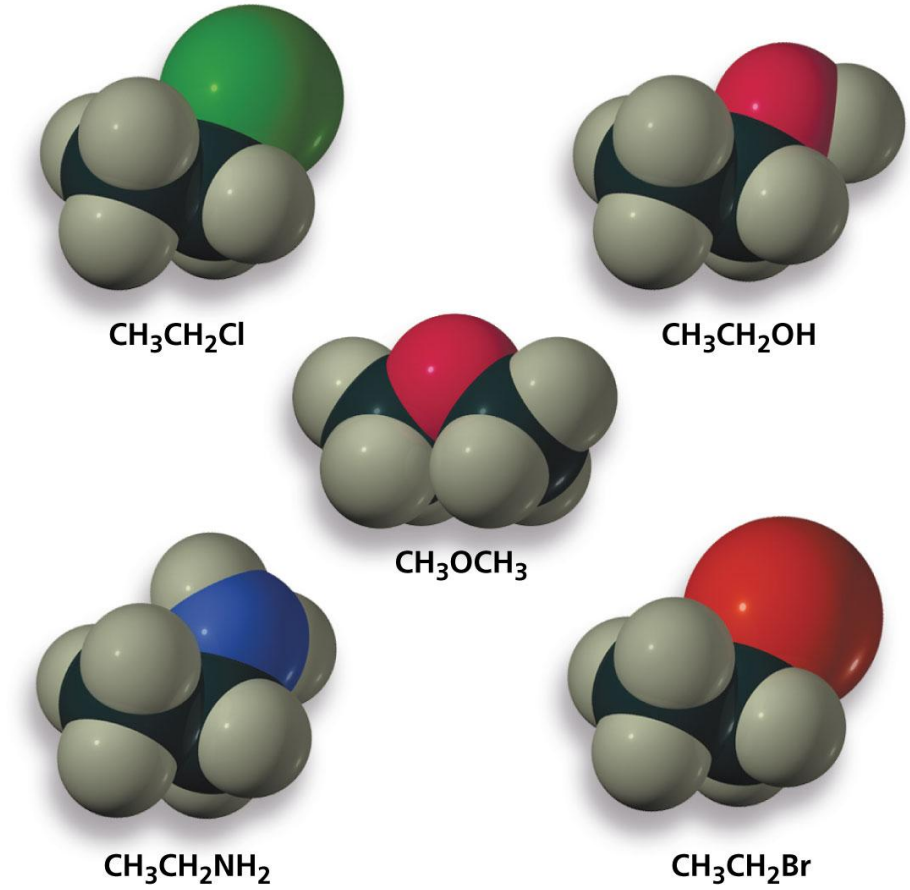
Organic Chemistry
2th Edition
Paula Yurkanis Bruice



Chapter 3

An Introduction to Organic Compounds

Nomenclature, Physical Properties, and Representation of Structure

Alkanes are hydrocarbons containing only single Bonds saturated (no more H's can be added)

General formula: C*n*H2*n*+2

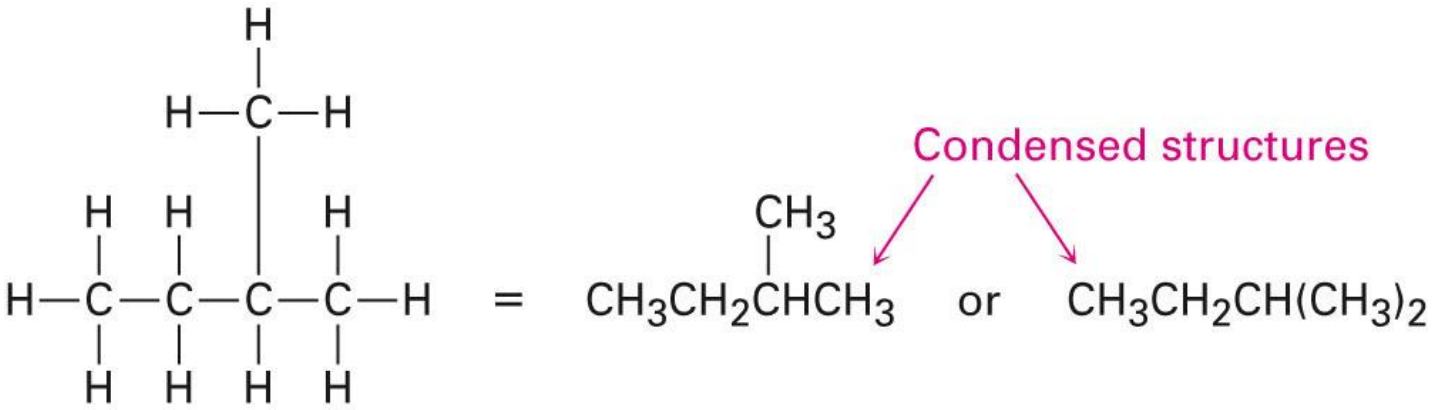
Table 2.1 Nomenclature and Physical Properties of Straight-Chain Alkanes

Number of carbons	Molecular formula	Name	Condensed structure	Boiling point (°C)	Melting point (°C)	Density[a] (g/mL)
1	CH_4	methane	CH_4	−167.7	−182.5	
2	C_2H_6	ethane	CH_3CH_3	−88.6	−183.3	
3	C_3H_8	propane	$CH_3CH_2CH_3$	−42.1	−187.7	
4	C_4H_{10}	butane	$CH_3CH_2CH_2CH_3$	−0.5	−138.3	
5	C_5H_{12}	pentane	$CH_3(CH_2)_3CH_3$	36.1	−129.8	0.5572
6	C_6H_{14}	hexane	$CH_3(CH_2)_4CH_3$	68.7	−95.3	0.6603
7	C_7H_{16}	heptane	$CH_3(CH_2)_5CH_3$	98.4	−90.6	0.6837
8	C_8H_{18}	octane	$CH_3(CH_2)_6CH_3$	125.7	−56.8	0.7026
9	C_9H_{20}	nonane	$CH_3(CH_2)_7CH_3$	150.8	−53.5	0.7177
10	$C_{10}H_{22}$	decane	$CH_3(CH_2)_8CH_3$	174.0	−29.7	0.7299
11	$C_{11}H_{24}$	undecane	$CH_3(CH_2)_9CH_3$	195.8	−25.6	0.7402
12	$C_{12}H_{26}$	dodecane	$CH_3(CH_2)_{10}CH_3$	216.3	−9.6	0.7487
13	$C_{13}H_{28}$	tridecane	$CH_3(CH_2)_{11}CH_3$	235.4	−5.5	0.7546
⋮	⋮	⋮	⋮	⋮	⋮	⋮
20	$C_{20}H_{42}$	eicosane	$CH_3(CH_2)_{18}CH_3$	343.0	36.8	0.7886
21	$C_{21}H_{44}$	heneicosane	$CH_3(CH_2)_{19}CH_3$	356.5	40.5	0.7917
⋮	⋮	⋮	⋮	⋮	⋮	⋮
30	$C_{30}H_{62}$	triacontane	$CH_3(CH_2)_{28}CH_3$	449.7	65.8	0.8097

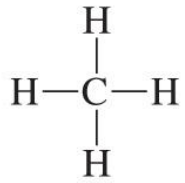
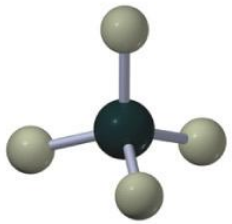
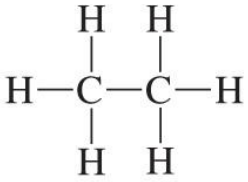
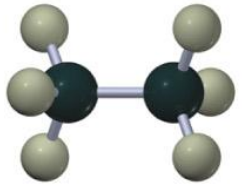
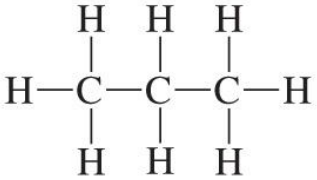
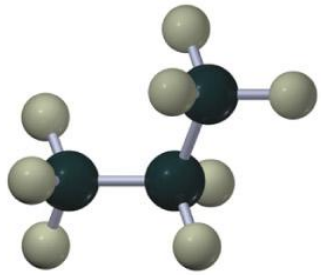
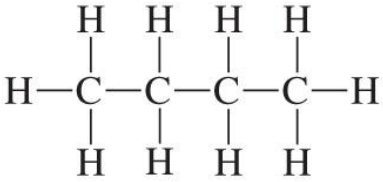
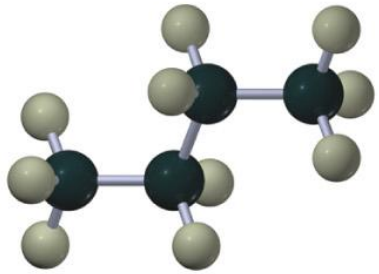
[a]Density is temperature dependent. The densities given are those determined at 20 °C ($d^{20°}$).

