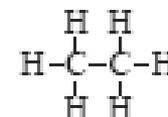
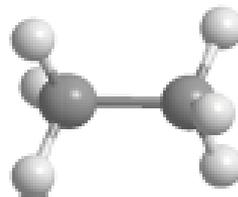


Alkany a cykloalkany

Alkany a cykloalkany jsou hlavní složky zemního plynu a ropy, které jsou převážným zdrojem energie

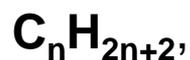
Nasycené alkany a cykloalkany mají pouze **jednoduché vazby** uhlík-vodík (C-H) a uhlík-uhlík (C-C).

Struktura alkanů

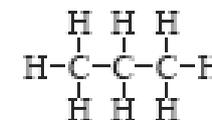
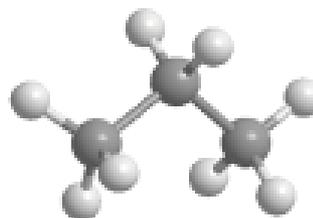


ethan

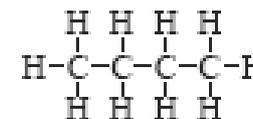
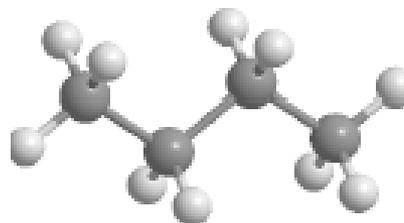
Alkany mají obecný molekulární vzorec:



kde n je počet atomů uhlíku.



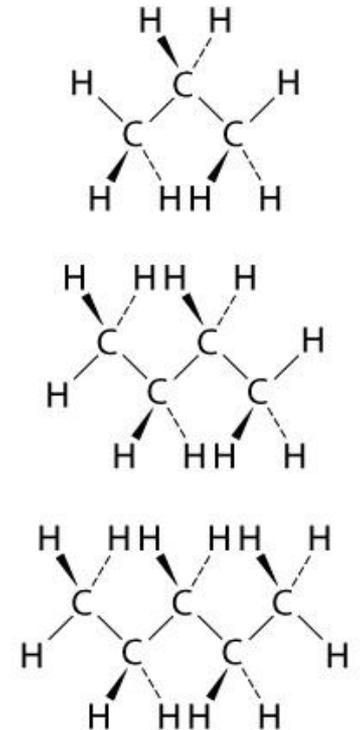
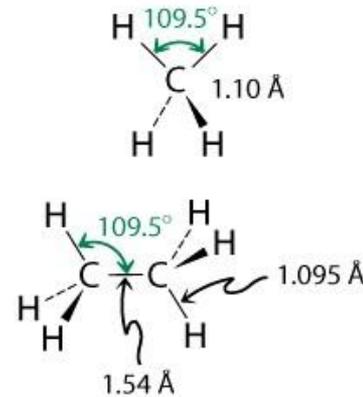
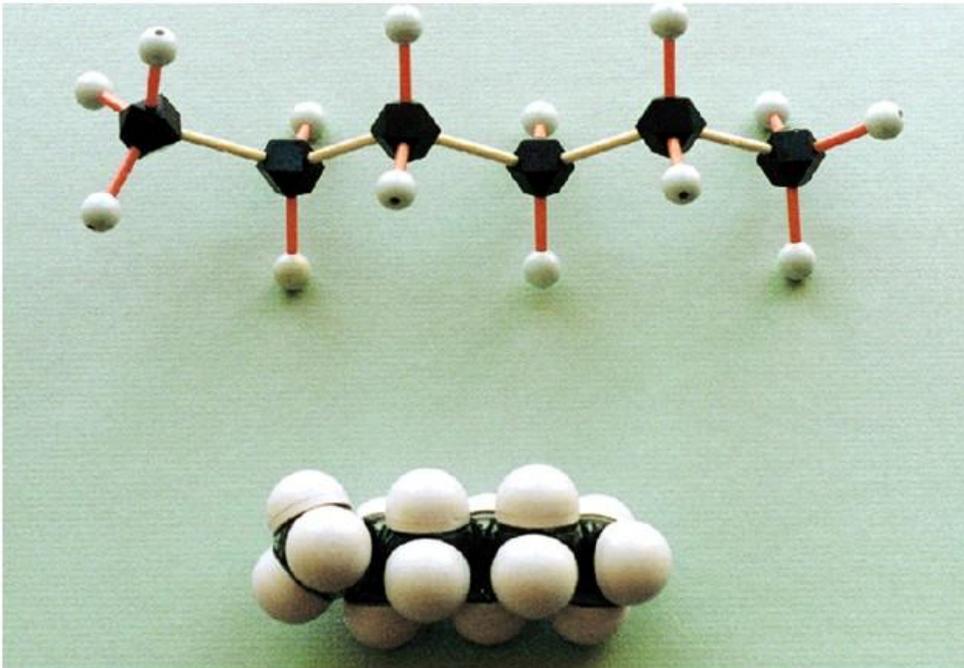
propan



butan

Struktura a fyzikální vlastnosti alkanů

Struktura alkanů je pravidelná. Uhlíkové atomu jsou tetraedrální v hybridizaci sp^3 (vazebné úhly cca. 109°), délka vazby C-C je $\sim 1.54 \text{ \AA}$ a C-H vazby $\sim 1.10 \text{ \AA}$.

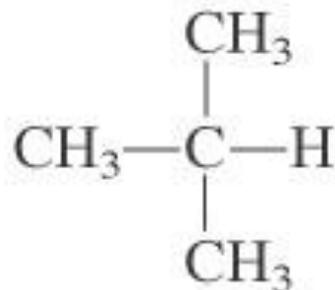


Lineární alkan



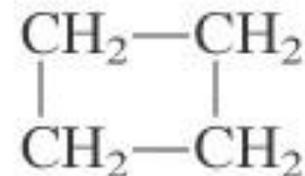
Butane, C₄H₁₀

Rozvětvený alkan



2-Methylpropane, C₄H₁₀
(Isobutane)

Cykloalkan

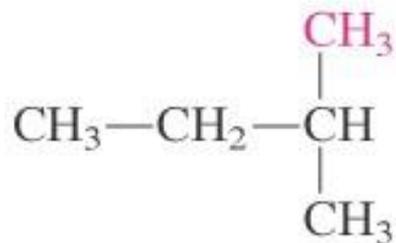


Cyclobutane, C₄H₈

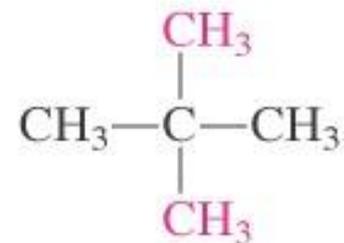
Lineární a rozvětvené alkany - izomery



Pentane



2-Methylbutane
(Isopentane)



2,2-Dimethylpropane
(Neopentane)

TABLE 2-4

Number of Possible
Isomeric Alkanes, $\text{C}_n\text{H}_{2n+2}$

n	Isomers
1	1
2	1
3	1
4	2
5	3
6	5
7	9
8	18
9	35
10	75
15	4,347
20	366,319

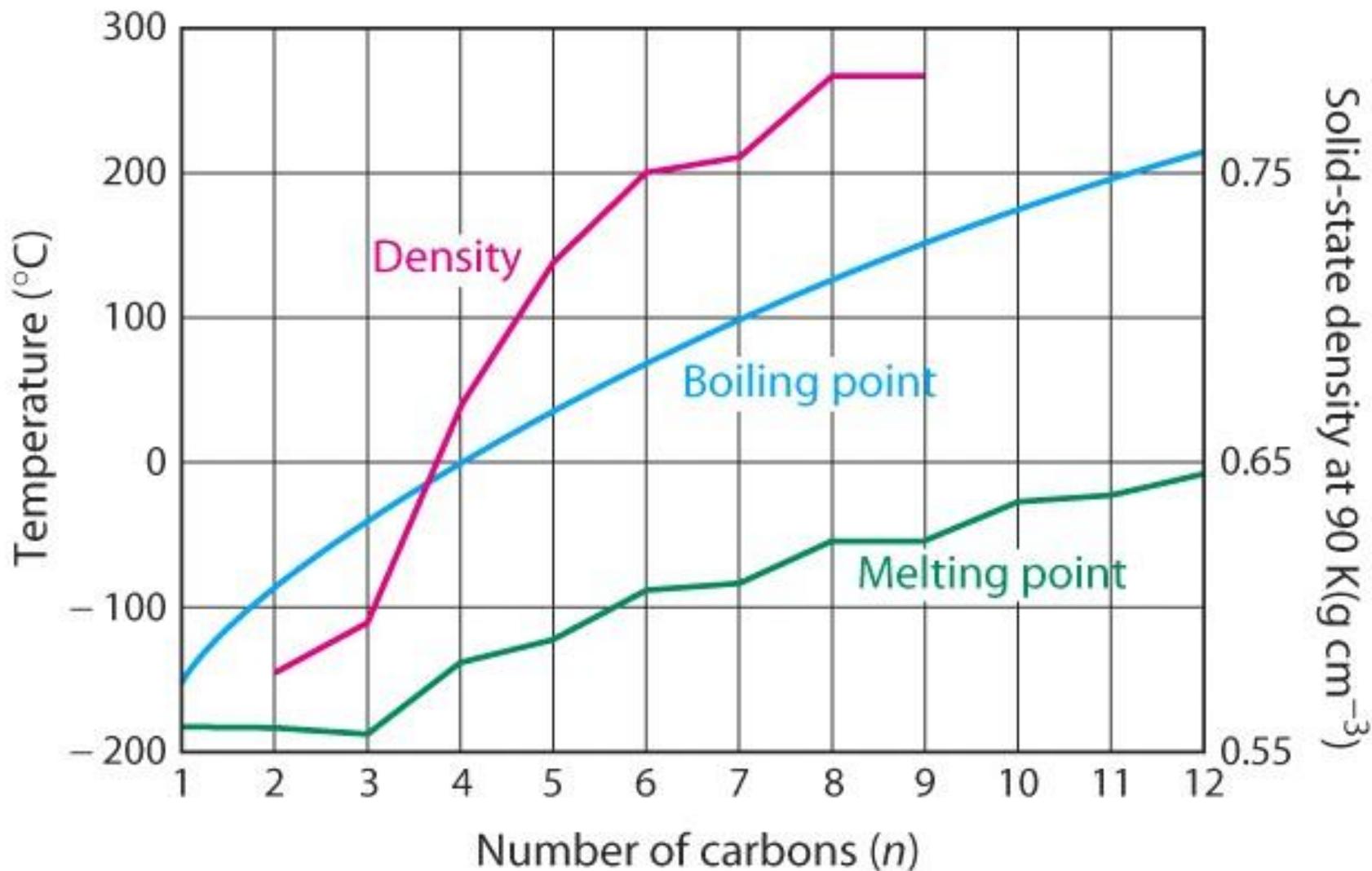
TABLE 2-5**Names and Physical Properties of Straight-Chain Alkanes, C_nH_{2n+2}**

<i>n</i>	Name	Formula	Boiling point (°C)	Melting point (°C)	Density at 20°C (g ml ⁻¹)
1	Methane	CH ₄	-161.7	-182.5	0.466 (at -164°C)
2	Ethane	CH ₃ CH ₃	-88.6	-183.3	0.572 (at -100°C)
3	Propane	CH ₃ CH ₂ CH ₃	-42.1	-187.7	0.5853 (at -45°C)
4	Butane	CH ₃ CH ₂ CH ₂ CH ₃	-0.5	-138.3	0.5787
5	Pentane	CH ₃ (CH ₂) ₃ CH ₃	36.1	-129.8	0.6262
6	Hexane	CH ₃ (CH ₂) ₄ CH ₃	68.7	-95.3	0.6603
7	Heptane	CH ₃ (CH ₂) ₅ CH ₃	98.4	-90.6	0.6837
8	Octane	CH ₃ (CH ₂) ₆ CH ₃	125.7	-56.8	0.7026
9	Nonane	CH ₃ (CH ₂) ₇ CH ₃	150.8	-53.5	0.7177
10	Decane	CH ₃ (CH ₂) ₈ CH ₃	174.0	-29.7	0.7299

TABLE 2-5**Names and Physical Properties of Straight-Chain Alkanes, C_nH_{2n+2}**

<i>n</i>	Name	Formula	Boiling point (°C)	Melting point (°C)	Density at 20°C (g ml ⁻¹)
11	Undecane	CH ₃ (CH ₂) ₉ CH ₃	195.8	-25.6	0.7402
12	Dodecane	CH ₃ (CH ₂) ₁₀ CH ₃	216.3	-9.6	0.7487
13	Tridecane	CH ₃ (CH ₂) ₁₁ CH ₃	235.4	-5.5	0.7564
14	Tetradecane	CH ₃ (CH ₂) ₁₂ CH ₃	253.7	5.9	0.7628
15	Pentadecane	CH ₃ (CH ₂) ₁₃ CH ₃	270.6	10	0.7685
16	Hexadecane	CH ₃ (CH ₂) ₁₄ CH ₃	287	18.2	0.7733
17	Heptadecane	CH ₃ (CH ₂) ₁₅ CH ₃	301.8	22	0.7780
18	Octadecane	CH ₃ (CH ₂) ₁₆ CH ₃	316.1	28.2	0.7768
19	Nonadecane	CH ₃ (CH ₂) ₁₇ CH ₃	329.7	32.1	0.7855
20	Icosane	CH ₃ (CH ₂) ₁₈ CH ₃	343	36.8	0.7886

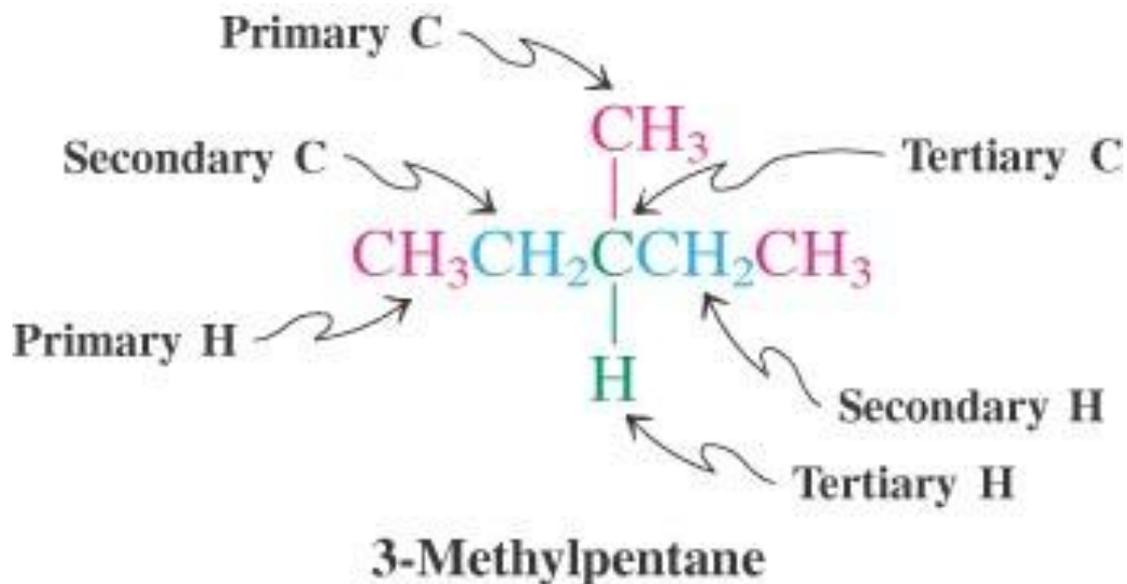
The physical constants of alkanes follow predictable trends:



Alkylová skupina (alkyl) je vytvořena formálním odstraněním vodíku z alkanu. Je pojmenována jako alkyl (přípona -yl).

