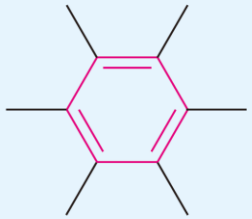
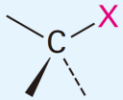
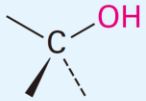
3 烷烃

3.1 官能团的概念

- 有机化合物成千上万，用官能团对其分类，并可预测性质。
- 官能团(Functional group)，是决定有机化合物的化学性质的原子和原子团。

Table 3.1 Structures of Some Common Functional Groups

Name	Structure*	Name ending	Example
Alkene (double bond)		*-ene*	$H_2C{=}CH_2$ Ethene
Alkyne (triple bond)	—C≡C—	*-yne*	HC≡CH Ethyne
Arene (aromatic ring)		None	 Benzene
Halide	 (X = F, Cl, Br, I)	None	CH_3Cl Chloromethane
Alcohol		*-ol*	CH_3OH Methanol

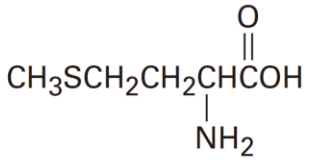
3.1 官能团的概念

- 课堂练习

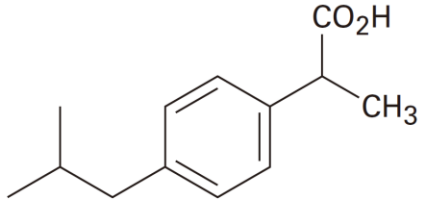
Problem 3.1

Identify the functional groups in each of the following molecules:

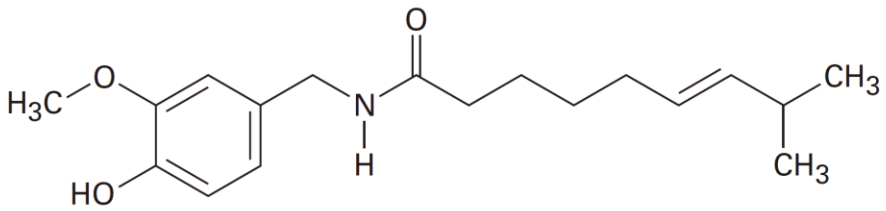
(a) Methionine, an amino acid:



(b) Ibuprofen, a pain reliever:

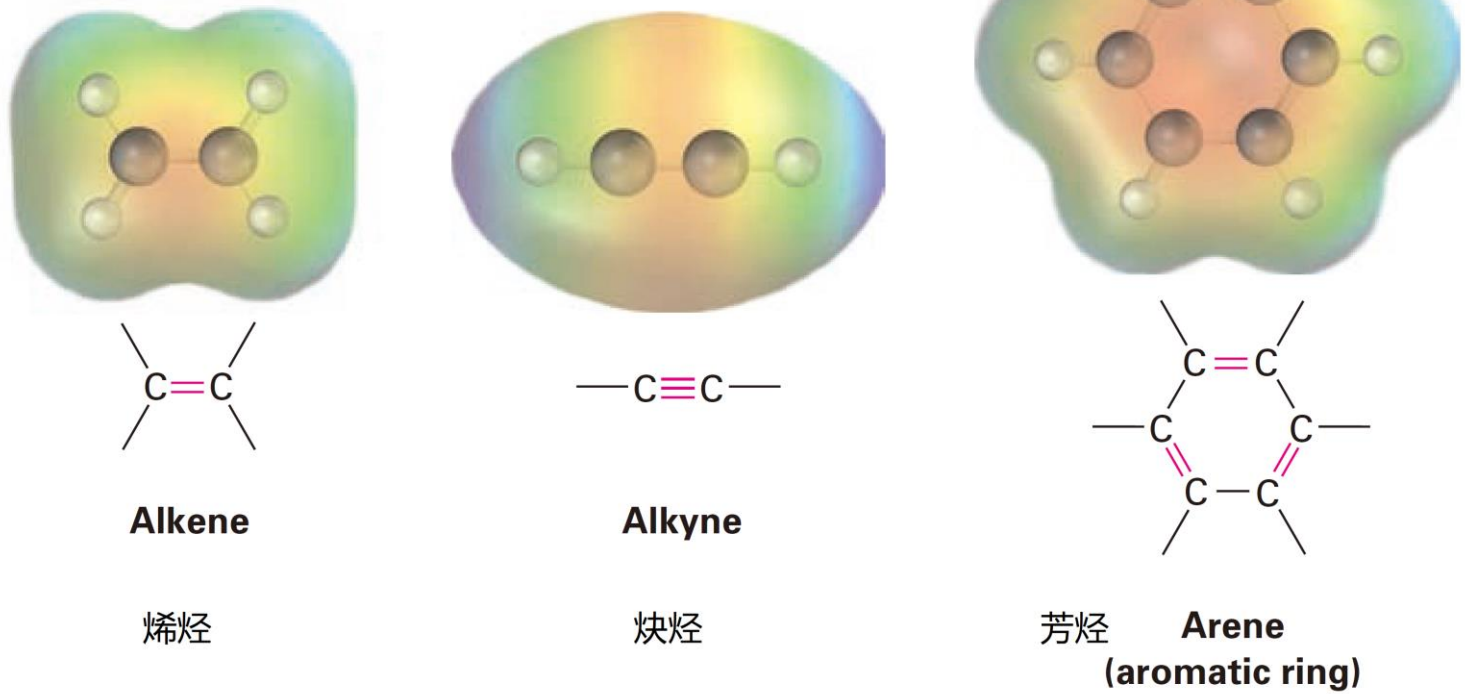


(c) Capsaicin, the pungent substance in chili peppers:



3.1 官能团的概念

- 基于碳碳多重建



Alkene

烯烃

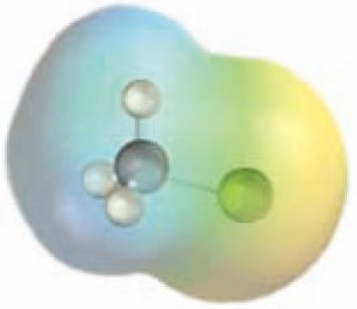
Alkyne

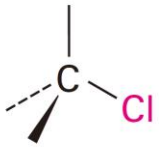
炔烃

芳烃 **Arene**
(aromatic ring)

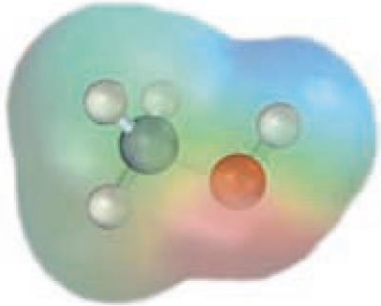
3.1 官能团的概念

- 基于碳杂原子键

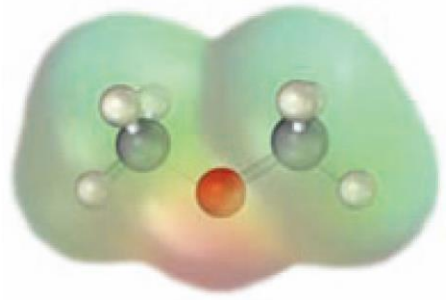


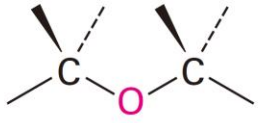


Alkyl halide 卤代烷
(haloalkane)