Drawing chemical structures

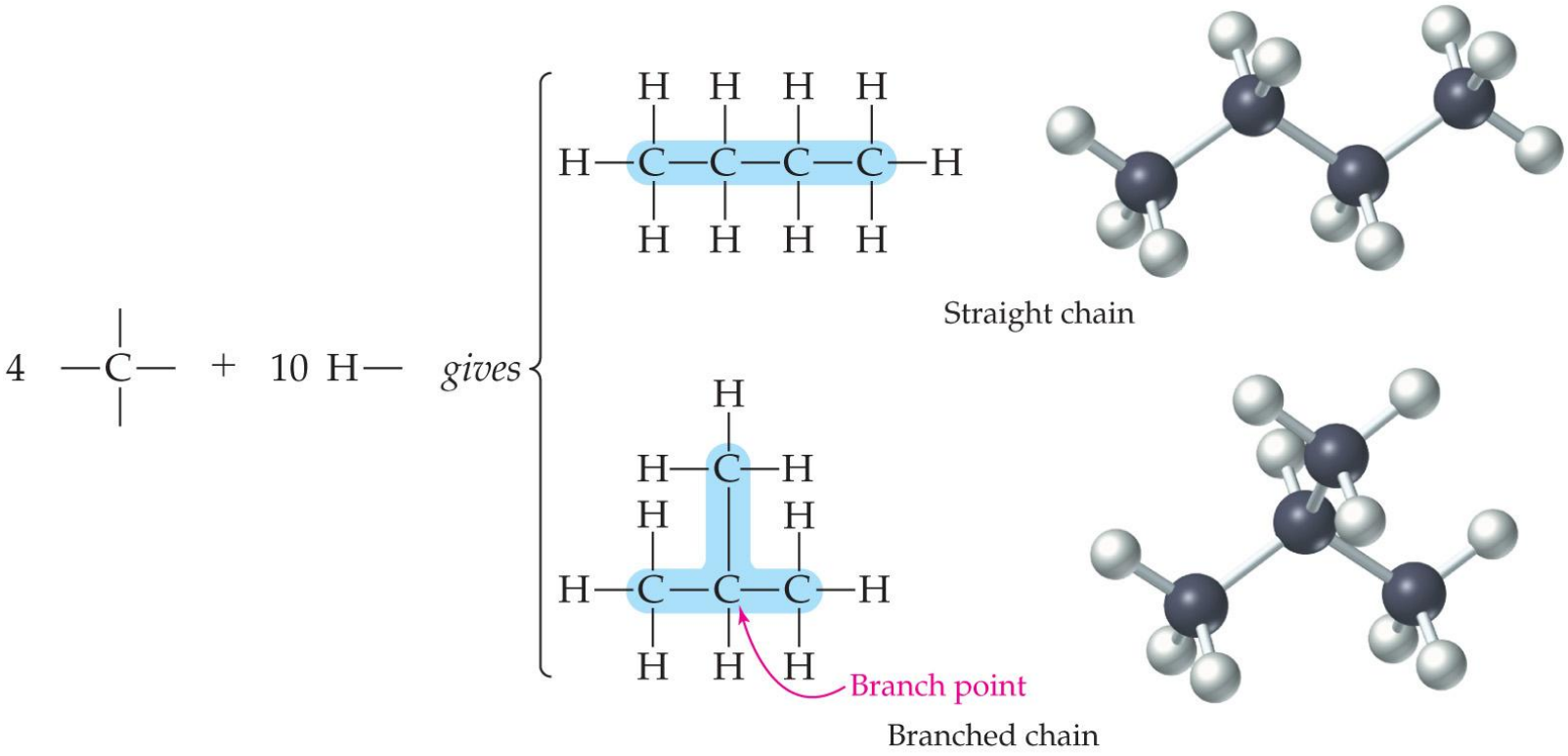
Several shorthand methods have been developed to write structures.
Condensed structures don't have C-H or C-C single bonds shown



2-Methylbutane

name	Kekulé structure	condensed structure	ball-and-stick model
methane		CH_4	
ethane		CH_3CH_3	
propane		$CH_3CH_2CH_3$	
butane		$CH_3CH_2CH_2CH_3$	

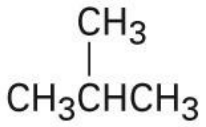
- **Straight-chain alkane:** An alkane that has all its carbons connected in a row (**normal alkanes)**.
- **Branched-chain alkane:** An alkane that has a branching connection of carbons.



Constitutional (Structural) Isomers

- Isomers that differ in how their atoms are arranged in chains are called **constitutional isomers**
- Compounds other than alkanes can be **constitutional isomers** of one another
- They must have the same molecular formula to be isomers

Different carbon skeletons
C_4H_{10}



2-Methylpropane (isobutane)

and

$CH_3CH_2CH_2CH_3$

Butane

Different functional groups
C_2H_6O

CH_3CH_2OH

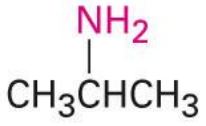
Ethanol

and

CH_3OCH_3

Dimethyl ether

Different position of functional groups
C_3H_9N



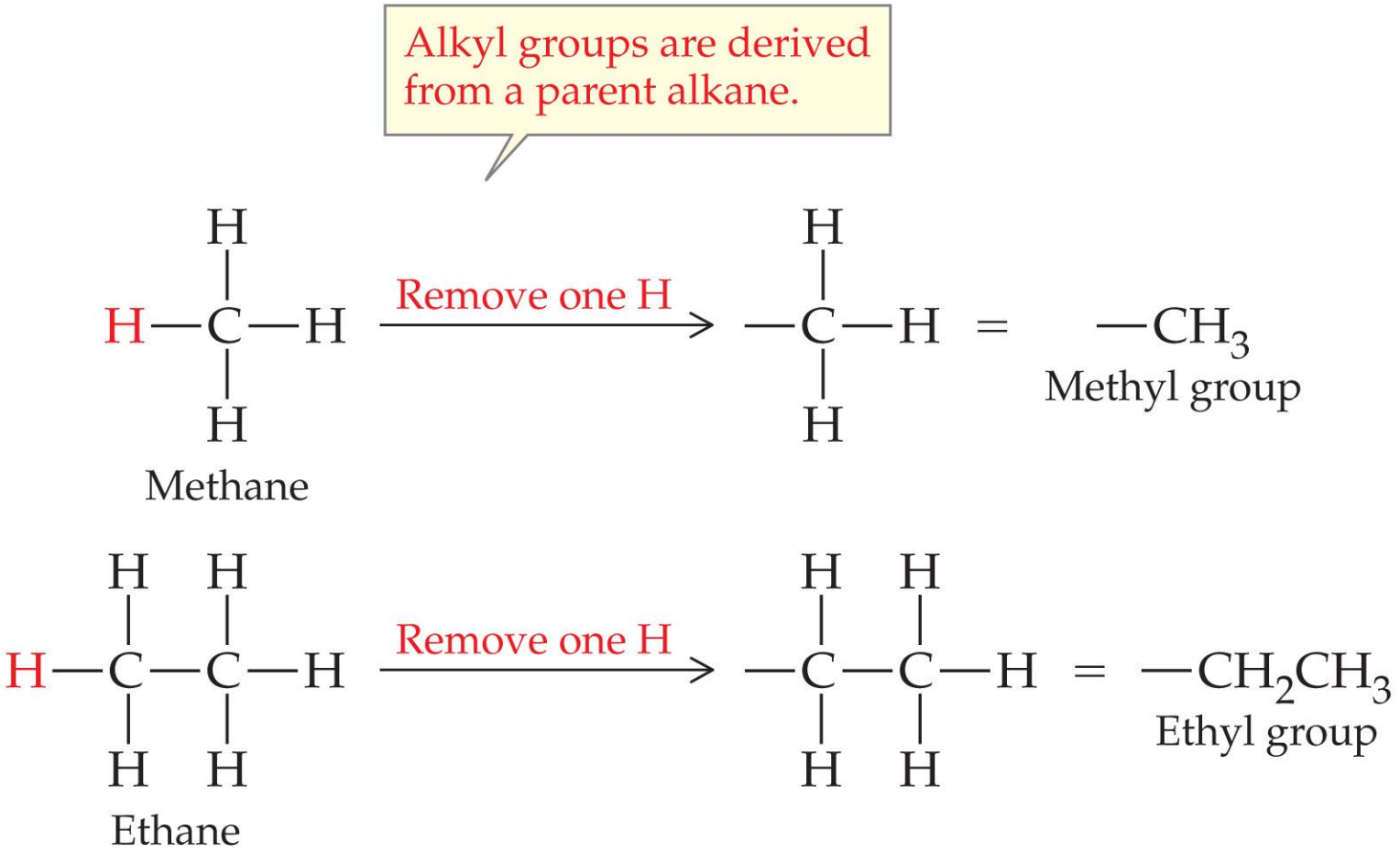
Isopropylamine

and

$CH_3CH_2CH_2NH_2$

Propylamine

- **Alkyl group (R) :** The part of an alkane that remains when a hydrogen atom is removed.



