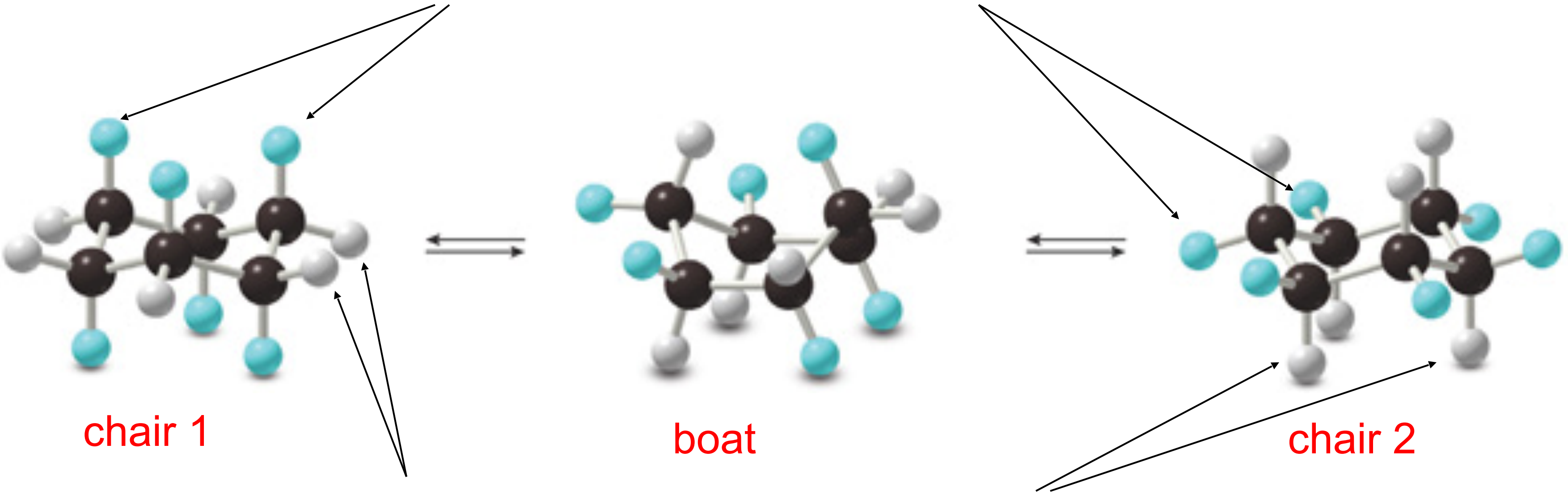
- There are 6 axial and 6 equatorial hydrogens in cyclohexane.

Ring Flipping

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



Ring Flipping



axial H become equatorial

chair 1

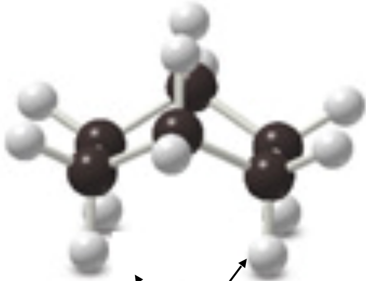
boat

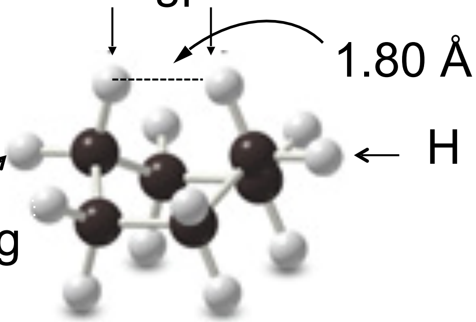
chair 2

equatorial H become axial

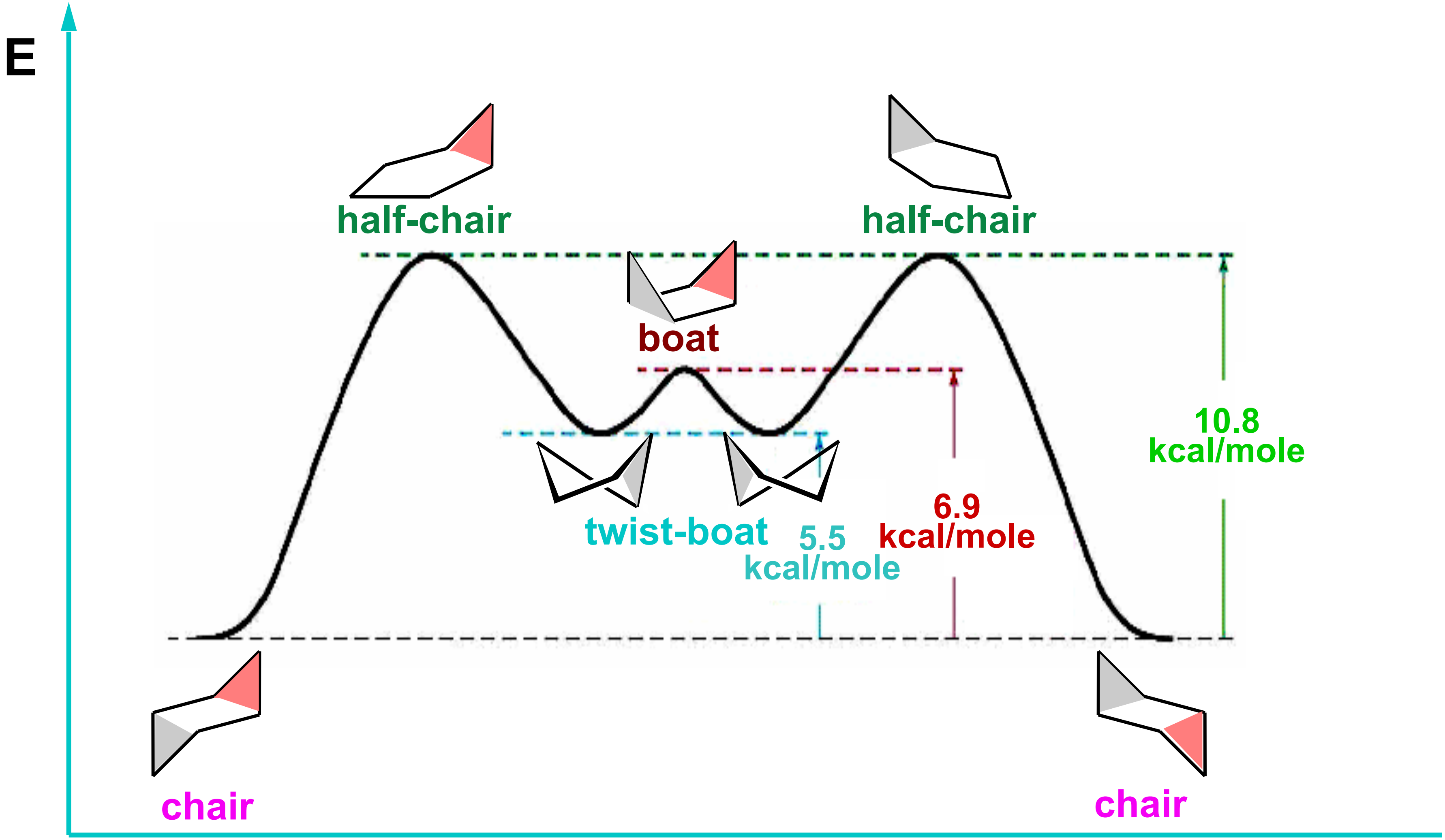
Conformations of Cyclohexane

- 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.