CH_3 - **methyl**; CH_3CH_2 - **ethyl**; $\text{CH}_3\text{CH}_2\text{CH}_2$ - **propyl**

Doplňující předpony jsou : **sec-** (nebo **s-**) pro sekundární a **tert-** (nebo **t-**) pro terciární. Sekundární uhlík je připojen k dalším dvěma uhlíkům, zatímco terciární ke třem uhlíkům a kvartérní ke čtyřem uhlíkům.



Vybrané rozvětvené alkyly:

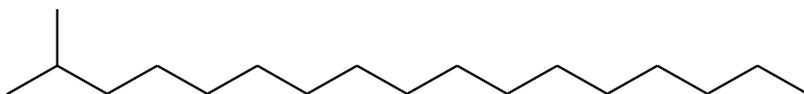
TABLE 2-6
Branched Alkyl Groups

Structure	Common name	Example of common name in use	Systematic name	Type of group
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \\ \\ \text{H} \end{array}$	Isopropyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{Cl} \text{ (Isopropyl chloride)} \\ \\ \text{H} \end{array}$	1-Methylethyl	Secondary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \\ \\ \text{H} \end{array}$	Isobutyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{CH}_3 \text{ (Isobutane)} \\ \\ \text{H} \end{array}$	2-Methylpropyl	Primary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{CH}_2 - \text{C} - \\ \\ \text{H} \end{array}$	<i>sec</i> -Butyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{CH}_2 - \text{C} - \text{NH}_2 \text{ (} \textit{sec}\text{-Butyl amine)} \\ \\ \text{H} \end{array}$	1-Methylpropyl	Secondary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \\ \\ \text{CH}_3 \end{array}$	<i>tert</i> -Butyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{Br} \text{ (} \textit{tert}\text{-Butyl bromide)} \\ \\ \text{CH}_3 \end{array}$	1,1-Dimethylethyl	Tertiary
$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \\ \\ \text{CH}_3 \end{array}$	Neopentyl	$\begin{array}{c} \text{CH}_3 \\ \\ \text{CH}_3 - \text{C} - \text{CH}_2 - \text{OH} \text{ (Neopentyl alcohol)} \\ \\ \text{CH}_3 \end{array}$	2,2-Dimethylpropyl	Primary

Výskyt alkanů v přírodě a jejich vlastnosti

Ropa je složitá směs organických sloučenin, z nichž větší část je tvořena alkany a cykloalkany. Složení ropy je závislé na místě původu.

Alkany se nacházejí i v přírodě a jsou produkovány některými rostlinami: cykloalkany a heptan tvoří hlavní složku terpenických silic.

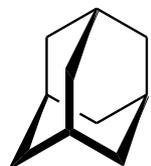


2-methylheptadekan



Grammia parthenice

©Paul A. Opler



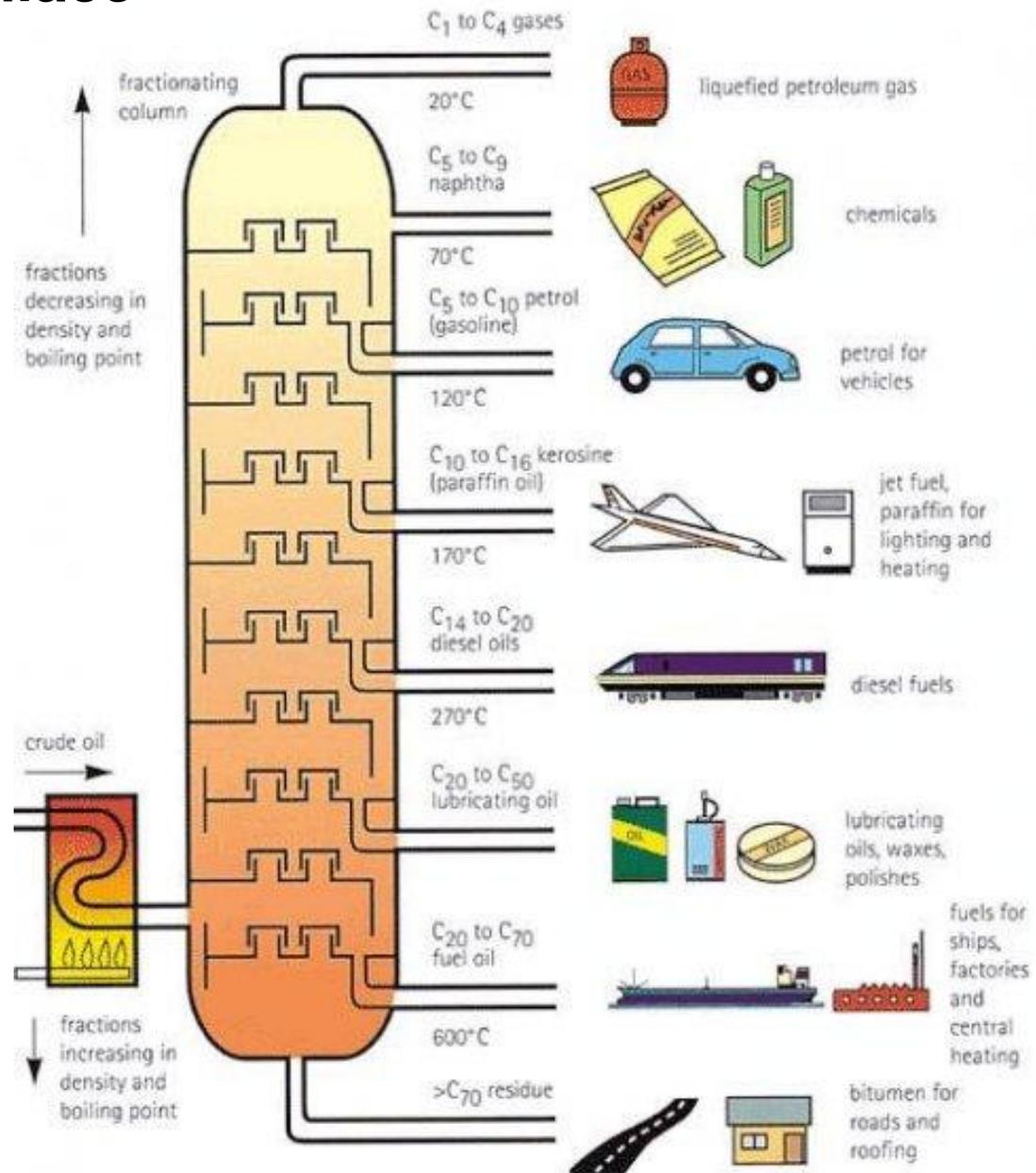
adamantan
tricyklo[3,3,1,1^{3,7}]dekan



diamantan

Izoloval Landa z Hodonínské ropy v roce 1932.

Ropa - destilace



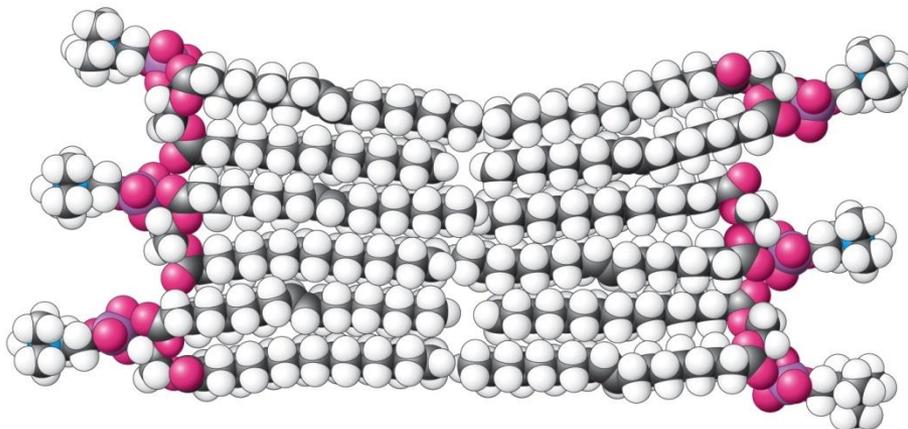
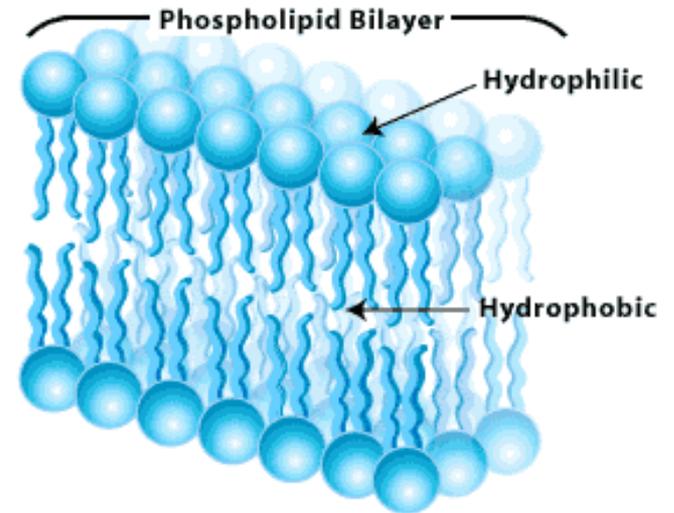
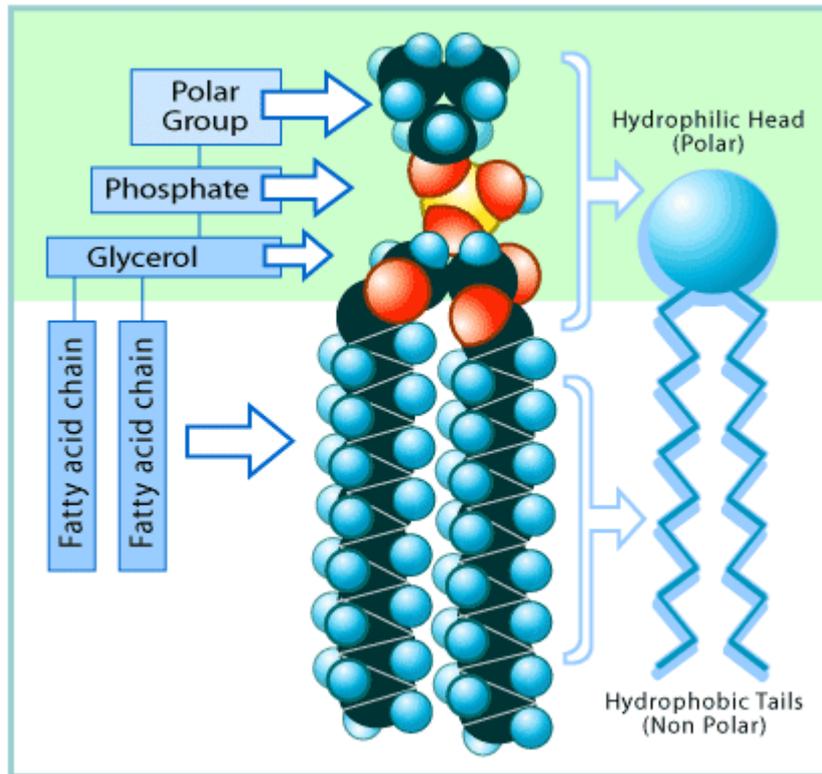
Vosky

Vyšší *n*-alkany jsou součástí nebo výhradní složkou přírodních vosků a tvoří ochrannou vrstvu na rostlinách: $C_{27}H_{56}$ a $C_{29}H_{60}$ (jablka), $C_{29}H_{60}$ (zelí, brokolice) a $C_{31}H_{64}$ (tabákové listy).