Common Alkyl Groups

One carbon

$CH_3—$

methyl group

Two carbons

$CH_3—CH_2—$

ethyl group

Three carbons

$CH_3—CH_2—CH_2—$

propyl group
(or "*n*-propyl group")

$CH_3—CH(CH_3)—$

isopropyl group

Four carbons

$CH_3—CH_2—CH_2—CH_2—$

butyl group
(or "*n*-butyl group")

$CH_3—CH(CH_3)—CH_2—$

isobutyl group

$CH_3—CH_2—CH(CH_3)—$

sec-butyl group

$CH_3—C(CH_3)_2—$

tert-butyl group
(or "*t*-butyl group")

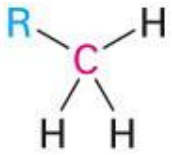
C_4H_{10}

$CH_3CH_2CH_2CH_3$ and $CH_3CH(CH_3)CH_3$

Butane

2-Methylpropane (isobutane)

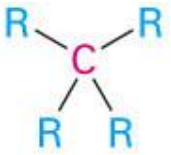
Types of Alkyl groups



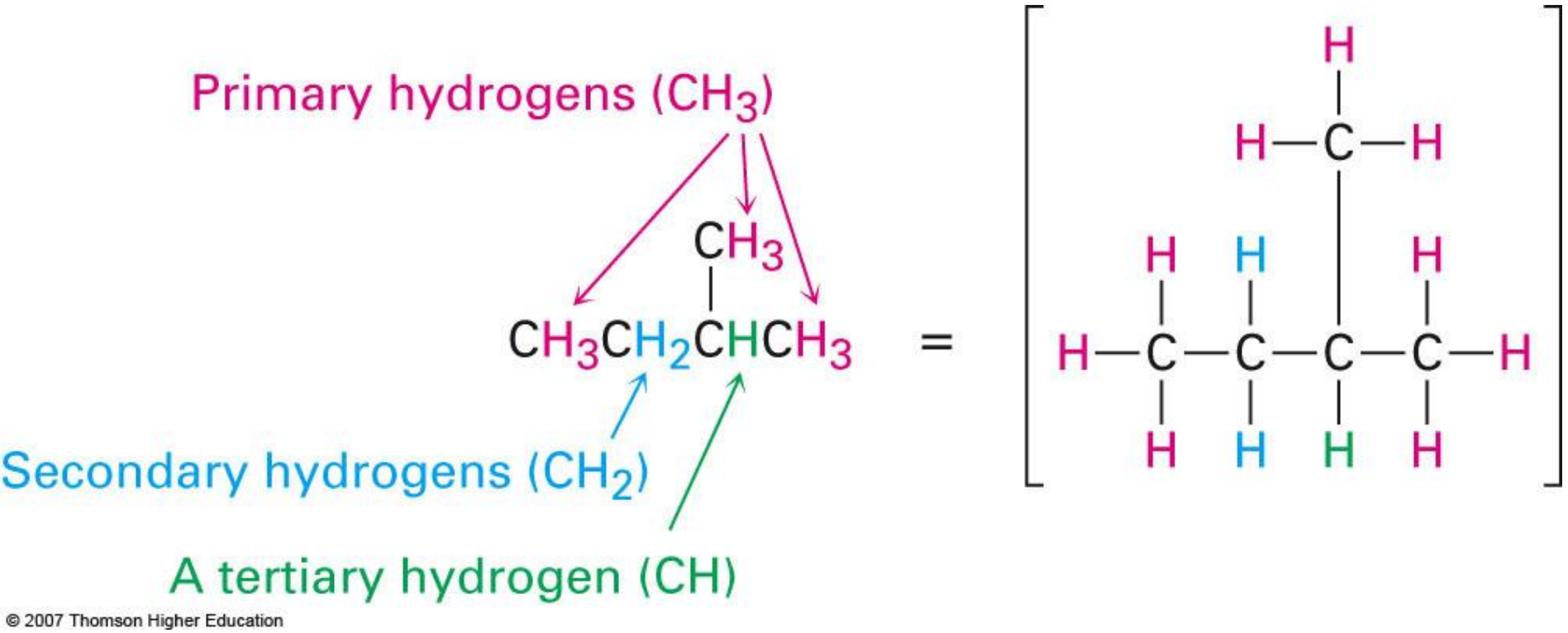
Primary **carbon (1°) is bonded to one other carbon.**

Secondary **carbon (2°) is bonded to two other carbons.**

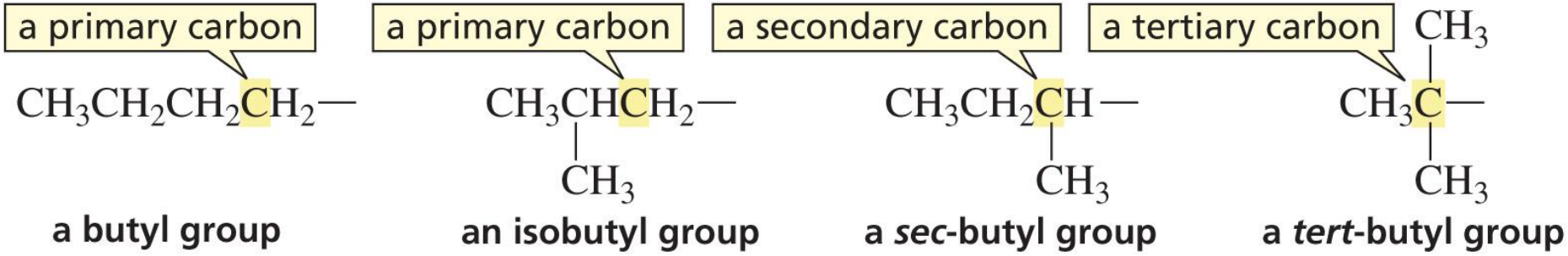
Tertiary **carbon (3°) is bonded to three other carbons.**

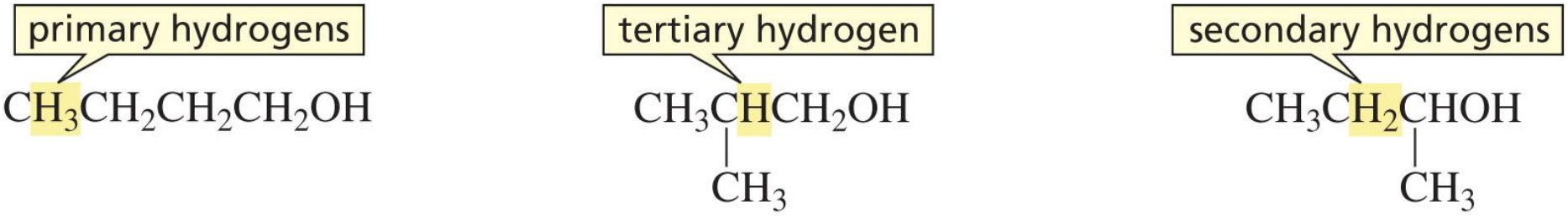


Quaternary **carbon (4°) is bonded to four other carbons.**



Different Kinds of Carbons and Hydrogens

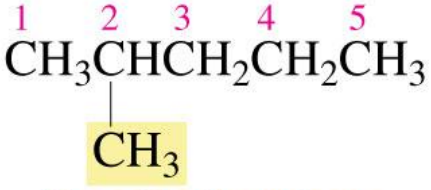




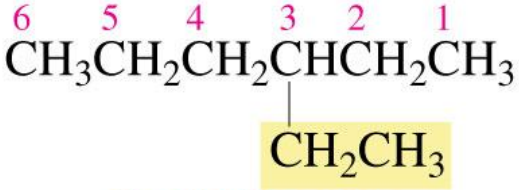
Nomenclature of Alkanes

The Name has Prefix+Parent + Suffix

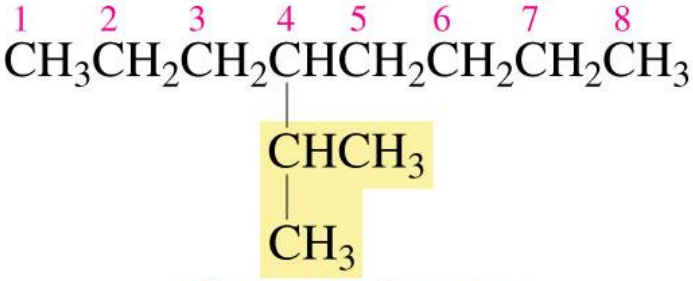
1. Determine the number of carbons in the longest continuous chain and Number the chain so that the substituent gets the lowest number



