Lecture 2

Classification, Representation & Nomenclature

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2020.11.05

Organic Compound Classification

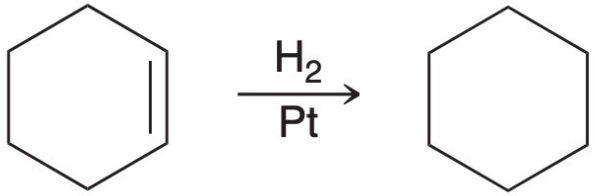
Functional Groups

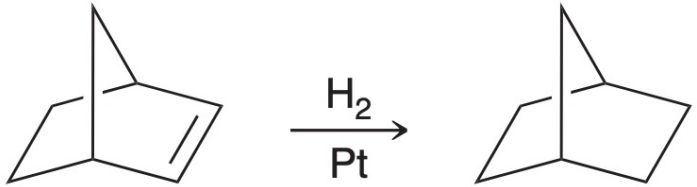
- B.M & M.P (states)
- Solubility
- The length of carbon chain
- The structure of carbon chain (linear, cyclic)

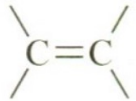
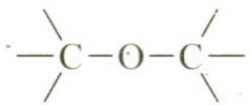
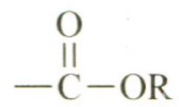
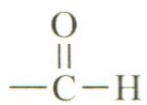
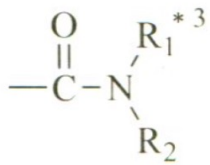
……

- **Functional group!**

- Functional group: An atom or group of atoms that determine the **chemical properties** of organic compounds

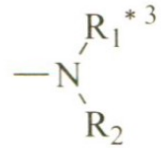
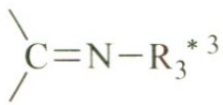
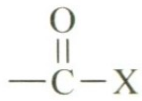
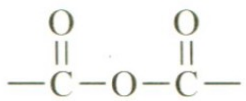




化合物类名	官能团结构	官能团名称	化合物类名	官能团结构	官能团名称
烯烃 alkene		碳碳双键 double bond	酚 phenol	—OH[*2]	羟基
炔烃 alkyne	—C≡C—	碳碳叁键 triple bond	硫醇 thio-alcohol	—SH[*1]	巯基 mercapto
卤代烃 halohydrocarbon	—X(F,Cl,Br,I)	卤原子 halogen atom	硫酚 thio-phenol	—SH[*2]	巯基
醇 alcohol	—OH[*1]	羟基 hydroxy	醚 ether		醚基 ether group
过氧化物 peroxide	—O—O—	过氧基 peroxy group	酯 ester		酯基 ester group
醛 aldehyde		醛基 aldehyde group	酰胺 amide		酰氨基 amide group

[*1] —OH 或—SH 与烃基直接相连。

[*2] —OH 或—SH 与芳环直接相连。

化合物类名	官能团结构	官能团名称	化合物类名	官能团结构	官能团名称
酮 ketone		羰基 carbonyl	胺 amine		氨基 amino
磺酸 sulfonic acid		磺(酸)基 sulfo	亚胺 imine		亚氨基 imino
羧酸 carboxylic acid		羧基 carboxy	硝基化合物 nitro compound		硝基 nitro
酰卤 acyl halide		酰卤基 acyl halide group	亚硝基化合物 nitroso compound		亚硝基 nitroso
酸酐 acid anhydride		酸酐基 acid anhydride group	腈 nitrile		氰基 cyano

*3 R_1, R_2, R_3 可以是氢也可以是烃基，R_1 与 R_2 可以相同也可以不同。

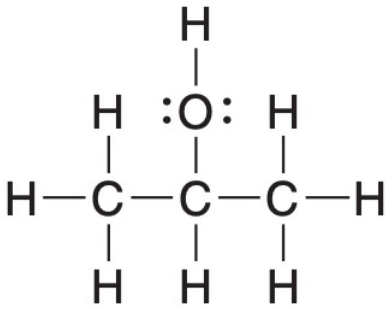
Molecular Representation

Skeletal Formula, Isomerism

Simple!

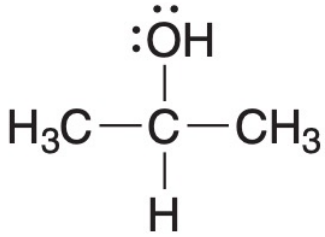
Simple!

Simple!



Lewis structure

Lewis结构式



Partially condensed structure

部分紧排式

$(CH_3)_2CHOH$

Condensed structure

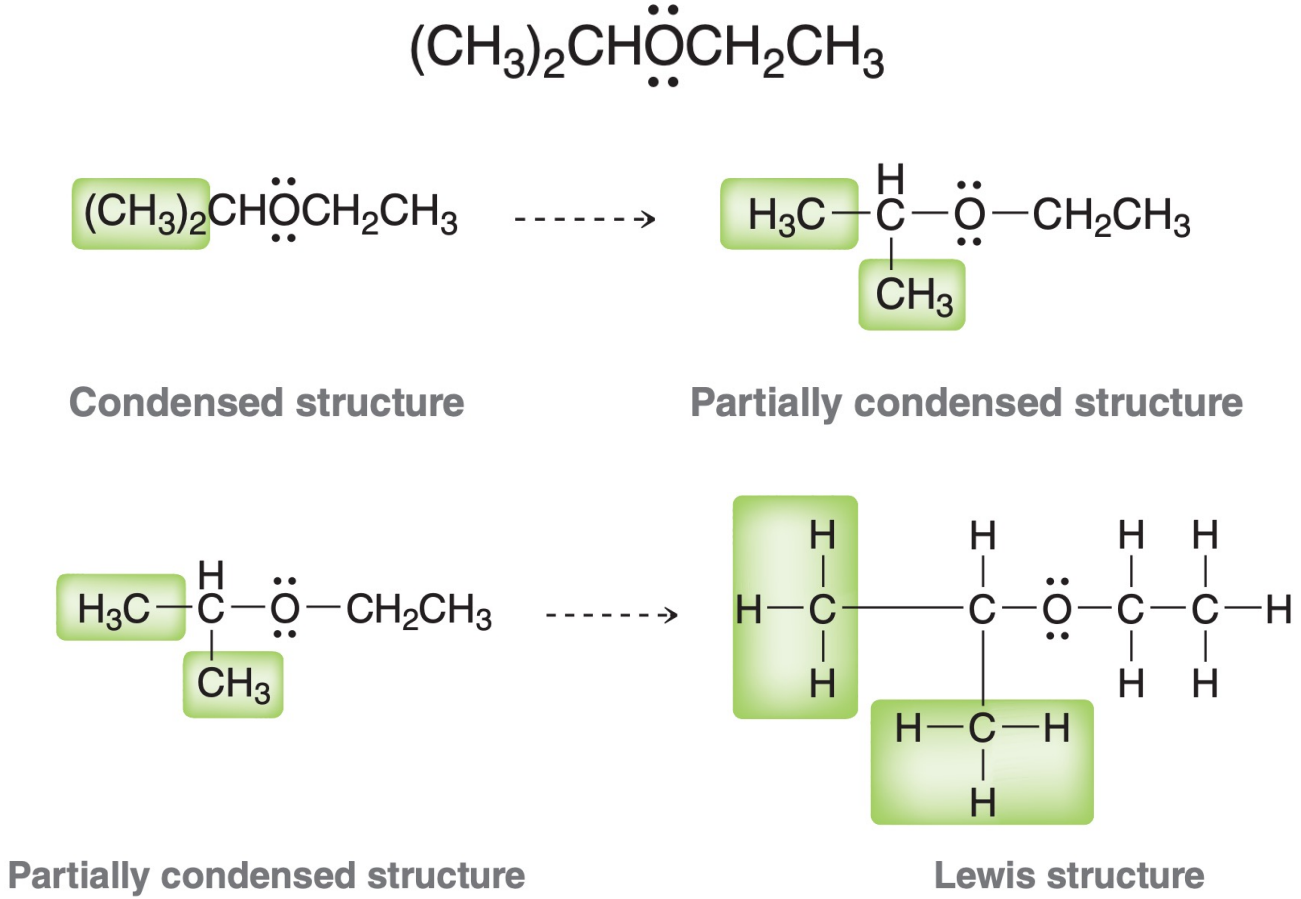
紧排式

C_3H_8O

Molecular formula

分子式

- Practice: draw a Lewis structure for the following compound:



- Practice: draw a Lewis structure for each of the compounds below:

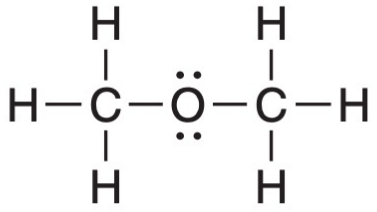
(a) $CH_2{=}CHOCH_2CH(CH_3)_2$

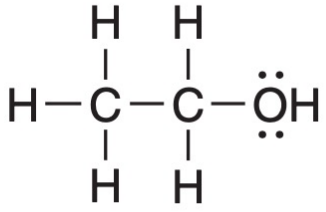
(b) $(CH_3CH_2)_2CHCH_2CH_2OH$

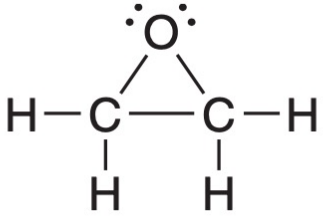
(c) $(CH_3CH_2)_3COH$

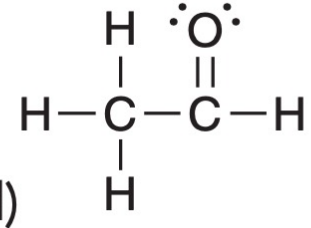
(d) $(CH_3)_2C{=}CHCH_2CH_3$

- Practice: draw a condensed structure for each of the compounds below:

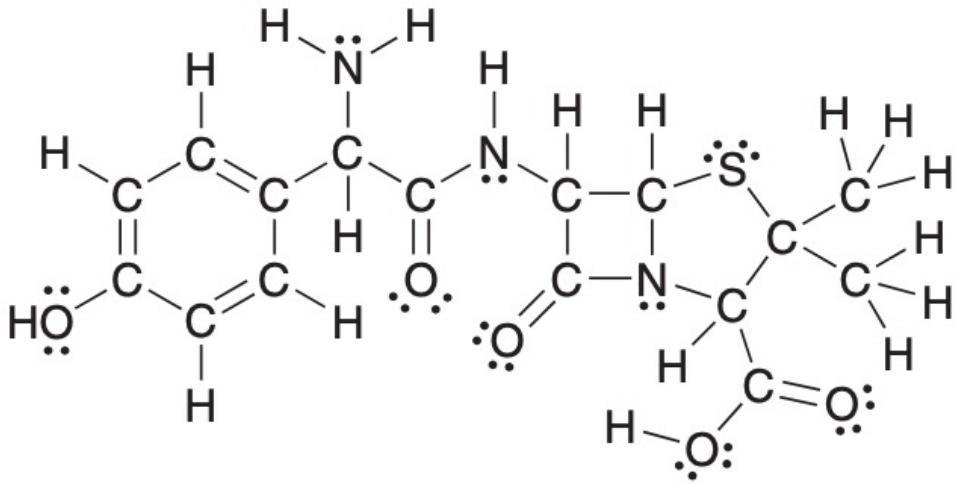
(a) 

(b) 

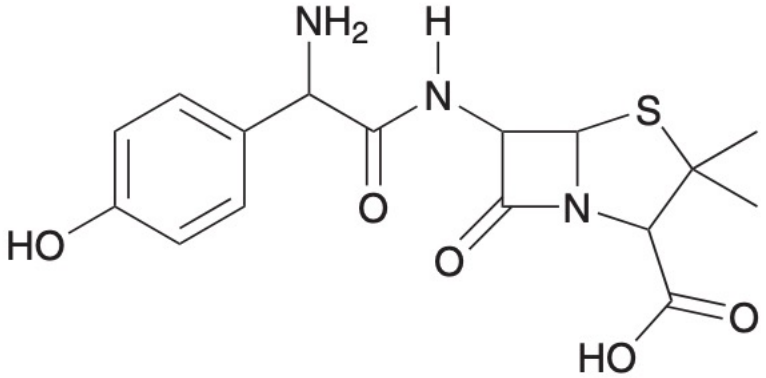
(c) 

(d) 

- Skeletal formula / bond-line structure

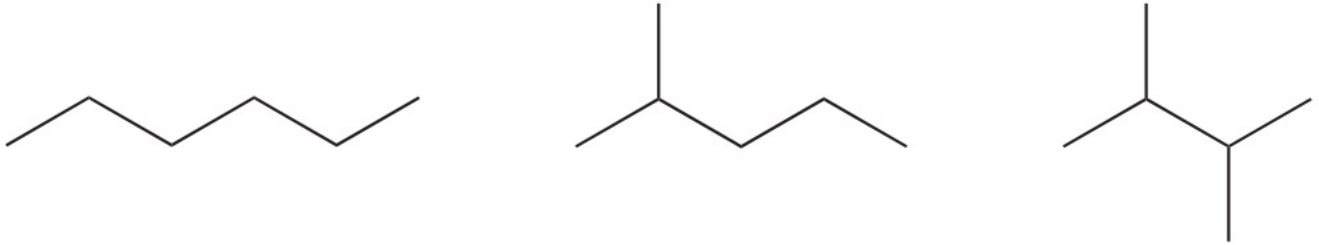


Amoxicillin



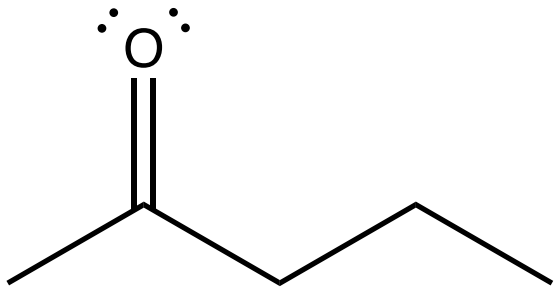
- 每一个拐角及端位为碳原子
- 碳原子上的氢被省略
- 杂原子（除C、H以外的所有原子，如O、Cl、S等）需要表示出来
- 杂原子上的氢不能省略