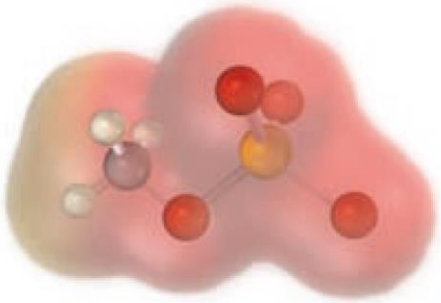


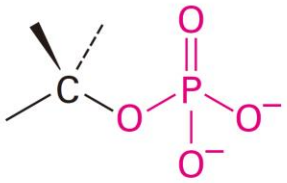
Alcohol 醇





Ether 醚

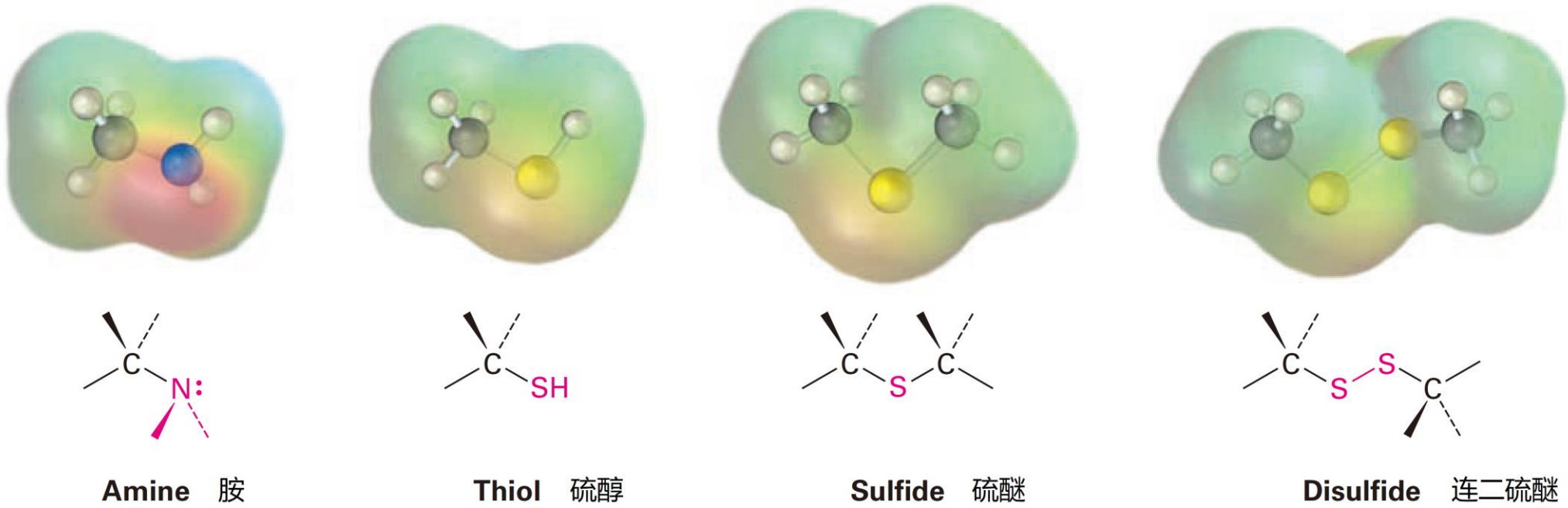




Phosphate 磷酸酯

3.1 官能团的概念

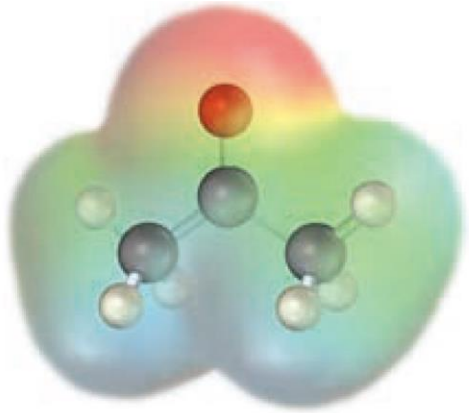
- 基于碳杂原子键

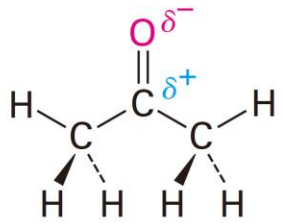


Amine 胺　　**Thiol** 硫醇　　**Sulfide** 硫醚　　**Disulfide** 连二硫醚

3.1 官能团的概念

- 基于碳氧双键



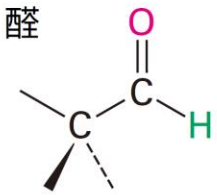


C=O

羰基化合物

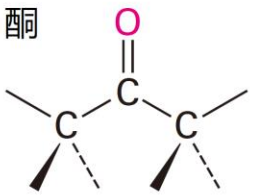
Acetone—a typical carbonyl compound

醛



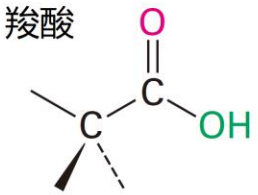
Aldehyde

酮



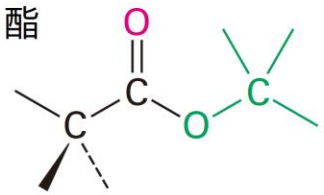
Ketone

羧酸



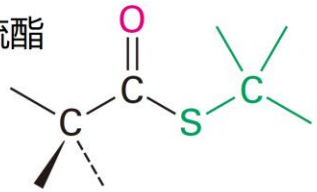
Carboxylic acid

酯



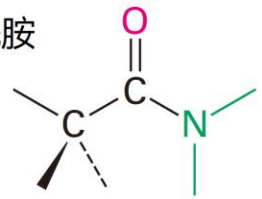
Ester

硫酯



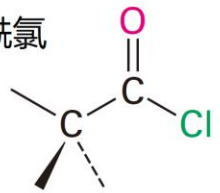
Thioester

酰胺



Amide

酰氯



Acid chloride

3.1 官能团的概念

- 课堂练习

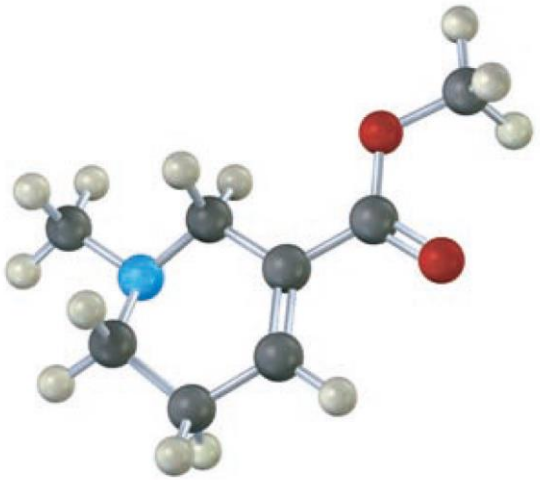
Problem 3.2

Propose structures for simple molecules that contain the following functional groups:

(a) Alcohol **(b)** Aromatic ring **(c)** Carboxylic acid
(d) Amine **(e)** Both ketone and amine **(f)** Two double bonds

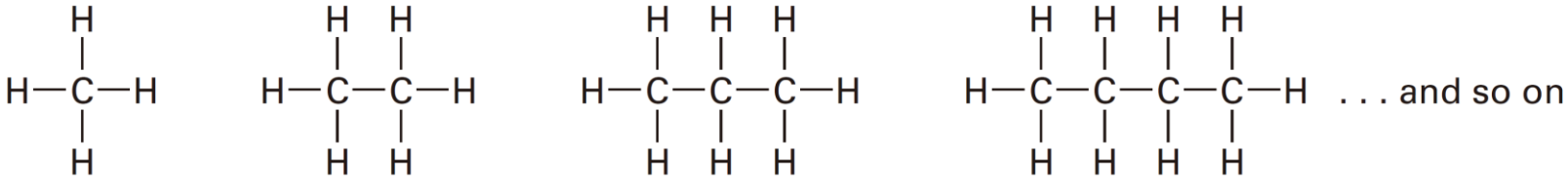
Problem 3.3

Identify the functional groups in the following model of arecoline, a veterinary drug used to control worms in animals. Convert the drawing into a line-bond structure and a molecular formula (red = O, blue = N).