2-methylpentane

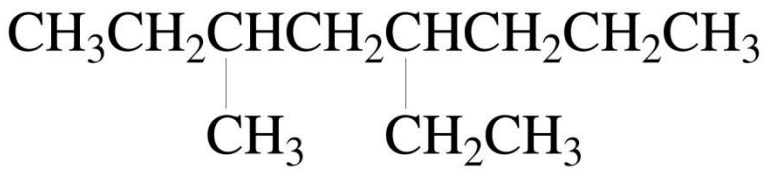


3-ethylhexane



4-isopropyloctane

2. Number the substituents to yield the lowest possible number in the number of the compound



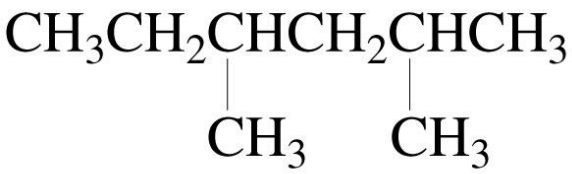
5-ethyl-3-methyloctane

not

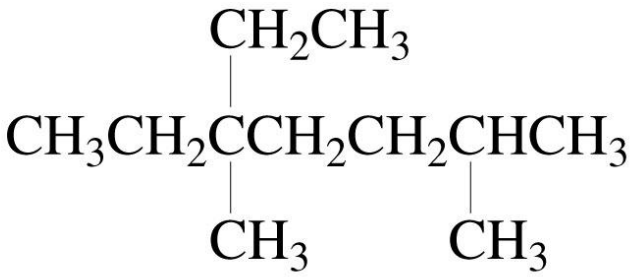
4-ethyl-6-methyloctane

because 3 < 4

substituents are listed in alphabetical order

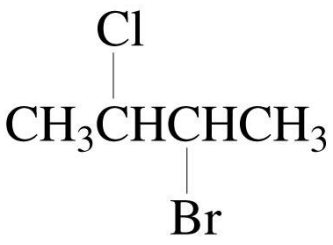


2,4-dimethylhexane

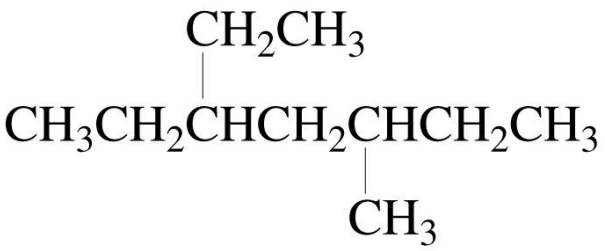


5-ethyl-2,5-dimethylheptane

3. If the same substituent numbers are obtained in both directions, the first group cited receives the lower number

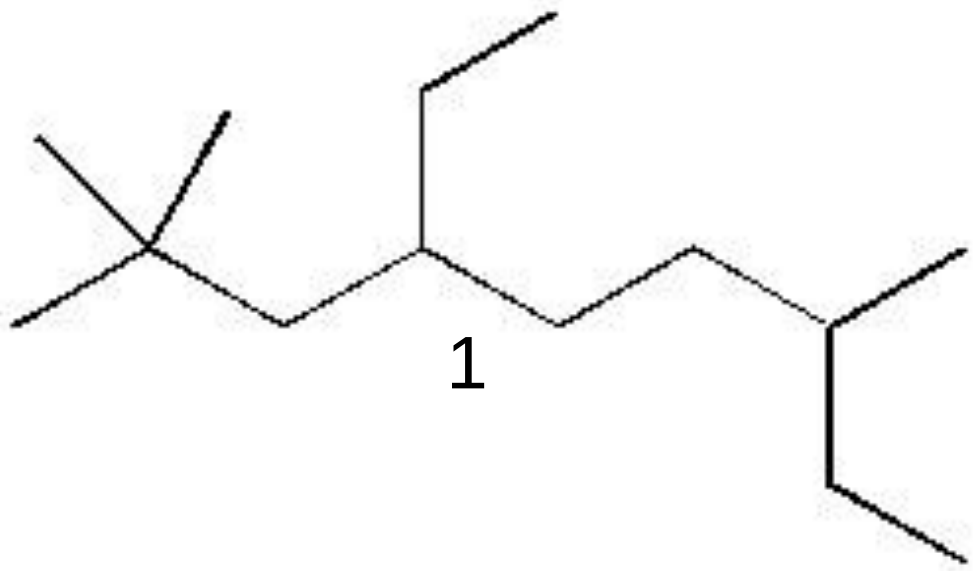


2-bromo-3-chlorobutane
not
3-bromo-2-chlorobutane



3-ethyl-5-methylheptane
not
5-ethyl-3-methylheptane

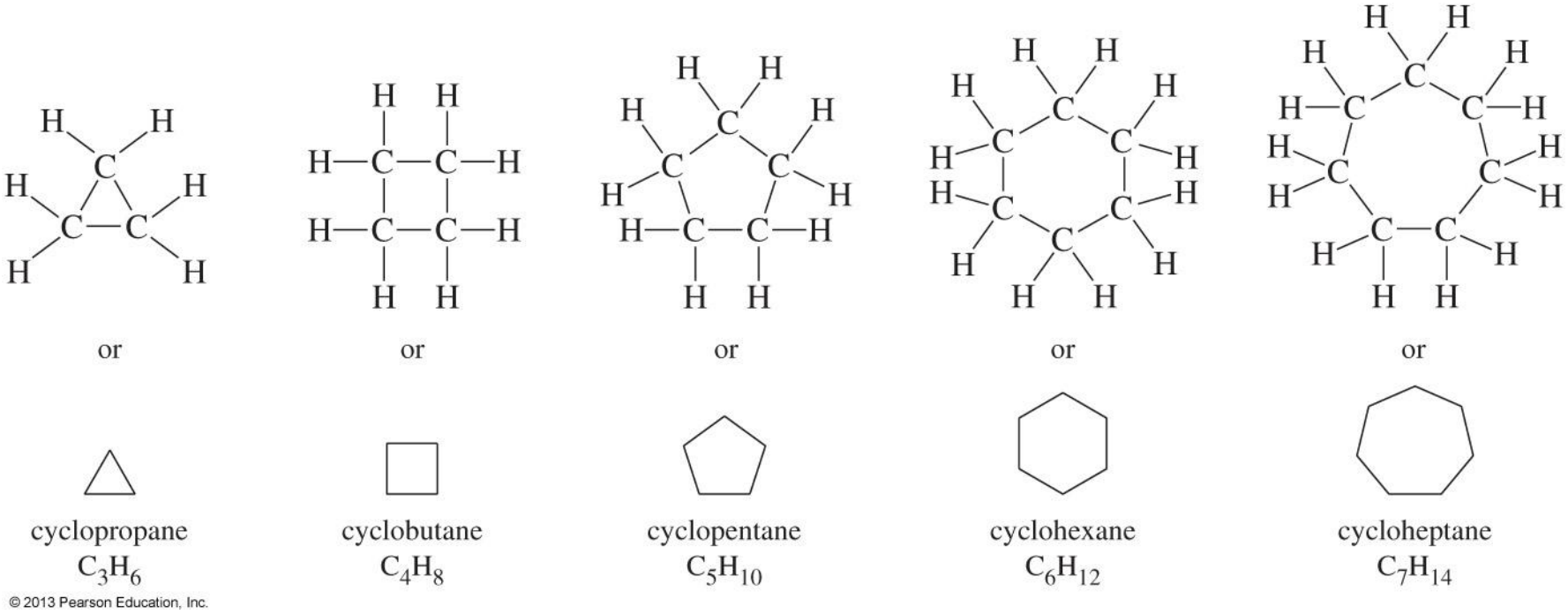
Give the systematic name of the alkanes shown below.



1

4-ethyl-2,2,7-trimethylnonane

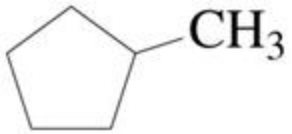
Cycloalkanes: C_nH_{2n}



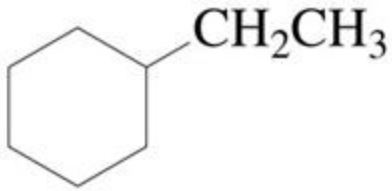
Cycloalkanes contain rings of carbon atoms.