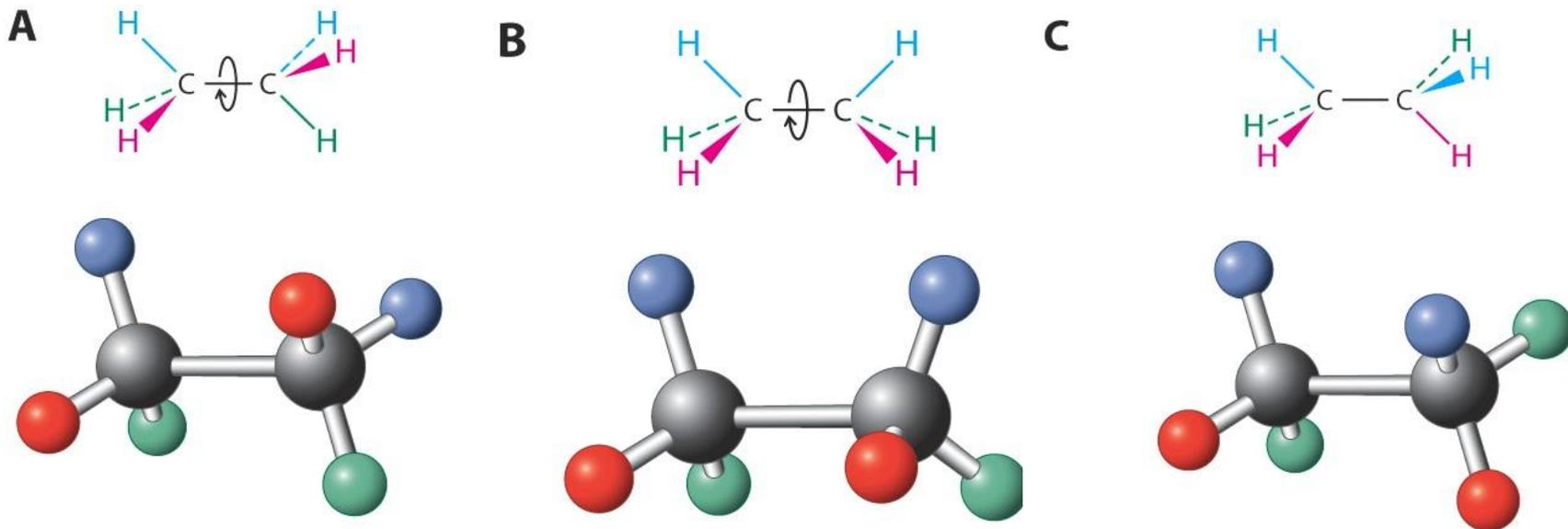


Hydrofobicita alkylových řetězců - membrány

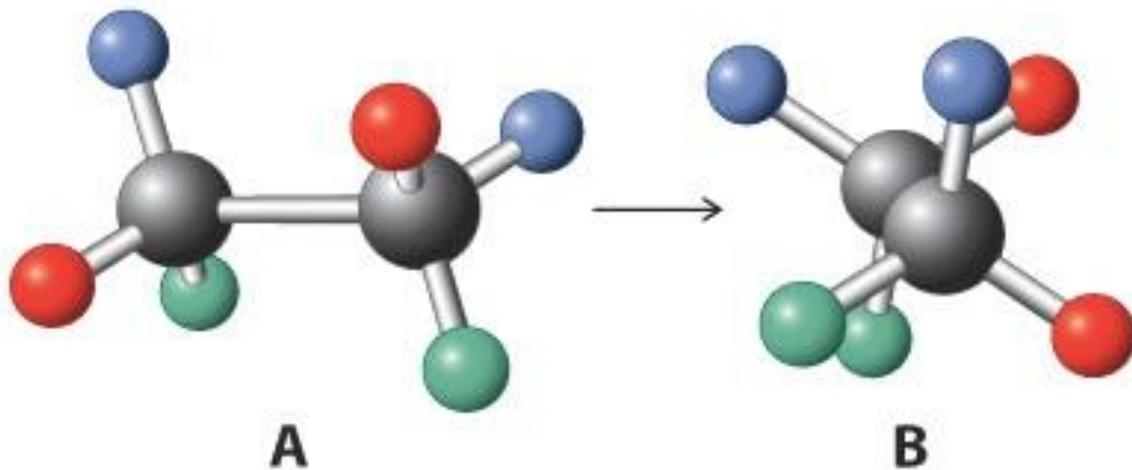
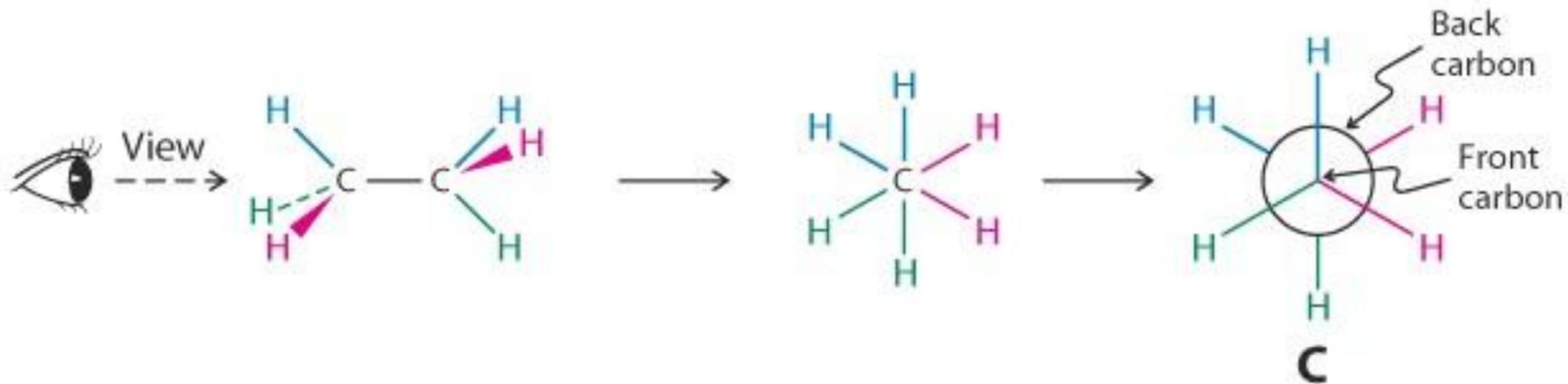


Rotace kolem jednoduché vazby: konformace

Rotační bariera kolem C-C vazby ethanu je 2.9 kcal/mol. Toto relativně nízké množství energie je k dispozici za pokojové teploty v důsledku molekulárních srážek, a proto se uvádí, že kolem C-C vazby ethanu je volná rotace.

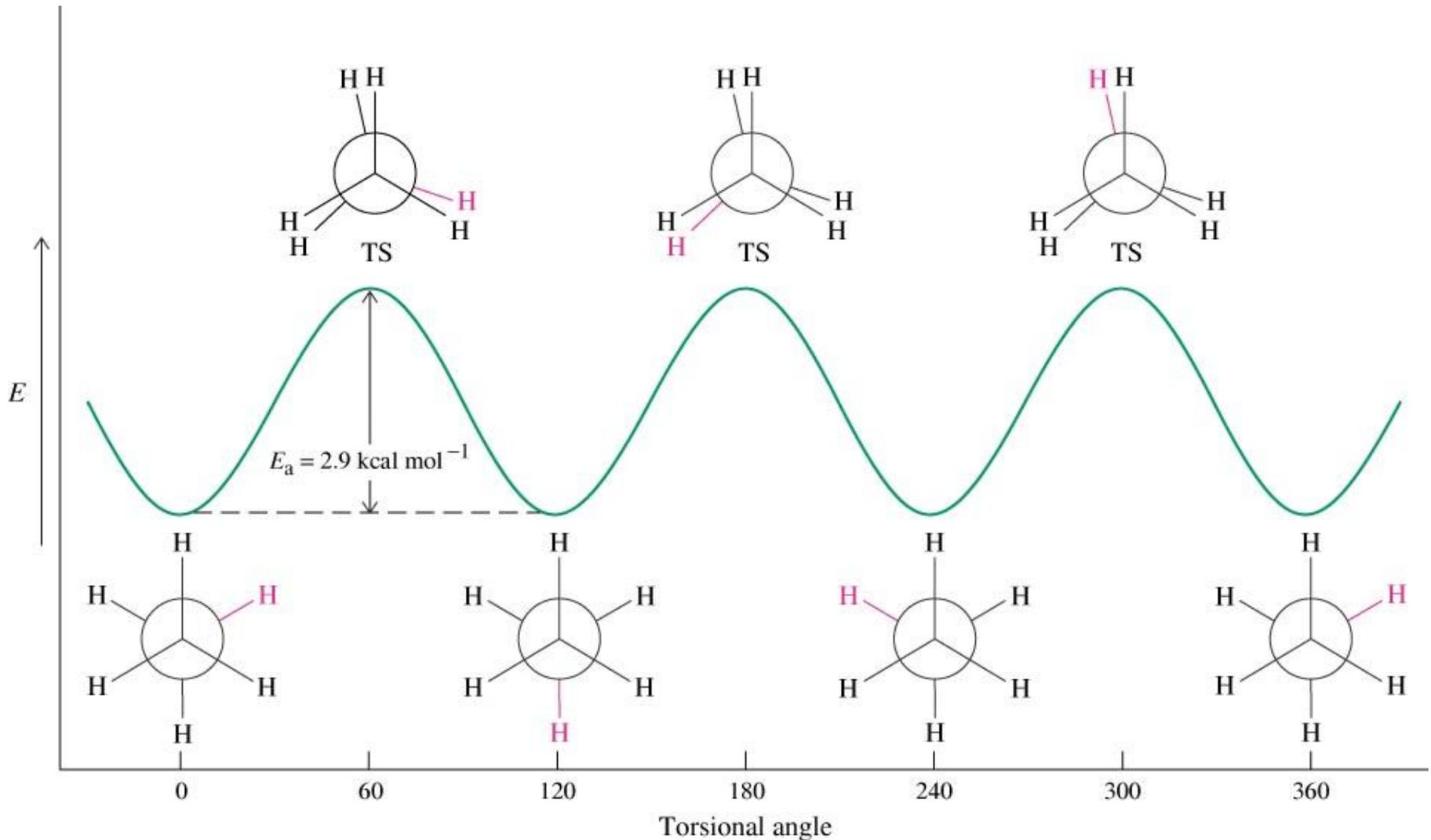


Newmanova projekce konformací ethanu.



Rotamery ethanu mají různou potenciální energii.

Nejnižší energii má střídavá konformace a nejvyšší zákrytová konformace (cca. 2.9 kcal/mole vyšší).

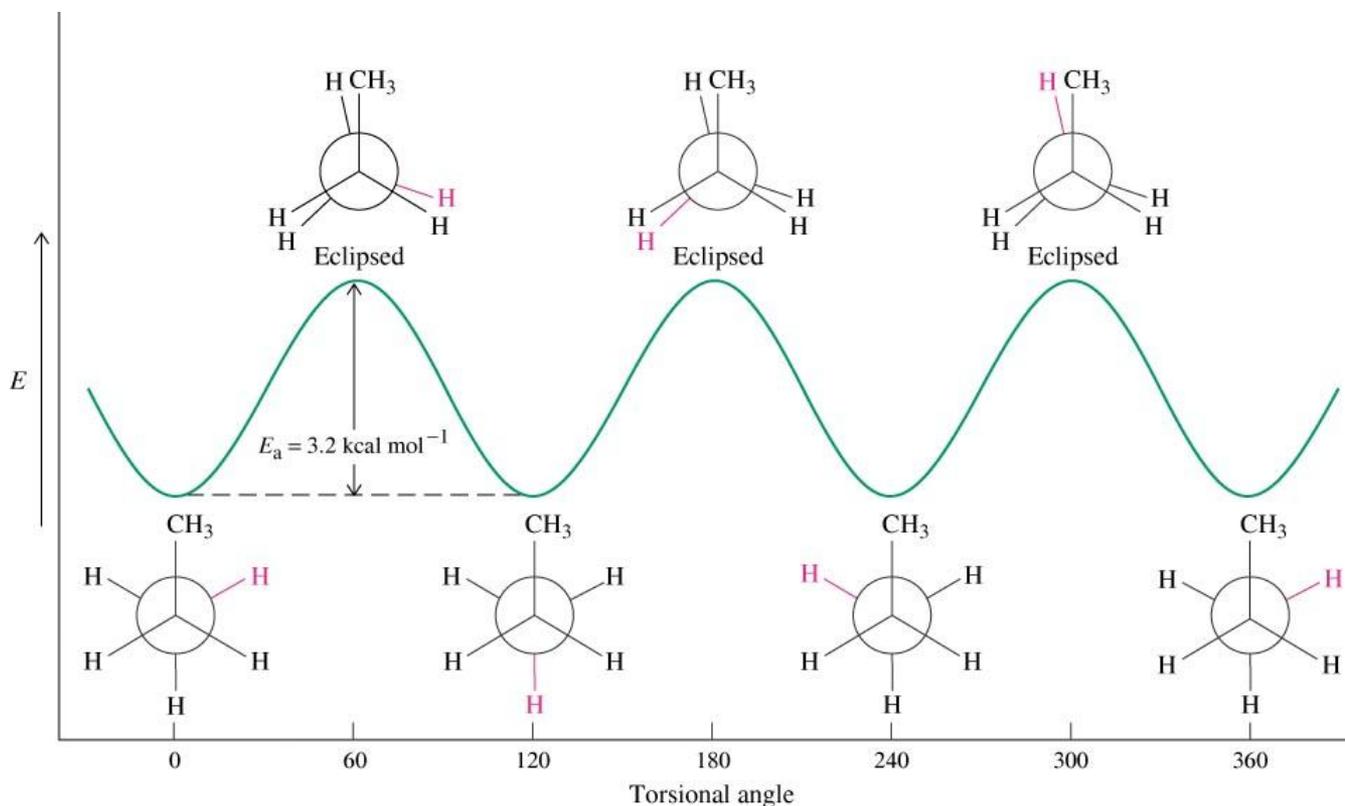


2-8

Rotation in Substituted Ethanes

Steric hindrance raises the energy barrier to rotation.