3.2 烷烃及其异构体

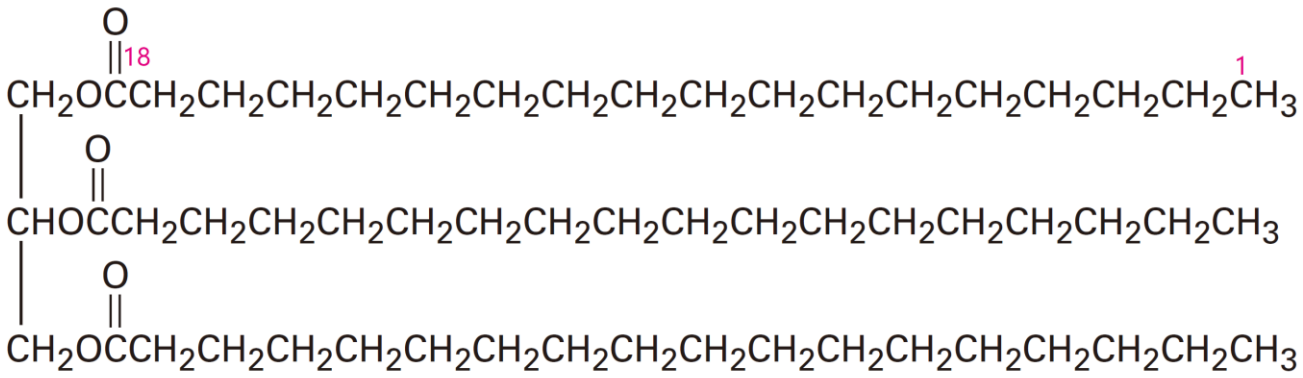
- 烷烃，俗称石蜡烃，又常简称为烷类，其整体构造大多仅由碳、氢两种原子构成，且只有碳–碳与碳–氢两种单键键结而成，是最简单的一种有机化合物。其下又可细分出链烷烃与环烷烃。



Methane **Ethane** **Propane** **Butane**

3.2 烷烃及其异构体

- 脂肪族化合物名称的由来(Aliphatic)



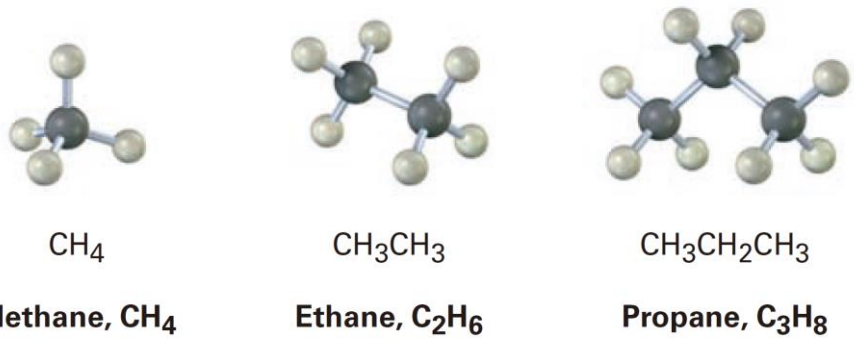
A typical animal fat

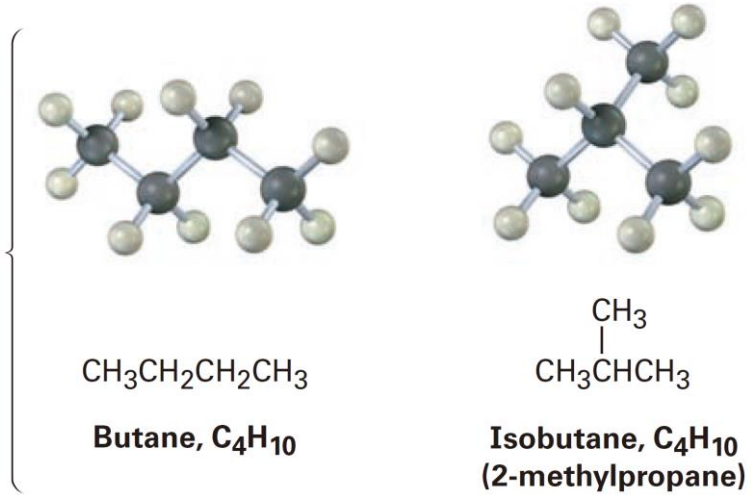
硬脂酸甘油三酯

硬脂酸，即十八酸。硬脂酸钠是肥皂的主要成分，具有很强的去污能力。

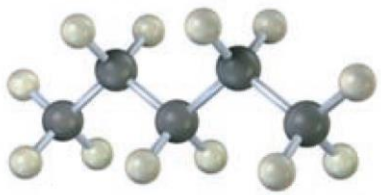
3.2 烷烃及其异构体

- 同分异构体是拥有相同分子式，但结构式却不相同的多种分子。其彼此间的化学性质并不相同，除非它们拥有相同的官能团。常见的两种主要的种类为结构异构以及立体异构。



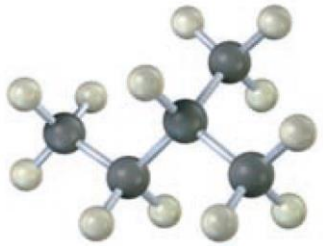


3.2 烷烃及其异构体



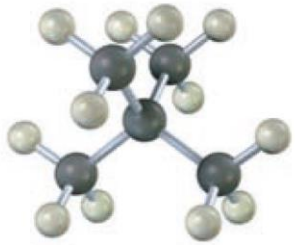
$CH_3CH_2CH_2CH_2CH_3$

Pentane, C_5H_{12}



$CH_3CH_2CHCH_3$ (CH₃ branch)

2-Methylbutane, C_5H_{12}



CH_3CCH_3 (CH₃ branches)

2,2-Dimethylpropane, C_5H_{12}

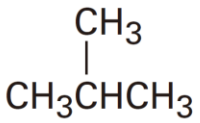
Table 3.2 Number of Alkane Isomers

Formula	Number of isomers
C_6H_{14}	5
C_7H_{16}	9
C_8H_{18}	18
C_9H_{20}	35
$C_{10}H_{22}$	75
$C_{15}H_{32}$	4,347
$C_{20}H_{42}$	366,319
$C_{30}H_{62}$	4,111,846,763

3.2 烷烃及其异构体

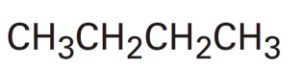
- 同分异构体之间化学性质可以不同，可以相近，取决于他们是否拥有相同的官能团。

Different carbon skeletons
C_4H_{10}



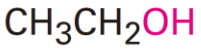
2-Methylpropane (isobutane)

and



Butane

Different functional groups
C_2H_6O

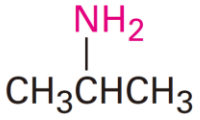


Ethanol

and

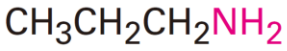
Dimethyl ether

Different position of functional groups
C_3H_9N



Isopropylamine

and



Propylamine

3.2 烷烃及其异构体

- 正构烷烃（直链烷烃）
- 中文：甲烷、乙烷，丙、丁、戊、己、庚、辛、壬、癸，十一烷，二十烷等。

Table 3.3 Names of Straight-Chain Alkanes

Number of carbons (n)	Name	Formula (C_nH_{2n+2})	Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4	9	Nonane	C_9H_{20}
2	Ethane	C_2H_6	10	Decane	$C_{10}H_{22}$
3	Propane	C_3H_8	11	Undecane	$C_{11}H_{24}$
4	Butane	C_4H_{10}	12	Dodecane	$C_{12}H_{26}$
5	Pentane	C_5H_{12}	13	Tridecane	$C_{13}H_{28}$
6	Hexane	C_6H_{14}	20	Icosane	$C_{20}H_{42}$
7	Heptane	C_7H_{16}	30	Triacontane	$C_{30}H_{62}$
8	Octane	C_8H_{18}			

3.2 烷烃及其异构体

- 课堂练习

Problem 3.4

Draw structures of the five isomers of C_6H_{14}.