Nomenclature of Cycloalkanes

1. No number is needed for a single substituent on a ring

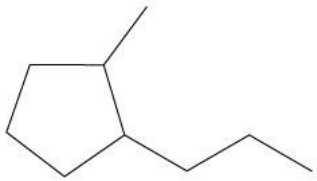


methylcyclopentane

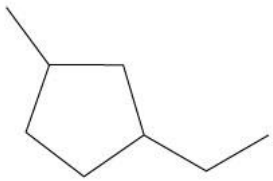


ethylcyclohexane

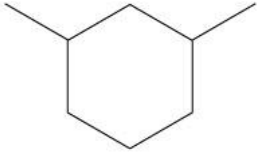
2. Name the two substituents in alphabetical order



1-methyl-2-propylcyclopentane



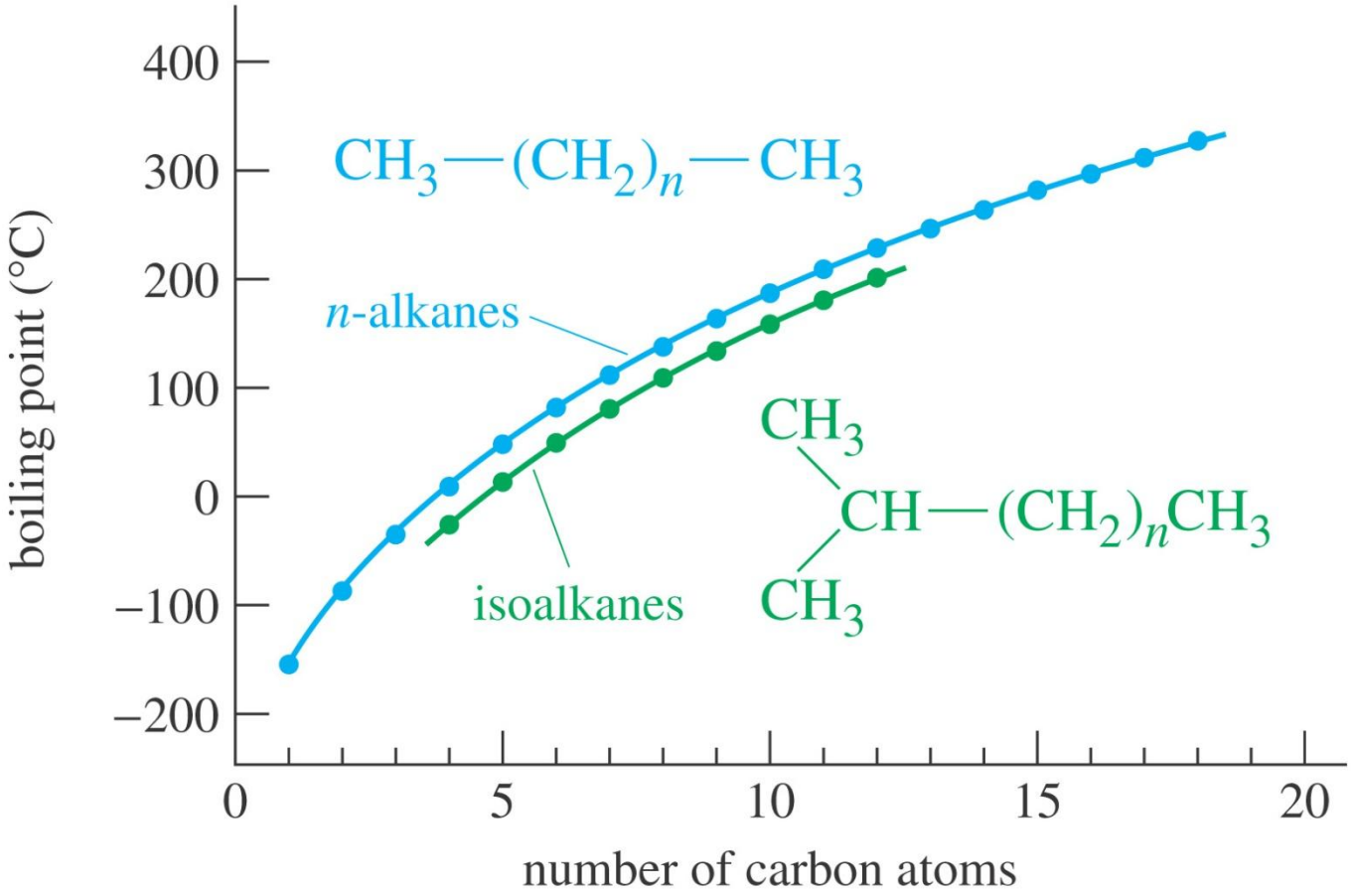
1-ethyl-3-methylcyclopentane



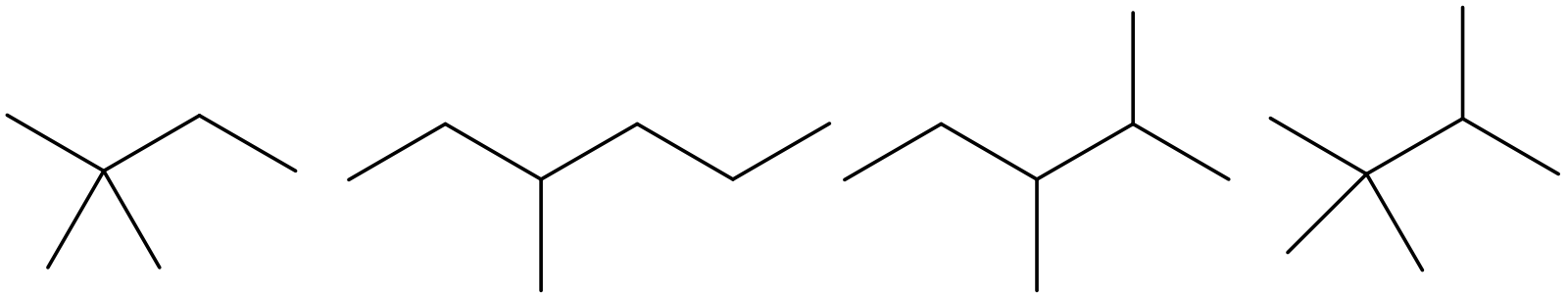
1,3-dimethylcyclohexane

Boiling Points of Alkanes

Branched alkanes have less surface area contact, so weaker intermolecular forces Less boiling points.



Arrange the following compounds in order of decreasing their <u>boiling points</u> ?



