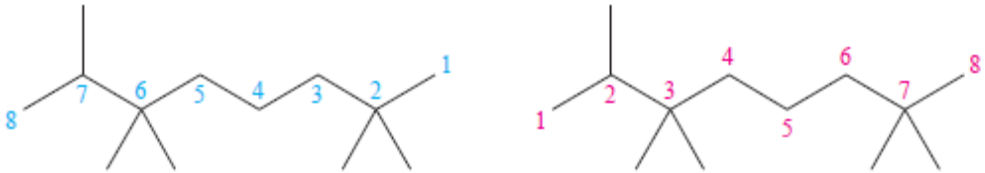
# Basics of Organic Chemistry (CH 111)

Organic Compounds: Classification, Nomenclature, Hybridization, Electronic Displacements: Inductive, electromeric, resonance and mesomeric effects, hyperconjugation, Dipole moment. Organic acids and bases. Homolytic and Heterolytic fission, arrow rules, Electrophiles and Nucleophiles; Carbocations, Carbanions, Free radicals and Carbenes. Introduction to types of organic reactions and their mechanism: Addition, Elimination and Substitution reactions.

| | | |
|---|---|---|
| **Q.5** | Q.1. Apply the IUPAC rules and write the names of the $C_6H_{14}$ Isomers.<br>Q.2. Which number is correct in the following structure. write the IUPAC name.<br>  | **2**<br>**2** |
| **Q. 9** | a) | **3+5** |
| **Books** | **Organic Chemistry, 7th Edition, Morrison, Boyd**<br>**Organic Chemistry, 7th Edition; Francis A Carey**<br>**Fundamentals of Organic Chemistry Solomons, John Wiley**<br>**Introduction to Organic Chemistry, Streitwiesser, Hathcock and Kosover, Macmillan.** | |

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# Organic Chemistry Grew with Historical Scientific Thoughts and Postulates

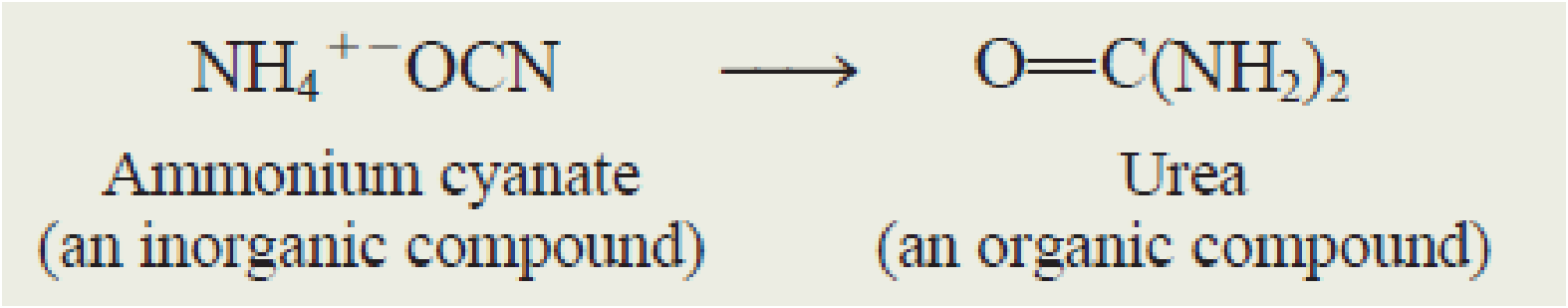
**Lavoisier (1743-1794)** **Law of Conservation of Mat**ter; how chemical compositions could be determined by identifying and measuring the amounts of water, carbon dioxide, and other materials produced when various substances were burned in air. By the time of Lavoisier's studies, two branches of chemistry were becoming recognized. It was **Berzelius** who in 1807 coined the term "organic chemistry" for the study of compounds ***derived from natural sources***. The other branch dealt with substances derived from nonliving matter—minerals and the like. It was called *inorganic chemistry.*
Combustion analysis: Natural sources contained carbon, and eventually a new definition of organic chemistry emerged: ***Organic chemistry is the study of carbon compounds*****.** This is the definition we still use today.


Lavoisier as portrayed on a 1943 French postage stamp.


A 1979 Swedish stamp honoring Berzelius.


This German stamp depicts a molecular model of urea and was issued in 1982 to commemorate the hundredth anniversary of Wöhler's death. The computer graphic at the top of this page is also a model of urea.