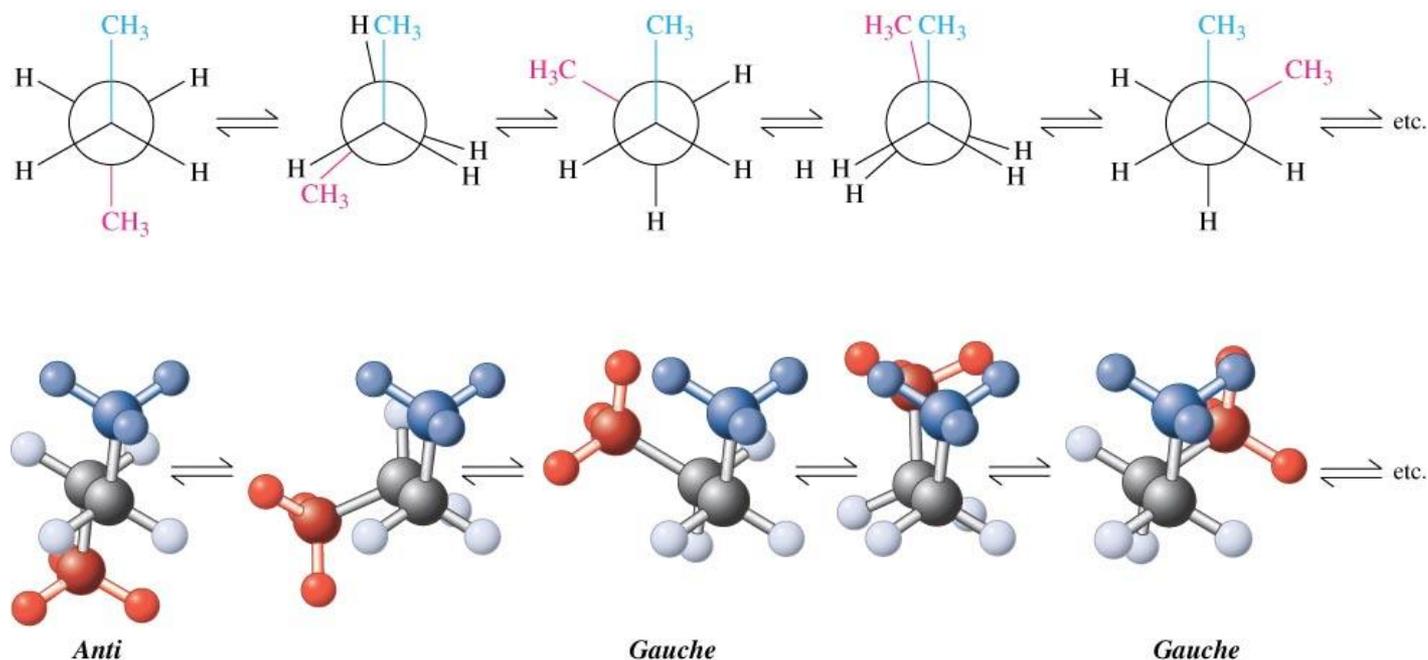
The potential energy diagram for C-C bond rotation in propane shows **steric hindrance**. The energy of the eclipsed conformation is 3.2 kcal/mole above that of the staggered conformation.



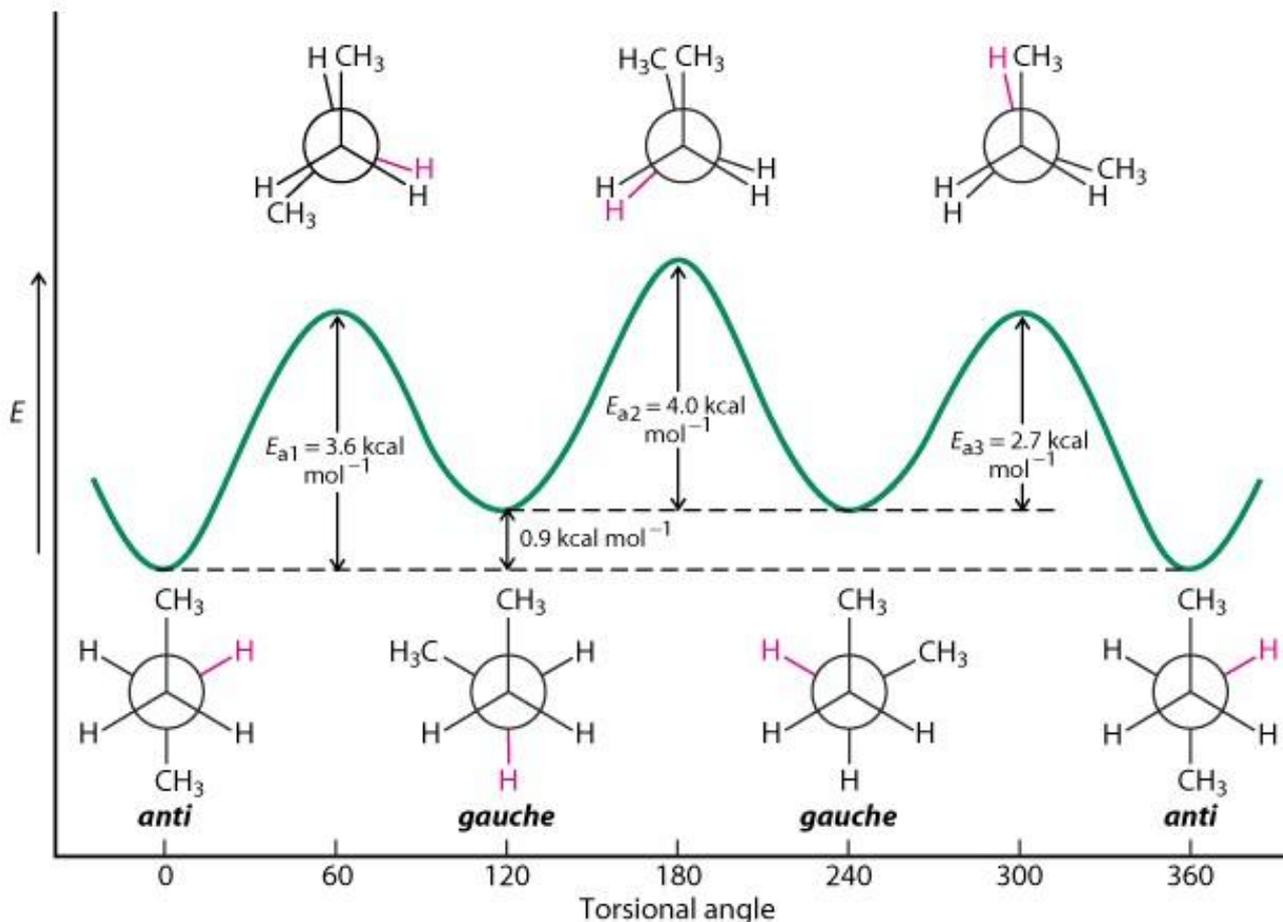
There can be more than one staggered and one eclipsed conformation: conformational analysis of butane.

There are two different types of staggered arrangements in butane. One in which the two terminal methyl groups are 180° apart (Anti), and two in which they are 30° apart (Gauche).

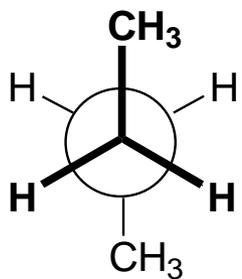
These are connected by two types of eclipsed conformations, one in which the two methyl groups pass each other, and two in which the methyl groups pass by hydrogen atoms:



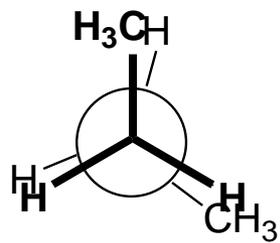
The transition state (eclipsed conformation) energies are 3.6 kcal/mol and 4.0 kcal/mol in butane:



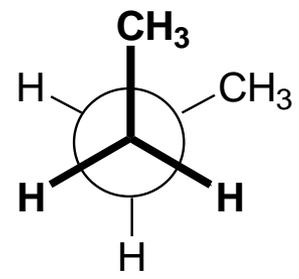
The most stable anti conformation represents about 72% of the conformers present at 25% while the less stable gauche conformation represents about 28% of the conformers present.



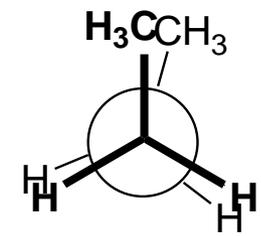
antiperiplanární



antiklinální



synperiplanární



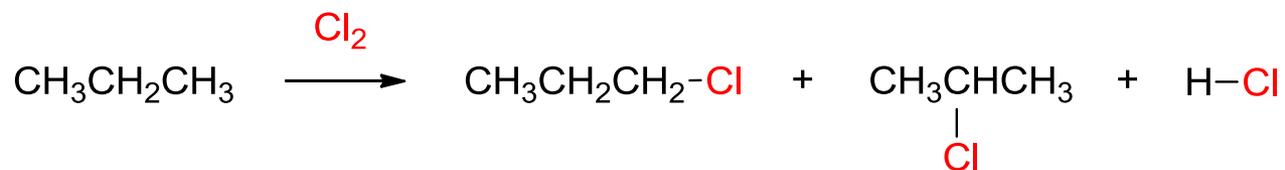
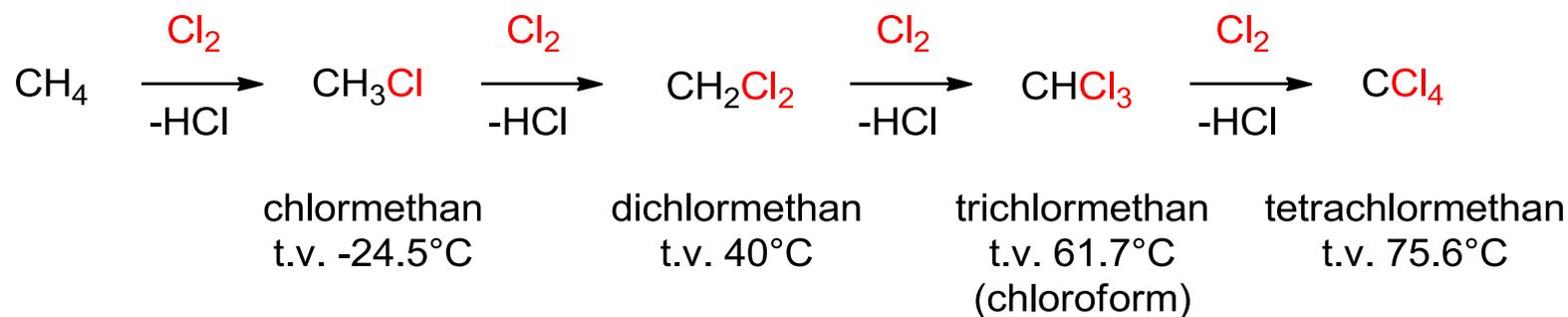
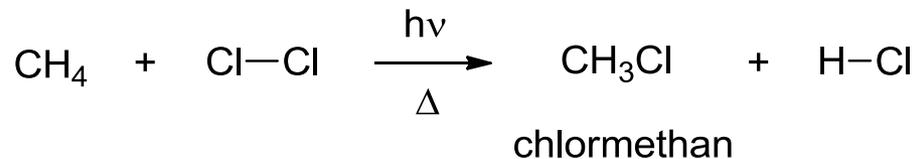
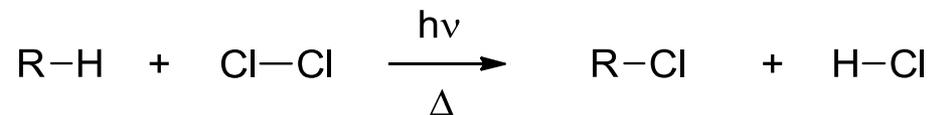
synklinální

3.9. Reakce alkanů

Oxidace (spalování)



Halogenace alkanů

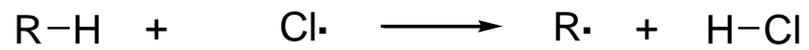


Mechanismus halogenace

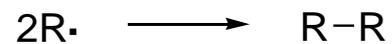
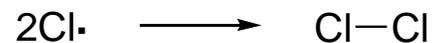
Iniciace