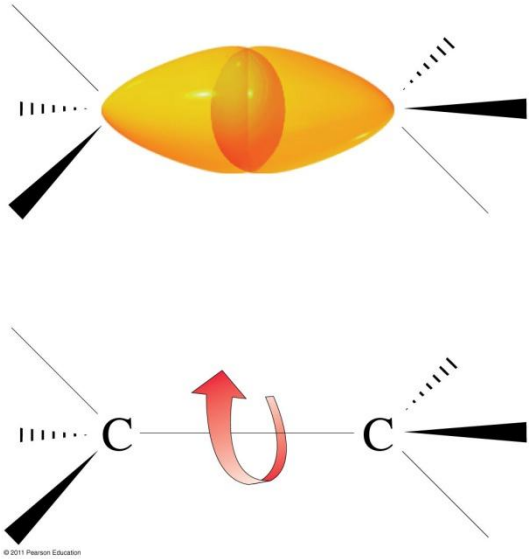
A) 1< 2 < 3<4

B) 1<4< 3 < 2

C) 2 < 3 < 1<4

D) 4<1 < 3 < 2

Conformations of Alkanes: Rotation about Carbon–Carbon Bonds



$H_3C—CH_3$

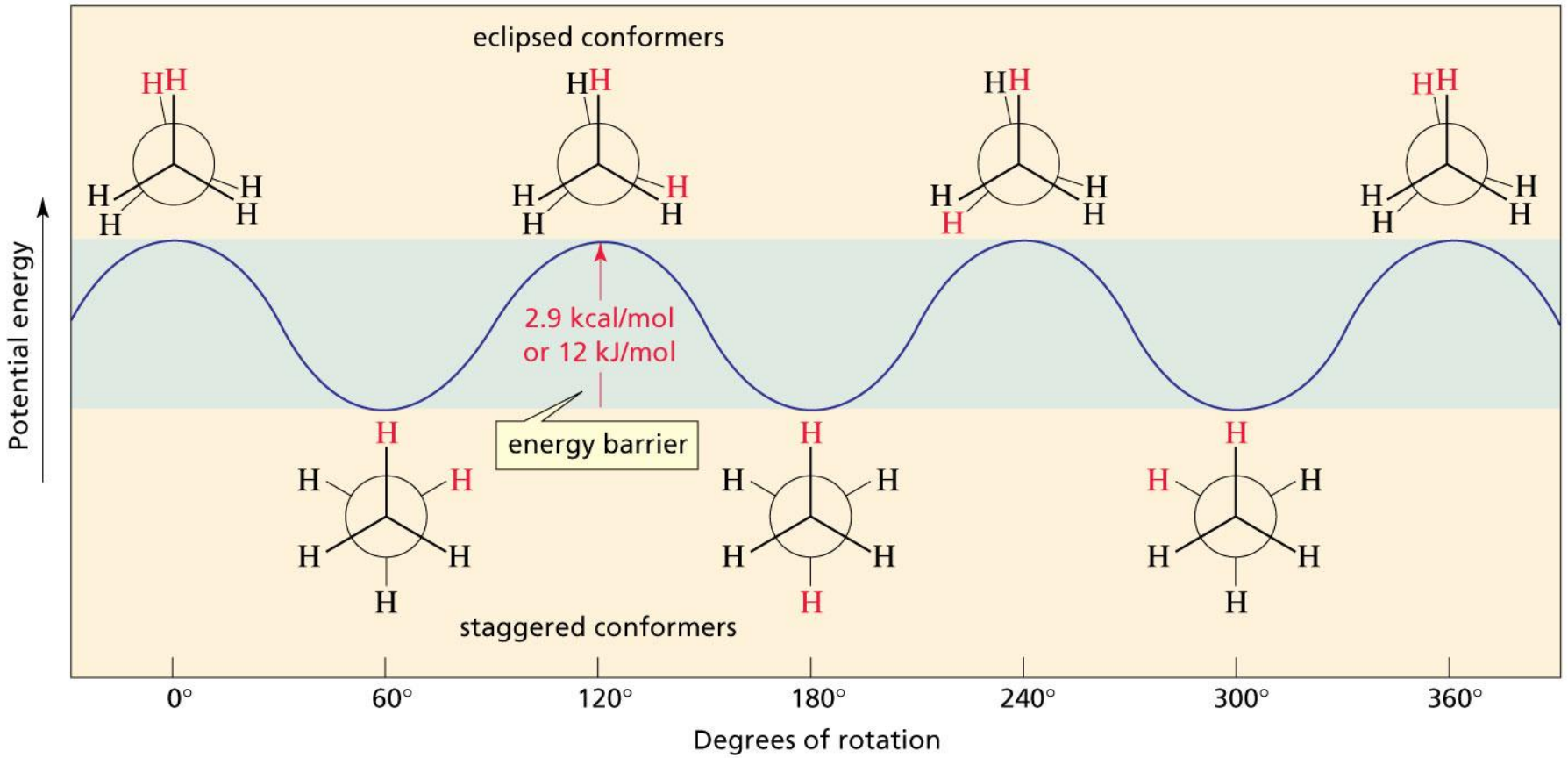
ethane

Newman projections

staggered conformer from rotation about the C—C bond in ethane

eclipsed conformer from rotation about the C—C bond in ethane

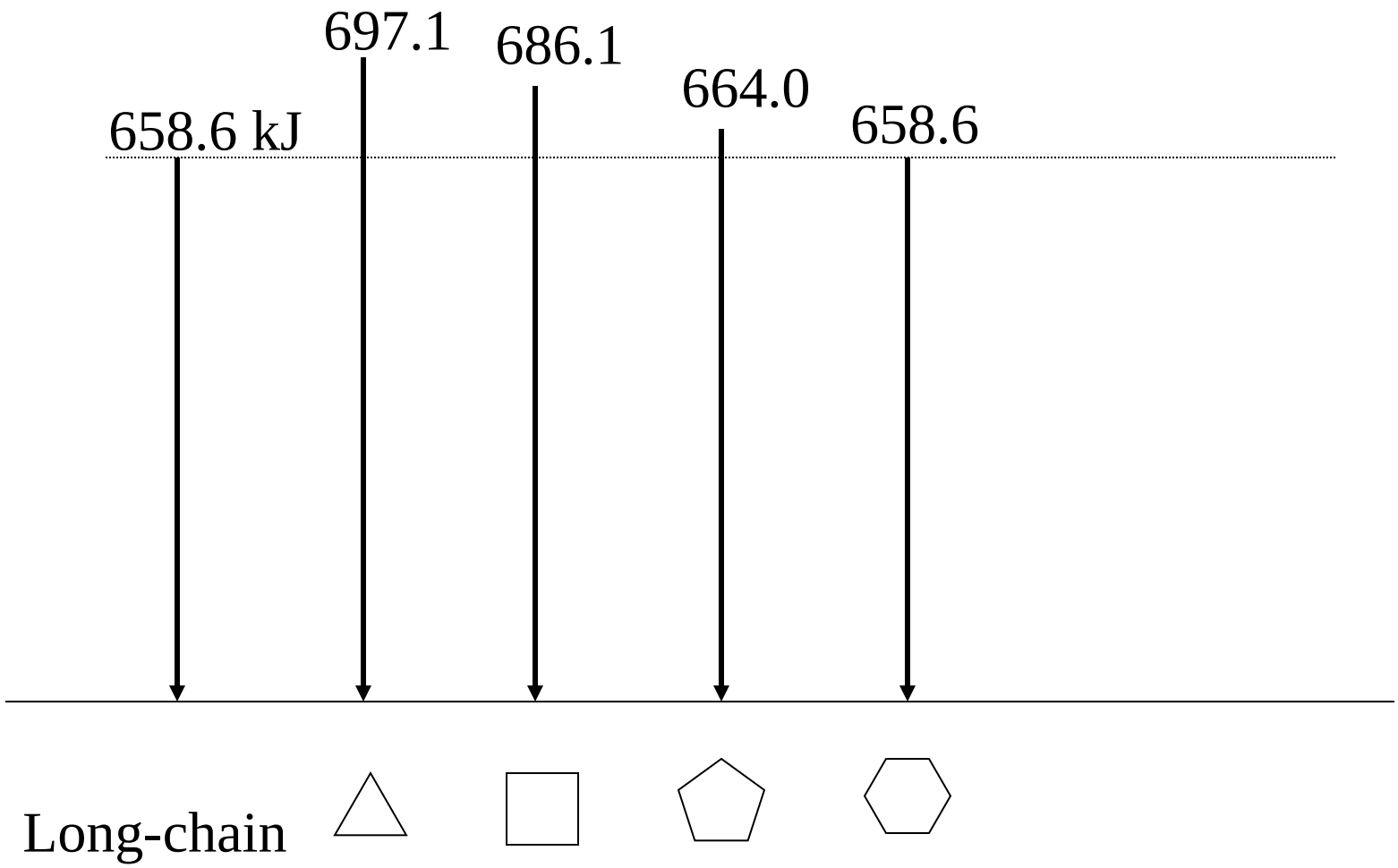
Different Conformations of Ethane



A staggered conformer is more stable than an eclipsed conformer

Heats of Combustion/CH_2

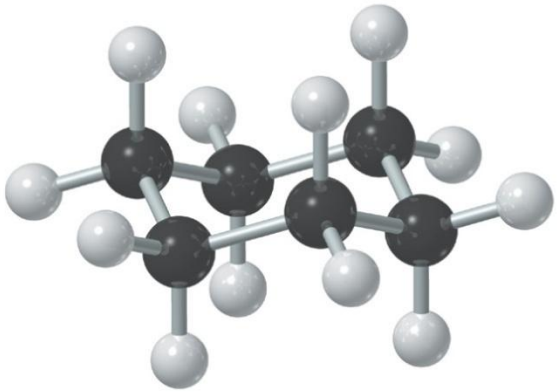
Alkane + $O_2 \rightarrow CO_2 + H_2O$



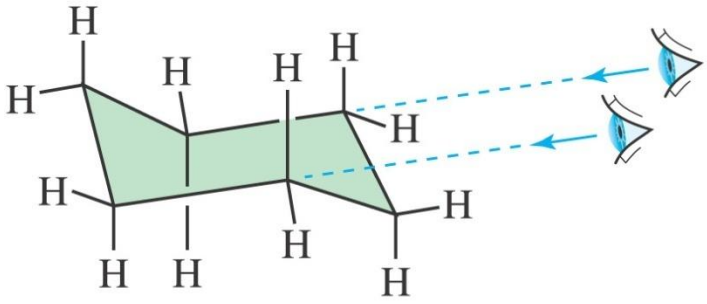
Q Which of the following correctly ranks the cycloalkanes in order of <u>increasing</u> ring strain per methylene?

- A) cyclopropane < cyclobutane < cyclohexane < cyclopentane
- B) cyclohexane < cyclopentane < cyclobutane < cyclopropane
- C) cyclohexane < cyclobutane < cyclopentane < cyclopropane
-
- D) cyclopentane < cyclopropane < cyclobutane < cyclohexane