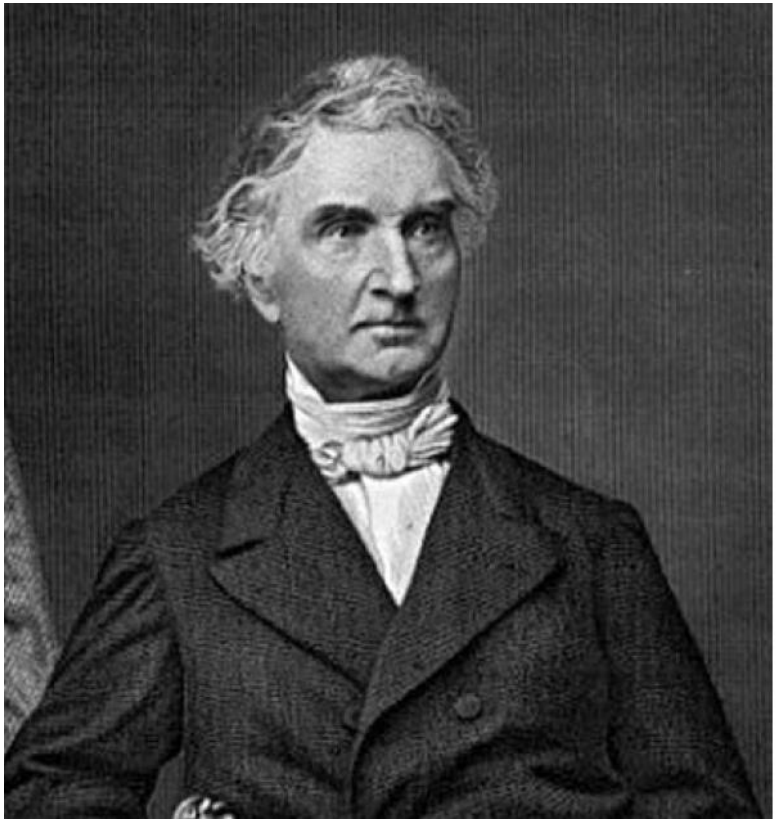
# *WOHLER DISCOVERY: Inorganic to Organic*



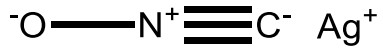

Wöhler brief paper, he published in 1828. Wöhler noted that when he evaporated an aqueous solution of ammonium cyanate, he obtained “colorless, clear crystals often more than an inch long,” which were not ammonium cyanate but were instead urea.