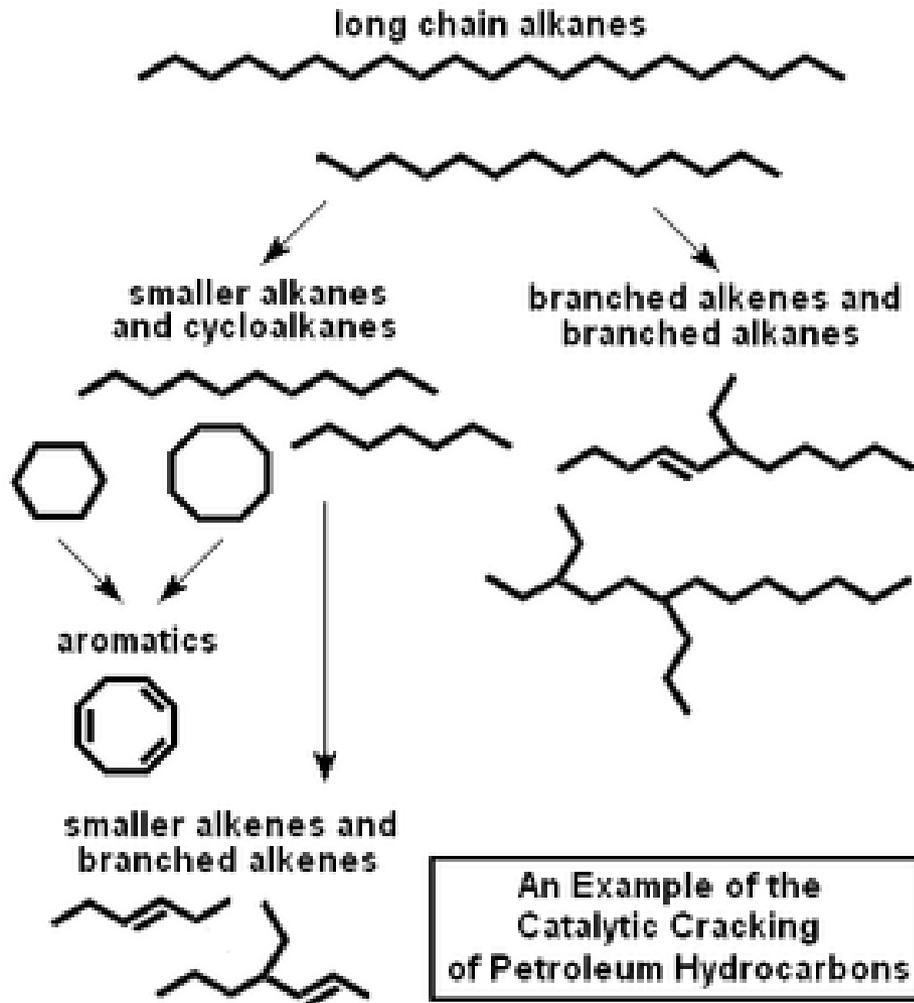
Propagace



Terminace

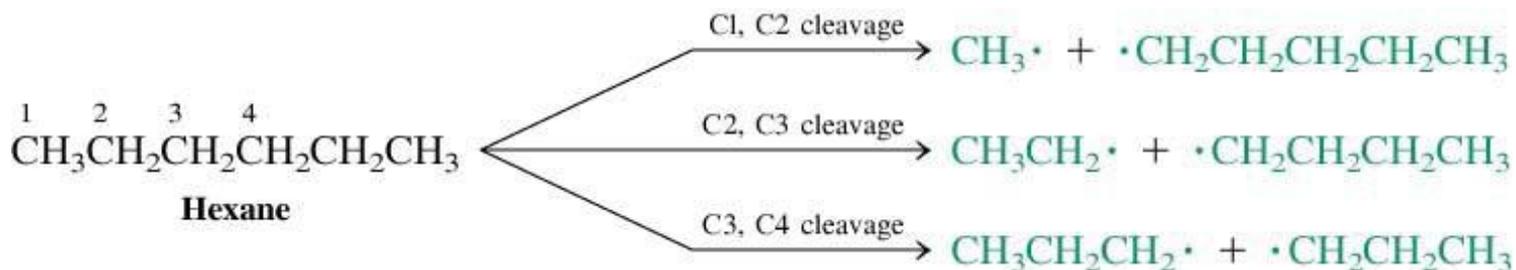


Krakování ropy - výroba benzínu

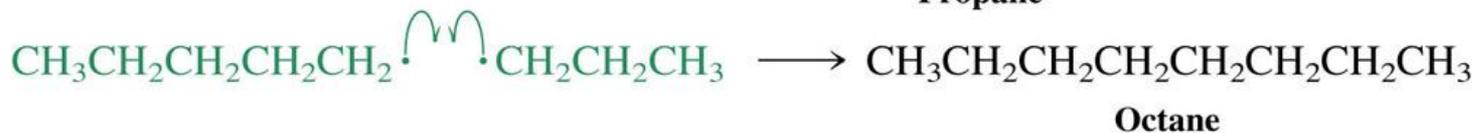
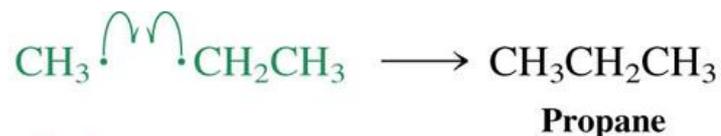


Krakování uhlovodíků – radikálová reakce

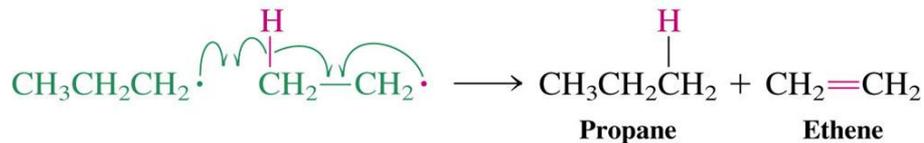
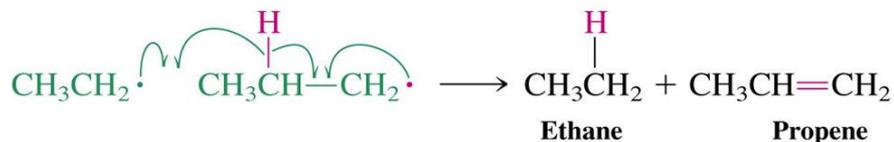
Homolytické štěpení



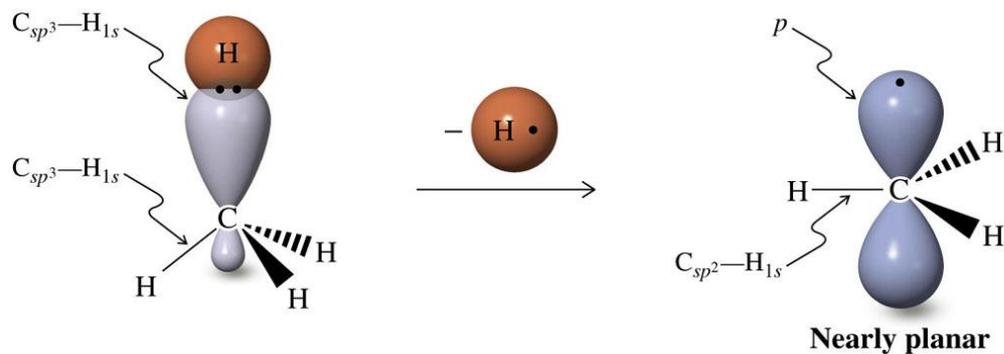
Rekombinace radikálů



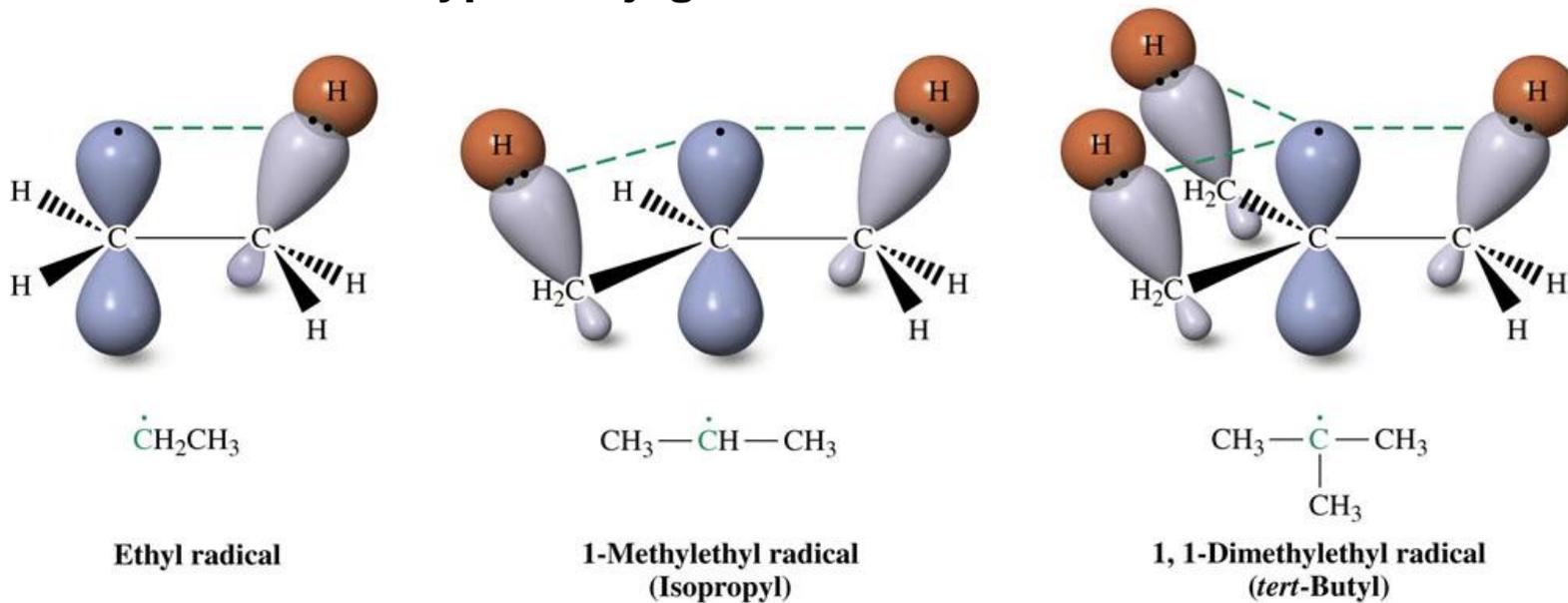
Abstrakce vodíku



Uhlíkové radikály



Hyperkonjugace



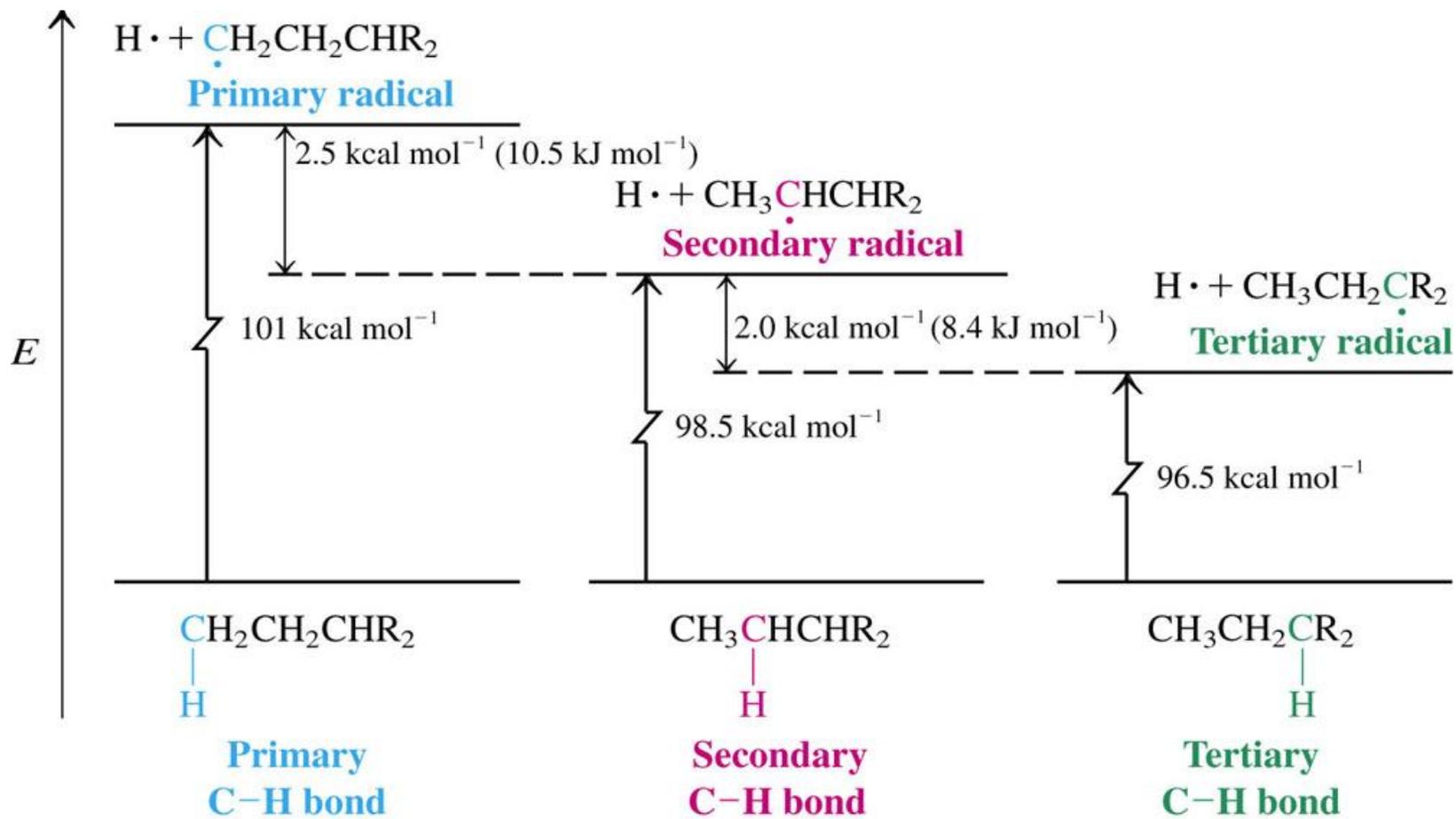


Table 3-2 Bond-Dissociation Energies for Some Alkanes

Compound	DH° [kcal mol ⁻¹ (kJ mol ⁻¹)]		Compound	DH° [kcal mol ⁻¹ (kJ mol ⁻¹)]	
CH ₃ -H	105 (439)	Decreasing DH° ↓	CH ₃ -CH ₃	90 (377)	Decreasing DH° ↓
C ₂ H ₅ -H	101 (423)		C ₂ H ₅ -CH ₃	89 (372)	
C ₃ H ₇ -H	101 (423)		C ₂ H ₅ -C ₂ H ₅	88 (368)	
(CH ₃) ₂ CHCH ₂ -H	101 (423)		(CH ₃) ₂ CH-CH ₃	88 (368)	
(CH ₃) ₂ CH-H	98.5 (412)		(CH ₃) ₃ C-CH ₃	87 (364)	
(CH ₃) ₃ C-H	96.5 (404)		(CH ₃) ₂ CH-CH(CH ₃) ₂	85.5 (358)	
			(CH ₃) ₃ C-C(CH ₃) ₃	78.5 (328)	

Note: See footnote for Table 3-1.