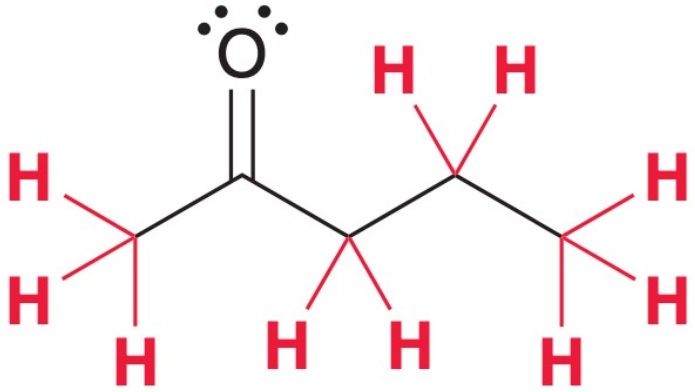
- Single bond



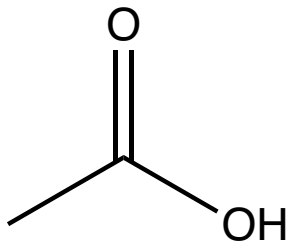
- Multiple bond

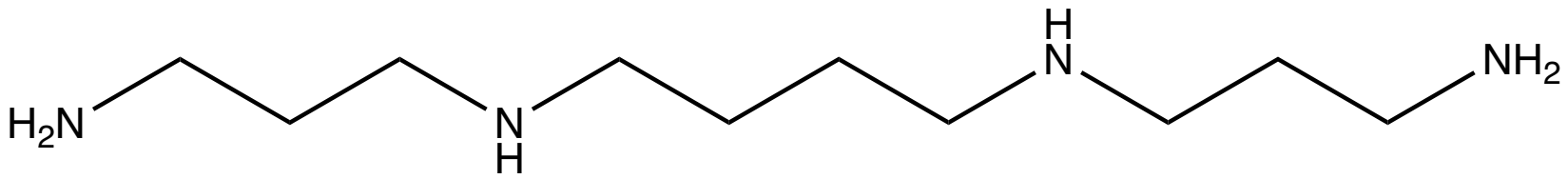
- 拐角用H补齐



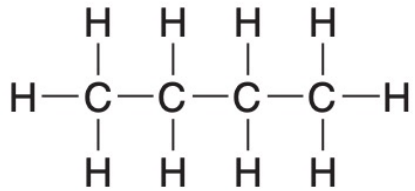


- 杂原子上的氢不能省



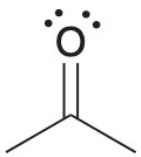


1. Carbon atoms in a straight chain should be drawn in a zigzag format:

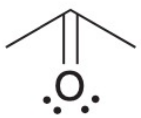


is drawn like this:

2. When drawing double bonds, draw all bonds as far apart as possible:

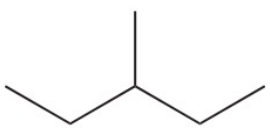


is much better than

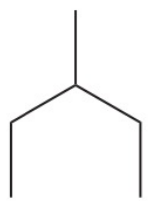


Bad

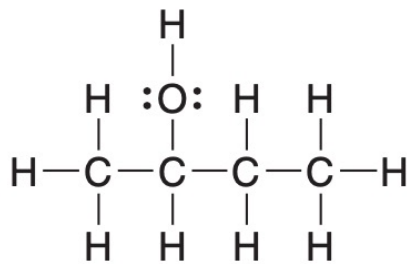
3. When drawing single bonds, the direction in which the bonds are drawn is irrelevant:



is the same as

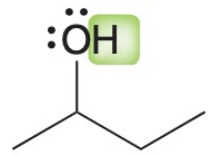


4. All *heteroatoms* (atoms other than carbon and hydrogen) must be drawn, and any hydrogen atoms attached to a heteroatom must also be drawn. For example:



is drawn like this:

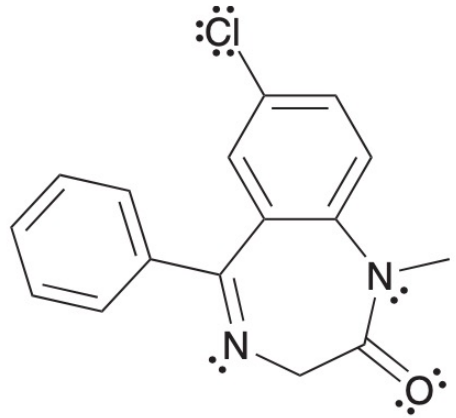
This H must be drawn:



5. Never draw a carbon atom with more than four bonds. Carbon only has four orbitals in its valence shell, and therefore carbon atoms can form a maximum of four bonds.

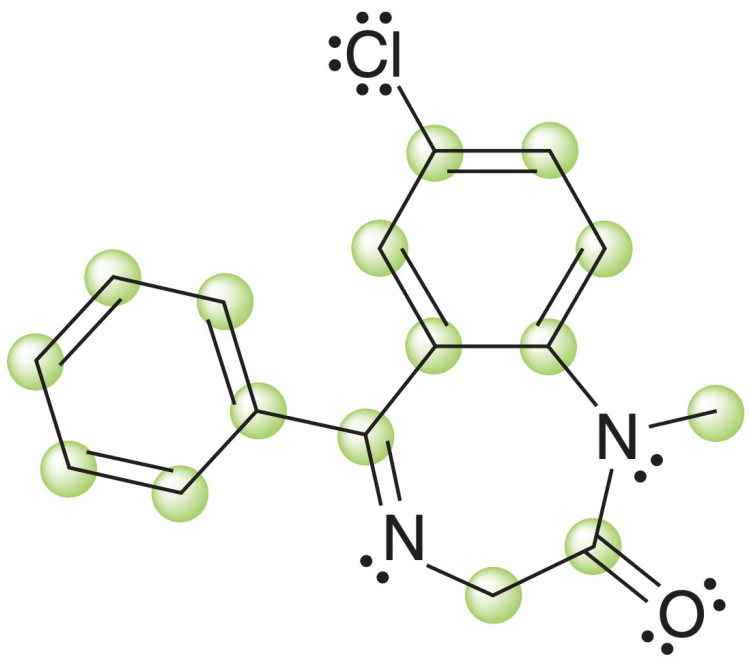
- Practice

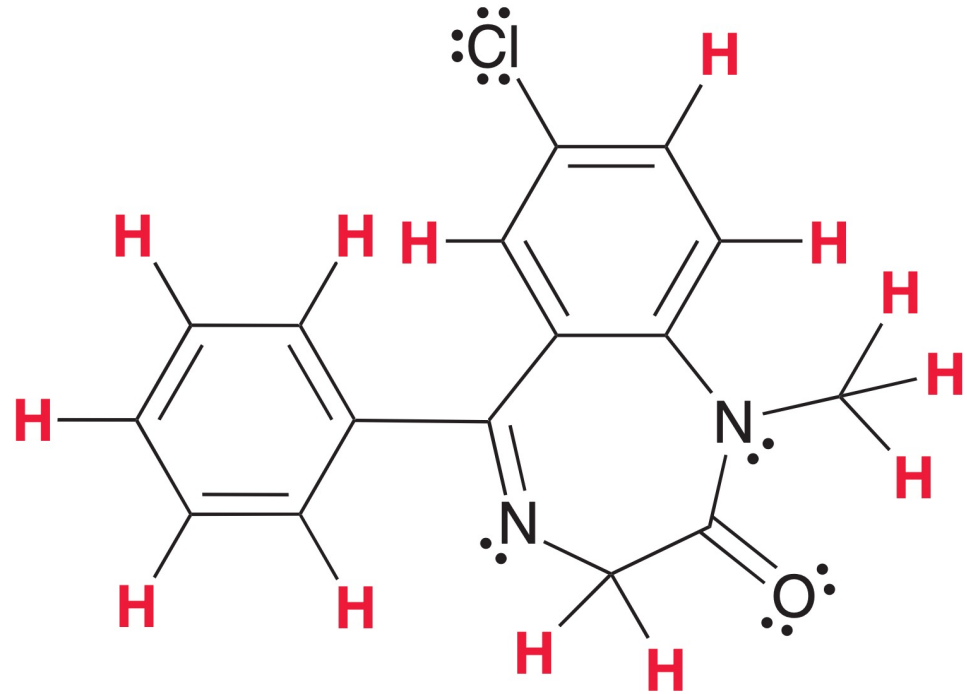
Consider the structure of diazepam, first marketed by the Hoffmann-La Roche Company under the trade name Valium. Diazepam is a sedative and muscle relaxant used in the treatment of anxiety, insomnia, and seizures. Identify the number of carbon atoms in diazepam, then fill in all the missing hydrogen atoms that are inferred by the drawing.



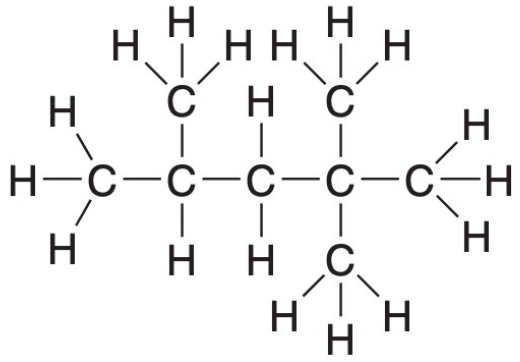
Diazepam (Valium)

Skeletal Formula

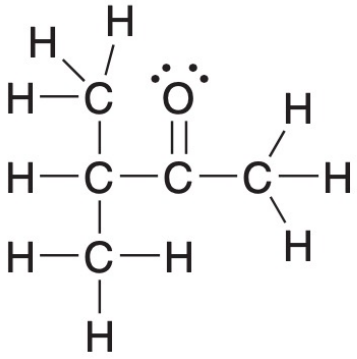




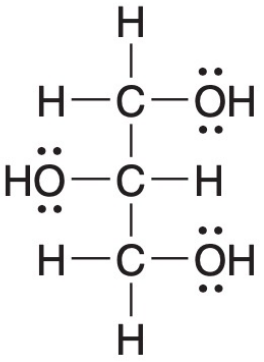
- Practice: draw a skeletal formula for the following compounds:



(a)



(b)



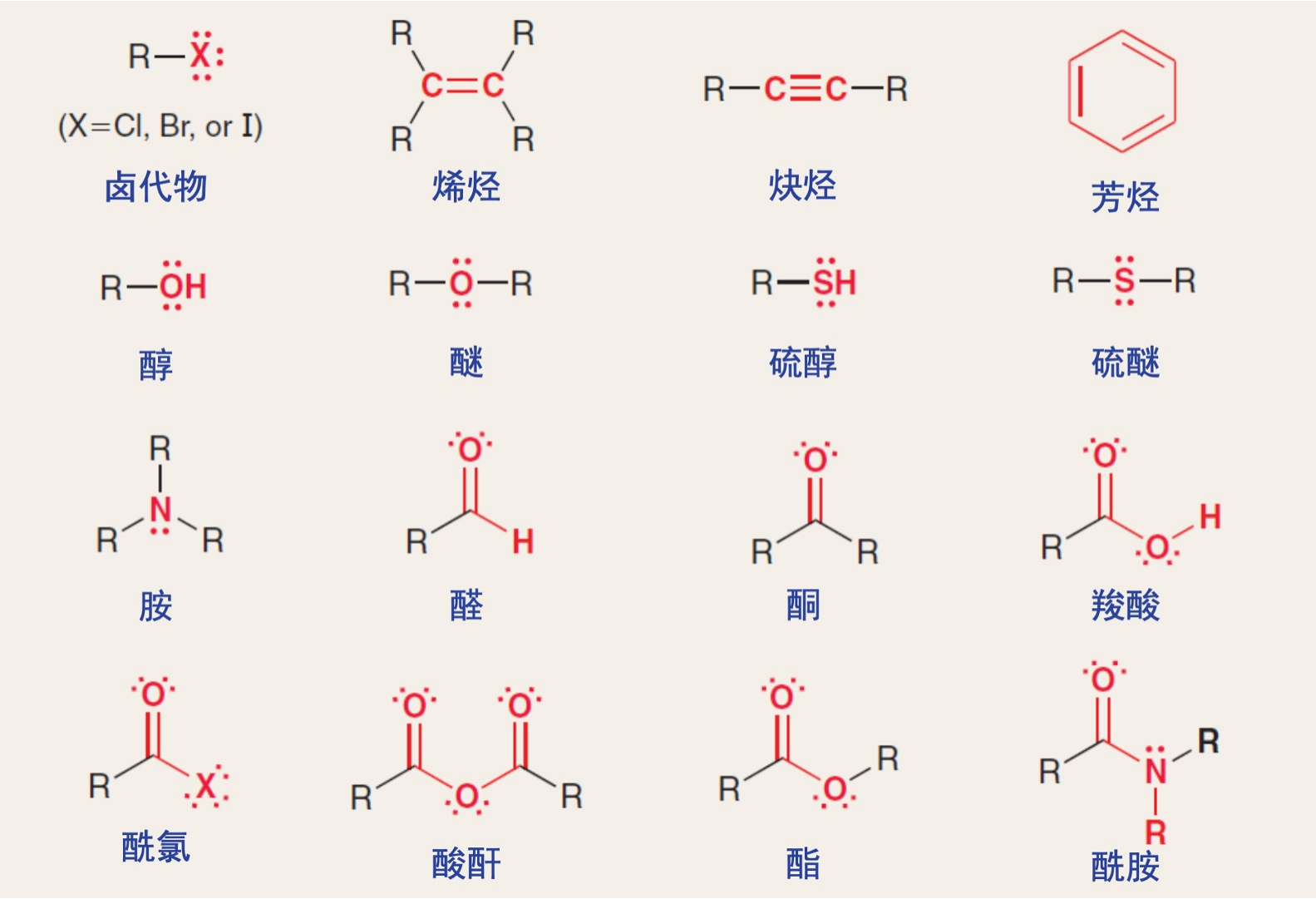
(c)