Problem 3.5

Propose structures that meet the following descriptions:

(a) Two isomeric esters with the formula $C_5H_{10}O_2$

(b) Two isomeric nitriles with the formula C_4H_7N

(c) Two isomeric disulfides with the formula $C_4H_{10}S_2$

Problem 3.6

How many isomers are there with the following descriptions?

(a) Alcohols with the formula C_3H_8O

(b) Bromoalkanes with the formula C_4H_9Br

(c) Thioesters with the formula C_4H_8OS

3.3 烷基基团

- 烷烃去掉一个氢即为烷基基团

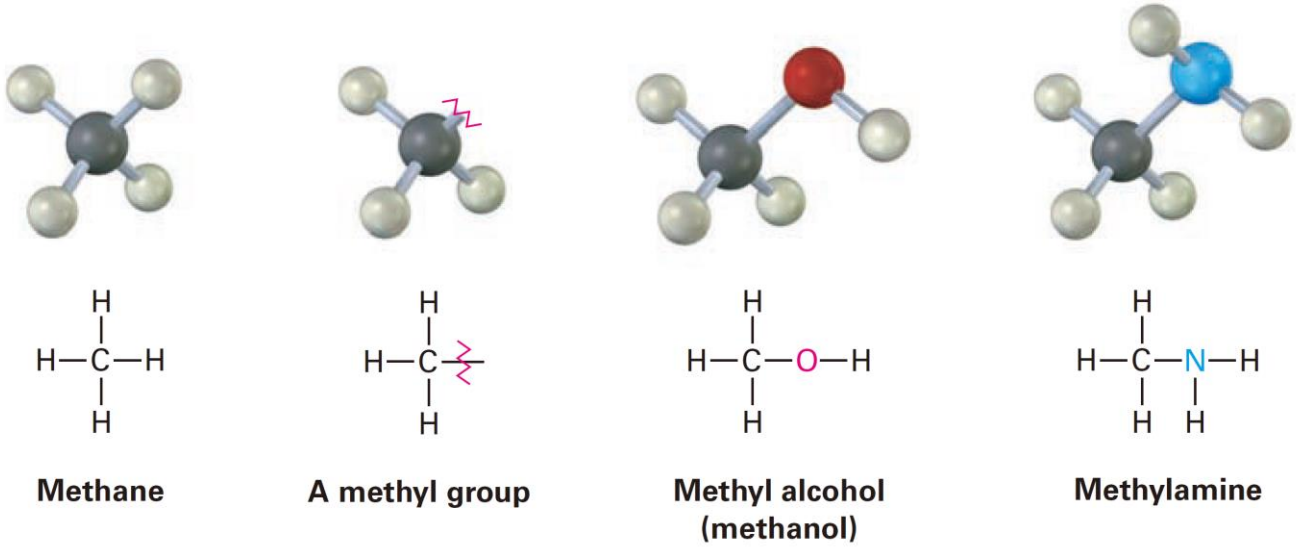


Table 3.4 Some Straight-Chain Alkyl Groups

Alkane	Name	Alkyl group	Name (abbreviation)
CH_4	Methane	$-CH_3$	Methyl (Me)
CH_3CH_3	Ethane	$-CH_2CH_3$	Ethyl (Et)
$CH_3CH_2CH_3$	Propane	$-CH_2CH_2CH_3$	Propyl (Pr)
$CH_3CH_2CH_2CH_3$	Butane	$-CH_2CH_2CH_2CH_3$	Butyl (Bu)
$CH_3CH_2CH_2CH_2CH_3$	Pentane	$-CH_2CH_2CH_2CH_2CH_3$	Pentyl, or amyl

3.3 烷基基团

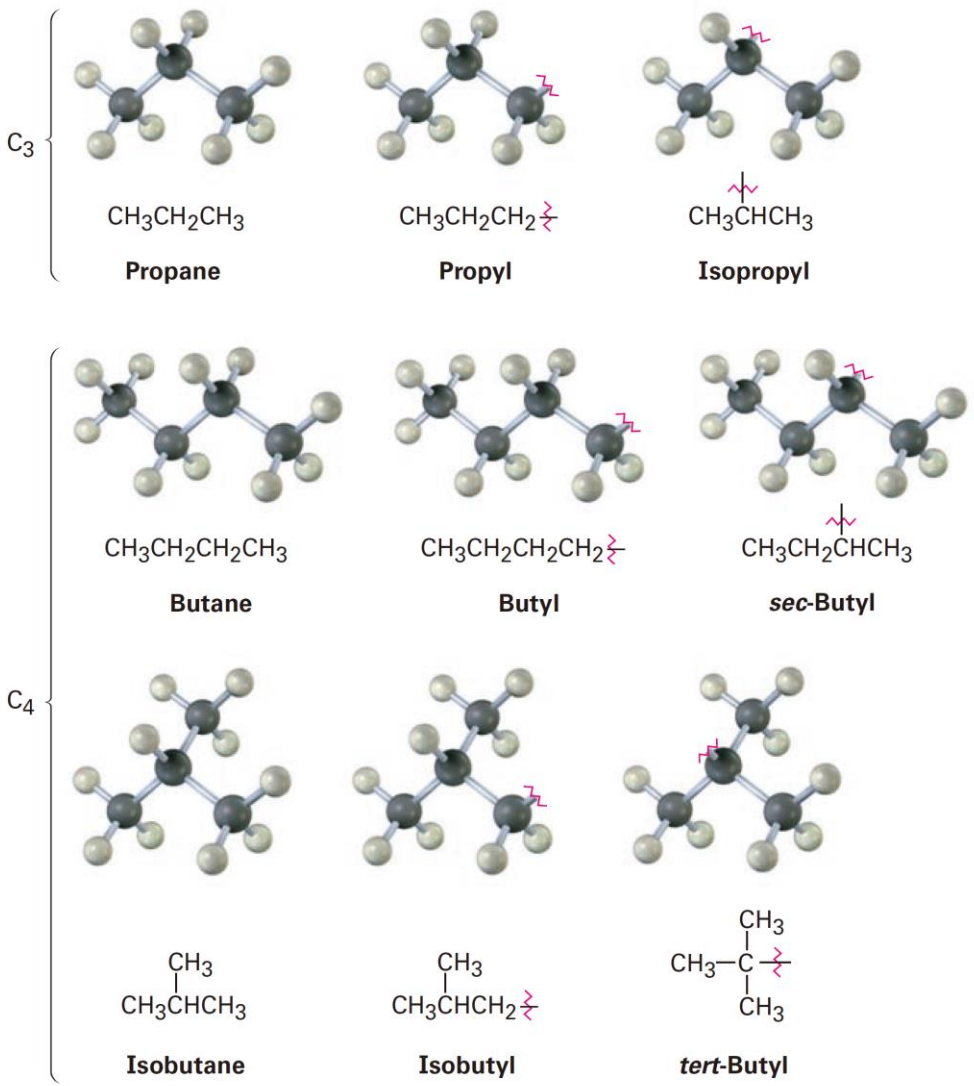
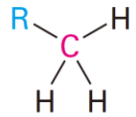


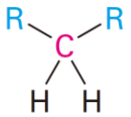
Figure 3.3 Alkyl groups generated from straight-chain alkanes.