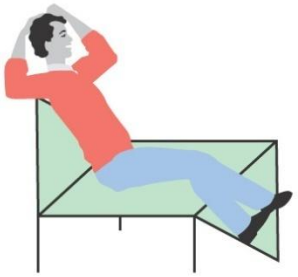
Chair Conformer

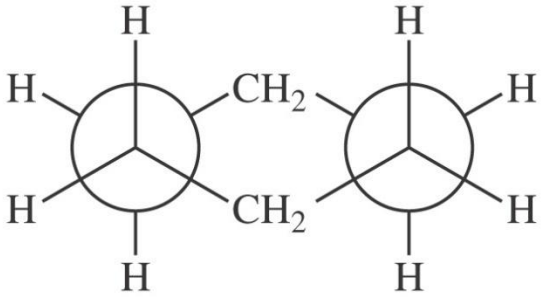


chair conformation



viewed along the “seat” bonds

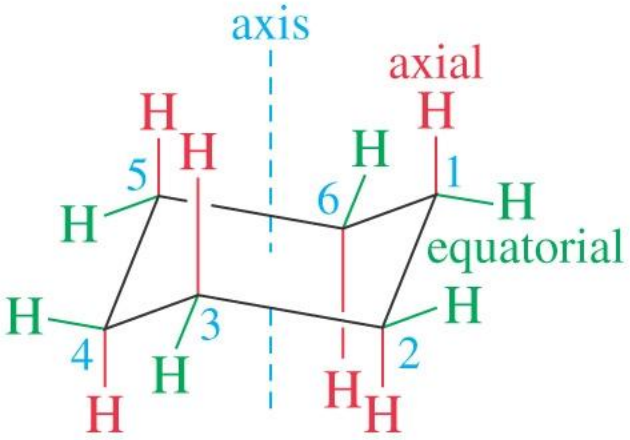


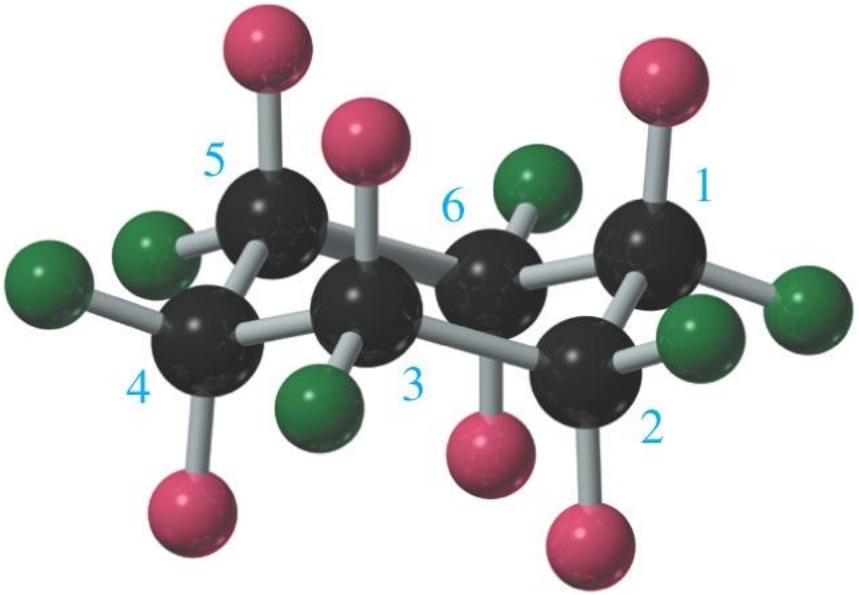


Newman projection

=>

Axial and Equatorial Positions





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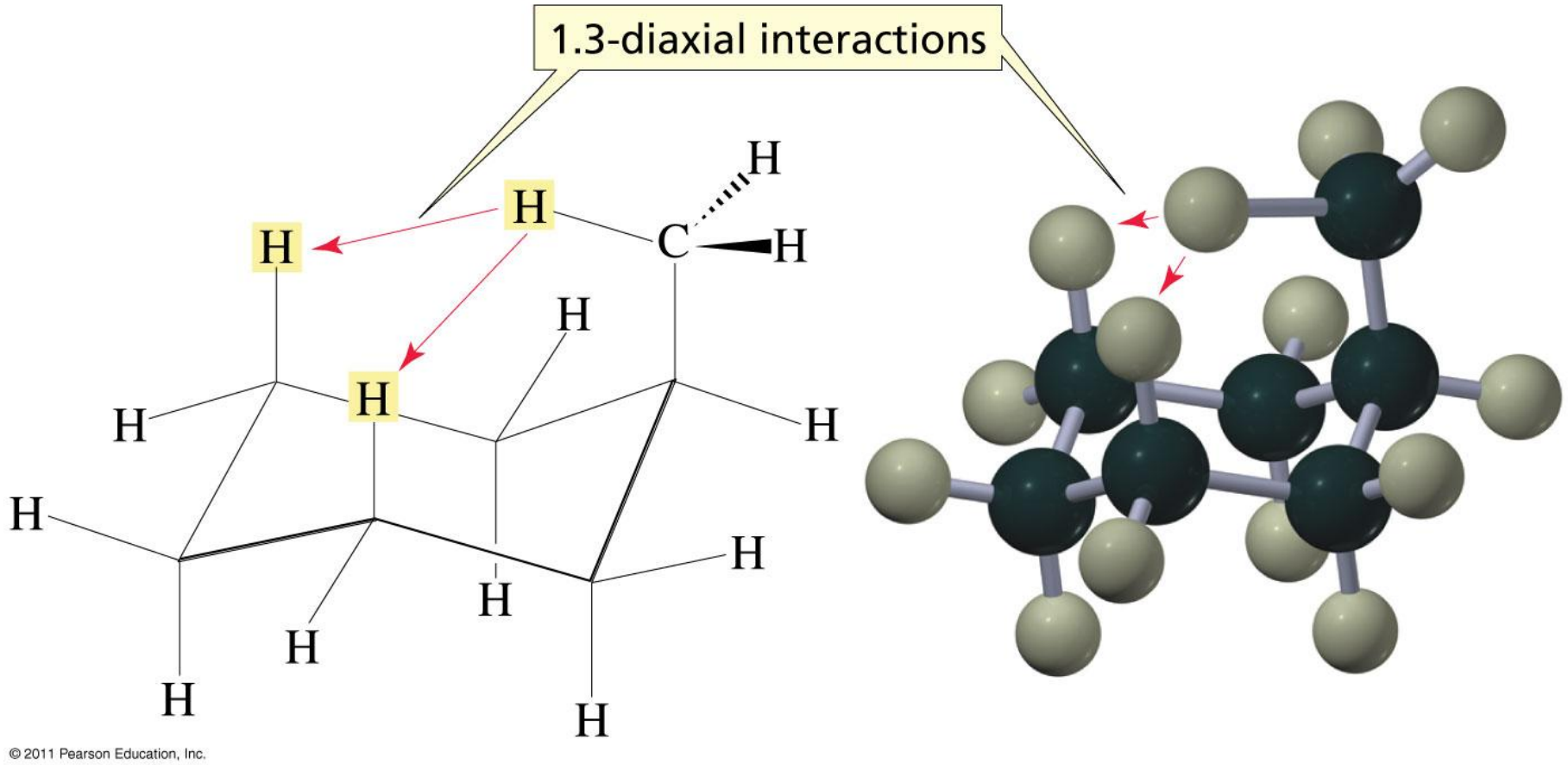
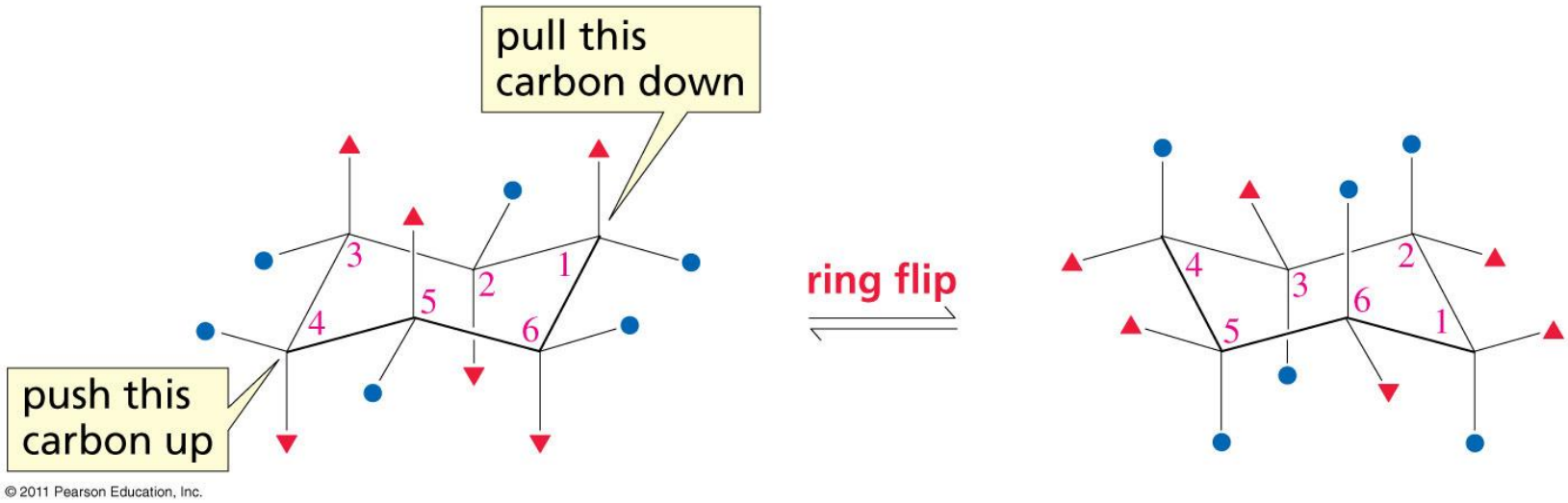
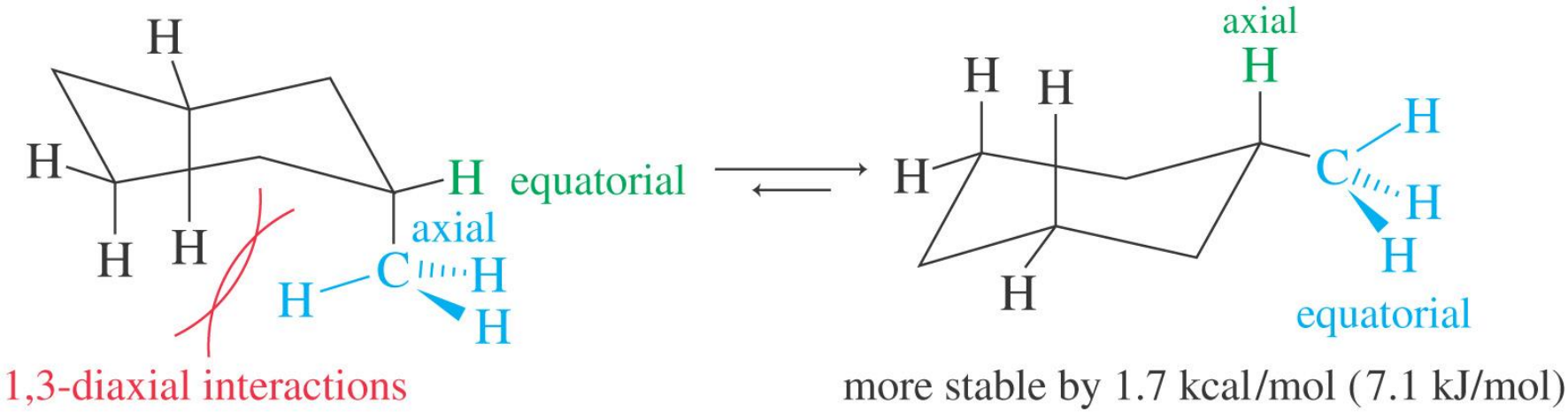
Steric Strain of 1,3-Diaxial Interaction in Methylcyclohexane