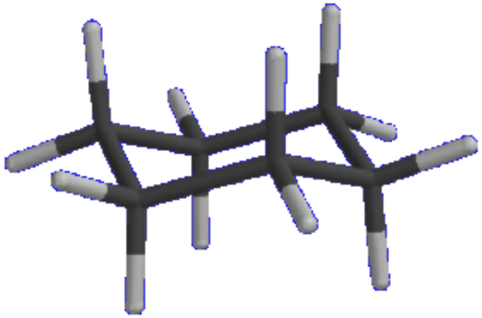




Conformations of Cyclohexane



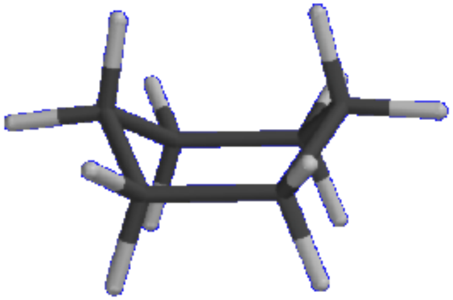
Conformations of Cyclohexane



chair

no ring strain

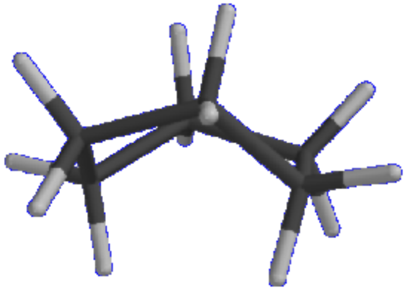
(99.99% at 25°C)



boat

- torsional strain
- steric strain

ring strain: ~ 7 kcal



twist-boat

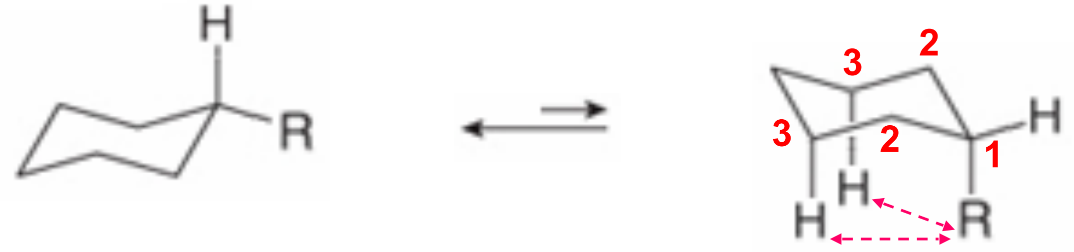
~ 1.5 kcal more stable

than the boat

(0.01% at 25°C)

Substitued Cyclohexanes

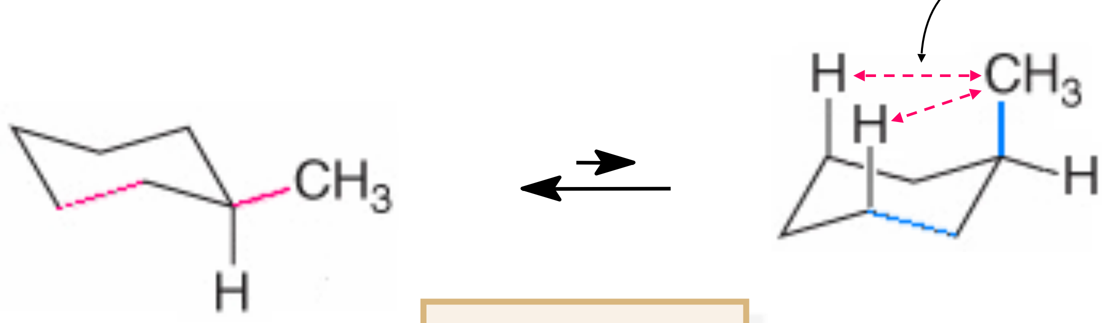
- The chair conformations are no longer equivalent: they have different energies.



- 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



1,3-diaxial
interactions

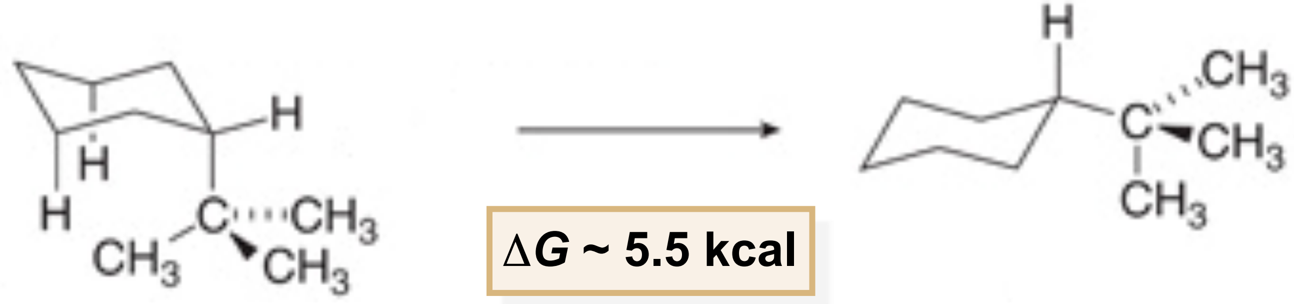
axial
(5%)
steric
repulsion

Δ*G* ~ 1.8 kcal

Each CH_3 / 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.



Δ*G* ~ 5.5 kcal

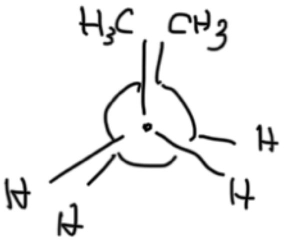
< 0.01%

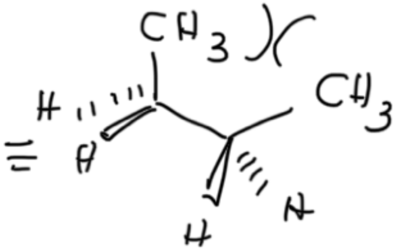
> 99.99%

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

Steric Strain and Torsional Strain

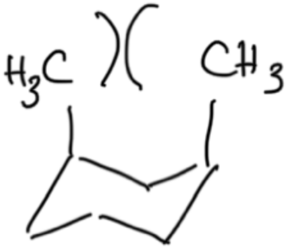
sostituenti separati da 3 legami





strain torsionale

sostituenti separati da >3 legami



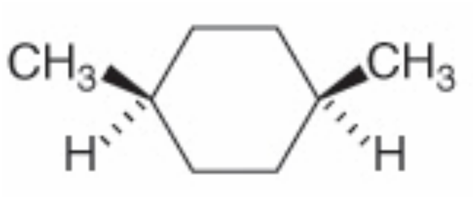
strain sterico

- Steric strain results from VdW repulsions between non bonded atoms or groups.

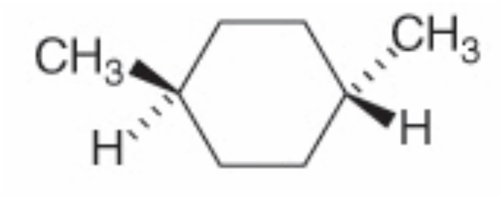
- Torsional strain is steric strain between atoms or groups that are separated by 3 bonds and depends on the dihedral angle between the adjacent groups (conformation = rotation around a single bond)

Disubstitued Cyclohexanes. Geometrical Stereoisomerism

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



cis

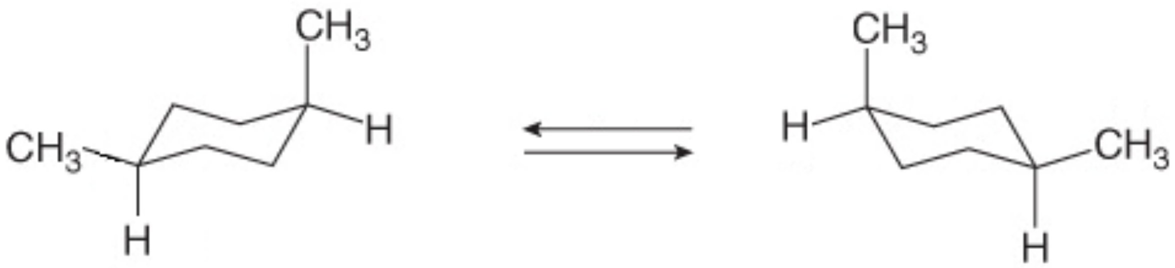


trans

- Each geometrical isomer has two possible chair conformations.