(d) $(CH_3)_3C—C(CH_3)_3$

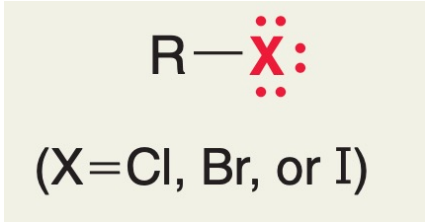
(e) $CH_3CH_2CH(CH_3)_2$

(f) $(CH_3CH_2)_3COH$

- Skeletal formula: functional groups

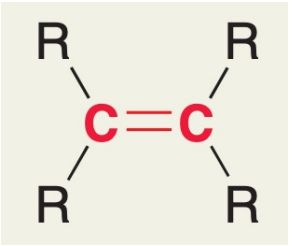


- 卤素(halogen)



卤代烃
alkyl halide

- 碳碳双键(carbon-carbon double bond)



烯烃
alkene

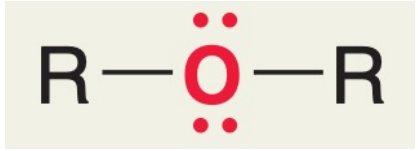
- 碳碳三键(carbon-carbon triple bond)

炔烃
alkyne

- 羟基(hydroxyl)

醇/酚
alcohol/phenol

- 醚键(ether group)

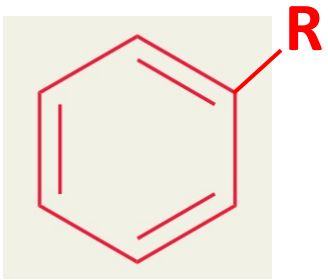


醚
ether

- 巯基(thiol/sulfhydryl)

硫醇
mercaptan/thiol-alcohol

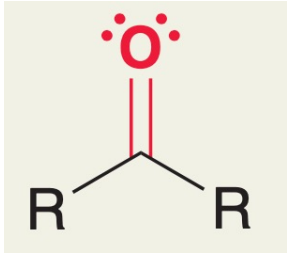
- 苯基(phenyl)

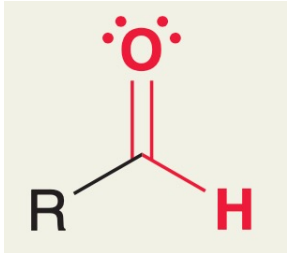


芳香化合物

aromatic compound

- 羰基(carbonyl)



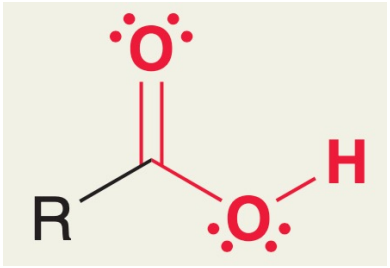


羰基化合物（酮/醛）

carbonyl compound

(ketone/aldehyde)

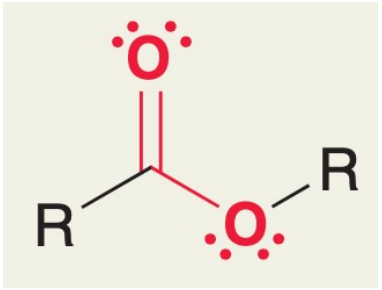
- 羧基(carboxyl)



羧酸

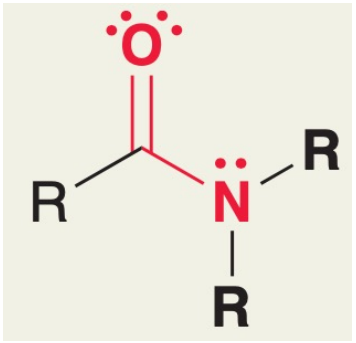
carboxylic acid

- 酯基(ester group)



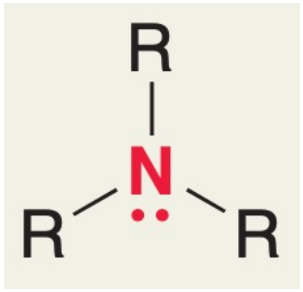
酯
ester

- 酰胺基(amide group)



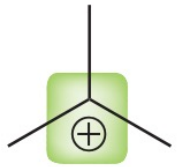
酰胺
amide

- 氨基(amino)



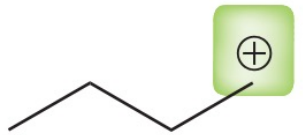
胺
amine

- Skeletal formula: charges on carbon

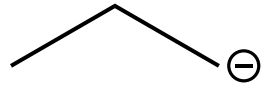


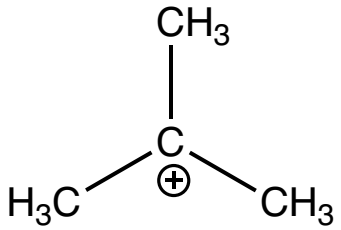
No hydrogen atoms on this C^+

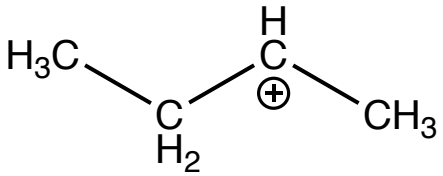
One hydrogen atom on this C^+

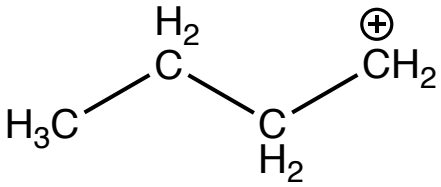


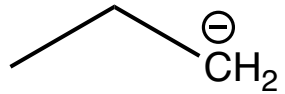
Two hydrogen atoms on this C^+



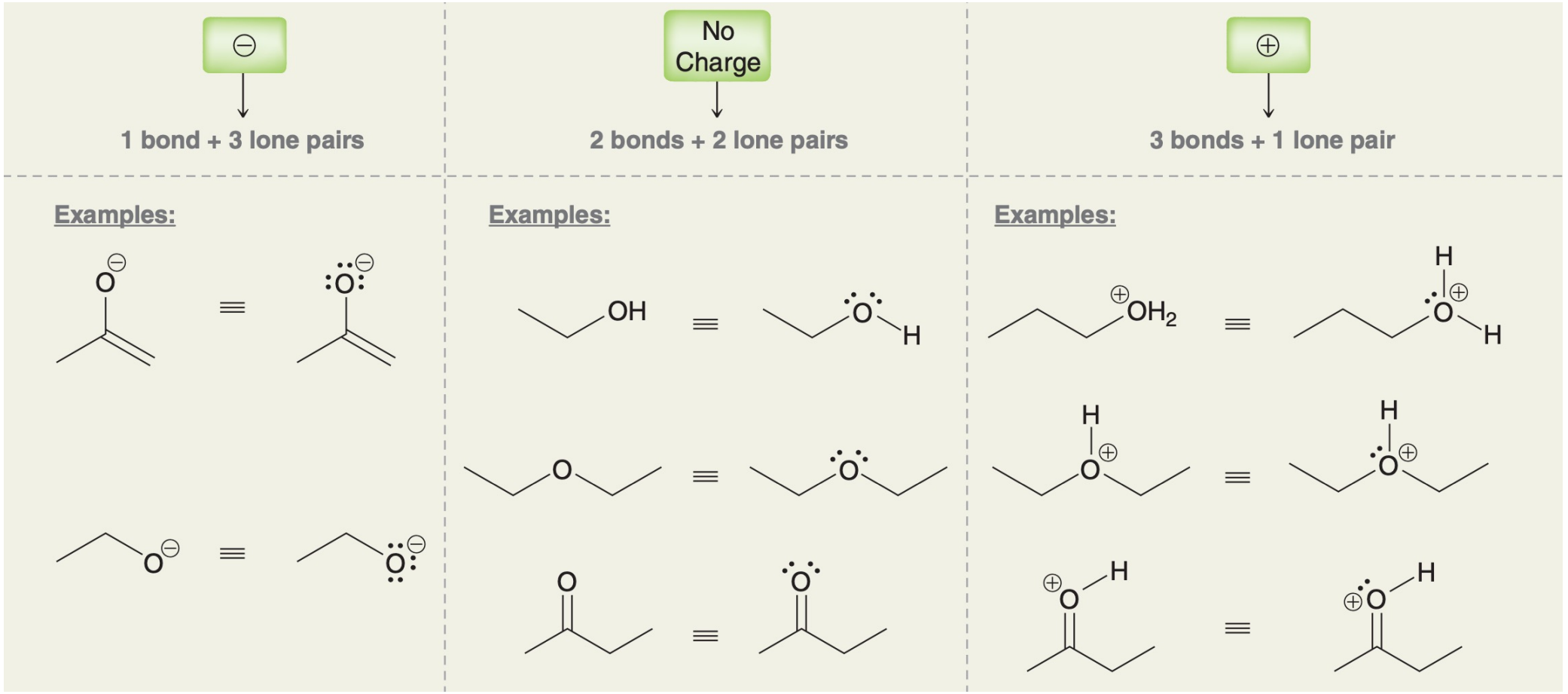




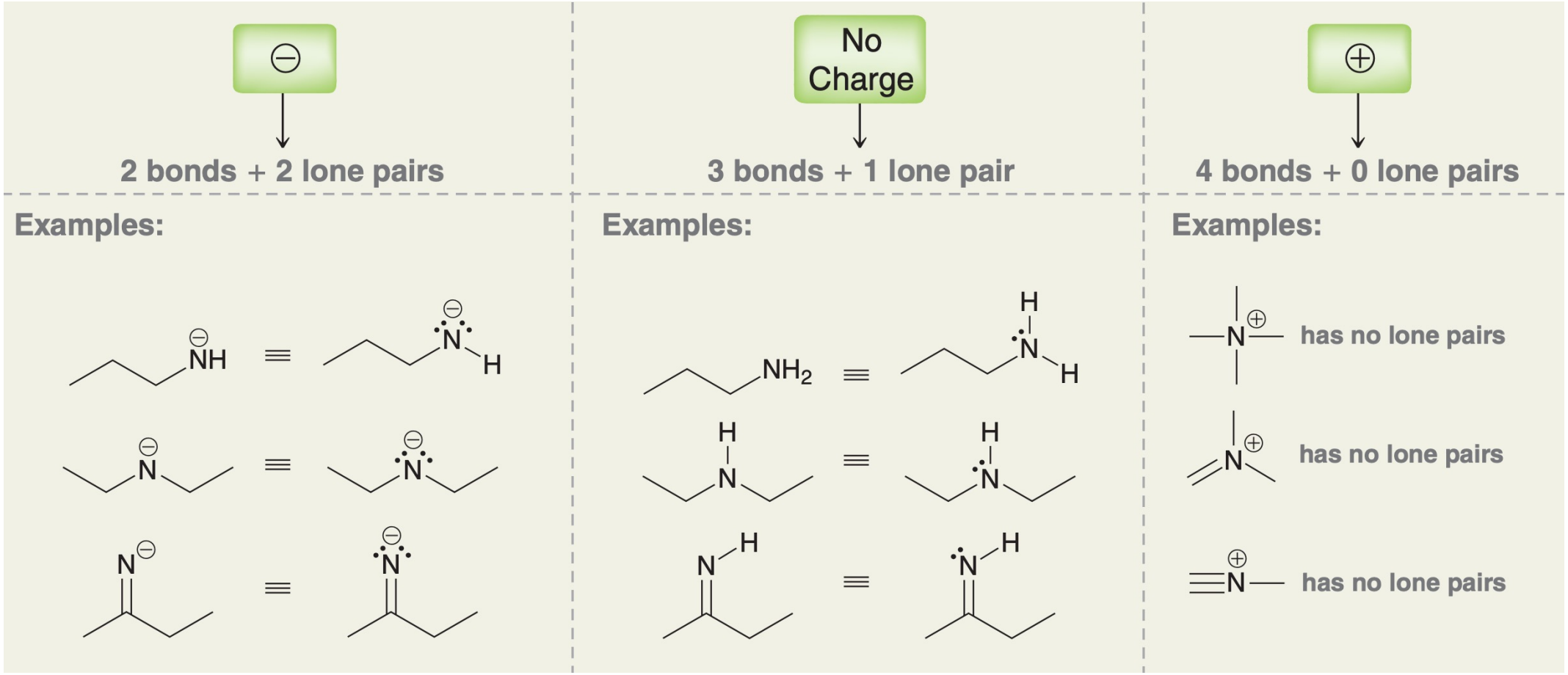




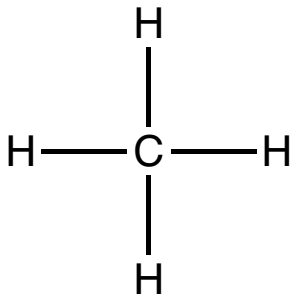
- Skeletal formula: charges on oxygen

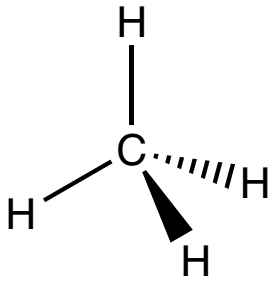


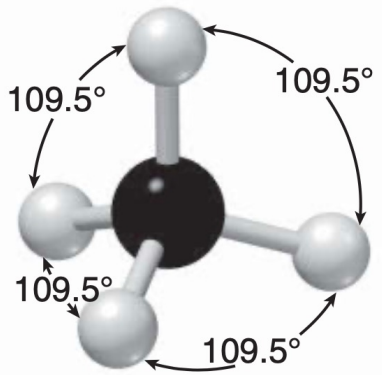
- Skeletal formula: charges on nitrogen

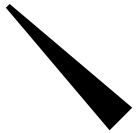


- 伞形式：立体空间中的分子





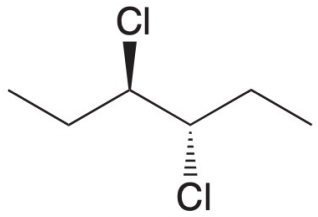




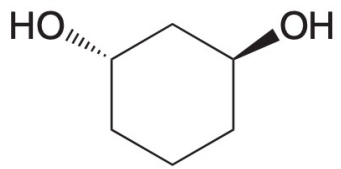
楔形实线：伸向纸面外
wedge

楔形虚线：伸向纸面内
dash

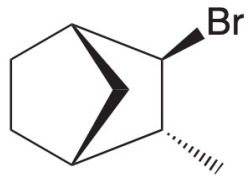
- Special representations of cyclic compounds