3.3 烷基基团

- 一级碳，二级碳，三级碳，四级碳



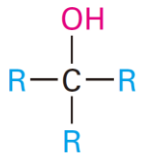
Primary **carbon (1°) is bonded to one other carbon.**



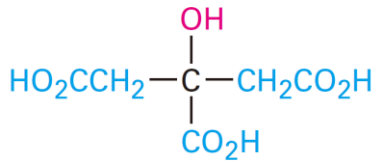
Secondary **carbon (2°) is bonded to two other carbons.**

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

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



General class of tertiary alcohols, R_3COH



Citric acid—a specific tertiary alcohol

3.3 烷基基团

- 课堂练习

Problem 3.10

Draw structures of alkanes that meet the following descriptions:

(a) An alkane with two tertiary carbons

(b) An alkane that contains an isopropyl group

(c) An alkane that has one quaternary and one secondary carbon

3.4 烷烃的命名

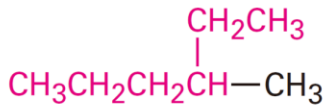
A chemical name typically has four parts in the IUPAC system of nomenclature: prefix, parent, locant, and suffix. The prefix identifies the various **substituent** groups in the molecule, the parent selects a main part of the molecule and tells how many carbon atoms are in that part, the locants give the positions of the functional groups and substituents, and the suffix identifies the primary functional group.

3.4 烷烃的命名

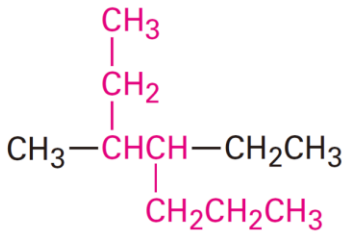
STEP 1

Find the parent hydrocarbon.

(a) Find the longest continuous chain of carbon atoms in the molecule, and use the name of that chain as the parent name. The longest chain may not always be apparent from the manner of writing; you may have to "turn corners."

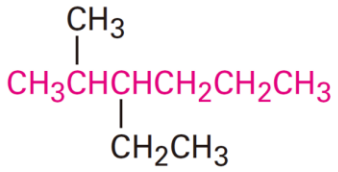


Named as a substituted hexane



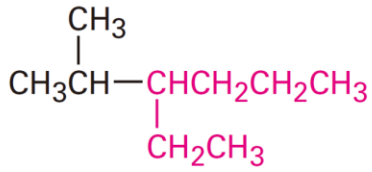
Named as a substituted heptane

(b) If two different chains of equal length are present, choose the one with the larger number of branch points as the parent.



Named as a hexane with *two* substituents

NOT



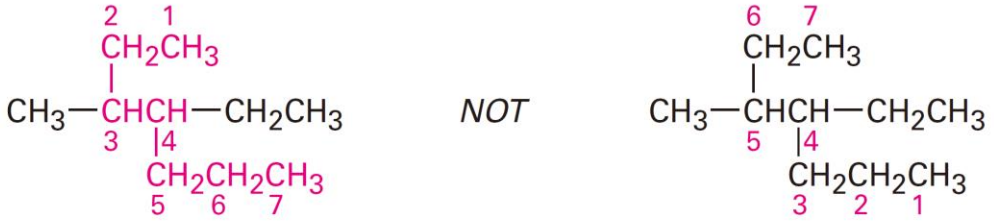
as a hexane with *one* substituent

3.4 烷烃的命名

STEP 2

Number the atoms in the longest chain.

(a) Beginning at the end nearer the first branch point, number each carbon atom in the parent chain.



The first branch occurs at C3 in the proper system of numbering, not at C4.

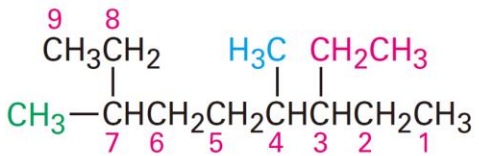
(b) If there is branching an equal distance away from both ends of the parent chain, begin numbering at the end nearer the second branch point.

3.4 烷烃的命名

STEP 3

Identify and number the substituents.

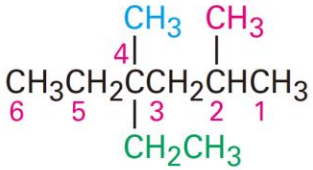
(a) Assign a number, or *locant,* to each substituent to locate its point of attachment to the parent chain.



Named as a nonane

Substituents: On C3, CH_2CH_3 (3-ethyl)
On C4, CH_3 (4-methyl)
On C7, CH_3 (7-methyl)

(b) If there are two substituents on the same carbon, give both the same number. There must be as many numbers in the name as there are substituents.



Named as a hexane

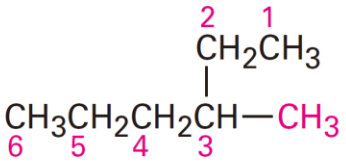
Substituents: On C2, CH_3 (2-methyl)
On C4, CH_3 (4-methyl)
On C4, CH_2CH_3 (4-ethyl)

3.4 烷烃的命名

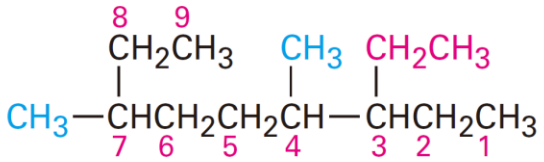
STEP 4

Write the name as a single word.

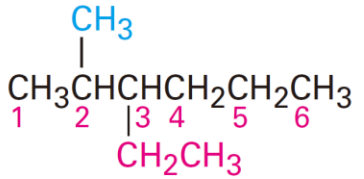
Use hyphens to separate the different prefixes, and use commas to separate numbers. If two or more different substituents are present, cite them in alphabetical order. If two or more identical substituents are present on the parent chain, use one of the multiplier prefixes *di-*, *tri-*, *tetra-*, and so forth, but don't use these prefixes for alphabetizing. Full names for some of the examples we have been using follow.



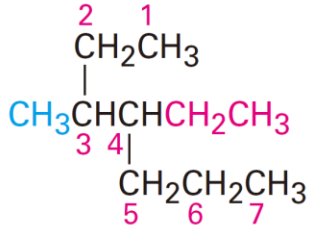
3-Methylhexane



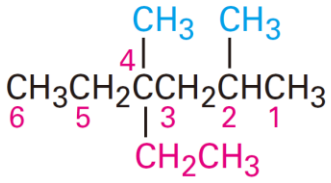
3-Ethyl-4,7-dimethylnonane



3-Ethyl-2-methylhexane



4-Ethyl-3-methylheptane



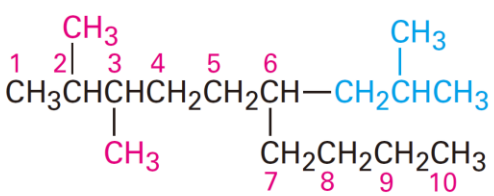
4-Ethyl-2,4-dimethylhexane

3.4 烷烃的命名

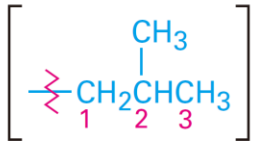
STEP 5

Name a complex substituent as though it were itself a compound.

In some particularly complex cases, a fifth step is necessary. It occasionally happens that a substituent on the main chain has sub-branching. In the following case, for instance, the substituent at C6 is a three-carbon chain with a methyl sub-branch. To name the compound fully, the complex substituent must first be named.