1,4-Dimethylcyclohexane

cis

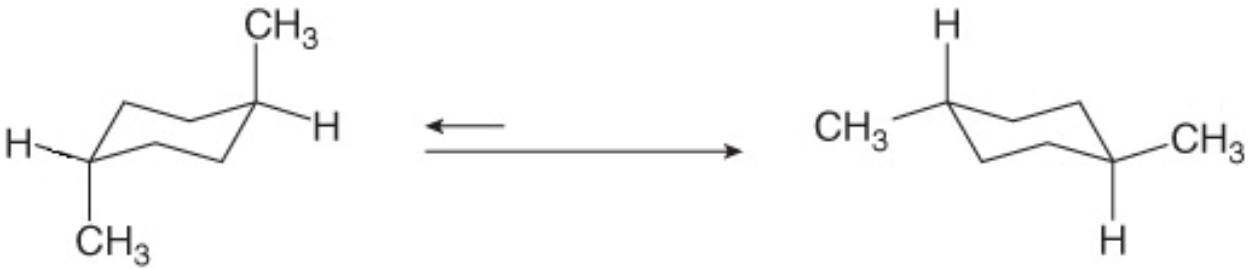


equatorial-axial
2 1,3-diaxial interactions
2 x 0.9 = 1.8 kcal

axial-equatorial
2 1,3-diaxial interactions
2 x 0.9 = 1.8 kcal

ΔG = 0 kcal

trans

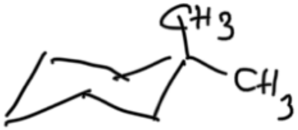


bisaxial
4 1,3-diaxial interactions
4 x 0.9 = 3.6 kcal

bisequatorial
no repulsions

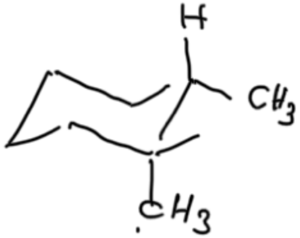
ΔG ~ 3.6 kcal

Dimethylcyclohexanes

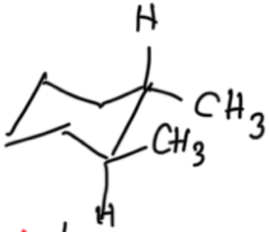


1,1

1,2:



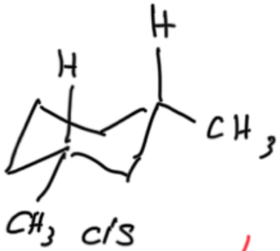
cis



trans

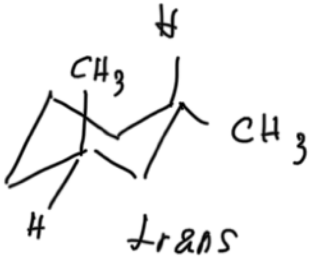
+ stabile

1,3



cis

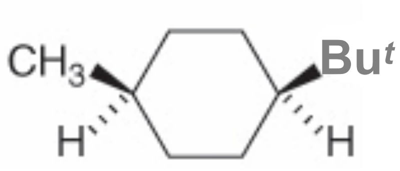
+ stabile

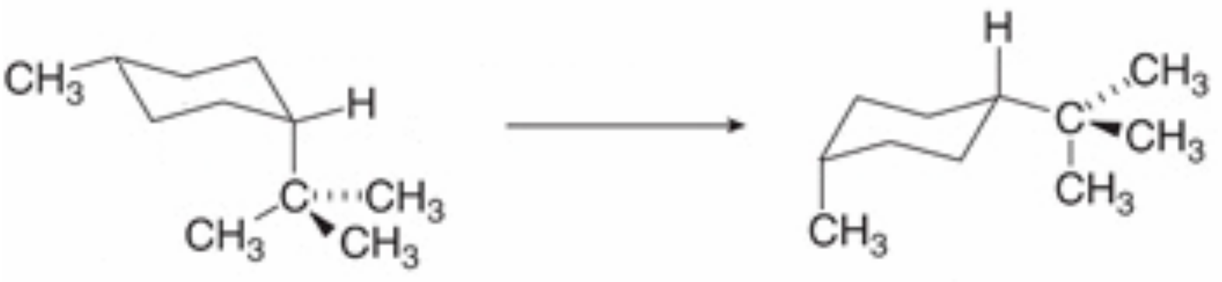


trans

cis-1-t-Butyl-4-methylcyclohexane

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

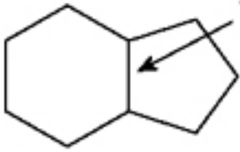




5.5 kcal/mol 1.8 kcal/mole **Δ*G* ~ 3.7 kcal**

Polycyclic compounds

A fused bicyclic system



This C–C bond is **shared** by both rings.

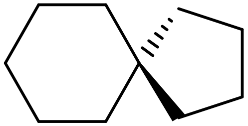
- One bond is shared by two rings.
- The shared C's are adjacent.

A bridged bicyclic system

These C's are **shared** by two rings.

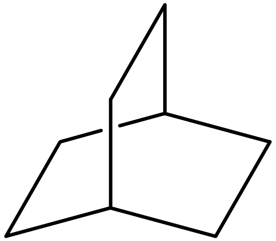
- Two non-adjacent atoms are shared by both rings.

A spiro bicyclic system

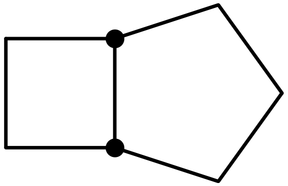


- One atom is shared by two rings

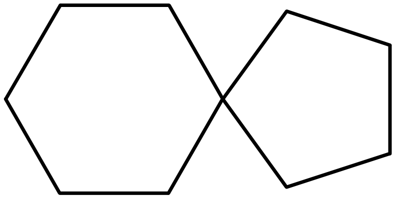
Polycyclic compounds



bicyclo[2.2.2]octane



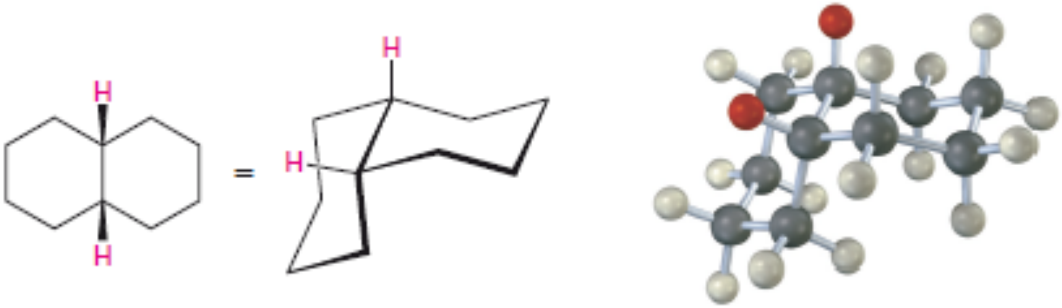
bicyclo[3.2.0]heptane



spiro[4,5]decane

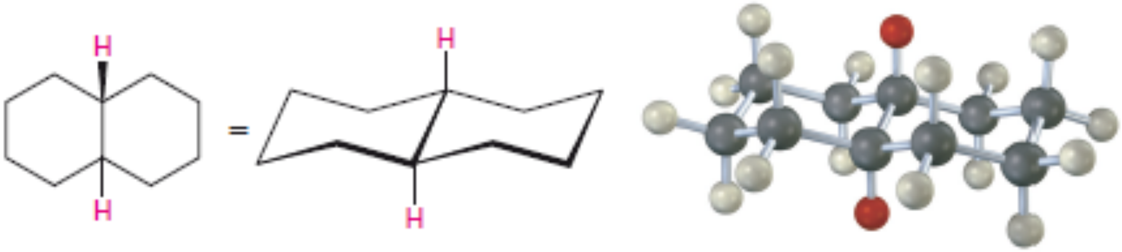
Polycyclic Hydrocarbons

less stable
(1 axial substituent)



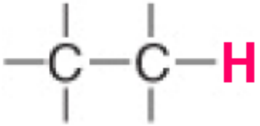
cis-decaline

more stable
(equatorial substituents)



trans-decaline

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.

$$\boxed{\text{R–H} + \text{X}_2 \xrightarrow{\Delta \text{ or } h\nu} \text{R–X} + \text{HX}}$$