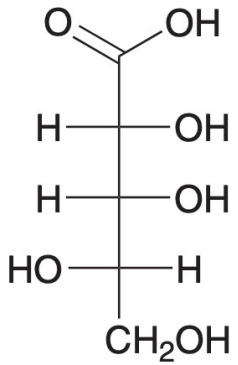
Acyclic
(No ring)



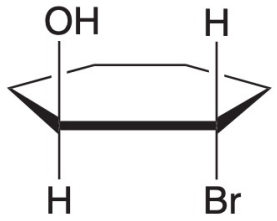
Cyclic
(One ring)



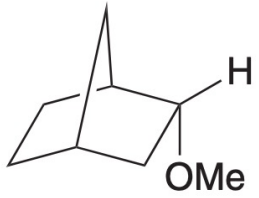
Bicyclic
(Two rings)



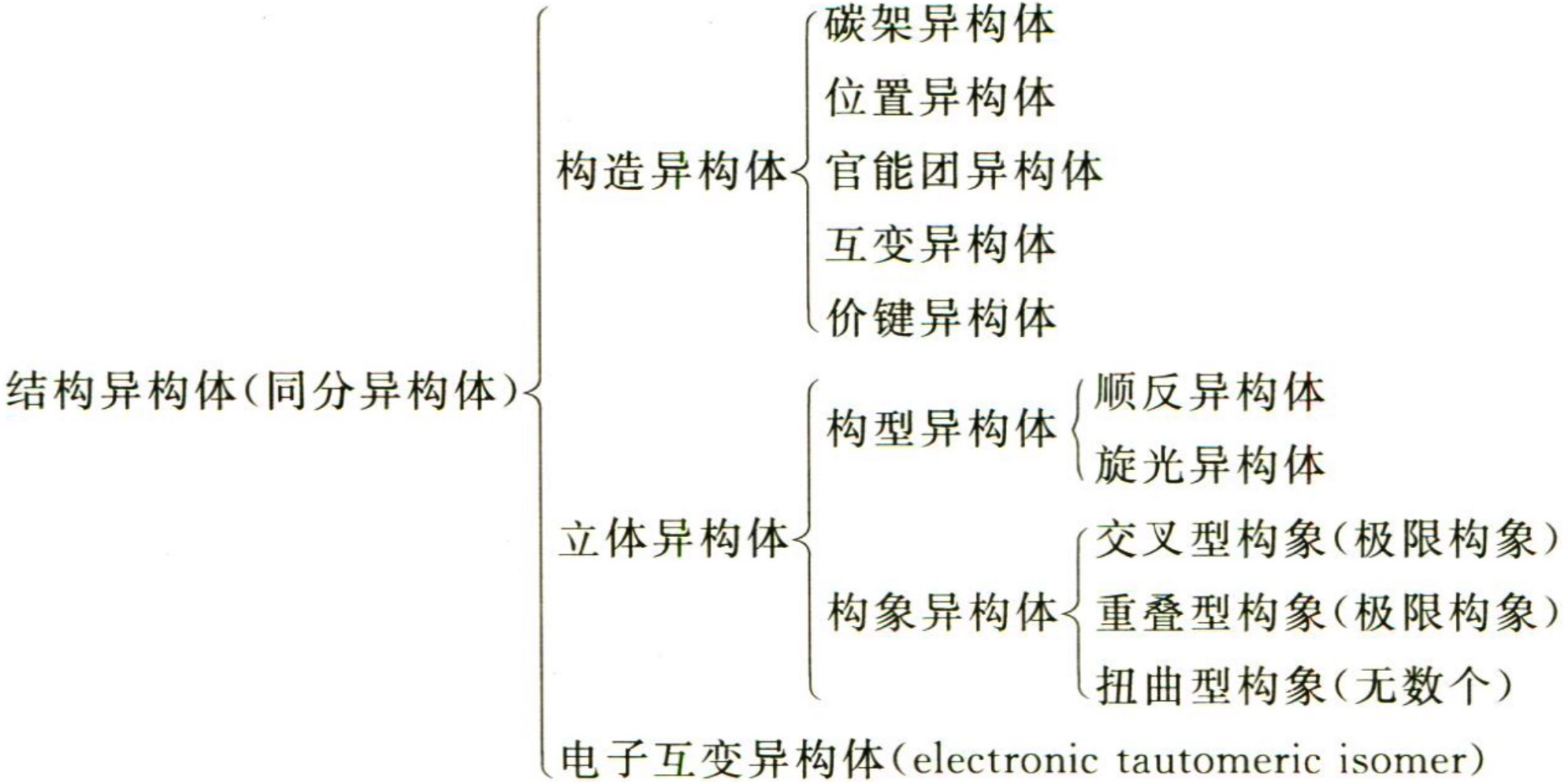
Fischer projection
(Used only for
acyclic compounds)



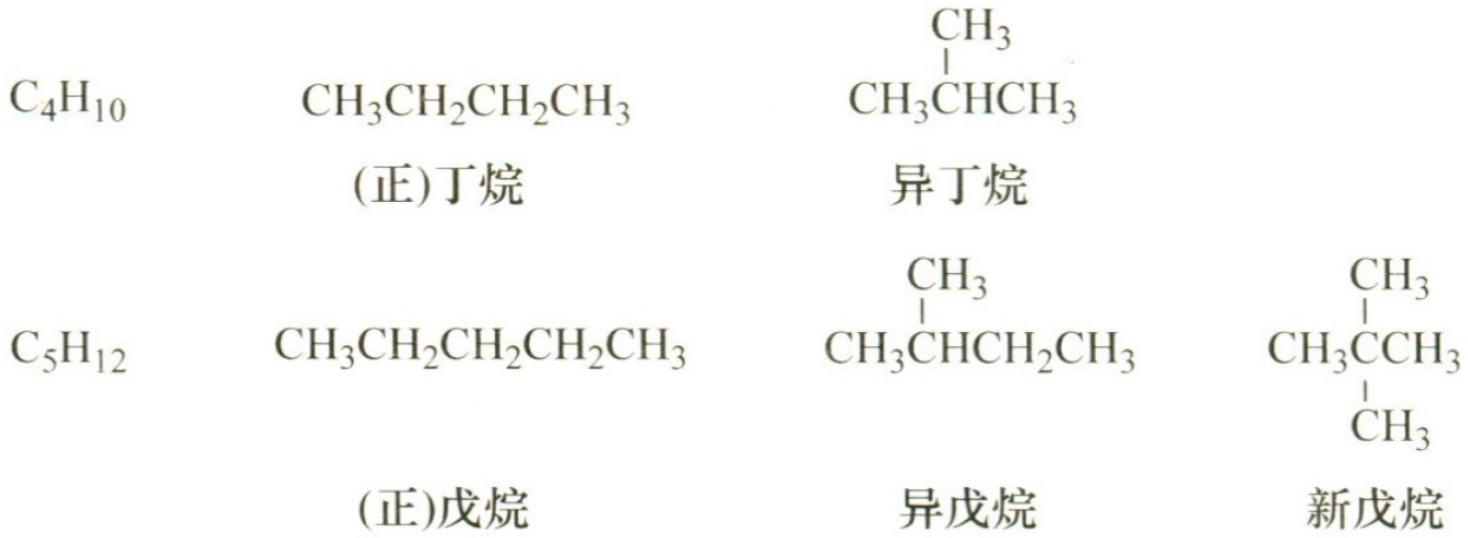
Haworth projection
(Used only for
cyclic compounds)



(Used only for
bicyclic compounds)


结构异构体(同分异构体)
构造异构体
碳架异构体
位置异构体
官能团异构体
互变异构体
价键异构体
立体异构体
构型异构体
顺反异构体
旋光异构体
构象异构体
交叉型构象(极限构象)
重叠型构象(极限构象)
扭曲型构象(无数个)
电子互变异构体(electronic tautomeric isomer)

- 碳架异构体(carbon skeleton isomer)



- 位置异构体(position isomer)

C_3H_8O

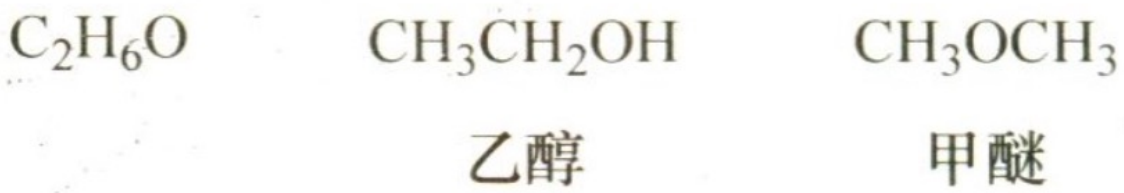
$CH_3CH_2CH_2OH$

正丙醇

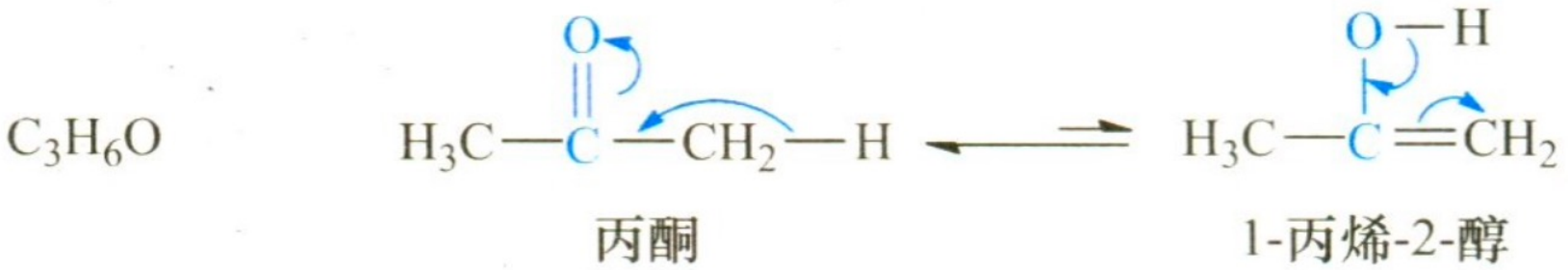
CH_3CHCH_3
|
OH

异丙醇

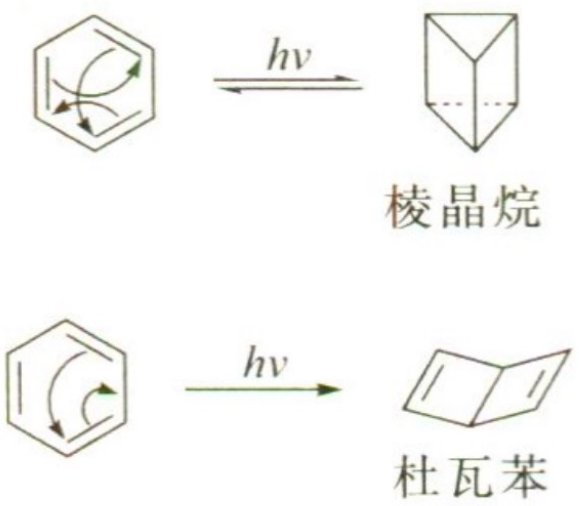
- 官能团异构体(functional group isomer)



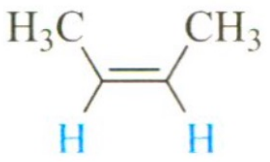
- 互变异构体(tautomeric isomer)



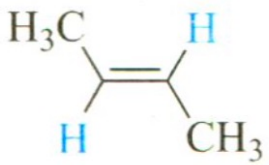
- 价键异构体(valence bond isomer)



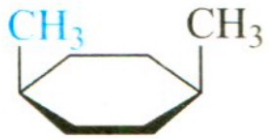
- 构型异构体(configuration isomer)