Ring Flipping in Cyclohexane



1,3-Diaxial Interactions



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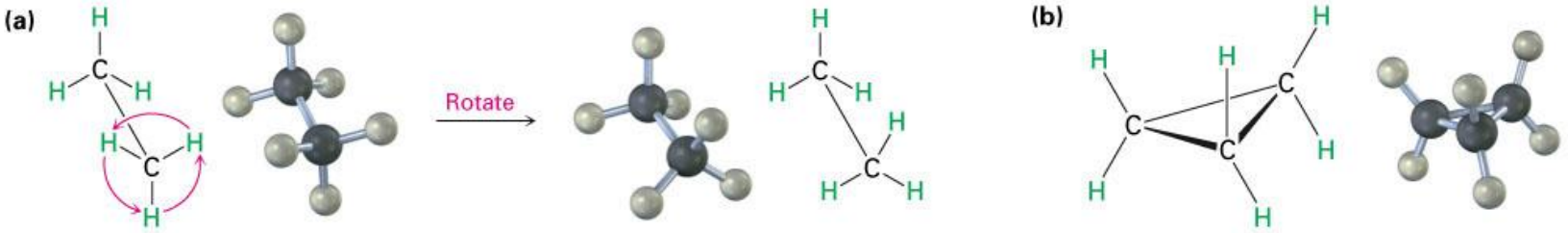
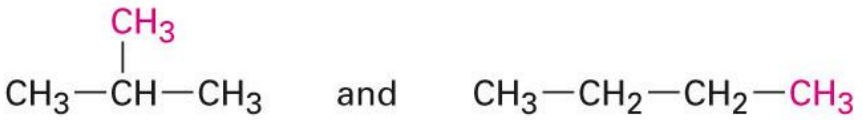
Cis-Trans Isomerism in Cycloalkanes

- Cycloalkanes are less flexible than open-chain alkanes.
- Much less conformational freedom in cycloalkanes.
- Therefore, isomerism is possible in substituted cycloalkanes
- There are two different 1,2-dimethyl-cyclopropane isomers

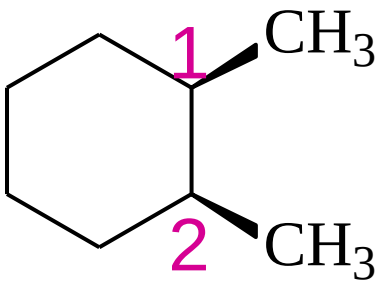


Constitutional isomers
(different connections between atoms)



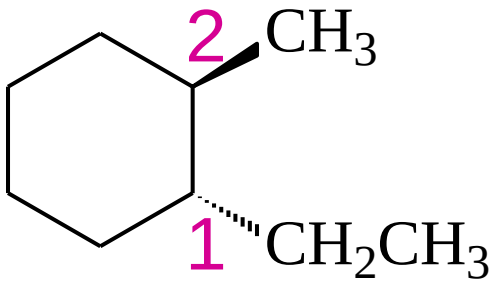
Stereoisomers
(same connections but different three-dimensional geometry)

Geometric Isomers



Same side: *cis*-

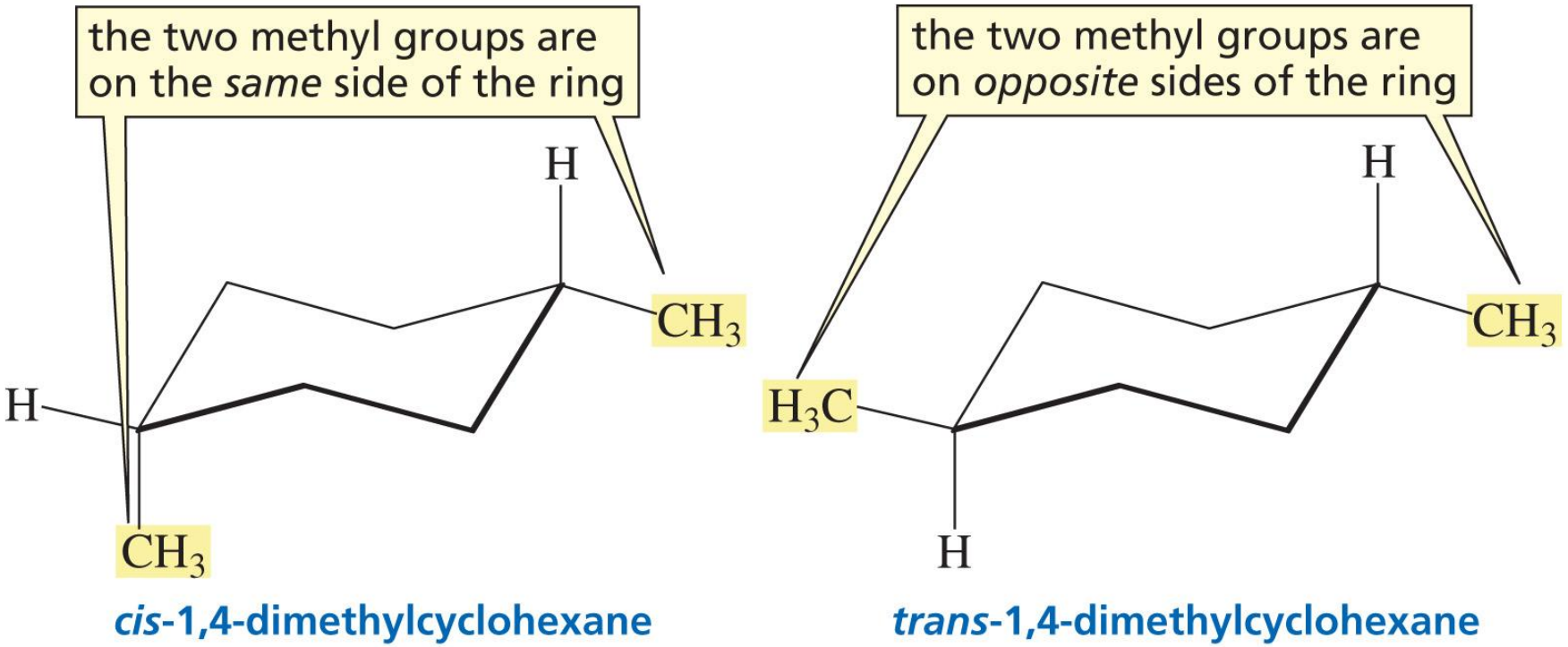
cis-1,2-dimethylcyclohexane



Opposite side: *trans*-

trans-1-ethyl-2-methylcyclohexane

Cis-Trans Isomerism



- Cis: like groups on same side of ring
- Trans: like groups on opposite sides of ring

Cis-trans Isomerism of Di-substituted cyclohexane

- **1,2 disubstituted**

-Trans is **diax** or **dieq** (most stable)

-Cis is one is **ax** and one is eq

- **1,3 disubstituted**

-Trans is one is **ax** and one is eq

-Cis is **diax** or **dieq** (most stable)

- **1,4 disubstituted (as 1,2)**