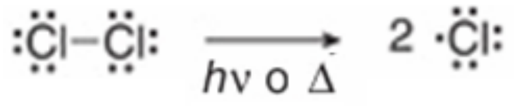
radical substitution

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

Halogenation of Methane

Initiation

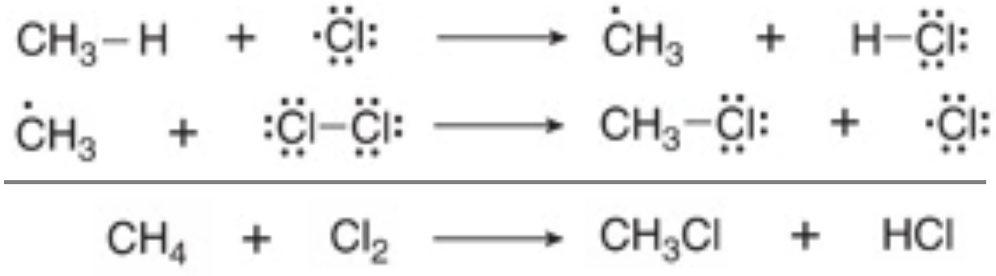
Stage [1]: formation of Cl· radicals



$$:\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}-\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}: \xrightarrow[h\nu \text{ o } \Delta]{} 2\ \cdot\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}:$$

Propagation

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



$$\mathrm{CH_3{-}H} + \cdot\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}: \longrightarrow \dot{\mathrm{C}}\mathrm{H_3} + \mathrm{H}-\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}:$$

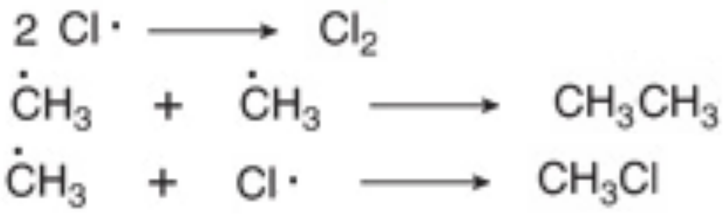
$$\dot{\mathrm{C}}\mathrm{H_3} + :\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}-\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}: \longrightarrow \mathrm{CH_3}-\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}: + \cdot\underset{\cdot\cdot}{\ddot{\mathrm{Cl}}}:$$

$$\mathrm{CH_4} + \mathrm{Cl_2} \longrightarrow \mathrm{CH_3Cl} + \mathrm{HCl}$$

thousands of cycles.
Chain reaction

Termination

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



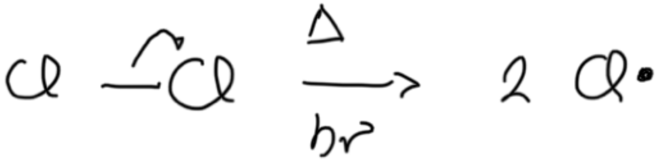
$$2\ \mathrm{Cl}\cdot \longrightarrow \mathrm{Cl_2}$$

$$\dot{\mathrm{C}}\mathrm{H_3} + \dot{\mathrm{C}}\mathrm{H_3} \longrightarrow \mathrm{CH_3CH_3}$$

$$\dot{\mathrm{C}}\mathrm{H_3} + \mathrm{Cl}\cdot \longrightarrow \mathrm{CH_3Cl}$$

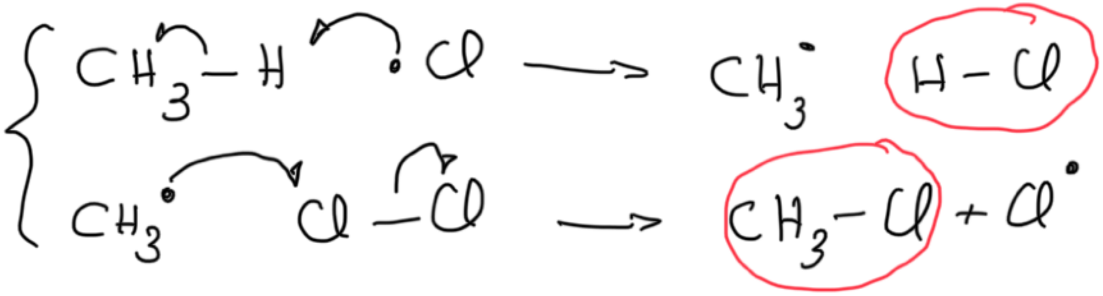
Halogenation of Methane

Initiation



$$Cl-Cl \xrightarrow[h\nu]{\Delta} 2\,Cl^{\bullet}$$

Propagation



$$CH_3-H \quad {}^{\bullet}Cl \longrightarrow CH_3^{\bullet} \quad H-Cl$$

$$CH_3^{\bullet} \quad Cl-Cl \longrightarrow CH_3-Cl + Cl^{\bullet}$$

Energetics

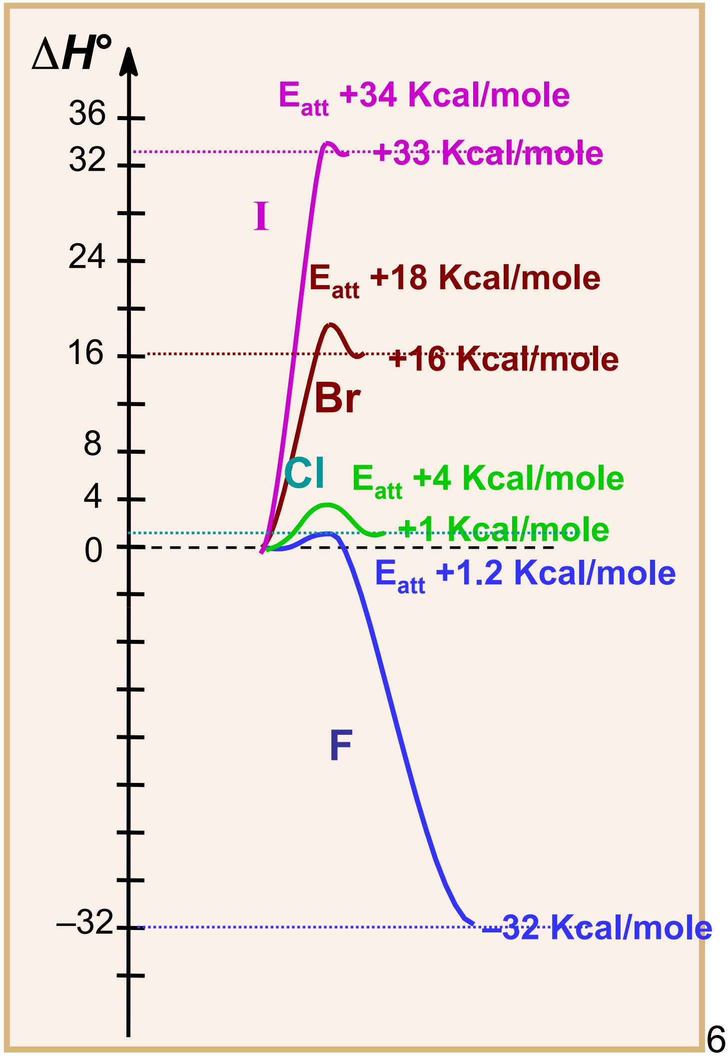
Stage [2] is the slow step:

$$CH_4 + X\cdot \longrightarrow \dot{C}H_3 + HX$$

$$\Delta H° = \Delta H°(C\text{-}H) - \Delta H°(X\text{-}H)$$

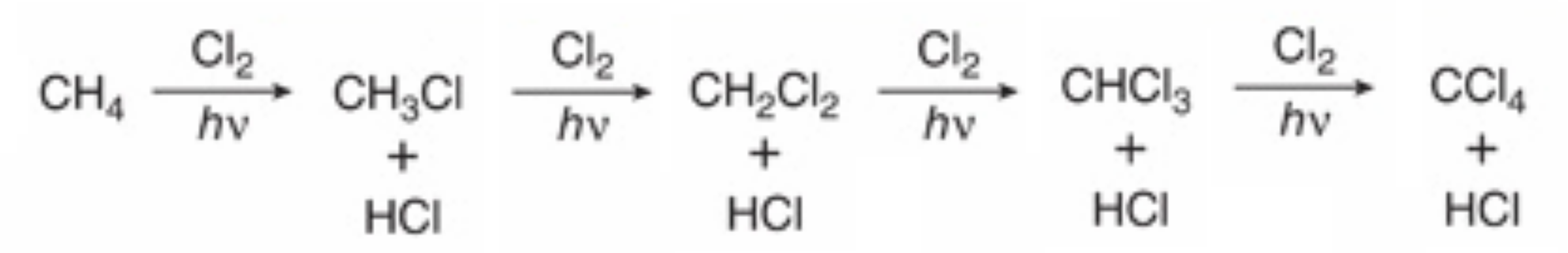
ΔH°, Kcal/mole

ΔH°(C-H)	104			
X =	F	Cl	Br	I
ΔH°(X-H)	136	103	88	71
ΔH°	-32	+1	+16	+33



Halogenation of Alkanes

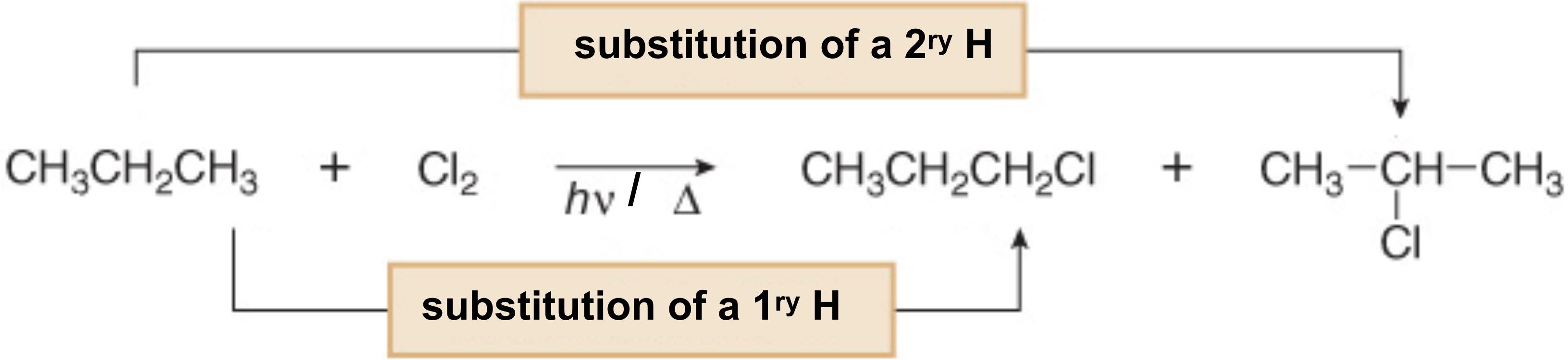
- ❑ Monohalogenation is only possible with an excess of substrate, otherwise polyhalogenation predominates.



- ❑ Problem: mixture of halogenated products.
- ❑ Solution: CH_4 in large excess and recycled.

Regioselectivity

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



$$CH_3CH_2CH_3 + Cl_2 \xrightarrow[h\nu\ /\ \Delta]{} CH_3CH_2CH_2Cl + CH_3-\underset{\displaystyle Cl}{\underset{|}{CH}}-CH_3$$

substitution of a 2ry H

substitution of a 1ry H

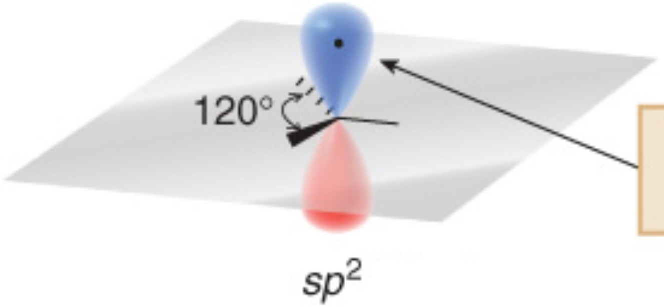
statistical ratio 3 : 1

observed ratio 1 : 1

Structure of Radicals

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

$\dot{C}H_3$	$R\dot{C}H_2$	$R_2\dot{C}H$	$R_3\dot{C}$
methyl radical	**1^{ry} radical**	**2^{ry} radical**	**3^{ry} radical**

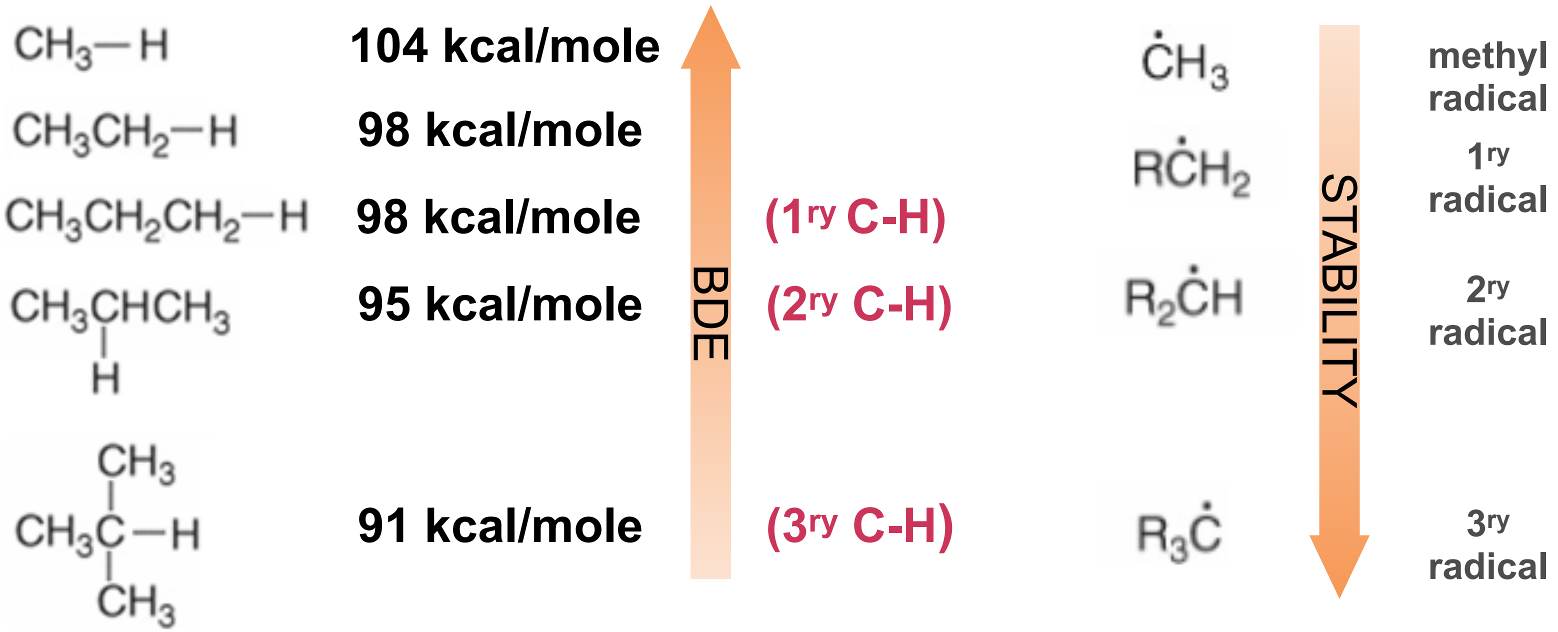


a single electron in the p orbital

C−H Bond Dissociation Energies

$R-H \rightarrow R\bullet + H\bullet$

D*H* = BDE bond dissociation energy

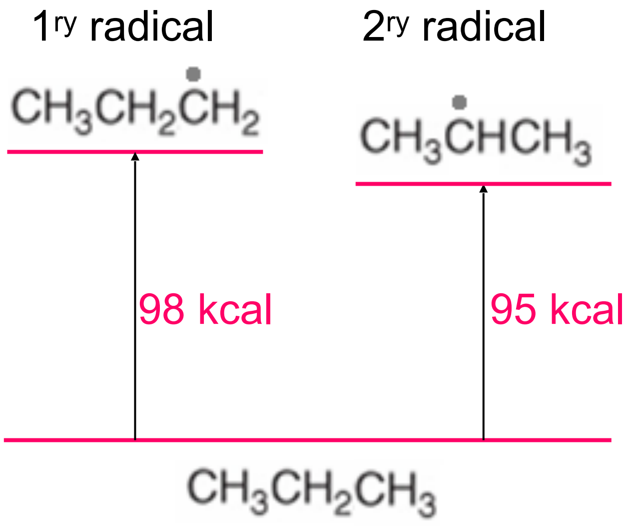


CH_3-H	**104 kcal/mole**	
CH_3CH_2-H	**98 kcal/mole**	
$CH_3CH_2CH_2-H$	**98 kcal/mole**	(1^{ry} C-H)
$CH_3\underset{H}{C}HCH_3$	**95 kcal/mole**	(2^{ry} C-H)
$CH_3\overset{CH_3}{\underset{CH_3}{C}}-H$	**91 kcal/mole**	(3^{ry} C-H)