Halogenace vyšších uhovodíků

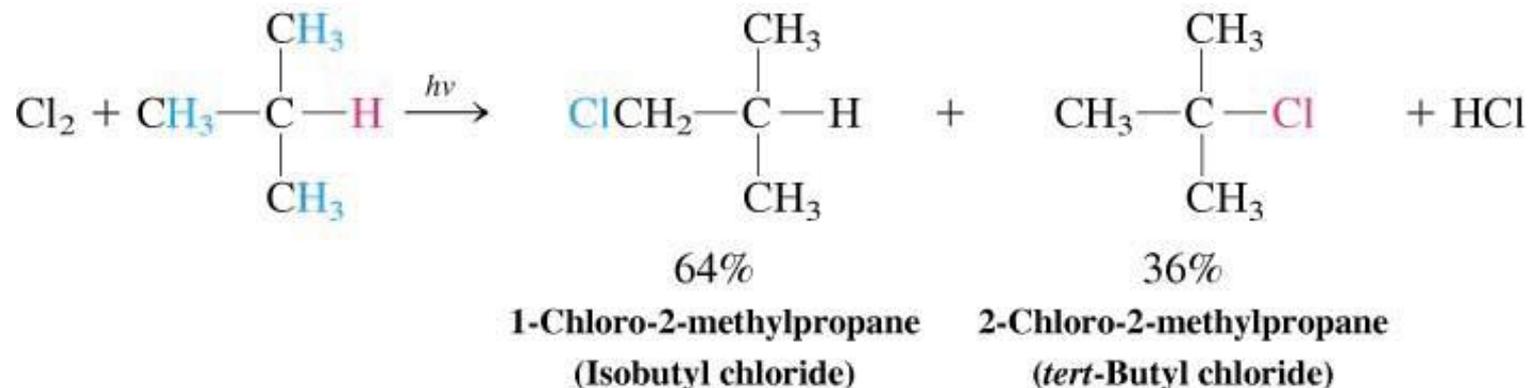
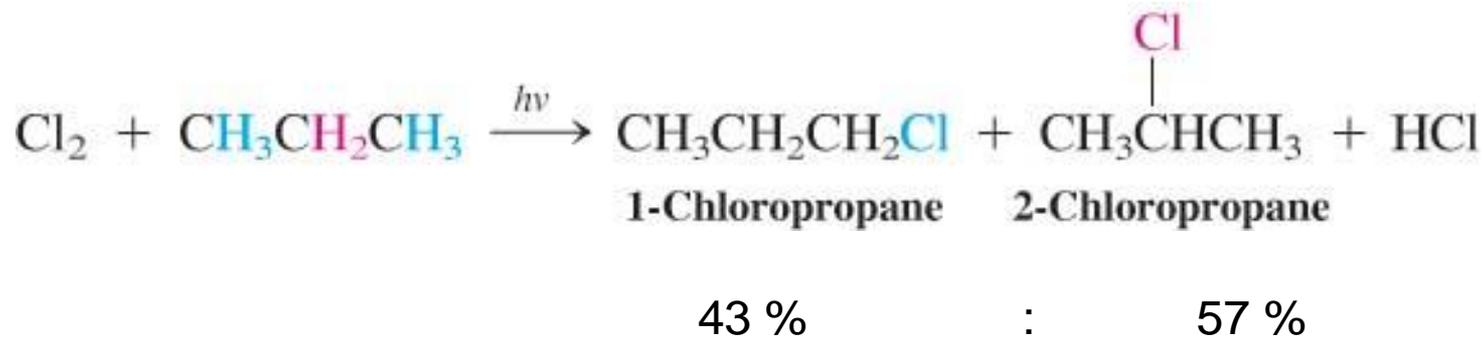
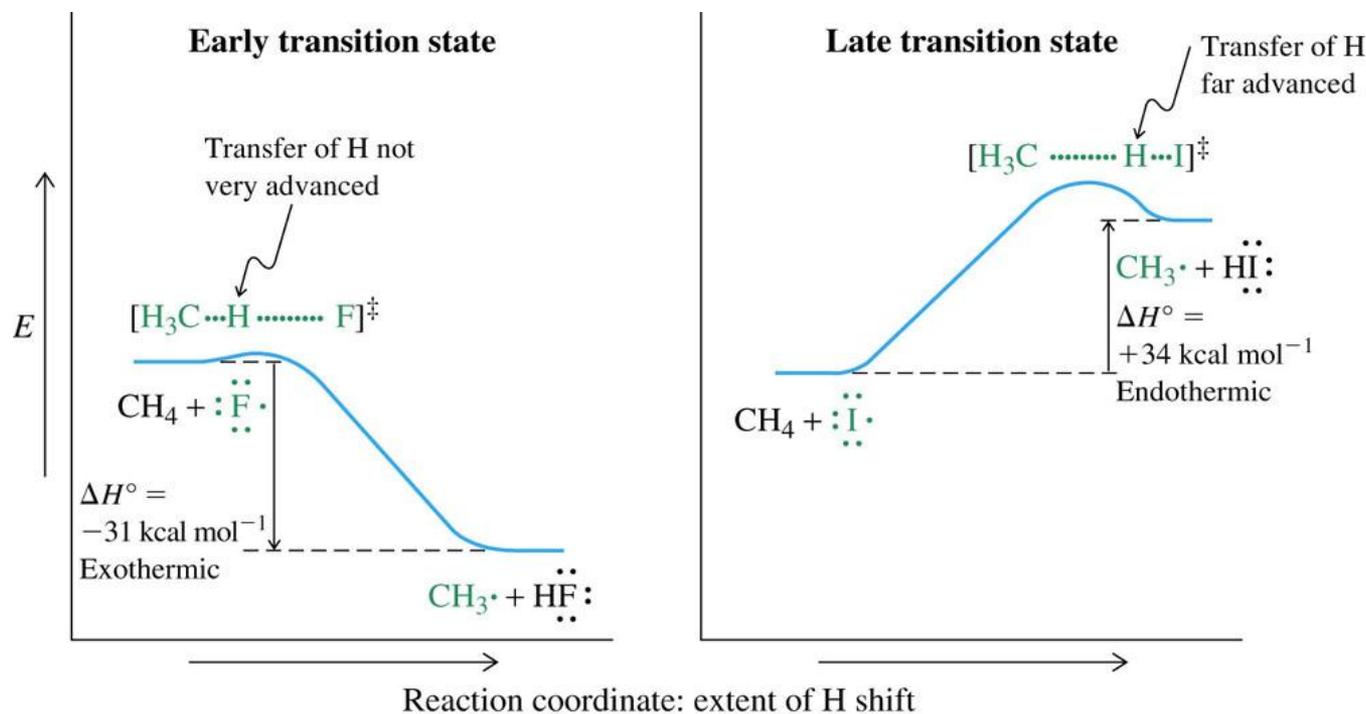
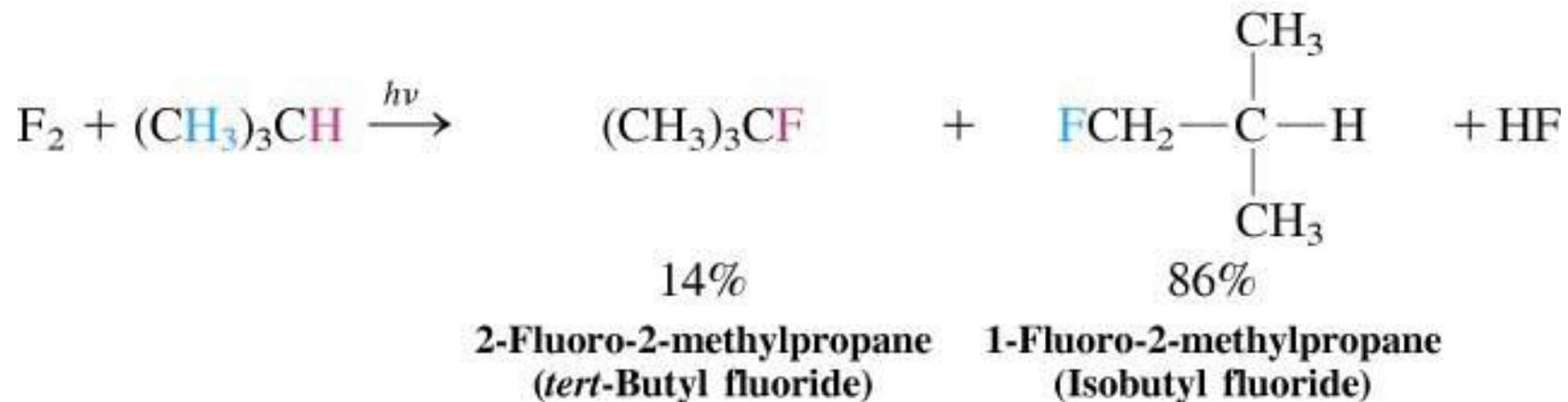


Table 3-5 Enthalpies of the Propagation Steps in the Halogenation of Methane [kcal mol⁻¹ (kJ mol⁻¹)]

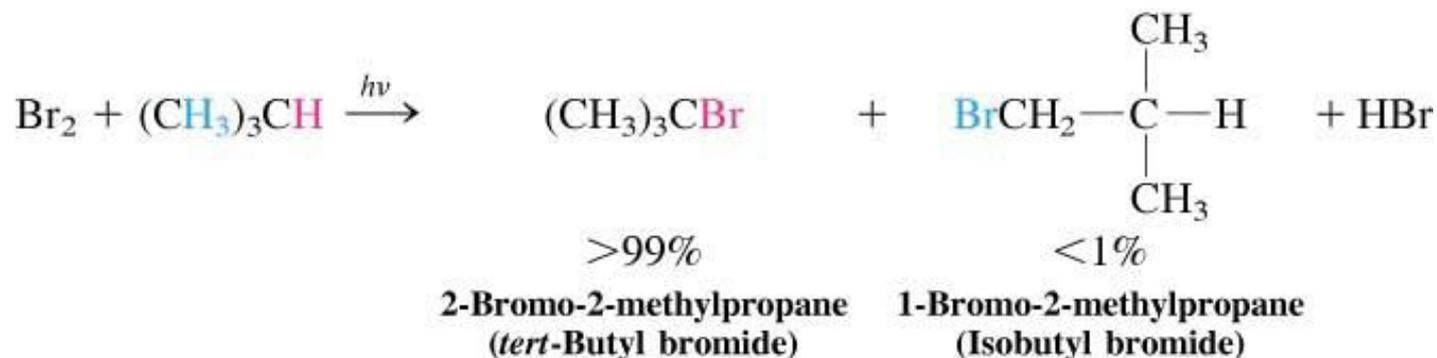
Reaction	F	Cl	Br	I
$\ddot{\text{X}}\cdot + \text{CH}_4 \longrightarrow \cdot\text{CH}_3 + \text{H}\ddot{\text{X}}:$	-31 (-130)	+2 (+8)	+18 (+75)	+34 (+142)
$\cdot\text{CH}_3 + \text{X}_2 \longrightarrow \text{CH}_3\ddot{\text{X}}: + \ddot{\text{X}}\cdot$	-72 (-301)	-27 (-113)	-24 (-100)	-21 (-88)
$\text{CH}_4 + \text{X}_2 \longrightarrow \text{CH}_3\ddot{\text{X}}: + \text{H}\ddot{\text{X}}:$	-103 (-431)	-25 (-105)	-6 (-25)	+13 (+54)



Fluorace 2-methylpropanu



Bromination of 2-Methylpropane



Cykloalkany



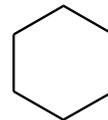
cyklopropan
t.v. -37.7°C



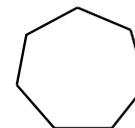
cyklobutan
t.v. 12°C



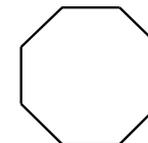
cyklopentan
t.v. 49.3°C



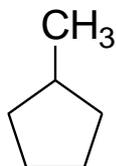
cyklohexan
t.v. 80.7°C



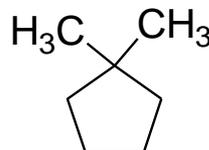
cykloheptan
t.v. 118.5°C



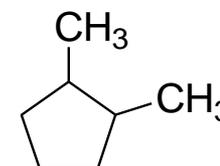
cyklooctan
t.v. 149°C



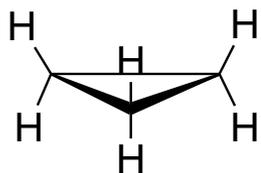
methylcyklopentan



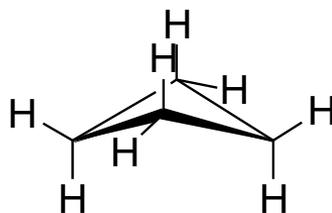
1,1-dimethylcyklopentan



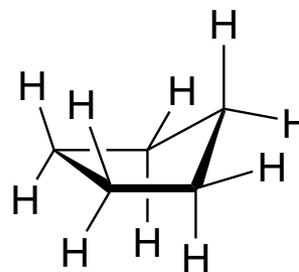
1,2-dimethylcyklopentan



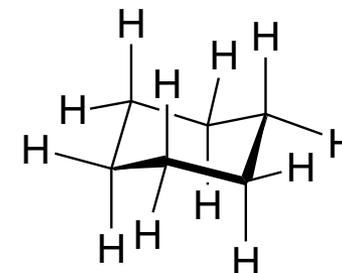
cyklopropan



cyklobutan



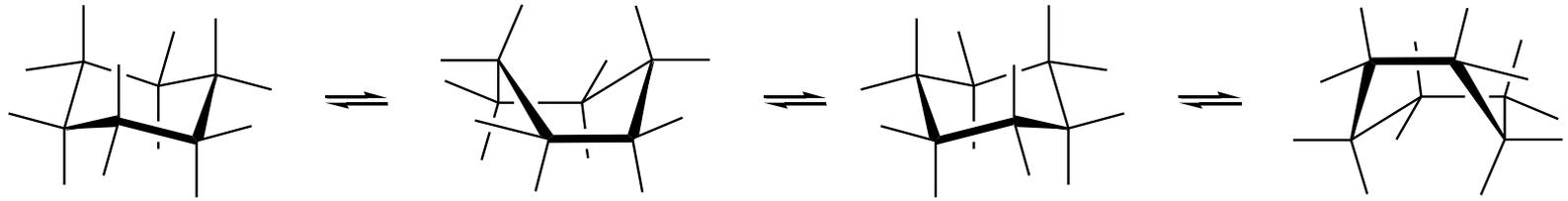
cyklopentan



cyklohexan

Počet atomů uhlíku kruhu n	ΔH (kJ·mol ⁻¹)	$\Delta H/n$ (kJ·mol ⁻¹)	$\Delta H - n \times 659$ (kJ·mol ⁻¹)
1 ^a	659	659	
2 ^b	1411	705	92
3	2093	697	115
4	2747	686	111
5	3322	664	27
6	3954	659	0
7	4639	662	26
8	5312	664	40

^a (hodnota získaná ze spalných tepel alkanů. ^b Pro ethen jako nejmenší kruh.