Named as a 2,3,6-trisubstituted decane



A 2-methylpropyl group

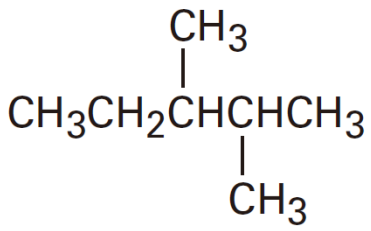
3.4 烷烃的命名

Problem 3.11

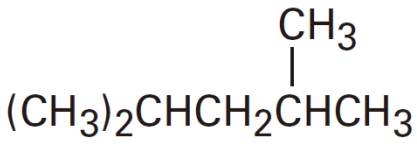
Give IUPAC names for the following compounds:

(a) The three isomers of C_5H_{12}

(b)



(c)



(d)

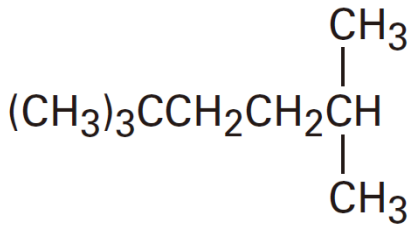


Table 3.3 Names of Straight-Chain Alkanes

Number of carbons (n)	Name	Formula (C_nH_{2n+2})
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$
11	Undecane	$C_{11}H_{24}$
12	Dodecane	$C_{12}H_{26}$
13	Tridecane	$C_{13}H_{28}$
20	Icosane	$C_{20}H_{42}$
30	Triacontane	$C_{30}H_{62}$

3.4 烷烃的命名

Problem 3.12

Draw structures corresponding to the following IUPAC names:

(a) 3,4-Dimethylnonane **(b)** 3-Ethyl-4,4-dimethylheptane

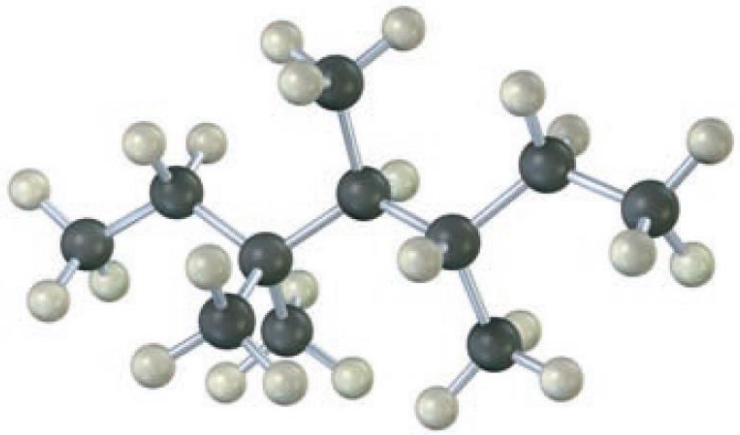
(c) 2,2-Dimethyl-4-propyloctane **(d)** 2,2,4-Trimethylpentane

Problem 3.13

Name the eight 5-carbon alkyl groups you drew in Problem 3.7.

Problem 3.14

Give the IUPAC name for the following hydrocarbon, and convert the drawing into a skeletal structure.



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4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octane	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$
11	Undecane	$C_{11}H_{24}$
12	Dodecane	$C_{12}H_{26}$
13	Tridecane	$C_{13}H_{28}$
20	Icosane	$C_{20}H_{42}$
30	Triacontane	$C_{30}H_{62}$

3.5 烷烃的性质

- 物理性质：熔点和沸点

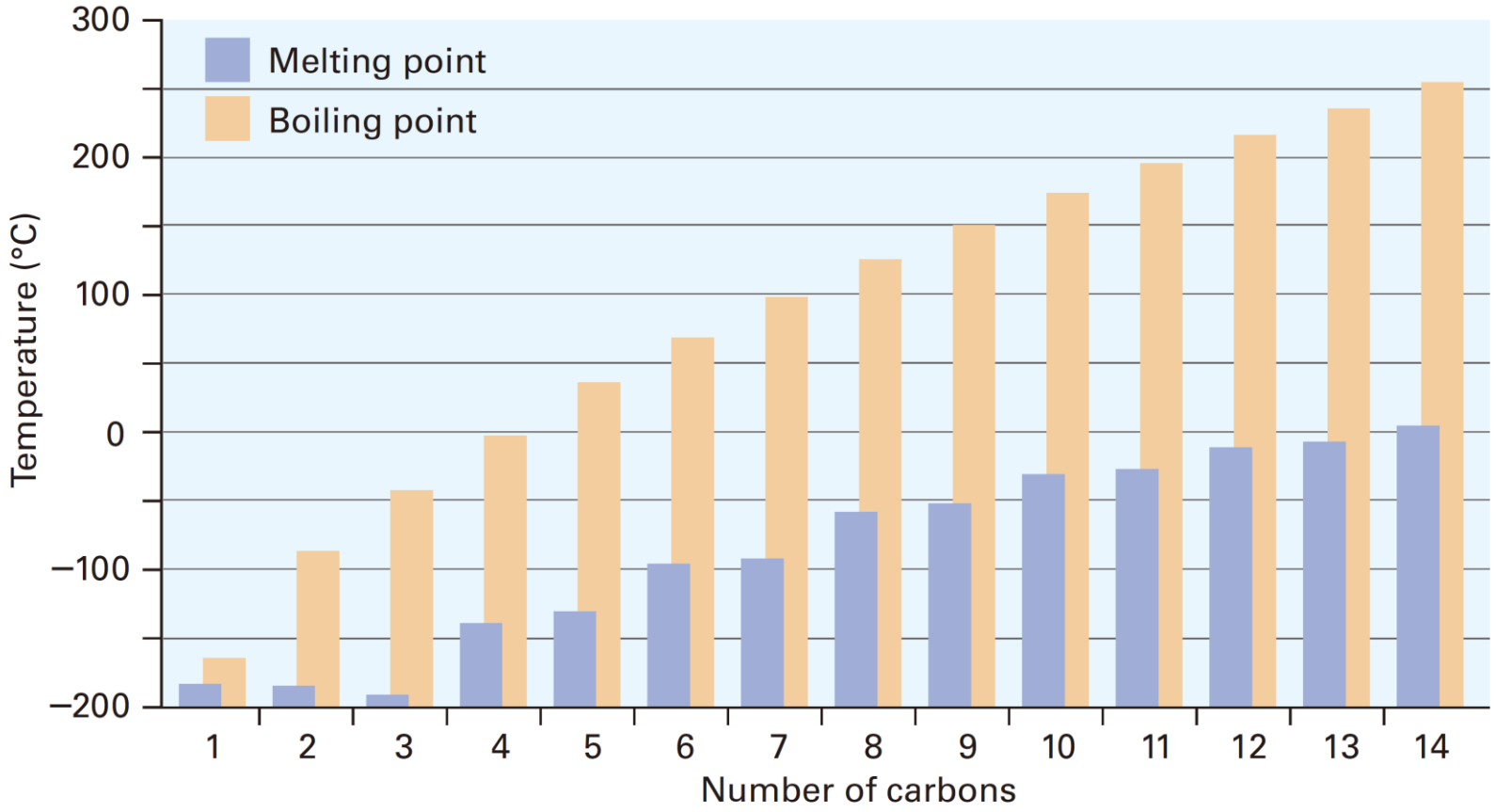


Figure 3.4 A plot of melting and boiling points versus number of carbon atoms for the C_1–C_{14} straight-chain alkanes. There is a regular increase with molecular size.