$\dot{C}H_3$	**methyl radical**
$R\dot{C}H_2$	**1^{ry} radical**
$R_2\dot{C}H$	**2^{ry} radical**
$R_3\dot{C}$	**3^{ry} radical**

Reactivity of C−H bonds:
$3^{ry} > 2^{ry} > 1^{ry} > CH_3-H$

Regioselectivity



1ry radical

$CH_3CH_2\dot{C}H_2$

2ry radical

$CH_3\dot{C}HCH_3$

98 kcal

95 kcal

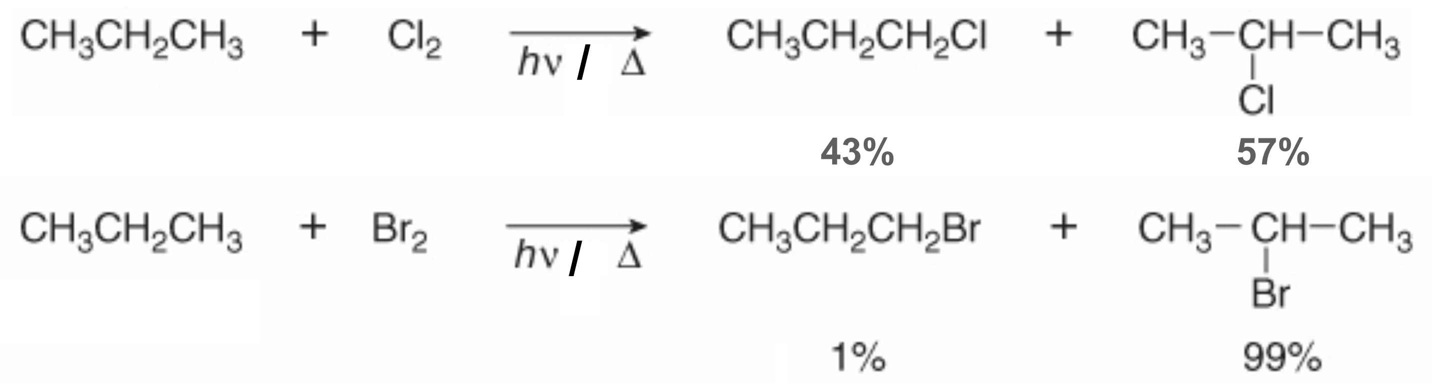
$CH_3CH_2CH_3$

Lower energy, more stable, weaker C-H bond.

- Radical stability: 3ry > 2ry > 1ry.
- Strength of C-H bonds: 3ry < 2ry < 1ry.

Reactivity and Selectivity

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



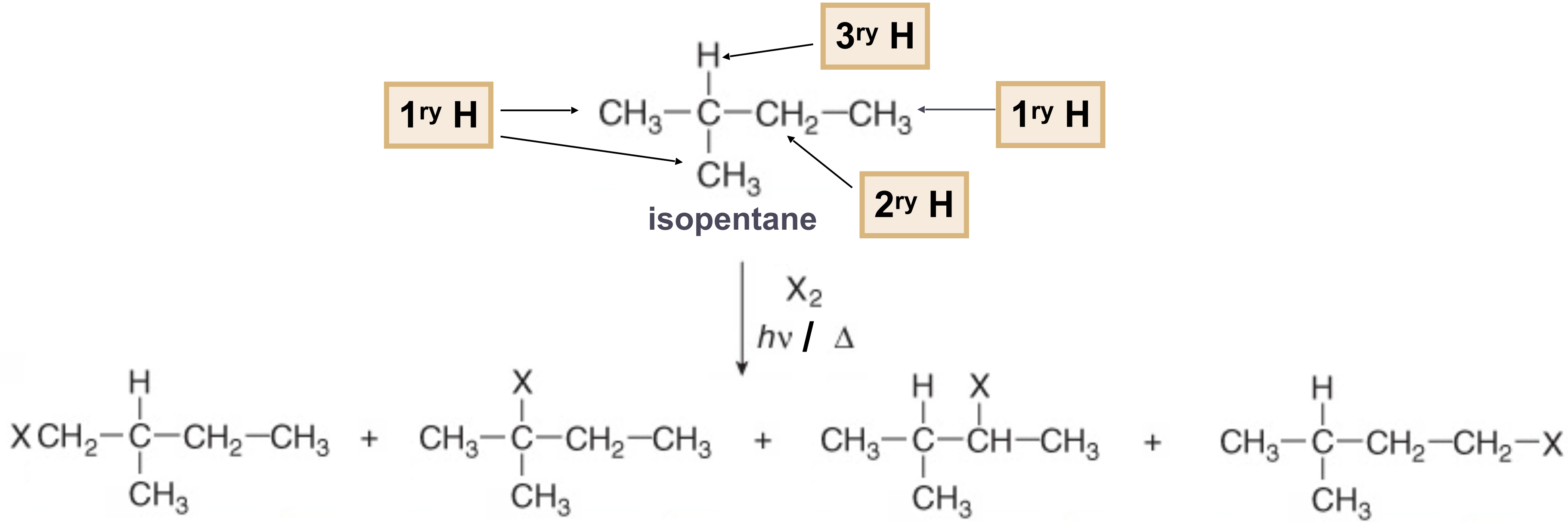
$$CH_3CH_2CH_3 + Cl_2 \xrightarrow[h\nu\ /\ \Delta]{} CH_3CH_2CH_2Cl + CH_3-\underset{\displaystyle Cl}{\underset{|}{CH}}-CH_3$$

43% 57%

$$CH_3CH_2CH_3 + Br_2 \xrightarrow[h\nu\ /\ \Delta]{} CH_3CH_2CH_2Br + CH_3-\underset{\displaystyle Br}{\underset{|}{CH}}-CH_3$$

1% 99%

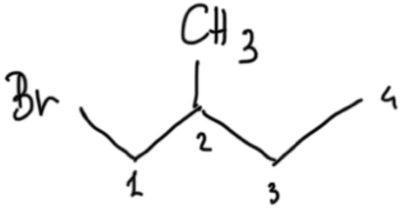
Regioselectivity



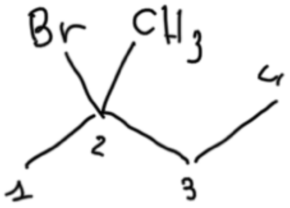
Cl_2:	**28%**	**23%**	**35%**	**14%**
Br_2:	**~0%**	**90%**	**9%**	**~0%**

C-H relative reactivity	**3ry**	**2ry**	**1ry**
with **Cl_2**	5.2	3.9	1
with **Br_2**	1640	82	1

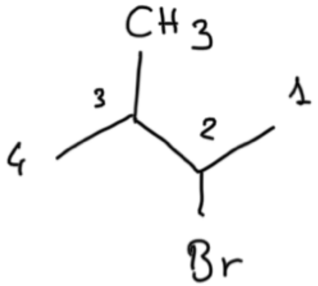
Nomenclatura dei bromo(metil)butani



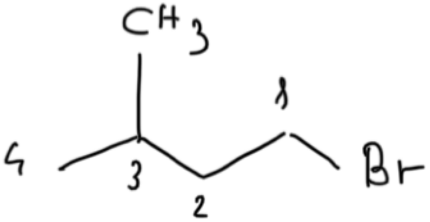
1-bromo-2-metilbutano



2-bromo-2-metilbutano

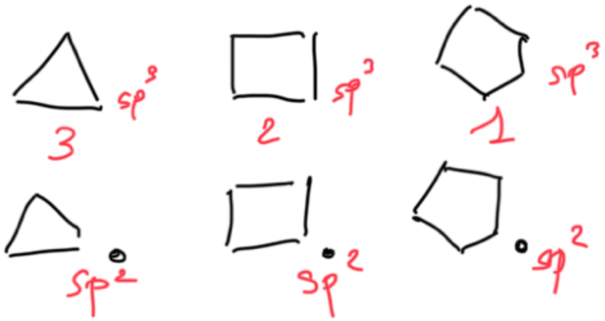


2-bromo-3-metilbutano



1-bromo-3-metilbutano

Bromurazione di cicloalcani



$\xrightarrow{Br_2,\, h\nu}$ ordine di reattività?