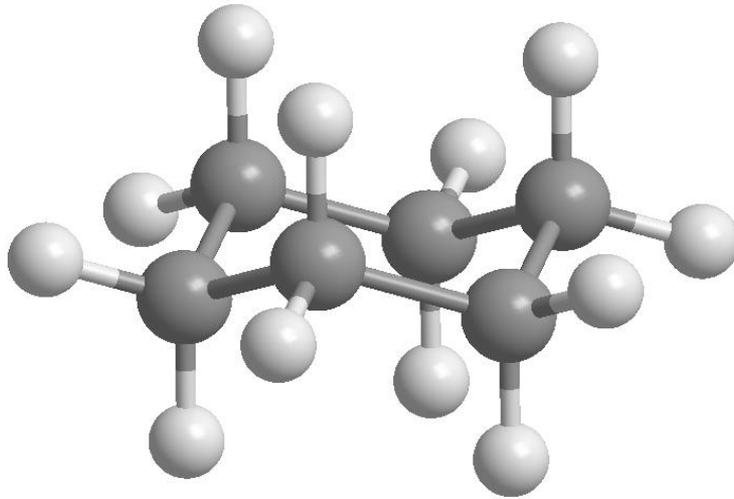


židličková konformace

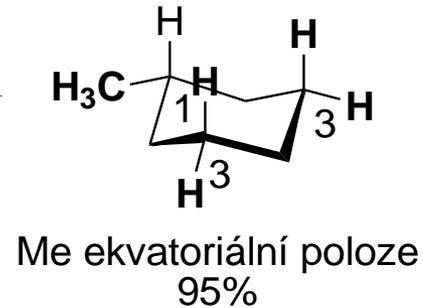
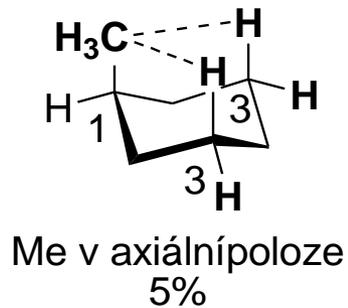
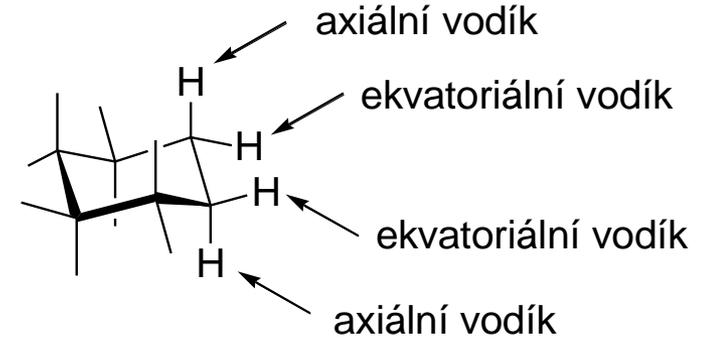
vaničková konformace

židličková konformace

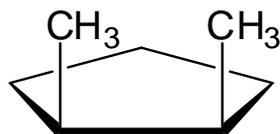
vaničková konformace



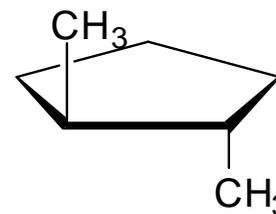
židličková konformace



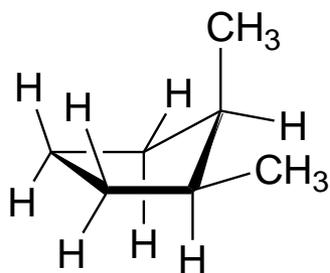
3.8. Cis a trans izomerie u cykloalkanů



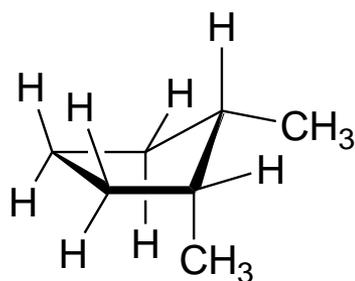
cis-1,2-dimethylcyklopentan
t.v. 99°C



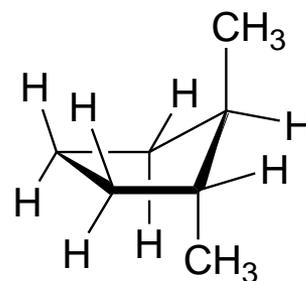
trans-1,2-dimethylcyklopentan
t.v. 92°C



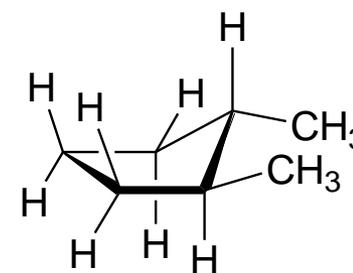
e,a



a,e

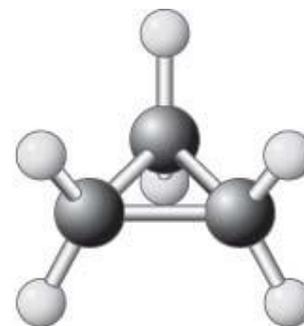


a,a

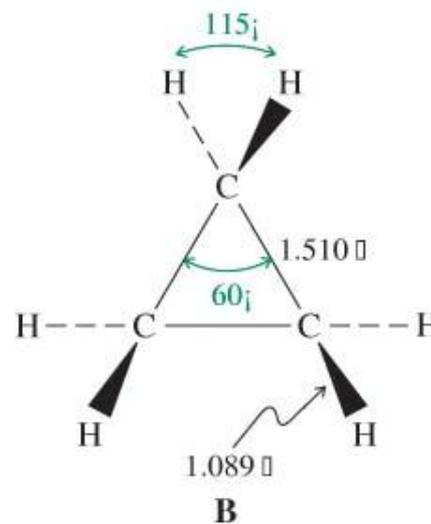


e,e

stabilnější

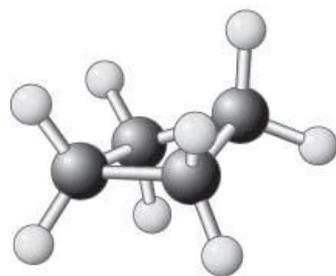


A

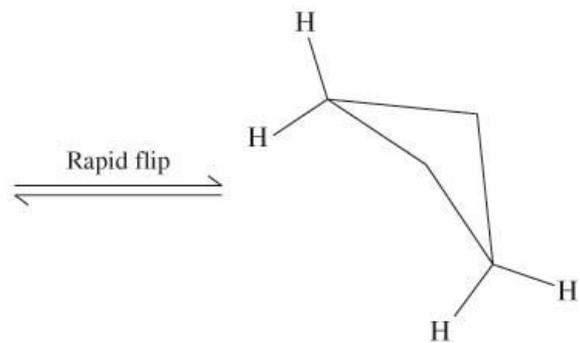
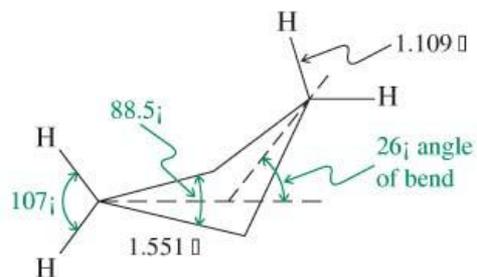


B

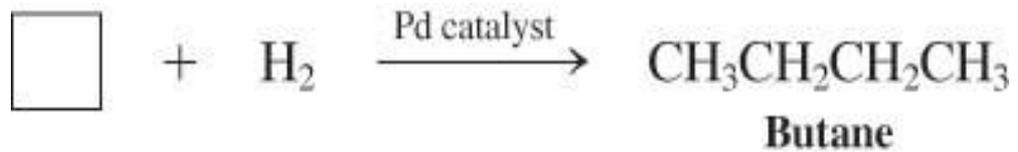


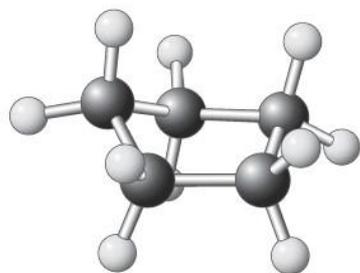


A

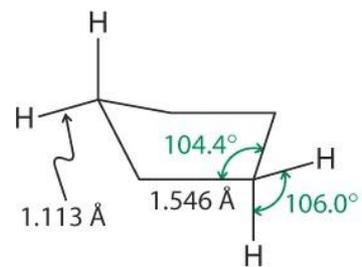


B

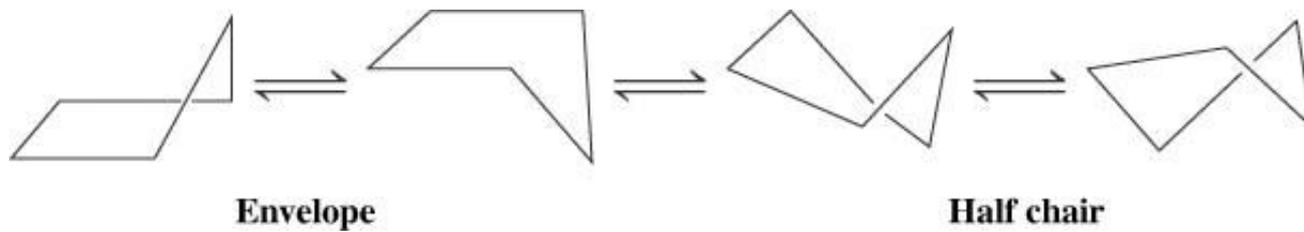


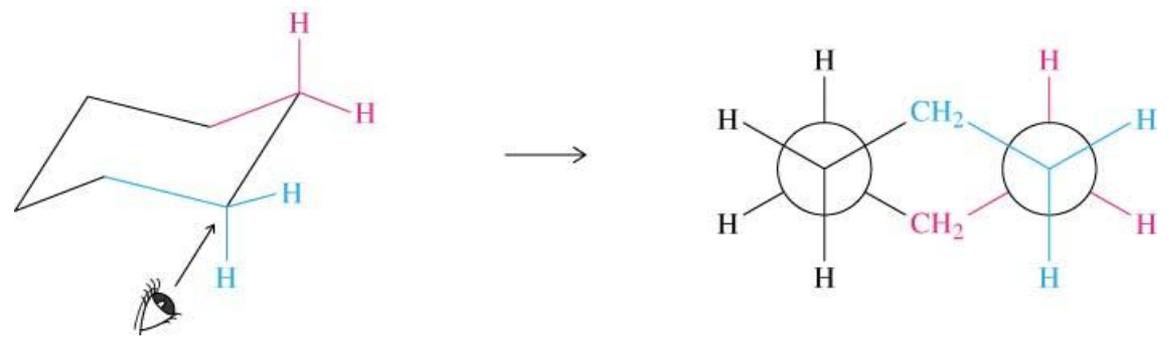
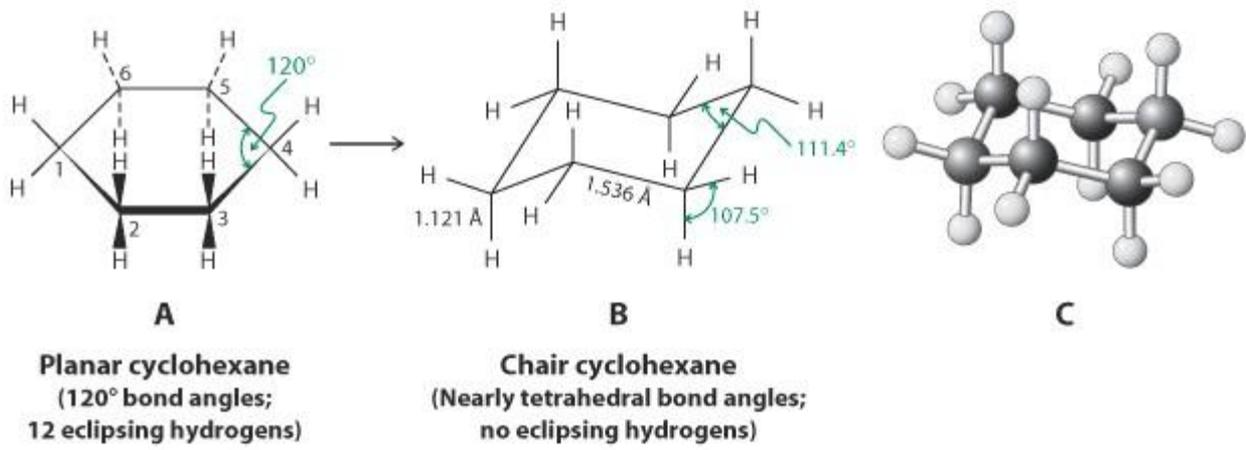