3.5 烷烃的性质

- 化学性质：燃烧和卤化

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O + 890\ kJ/mol\ (213\ kcal/mol)$$

$$CH_4 + Cl_2 \xrightarrow{h\nu} CH_3Cl + HCl$$

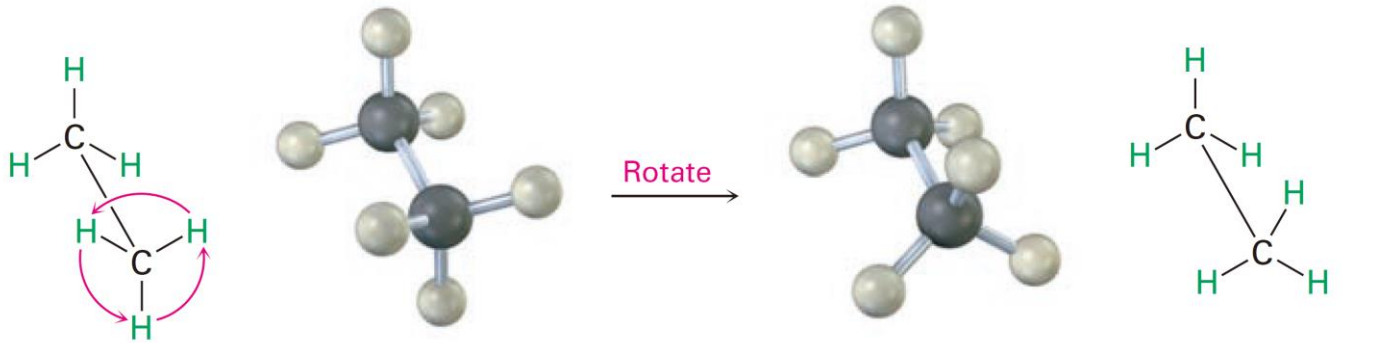
$$CH_3Cl \xrightarrow{Cl_2} CH_2Cl_2 + HCl$$

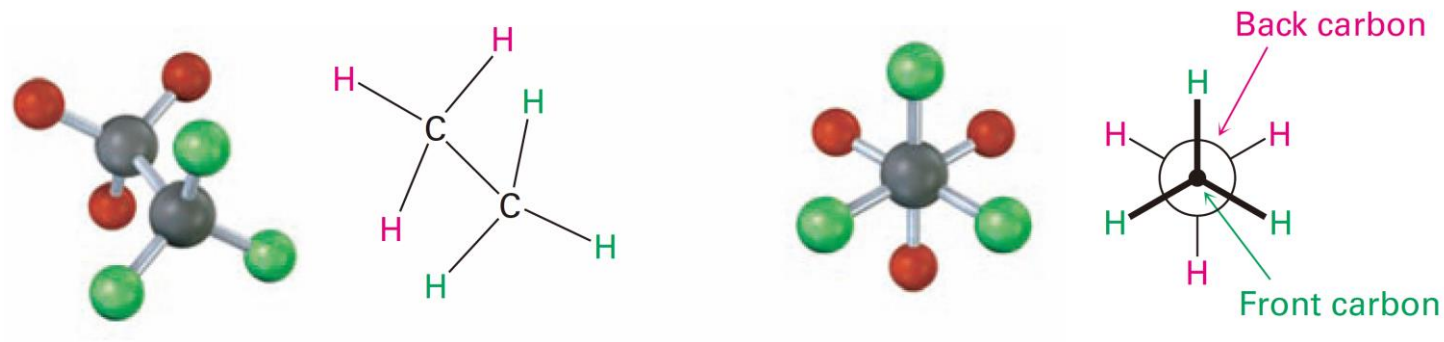
$$CH_2Cl_2 \xrightarrow{Cl_2} CHCl_3 + HCl$$