$R-H \xrightarrow{X^\bullet} R^\bullet + H-X$ lento

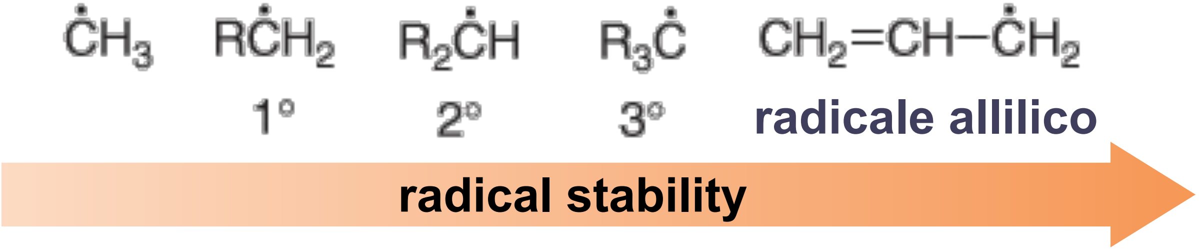
$R^\bullet + X-X \longrightarrow R-X + R^\bullet$ veloce

Halogenation of Allylic Carbons

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

$$CH_2{=}CH{-}CH_2{-}H \longrightarrow \underset{\text{allylic radical}}{CH_2{=}CH{-}\dot{C}H_2} + \cdot H \qquad \Delta H^\circ = +87\ \text{kcal/mol}$$

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

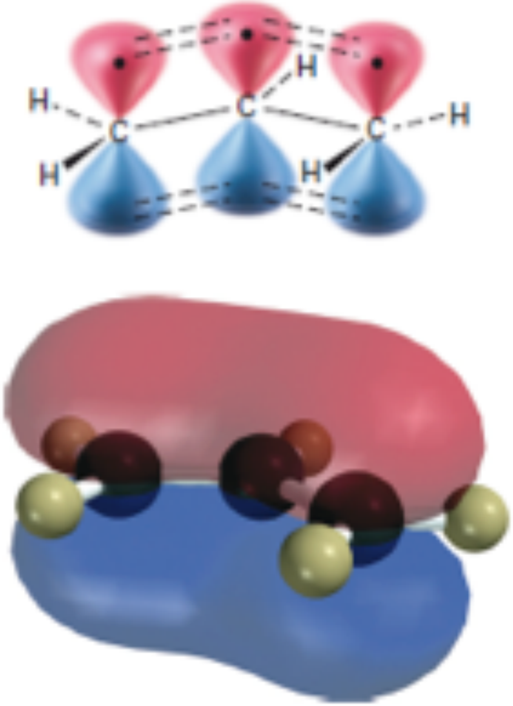


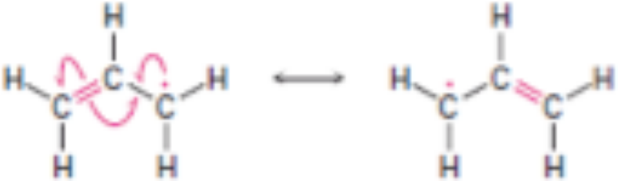
$\dot{C}H_3$ $R\dot{C}H_2$ $R_2\dot{C}H$ $R_3\dot{C}$ $CH_2{=}CH{-}\dot{C}H_2$