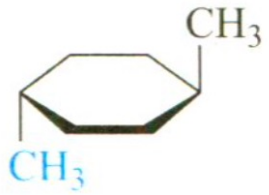
顺-2-丁烯



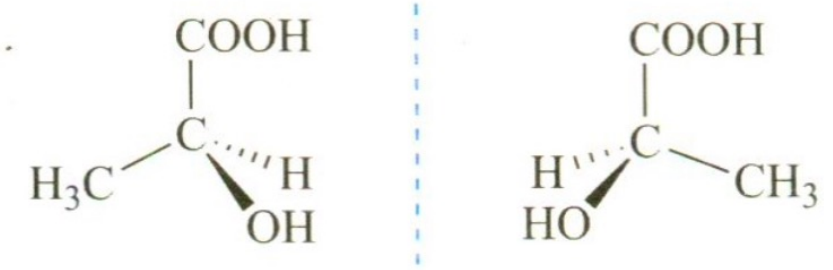
反-2-丁烯



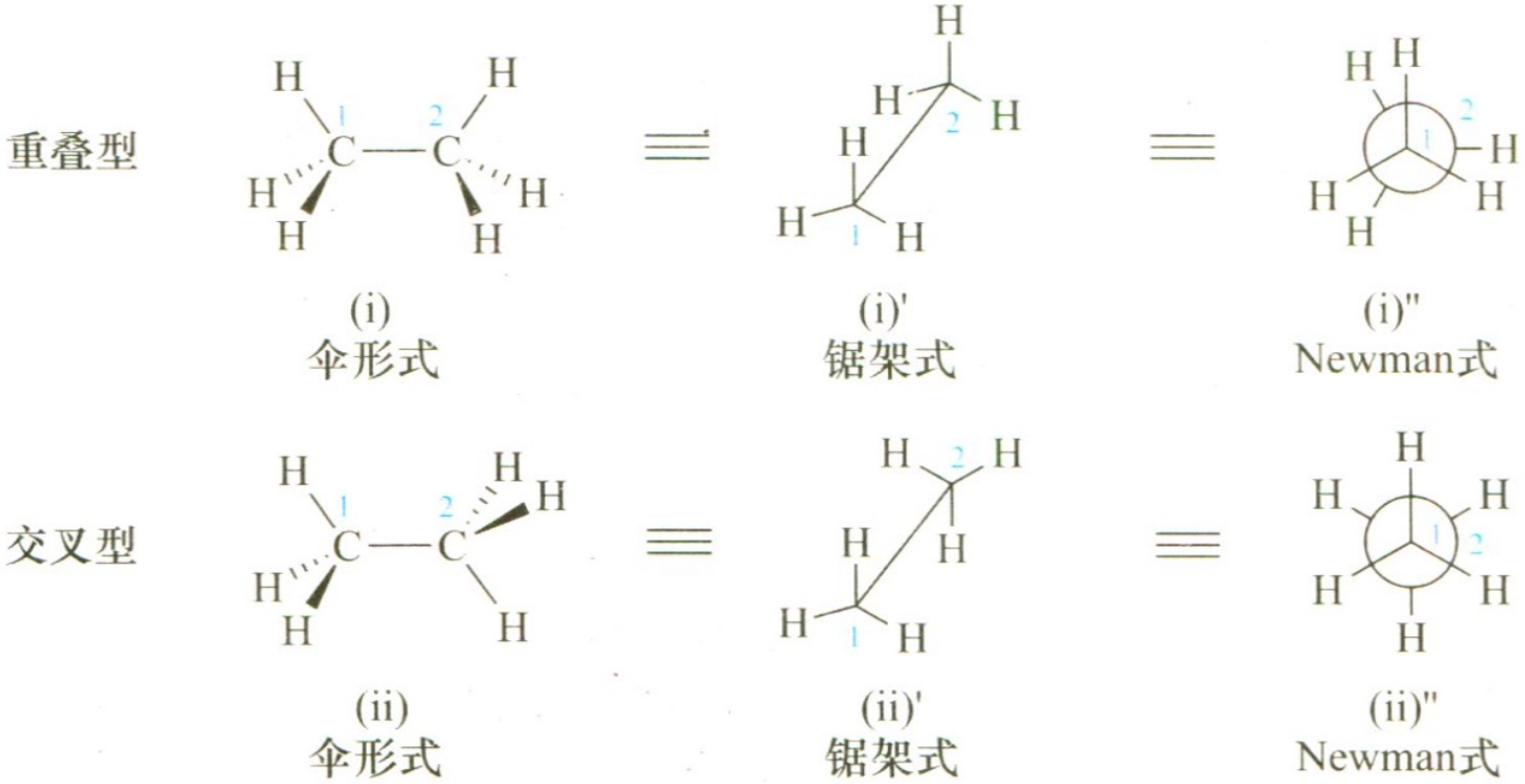
顺-1,4-二甲基环己烷



反-1,4-二甲基环己烷



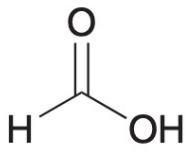
- 构象异构体(conformational isomer)



Nomenclature

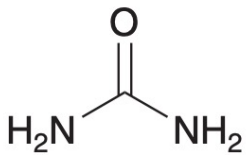
Common (Trivial) Nomenclature, Systematic Nomenclature

- 物质的俗名



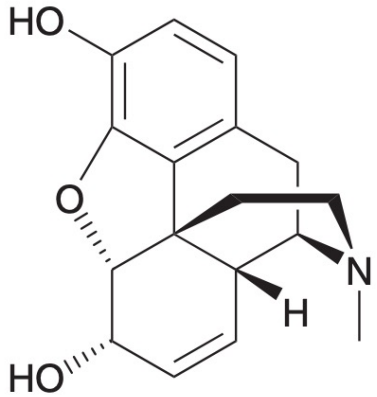
Formic acid
Isolated from ants
and named after the
Latin word for ant, *formica*

蚁酸



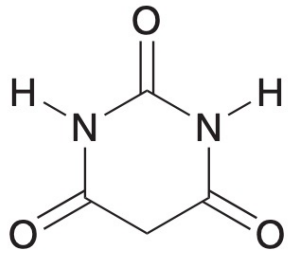
Urea
Isolated from urine

尿素



Morphine
A painkiller named after
the Greek god of dreams,
Morpheus

吗啡



Barbituric acid
Adolf von Baeyer named this
compound in honor of a
woman named Barbara

巴比妥酸

- 普通命名法

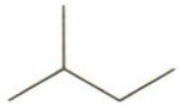
烷烃	相应的烷基	普通命名法 中文名称(英文名称)
甲烷 CH_4	CH_3-	甲基(methyl,缩写 Me)
乙烷 CH_3CH_3	CH_3CH_2-	乙基(ethyl,缩写 Et)
丙烷 $CH_3CH_2CH_3$	$CH_3CH_2CH_2-$	(正)丙基[*1](*n*-propyl,缩写 *n*-Pr)[*2]
	$CH_3\overset{1}{C}H\overset{2}{C}H_3$ (C1 上有一根向下的键)	异丙基(isopropyl,缩写 *i*-Pr)
(正)丁烷 $CH_3(CH_2)_2CH_3$	$CH_3CH_2CH_2CH_2-$	(正)丁基(*n*-butyl,缩写 *n*-Bu)
	$\overset{3}{C}H_3\overset{2}{C}H_2\overset{1}{C}HCH_3$ (C1 上有一根向下的键)	二级丁基或仲丁基 (*sec*-butyl,缩写 *s*-Bu)
异丁烷 CH_3CHCH_3 (中间 C 上连 CH_3)	$\overset{3}{C}H_3\overset{2}{C}H\overset{1}{C}H_2-$ (C2 上连 CH_3)	异丁基(isobutyl,缩写 *i*-Bu)
	$CH_3\overset{2}{C}CH_3$ (中间 C 上有一根向上的键,下连 CH_3)	三级丁基或叔丁基 (*tert*-butyl,缩写 *t*-Bu)

*1 括号中的正字可以省略。

*2 在英文命名时,正用 *n*-,异用 *iso*-或 *i*-,新用 neo,二级用词头 *sec*-(或 *s*-),三级用词头 *tert*-(或 *t*-)表示,后面有一短横线。

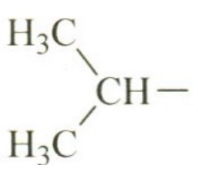
- 数出碳原子个数
- 按照天干顺序进行命名（甲、乙、丙、丁…）
- 支链按照正(*n*-)、异(*iso*-)、新(*neo*-)来表示
- eg.

(正)戊烷

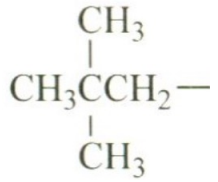


异戊烷

新戊烷

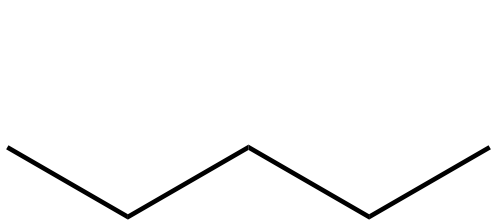


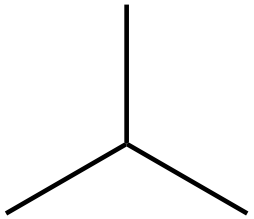
含“异”的碳链尾端结构

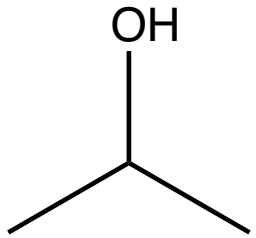


含“新”的碳链尾端结构

- Practice: 用普通命名法给下列化合物命名（中/英）：



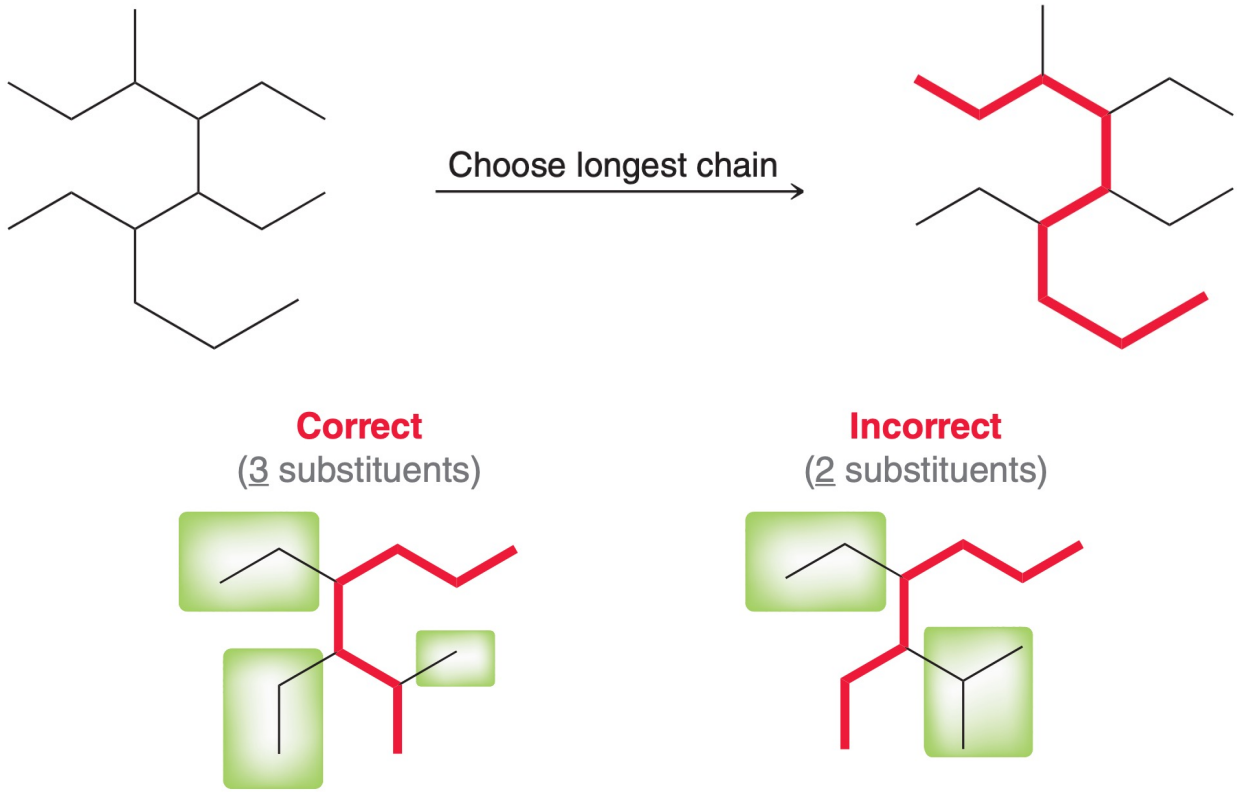




- 系统命名法 – Systematic Nomenclature ***by IUPAC***
- IUPAC – 国际纯粹与应用化学联合会
  International Union of Pure and Applied Chemistry