$$CHCl_3 \xrightarrow{Cl_2} CCl_4 + HCl$$

3.6 乙烷的构象

- 立体化学研究有机物在三维空间内的结构与变化。
- 构象指由于原子环绕于化学键四周，而导致结构式相同，却具有化学构象或构象异构体差异的分子现象。

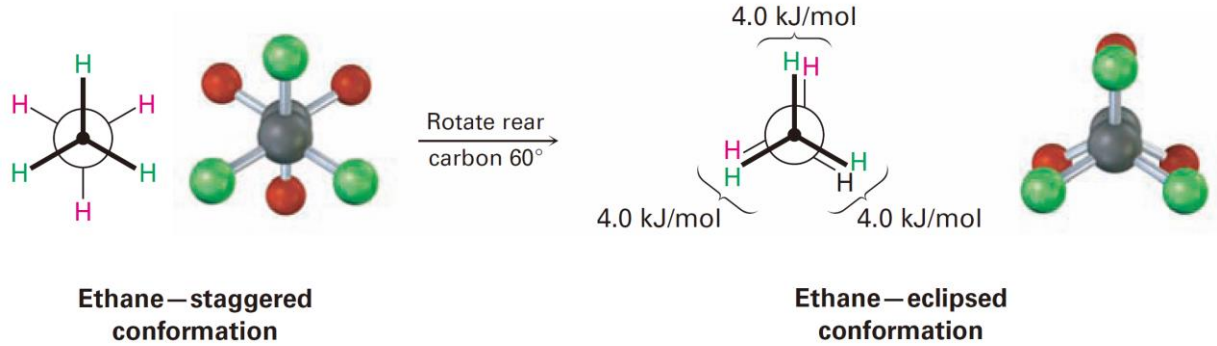


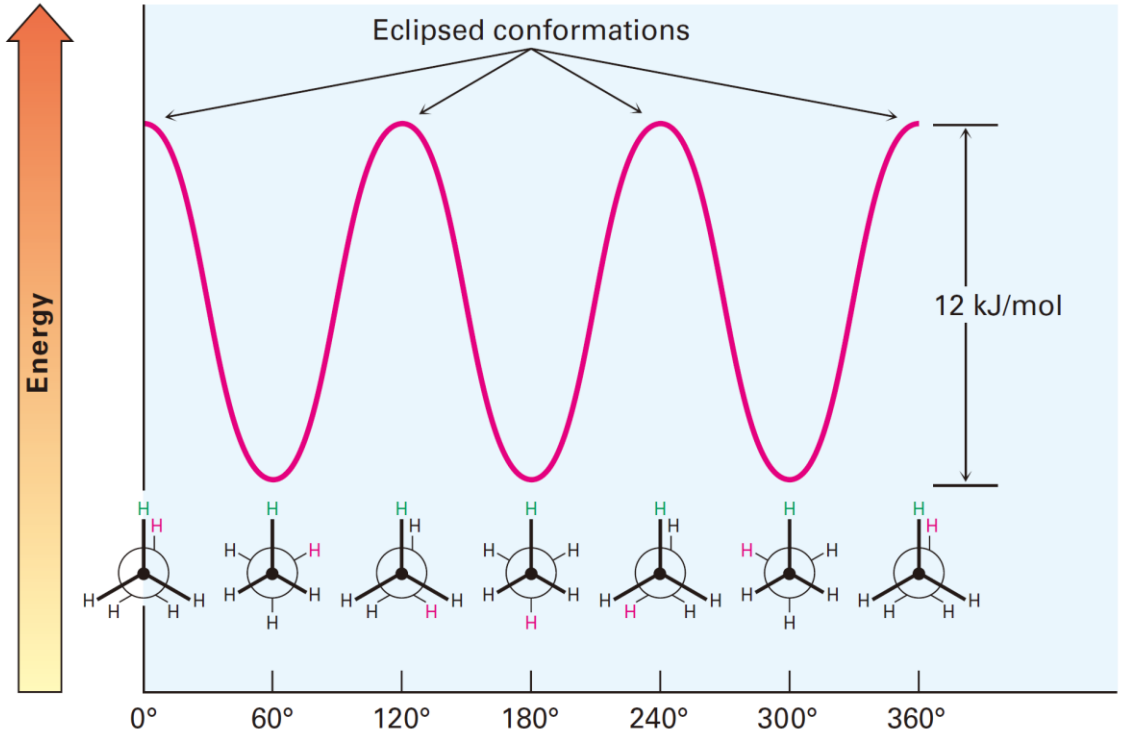


Sawhorse representation 锯架式

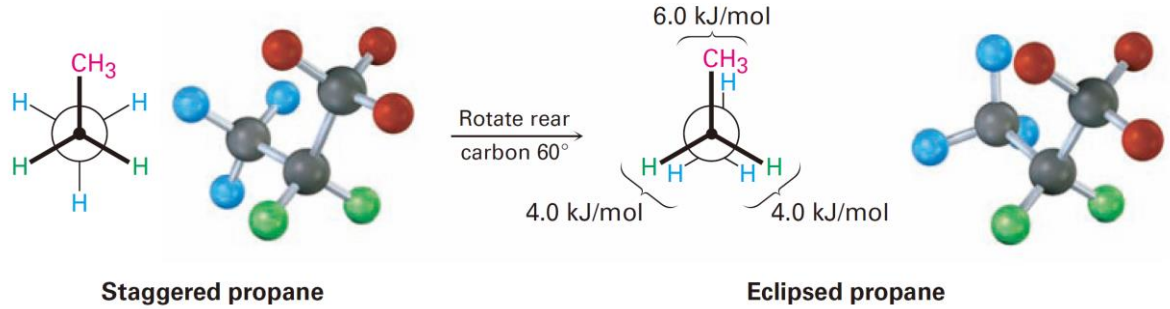
Newman projection 纽曼式

3.6 乙烷的构象

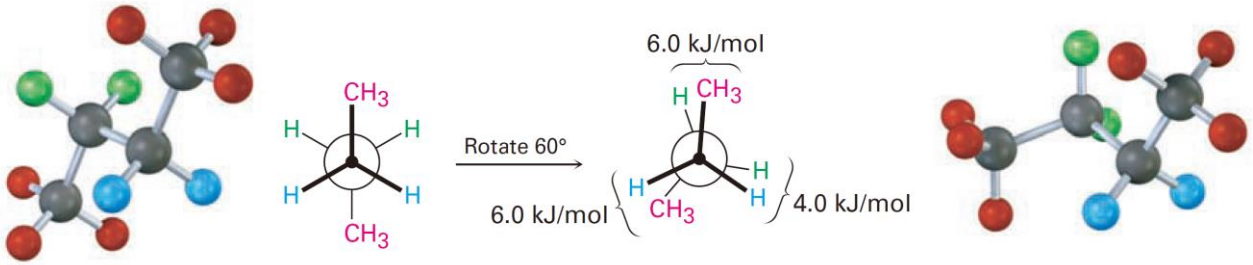

Rotate rear
carbon 60°
4.0 kJ/mol
4.0 kJ/mol
4.0 kJ/mol
Ethane—staggered conformation
Ethane—eclipsed conformation


Eclipsed conformations
Energy
12 kJ/mol
0°
60°
120°
180°
240°
300°
360°

3.7 丙烷和丁烷的构象

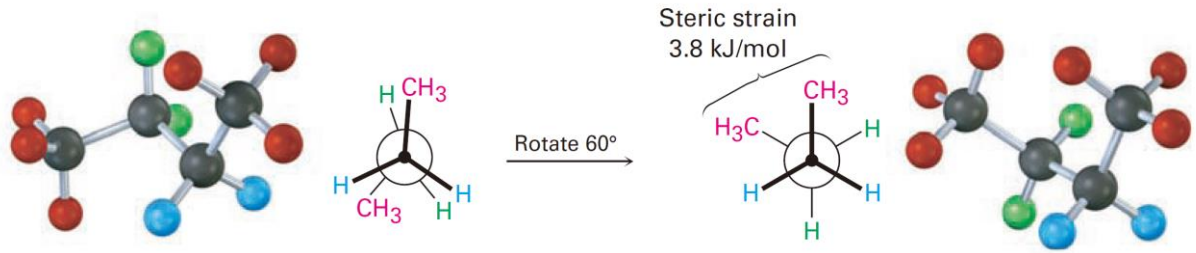


Staggered propane **Eclipsed propane**



Butane—anti conformation (0 kJ/mol)

Butane—eclipsed conformation (16 kJ/mol)



Butane—eclipsed conformation (16 kJ/mol)

Butane—gauche conformation (3.8 kJ/mol)

3.7 丙烷和丁烷的构象

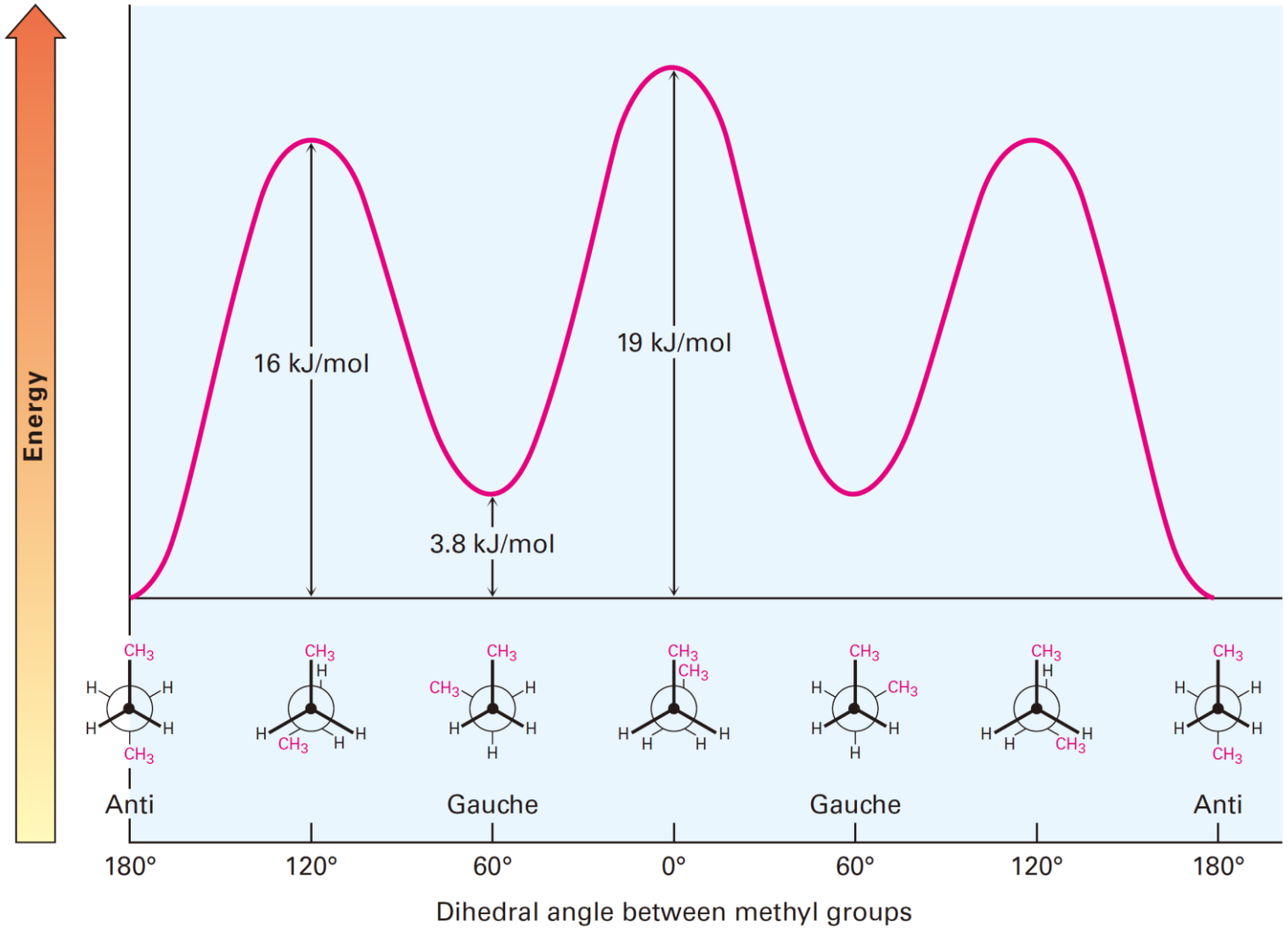


Figure 3.9 A plot of potential energy versus rotation for the C2—C3 bond in butane. The energy maximum occurs when the two methyl groups eclipse each other, and the energy minimum occurs when the two methyl groups are 180° apart (anti).

作业

- 3.48-3.53