1° 2° 3° **radicale allilico**

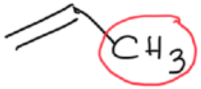
radical stability

The Allylic Radical

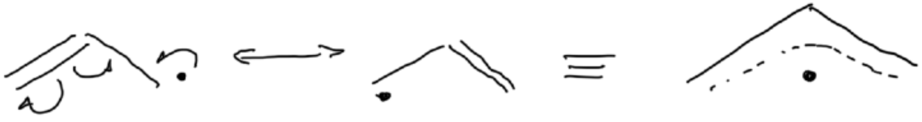


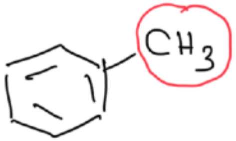


Delocalyzed Radicals

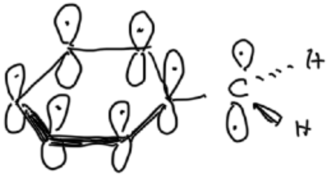


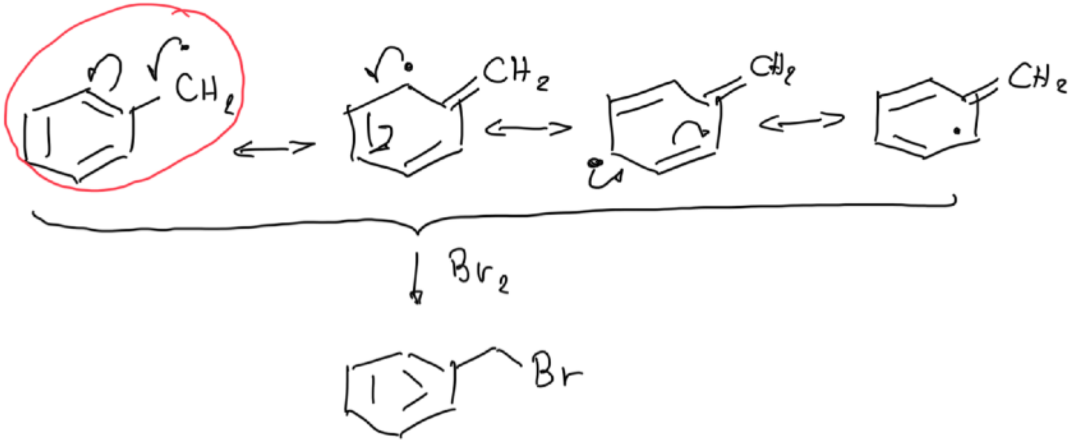
allilico



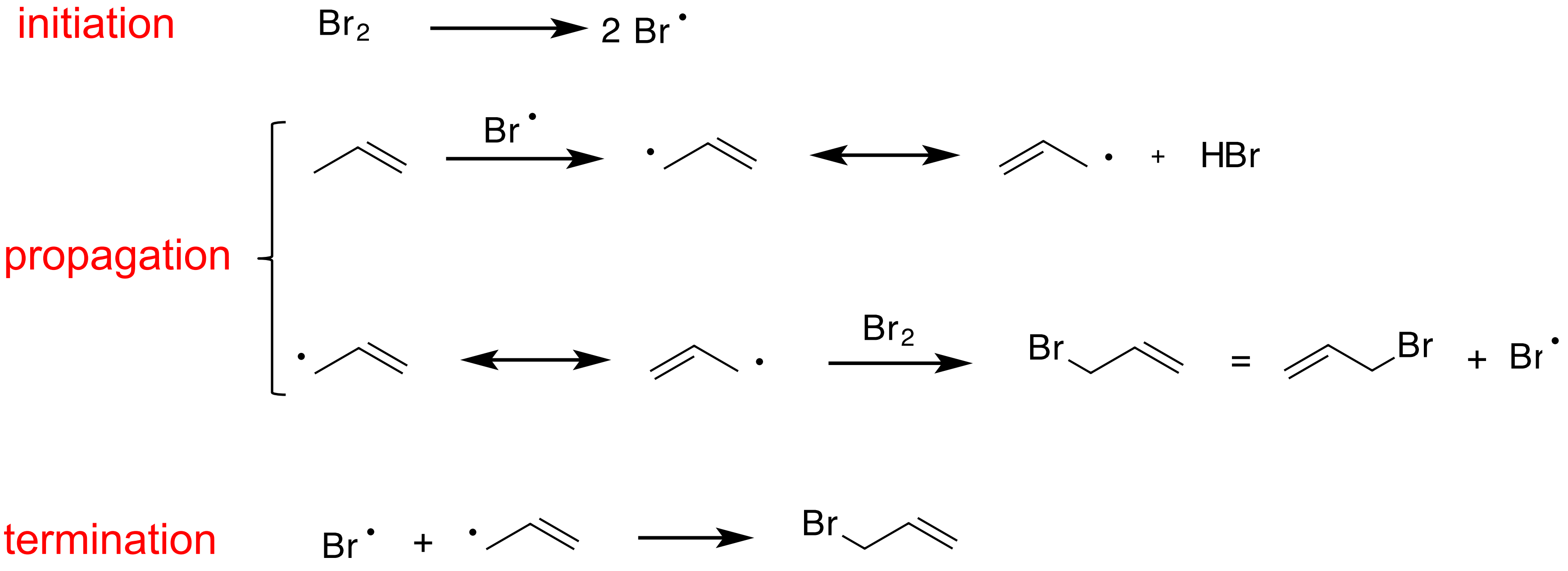


benzilico





Halogenation of Allylic Carbons



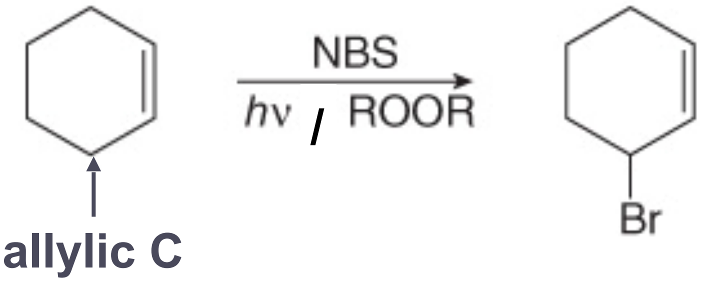
initiation

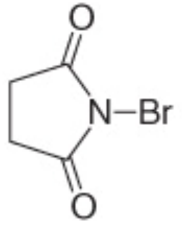
propagation

termination

Halogenation of Allylic Carbons

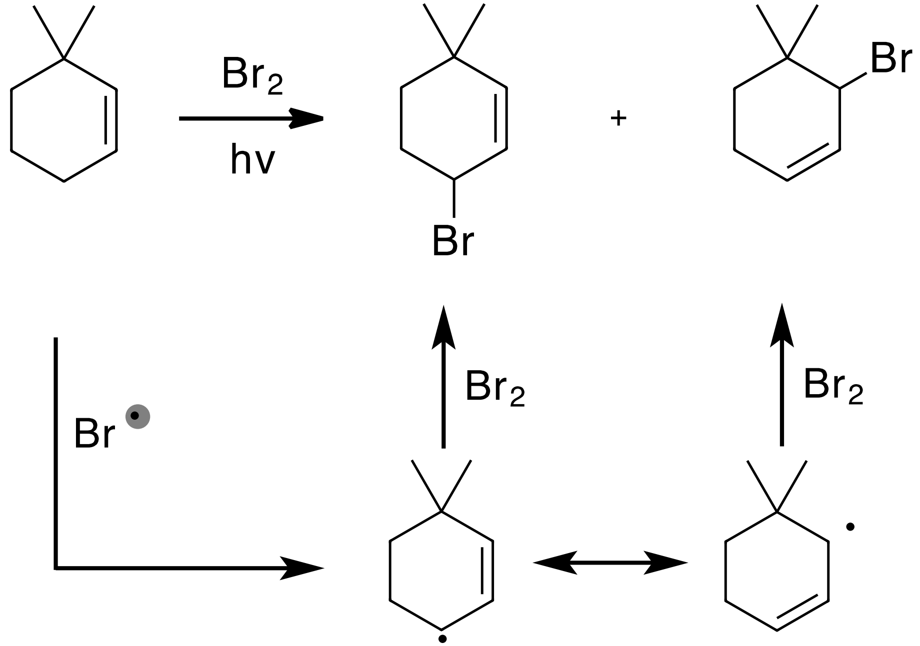
- Allylic carbons can be selectively brominated with NBS and UV irradiation or a radical initiator.
- Breaking of the weak N-Br bond of NBS initiates the radical chain reaction.





N-bromosuccinimide
NBS

Halogenation of Allylic Carbons



Combustion of Alkanes

- 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.

$$CH_4 + 2\,O_2 \longrightarrow CO_2 + 2\,H_2O + \text{heat}$$

$$(CH_3)_3CCH_2CH(CH_3)_2 + (25/2)\,O_2 \longrightarrow 8\,CO_2 + 9\,H_2O + \text{heat}$$

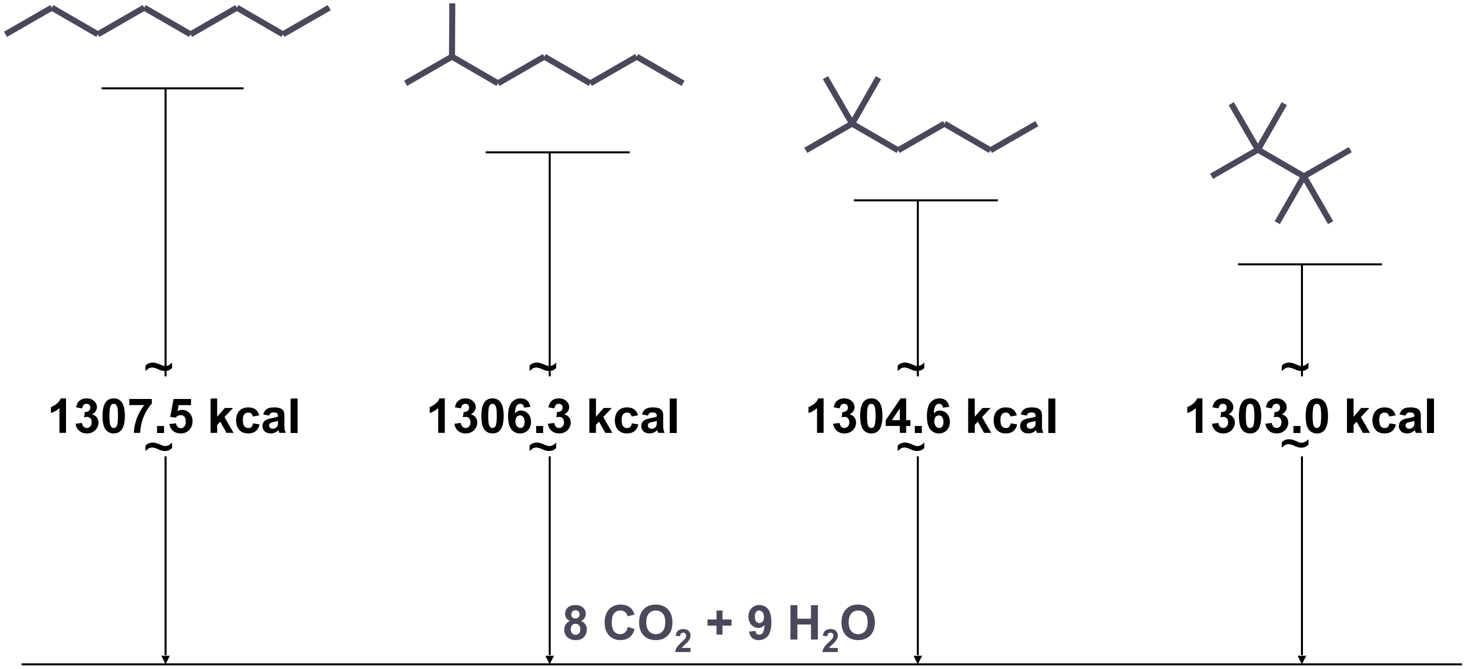
isoottano

$$C_nH_{2n+2} + \frac{3n+1}{2}O_2 \longrightarrow n\,CO_2 + (n+1)H_2O + \text{heat}$$

Every C atom is converted into CO_2

Stability of Isomers

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



1307.5 kcal

1306.3 kcal

1304.6 kcal

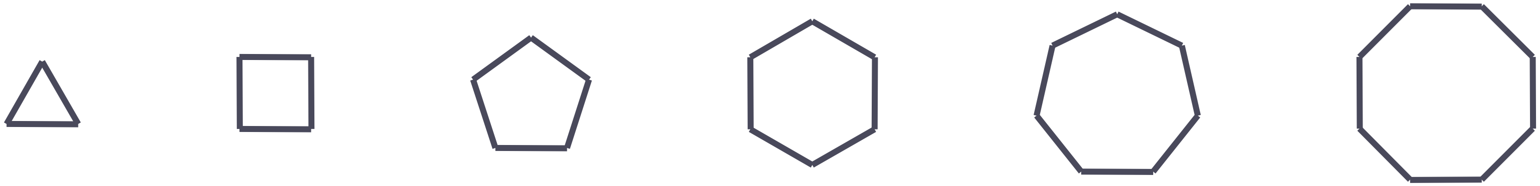
1303.0 kcal

$8\ CO_2 + 9\ H_2O$

Branched isomers are more stable than linear ones.

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