- 系统命名法的烷烃命名
  1. 确定主链：碳链最长、取代基最多
  2. 确定取代基种类
  3. 确定取代基编号
  4. 进行命名（天干：甲乙丙丁…）

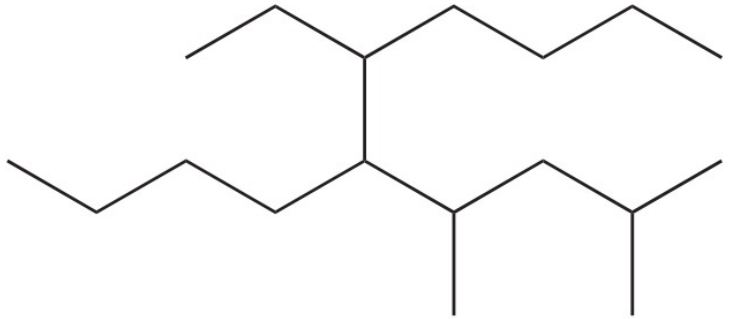
- 确定主链

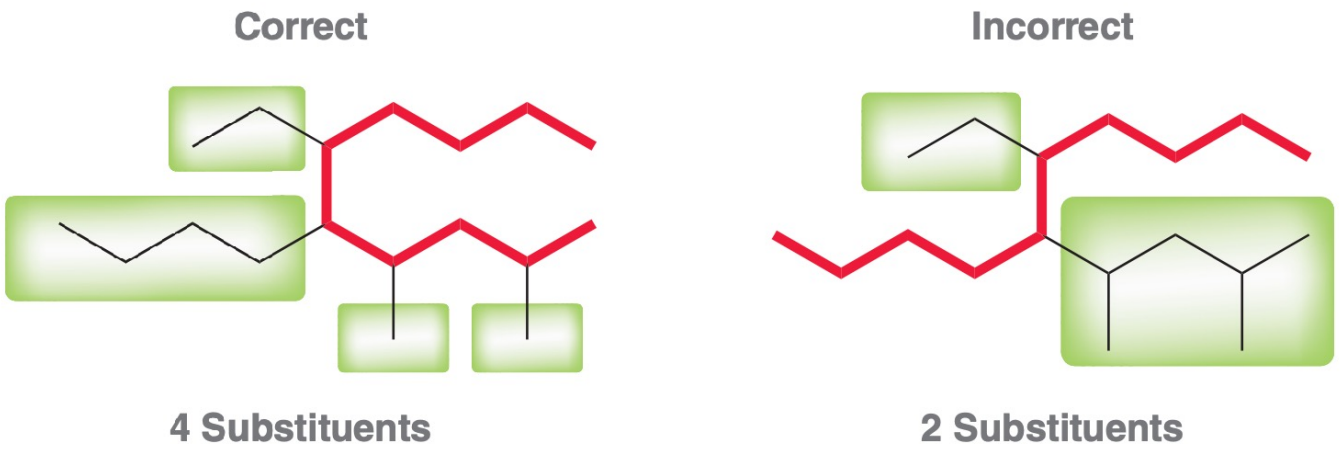

Choose longest chain
Correct
(3 substituents)
Incorrect
(2 substituents)

- 确定主链

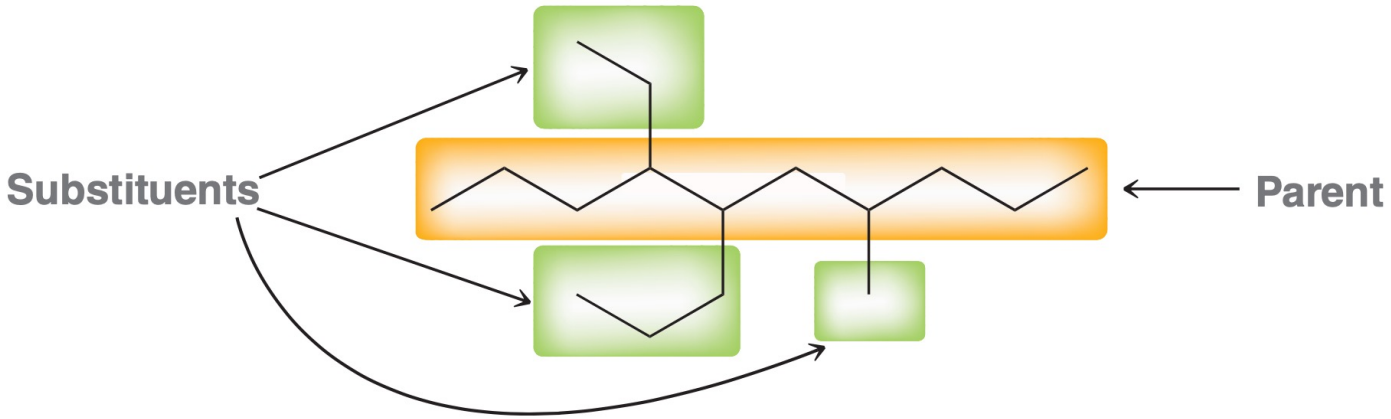
NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE	NUMBER OF CARBON ATOMS	PARENT	NAME OF ALKANE
1	*meth*	methane	11	*undec*	undecane
2	*eth*	ethane	12	*dodec*	dodecane
3	*prop*	propane	13	*tridec*	tridecane
4	*but*	butane	14	*tetradec*	tetradecane
5	*pent*	pentane	15	*pentadec*	pentadecane
6	*hex*	hexane	20	*eicos*	eicosane
7	*hept*	heptane	30	*triacont*	triacontane
8	*oct*	octane	40	*tetracont*	tetracontane
9	*non*	nonane	50	*pentacont*	pentacontane
10	*dec*	decane	100	*hect*	hectane

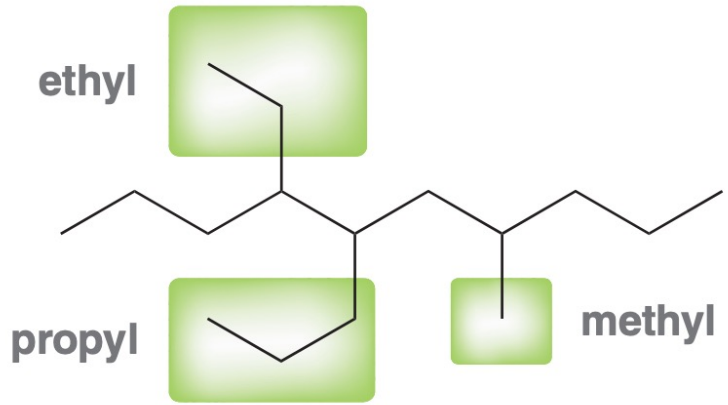
- Practice: identify and provide a name for the parent in the following compound:





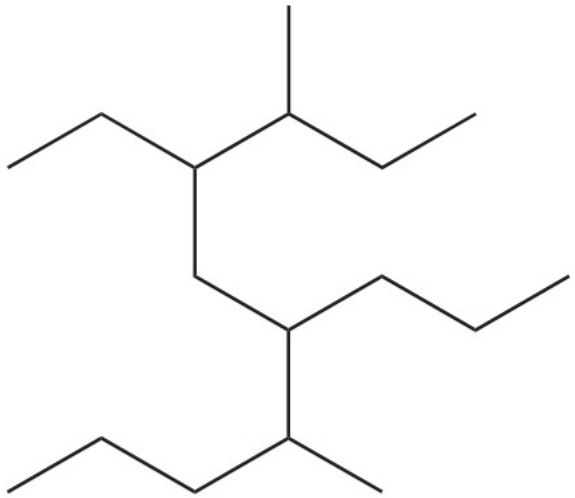
- 确定取代基种类

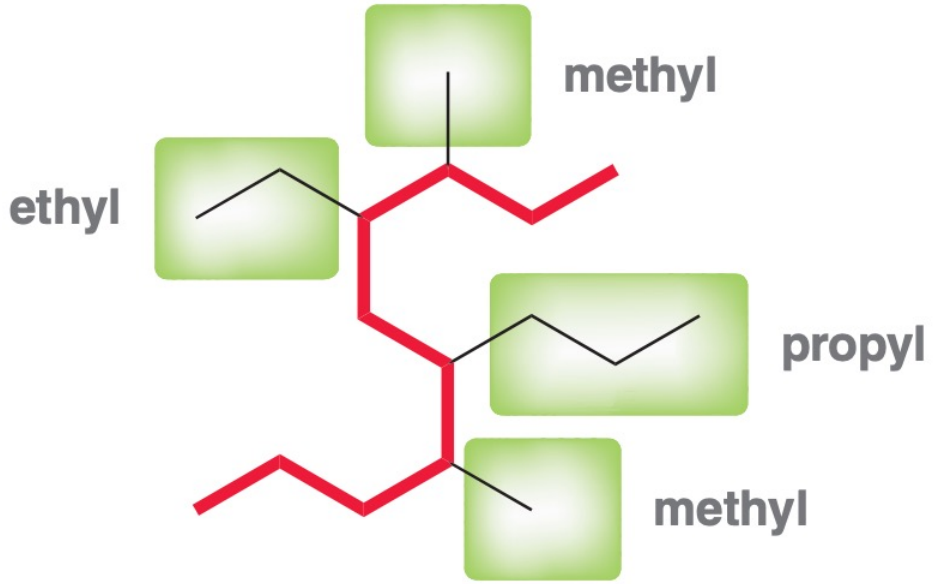




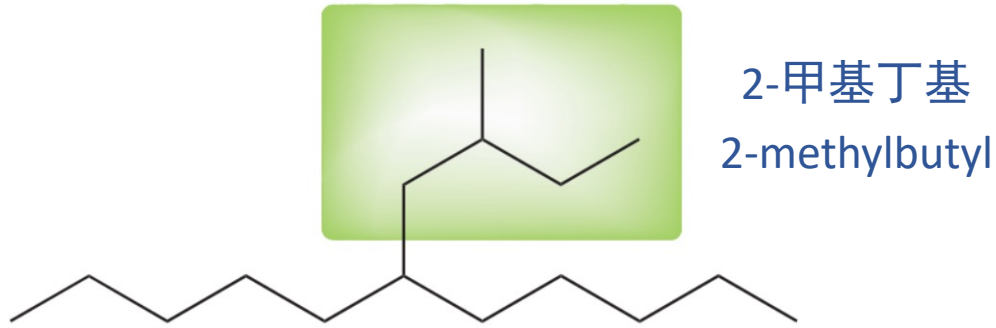
NUMBER OF CARBON ATOMS IN SUBSTITUENT	TERMINOLOGY
1	*methyl*
2	*ethyl*
3	*propyl*
4	*butyl*
5	*pentyl*
6	*hexyl*
7	*heptyl*
8	*octyl*
9	*nonyl*
10	*decyl*

- Practice: identify and name all substituents in the following compound:



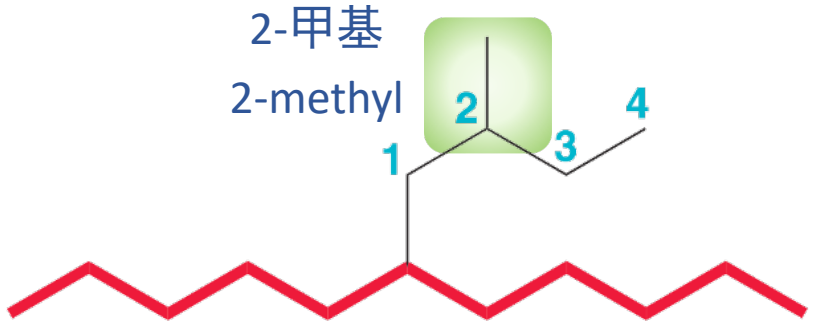


- 复杂的取代基

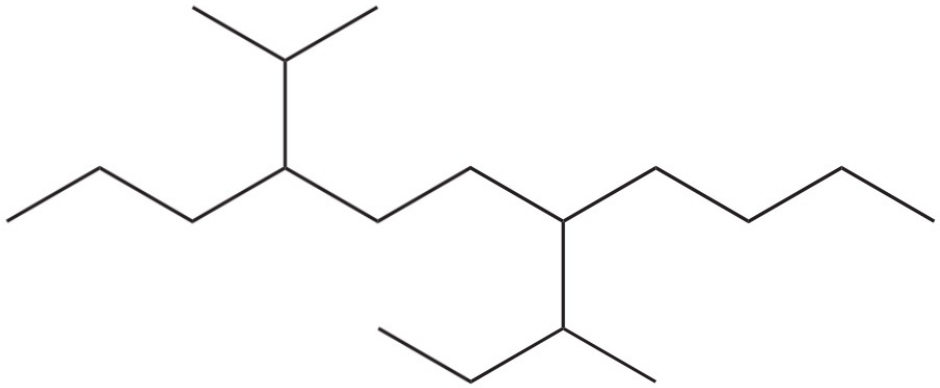


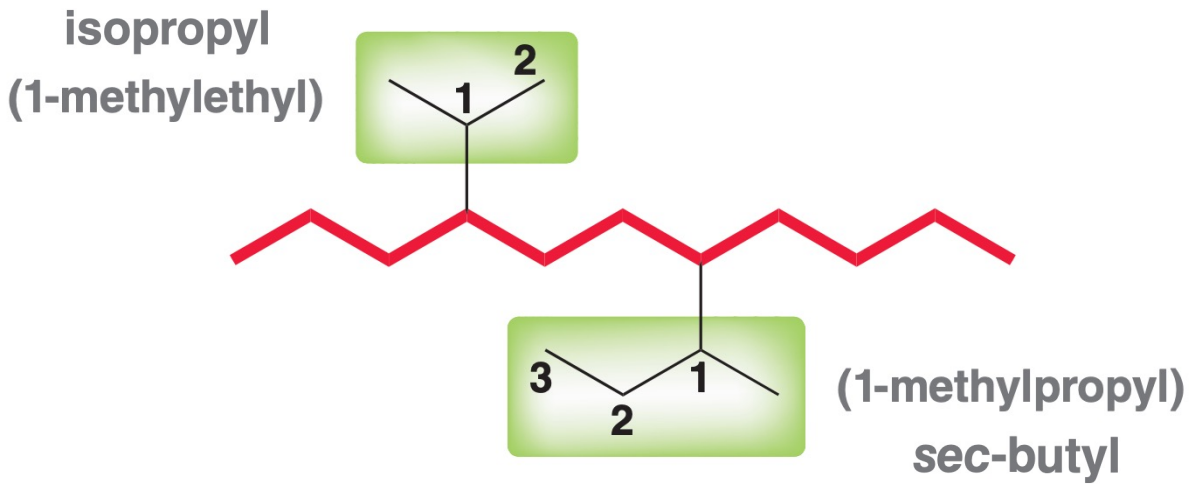
2-甲基丁基

2-methylbutyl

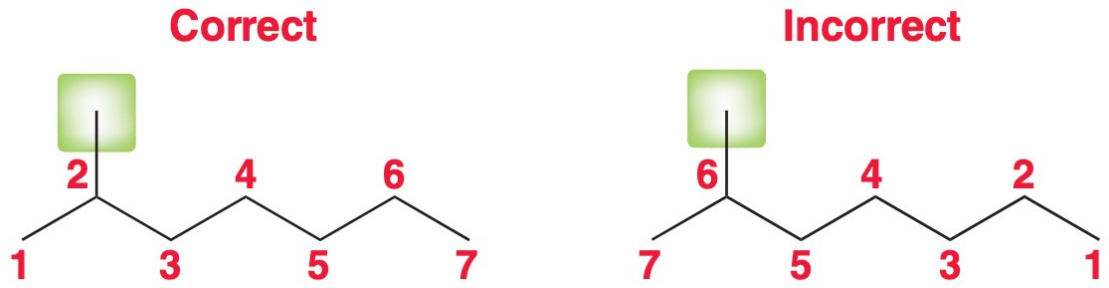


- Practice: in the following compound, identify all groups that would be considered substituents and then indicate the systematic name as well as the common name for each substituent:

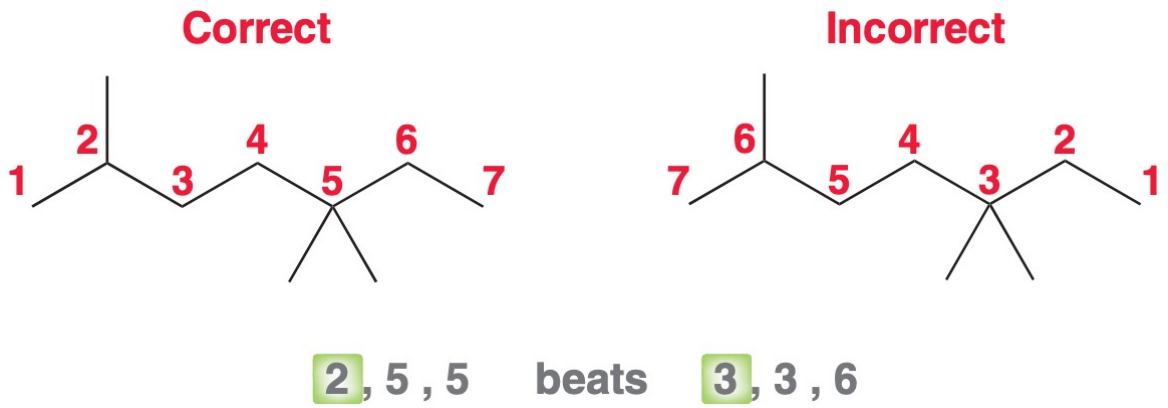




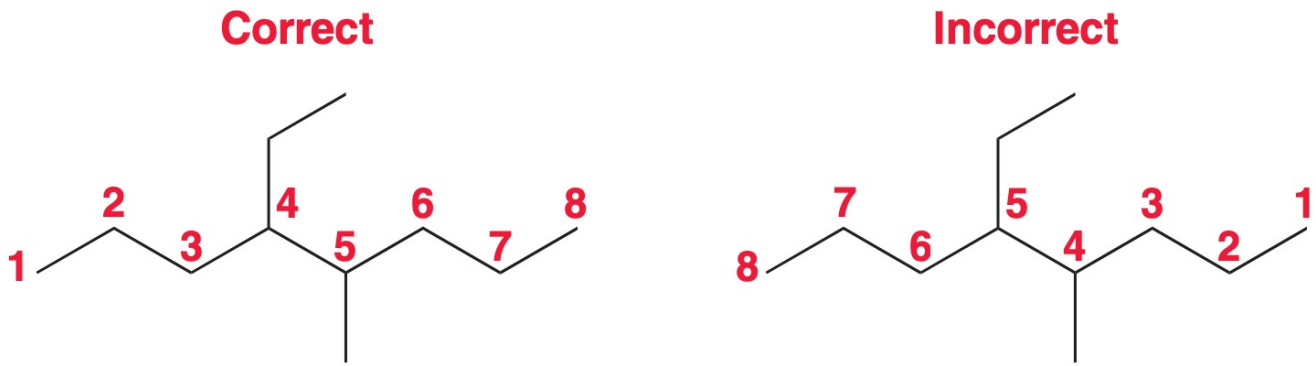
- 确定取代基编号
  - 单取代时，取代基编号尽量最小



  - 多取代时，第一个取代基编号尽量最小



- 若编号相同，则取代基按字母顺序排序



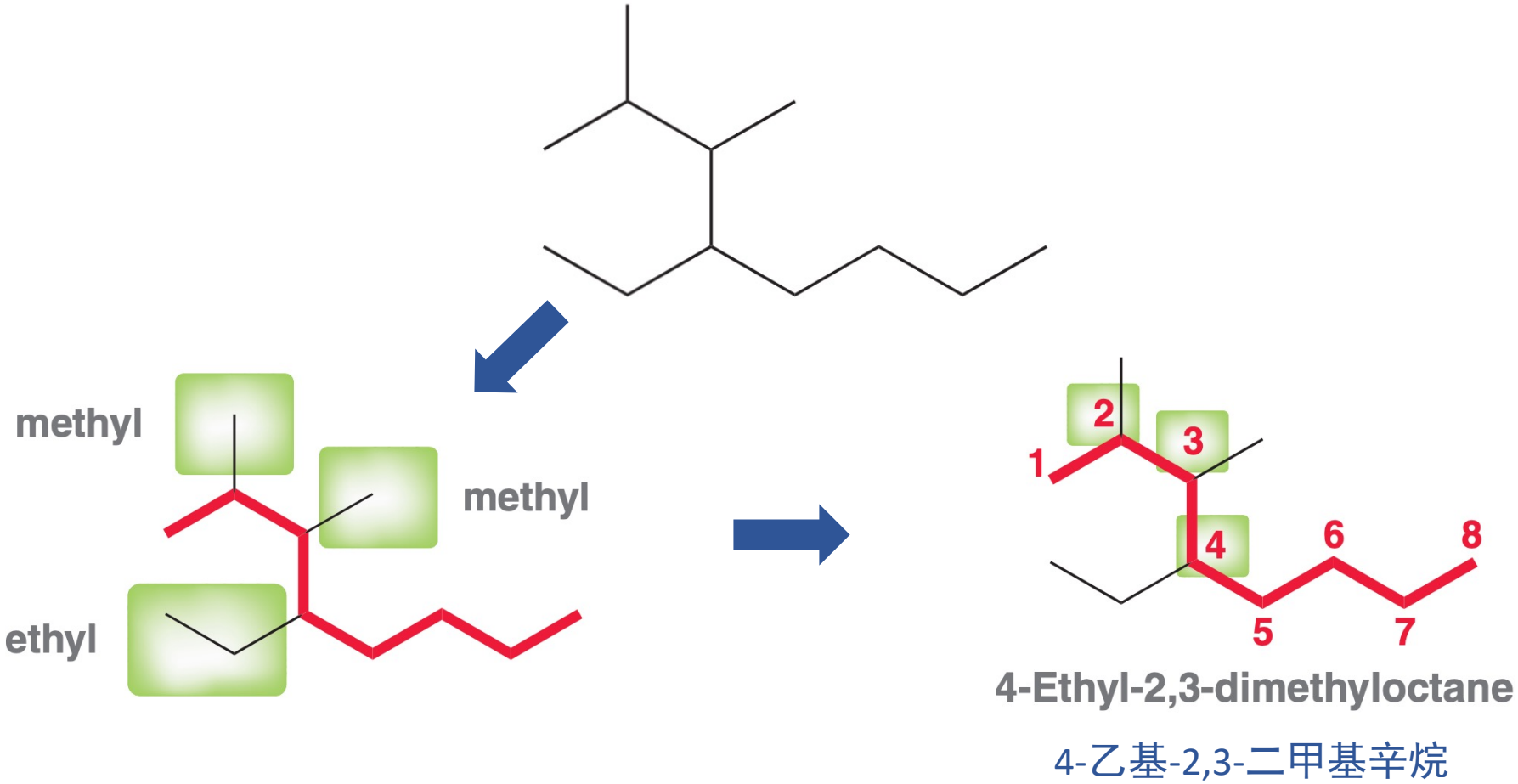
1. ***Identify the parent chain***: Choose the longest chain. For two chains of equal length, the parent chain should be the chain with the greater number of substituents.

2. ***Identify and name the substituents***.

3. ***Number the parent chain and assign a locant to each substituent***: Give the first substituent the lower possible number. If there is a tie, choose the chain in which the second substituent has the lower number.

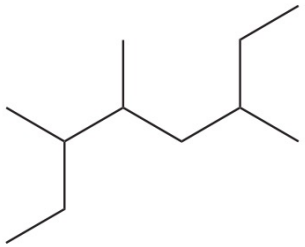
4. ***Arrange the substituents alphabetically***. Place locants in front of each substituent. For identical substituents, use di, tri, or tetra, which are ignored when alphabetizing.

- Practice: provide a systematic name for the following compound:



- Practice: provide a systematic name for each of the following compounds:

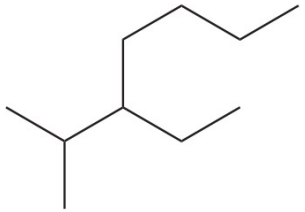
(a)



3,4,6-trimethyloctane

3,4,6-三甲基辛烷

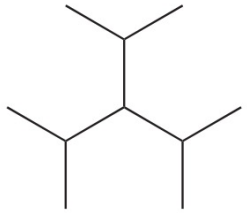
(c)



3-ethyl-2-methylheptane

3-乙基-2-甲基庚烷

(d)



3-isopropyl-2,4-dimethylpentane

or

3-(1-methylethyl)-2,4-dimethylpentane

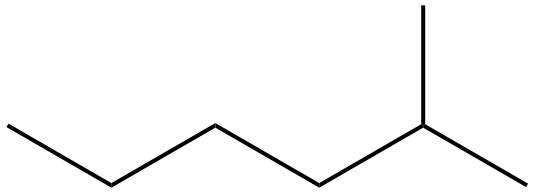
3-异丙基-2,4-二甲基戊烷

or

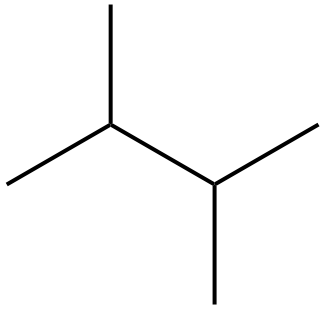
3-(1-甲基乙基)-2,4-二甲基戊烷

- Practice: draw a skeletal formula for each of the following compounds:

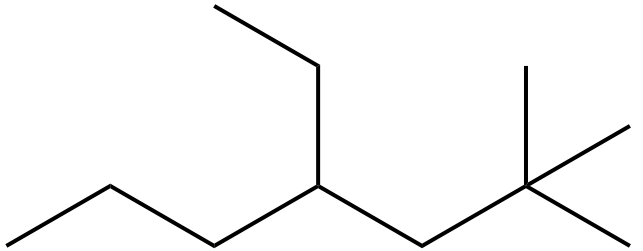
a. 2-methylhexane



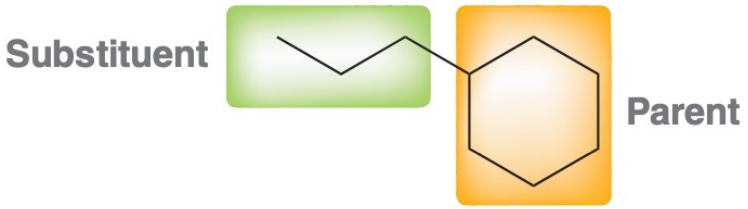
b. 2,3-dimethylbutane



c. 4-ethyl-2,2-dimethylheptane

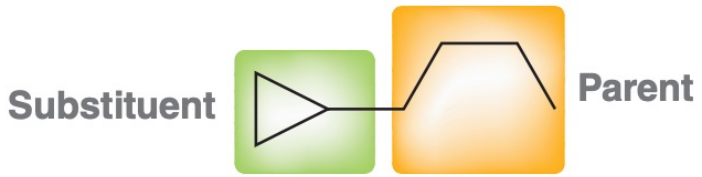


- 环烷烃的命名
  - 一般把环作为母体



Propylcyclohexane

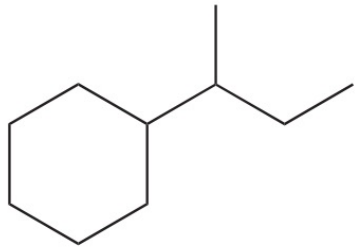
  - 特别地，当环比直链的碳原子少时，可把环当作取代基



1-Cyclopropylbutane

- Practice: provide a systematic name for each of the following compounds:

(b)



sec-butylcyclohexane

or

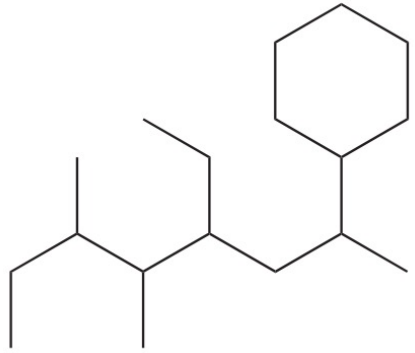
1-methylpropylcyclohexane

仲（二级）丁基环己烷

or

1-甲基丙基环己烷

(f)



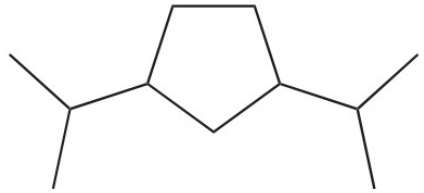
2-cyclohexyl-4-ethyl-5,6-dimethyloctane

(4-ethyl-5,6-dimethyloctan-2-yl)cyclohexane

2-环己基-4-乙基-5,6-二甲基辛烷

(4-乙基-5,6-二甲基辛烷-2-基)环己烷

(j)



1,3-diisopropylcyclopentane

or

1,3-di(1-methylethyl)cyclopentane

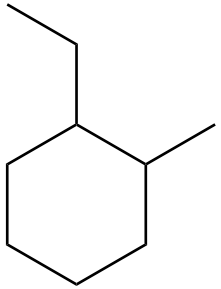
1,3-二异丙基环戊烷

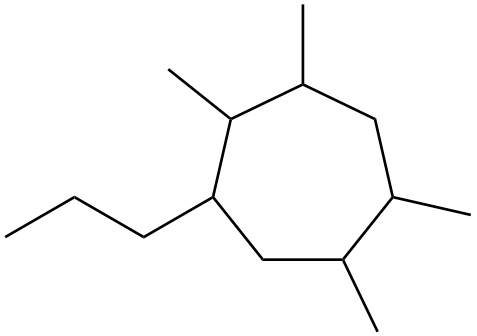
or

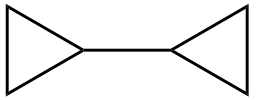
1,3-二(1-甲基乙基)环戊烷

- Practice: draw a skeletal formula for each of the following compounds:

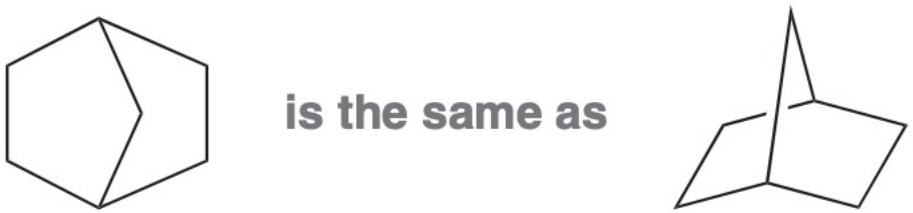
(a) 1-ethyl-2-methylcyclohexane (b) 1,2,5,6-tetramethyl-3-propylcycloheptane (c) 1-cyclopropylcyclopropane



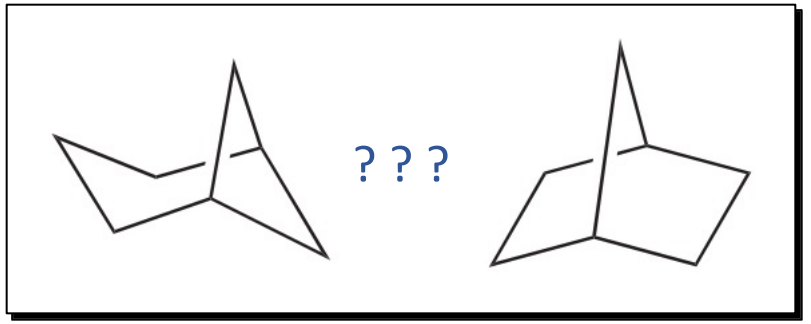




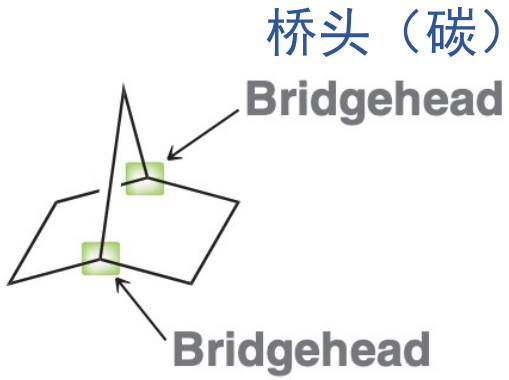
- 二环化合物(bicyclic compound)



bicycloheptane



- 二环化合物(bicyclic compound)



bicyclo[2.2.1]heptane

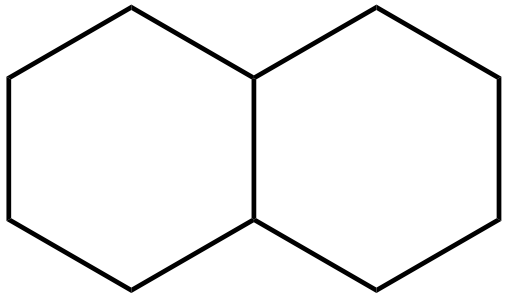
二环[2.2.1]庚烷

- 桥环烷烃的命名
  - 确定母体烃的碳原子数目
  - 确定两个环上分别的碳原子数目（不算桥头碳）
  - 确定桥上的碳原子数目（不算桥头碳）
  - 确定编号和取代基

Bicyclo[3.1.1]heptane

Bicyclo[2.2.1]heptane

- Practice: assign a name for the following compound:



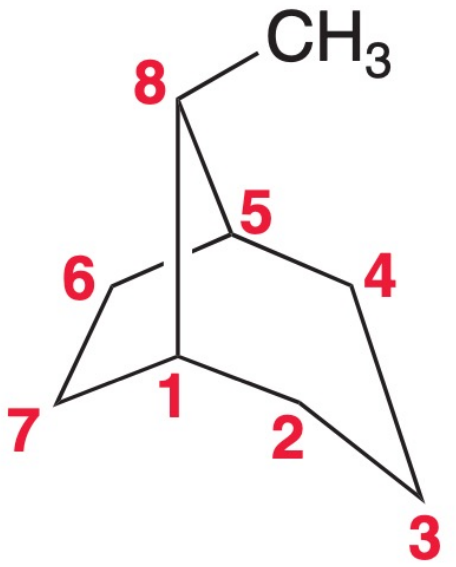
bicyclo[4.4.0]decane

二环[4.4.0]癸烷

decahydronaphthalene / naphthene

十氢化萘

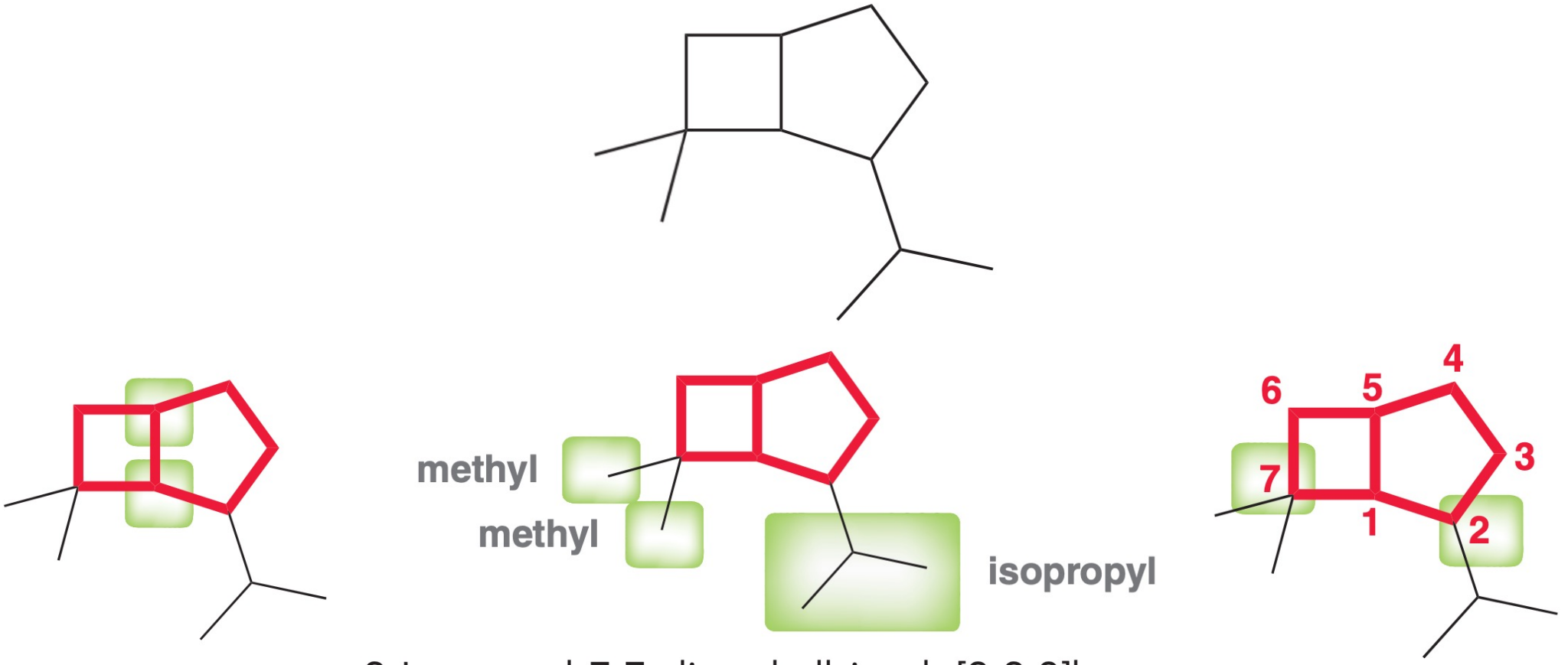
- 桥环上的取代基
- 编号规则：
  - 从桥头碳开始
  - 先走大环，经过另一桥头碳，再走小环
  - 最后走桥上返回第一个桥头碳



8-methylbicyclo[3.2.1]octane

8-甲基二环[3.2.1]辛烷

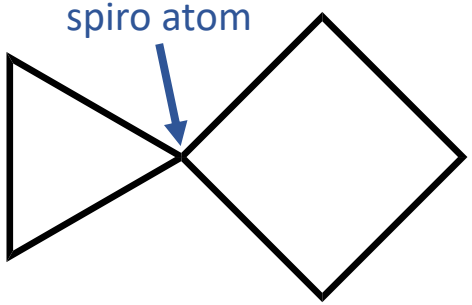
- Practice: assign a name for the following compound:



2-Isopropyl-7,7-dimethylbicyclo[3.2.0]heptane

2-异丙基-7,7-二甲基二环[3.2.0]庚烷

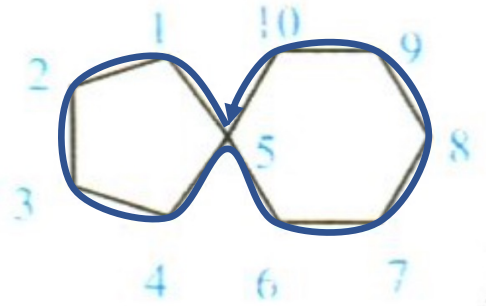
- 螺环烷烃的命名
  - 确定母体烃的碳原子数目
  - 确定两个环上分别的碳原子数目（不算螺原子）
  - 确定编号和取代基



spiro[2.3]hexane

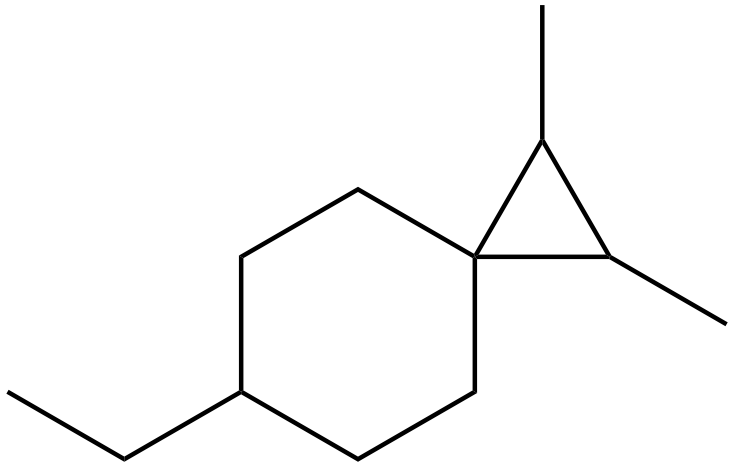
螺[2.3]己烷

- 螺环上的取代基
- 编号规则：
  - 从小环上最临近螺原子的碳开始
  - 先走小环，经过螺原子，再走大环
  - 回到螺原子
  - 编号顺序尽可能使取代基位序最小



螺[4. 5]癸烷
spiro[4. 5]decane

- Practice: assign a name for the following compound:



6-ethyl-1,2-dimethylspiro[2.5]octane

6-乙基-1,2-二甲基螺[2.5]辛烷

- 桥环、螺环的命名比较

比较内容	桥环 bridged ring	螺环 spiro ring
定义	环与环之间共用**两个或多个**碳原子的多环烷烃	环与环之间共用**一个**碳原子的多环烷烃
共用原子名称	桥头碳 bridgehead carbon	螺原子 spiro atom
格式	环+[　　]+母体名称 cyclo+[　　]+parent name	螺+[　　]+母体名称 spiro+[　　]+parent name
[　　]	[大环.小环.桥碳]	[小环.大环]
编号顺序	**桥头碳**→**大环**→另一桥头碳→**小环**→桥碳→首个桥头碳	**小环上临螺原子的碳**→**小环**→螺原子→**大环**