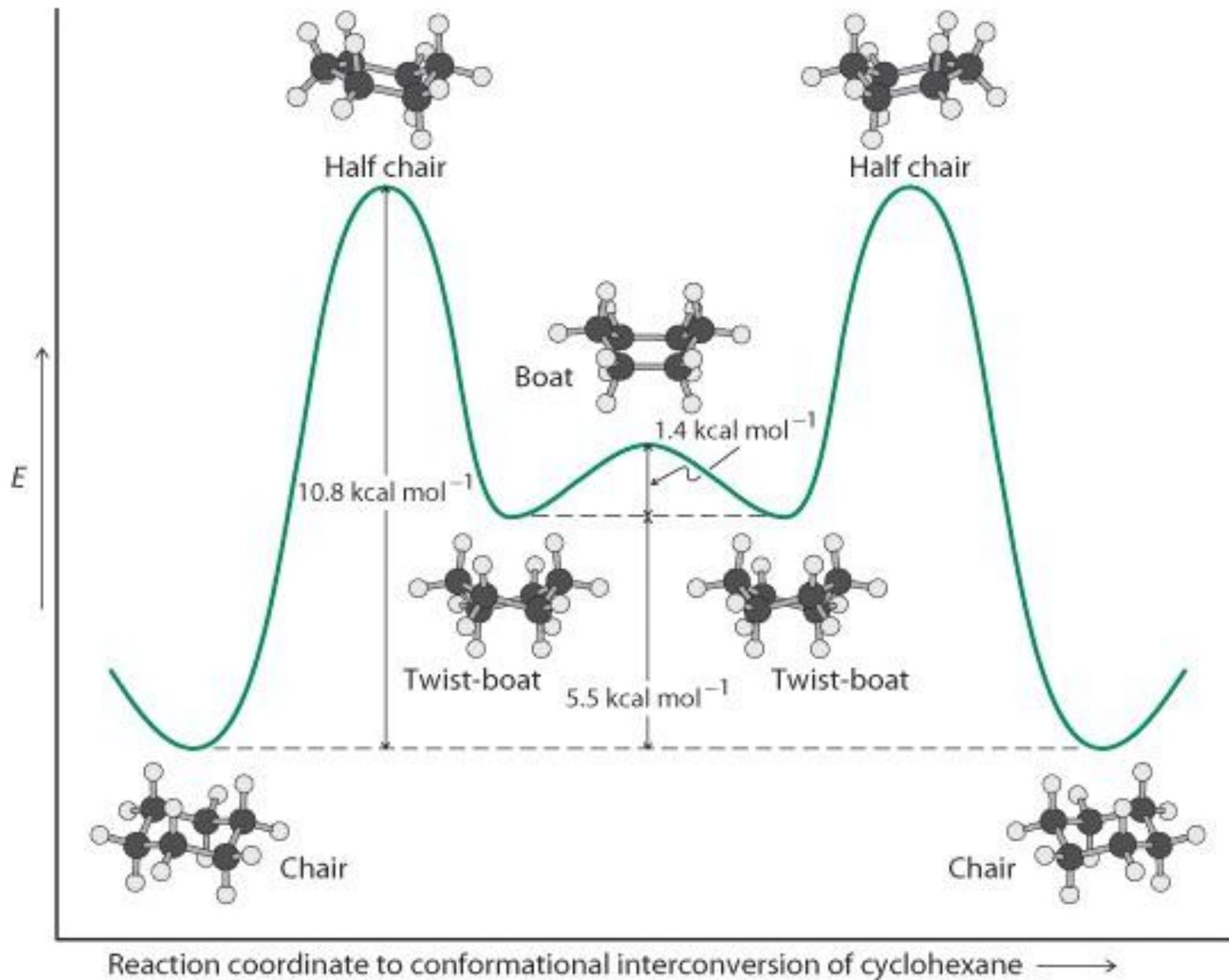
A

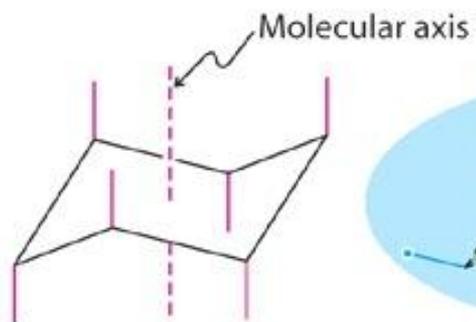


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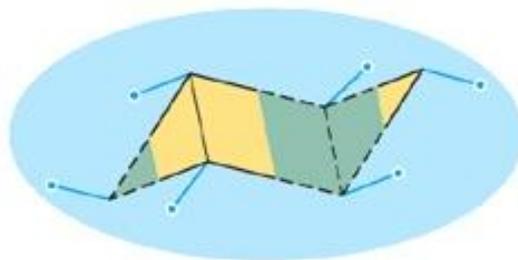




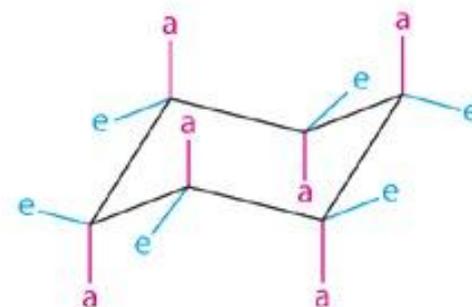




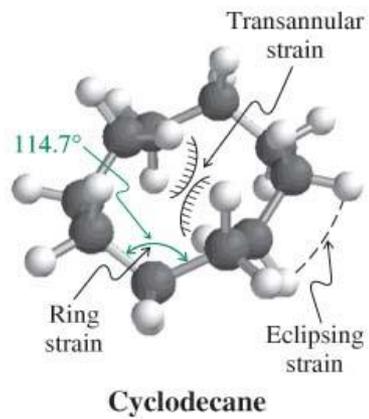
Axial
positions



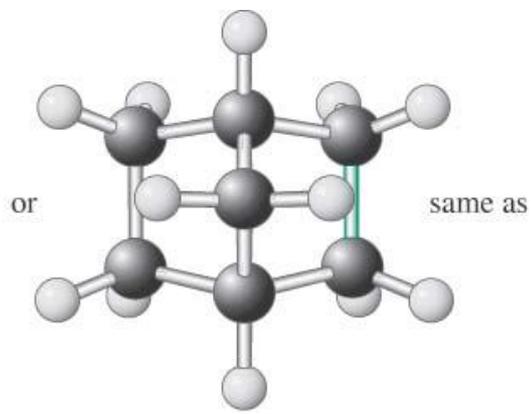
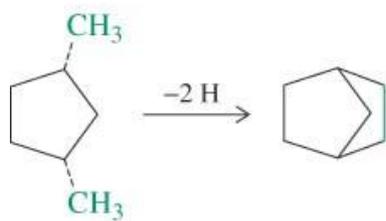
Equatorial
positions



Axial (a) and equatorial (e)
positions

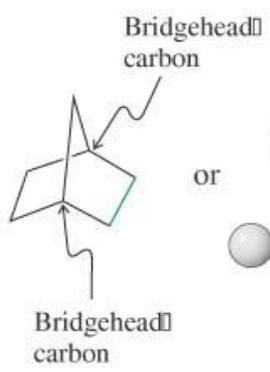


Strain energy of 14 kcal mol^{-1} .

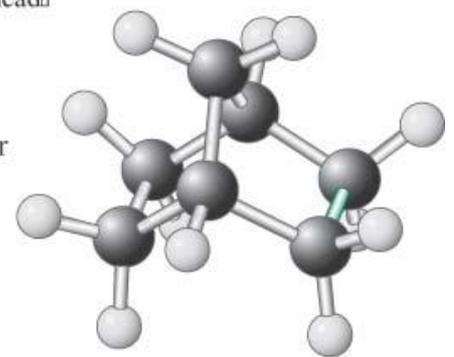


or

same as

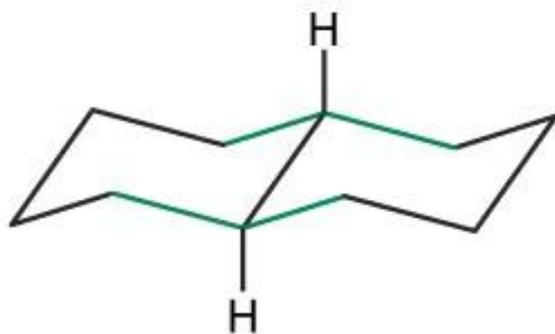
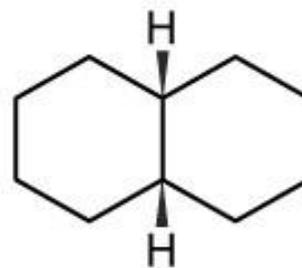
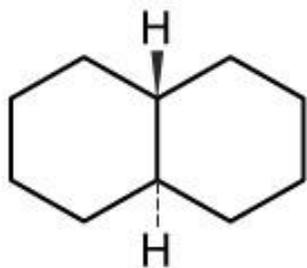


or



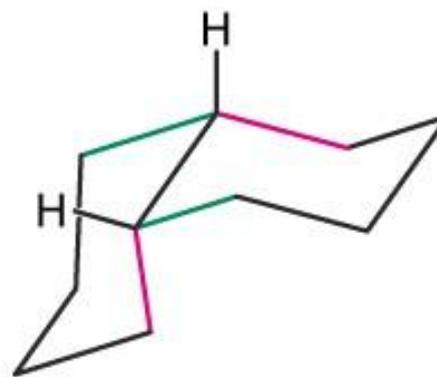
Norbornane

Norbornane



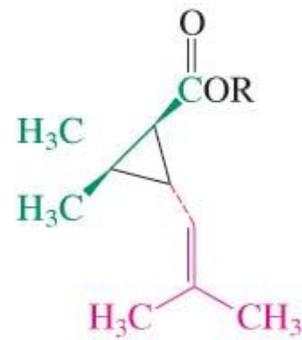
Equatorial C-C bonds

trans-Decalin

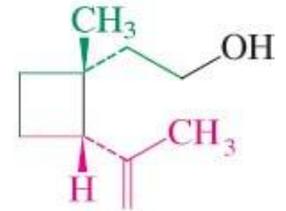


Axial C-C bonds Equatorial C-C bonds

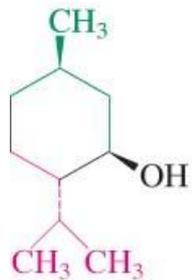
cis-Decalin



trans-Chrysanthemic acid (R = H)
trans-Chrysanthemic esters (R ≠ H)



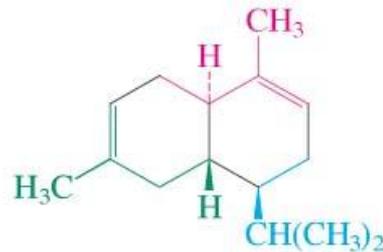
Grandisol



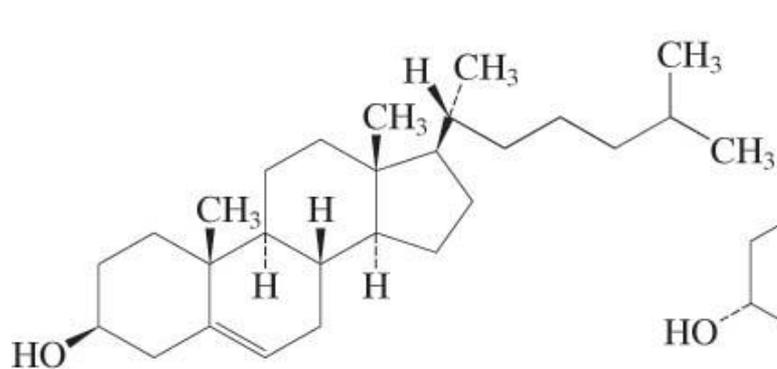
Menthol



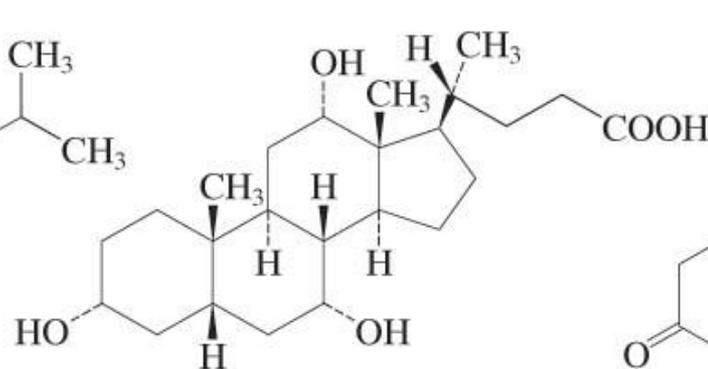
Camphor



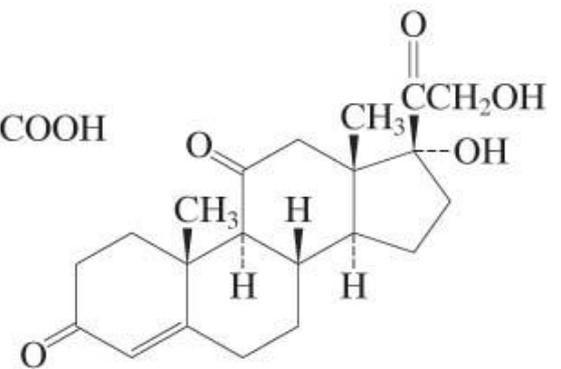
β -Cadinene



Cholesterol



Cholic acid



Cortisone