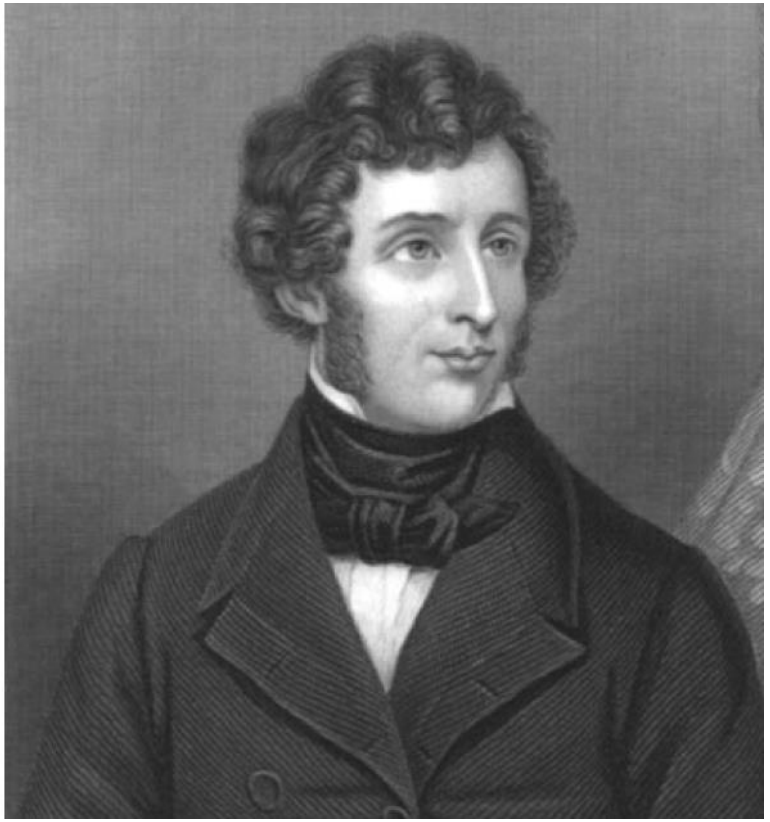
# FIGHT BETWEEN TWO CHEMIST: DISCOVERY OF ISOMERISM





Justus Liebig



Friedrich Wohler



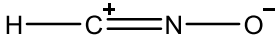


cyanic acid




isocyanic acid

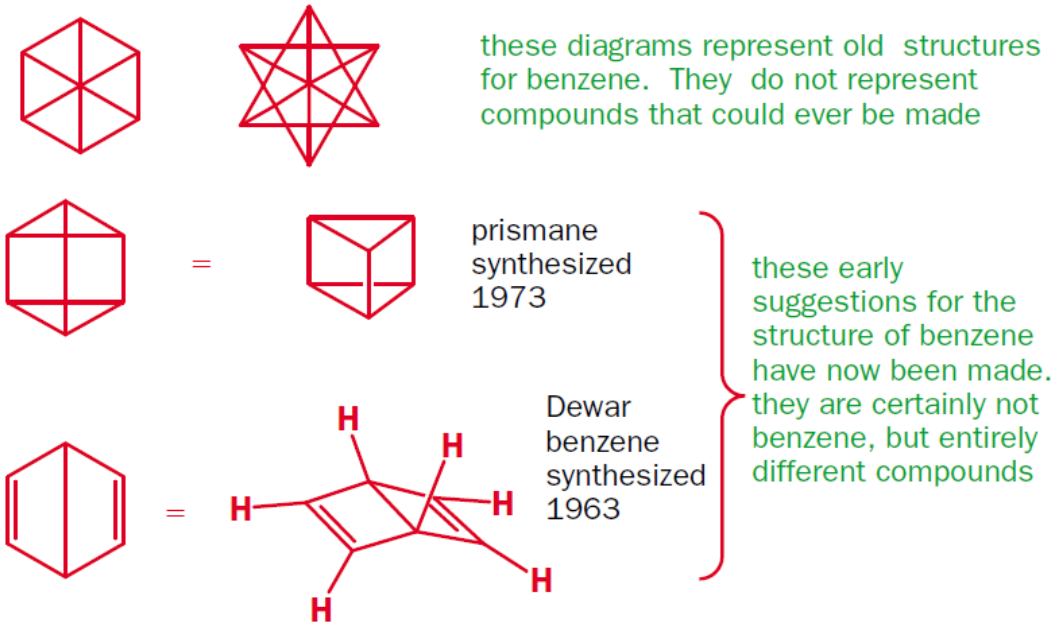

Fulminic Acid



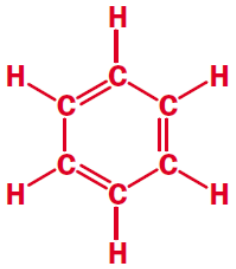

Fulminic Acid

# *Questions/Interesting Facts*

- **Benzene has been known since**
  - **1825:** when Michael Faraday first isolated and identified benzene from the oily residue. Thus the molecular formula were calculated by chemical analysis and it was $C_6H_6$.
- **What are those strange structure, which were suggested for Benzene**




- **Kekulé proposed the satisfactory structure in 1865**




Kekulé's structure for benzene

# *What's in a Name? Organic Nomenclature*

**Systematic Names and Common Names** *Systematic names are derived according to a prescribed set of rules, common names are not*. Many compounds are better known by **common names** than by their **systematic names**.

*A single compound can have* ***several acceptable systematic*** *names but no two compounds can have the same name*.

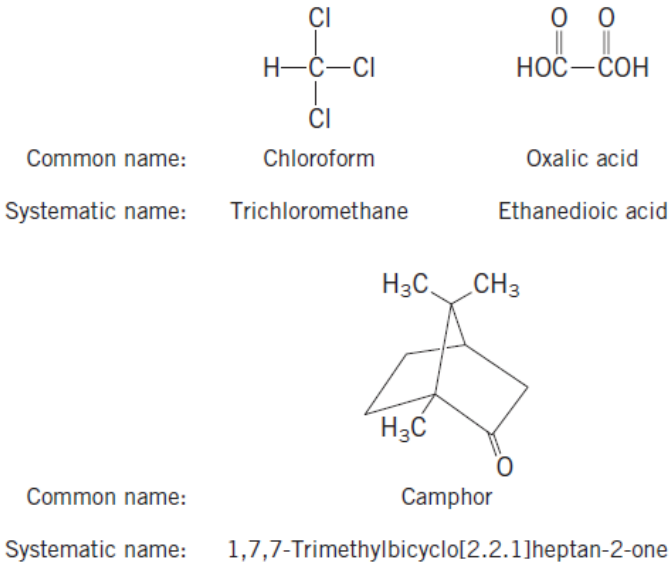
**1892**: a group of prominent chemists met in Geneva, Switzerland, where they formulated the principles on which our present system of organic nomenclature is based.

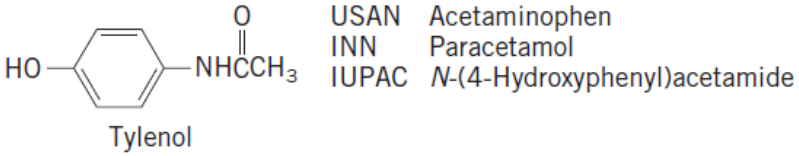
**20th Century**, ***International Union of Pure and Applied Chemistry*** **(IUPAC)** carried out major revisions and extensions of organic nomenclature: **IUPAC Rules**. 1979 and 1993 versions of these rules were joined in 2004.

2004 IUPAC recommendations: "preferred IUPAC name" **(PIN)**

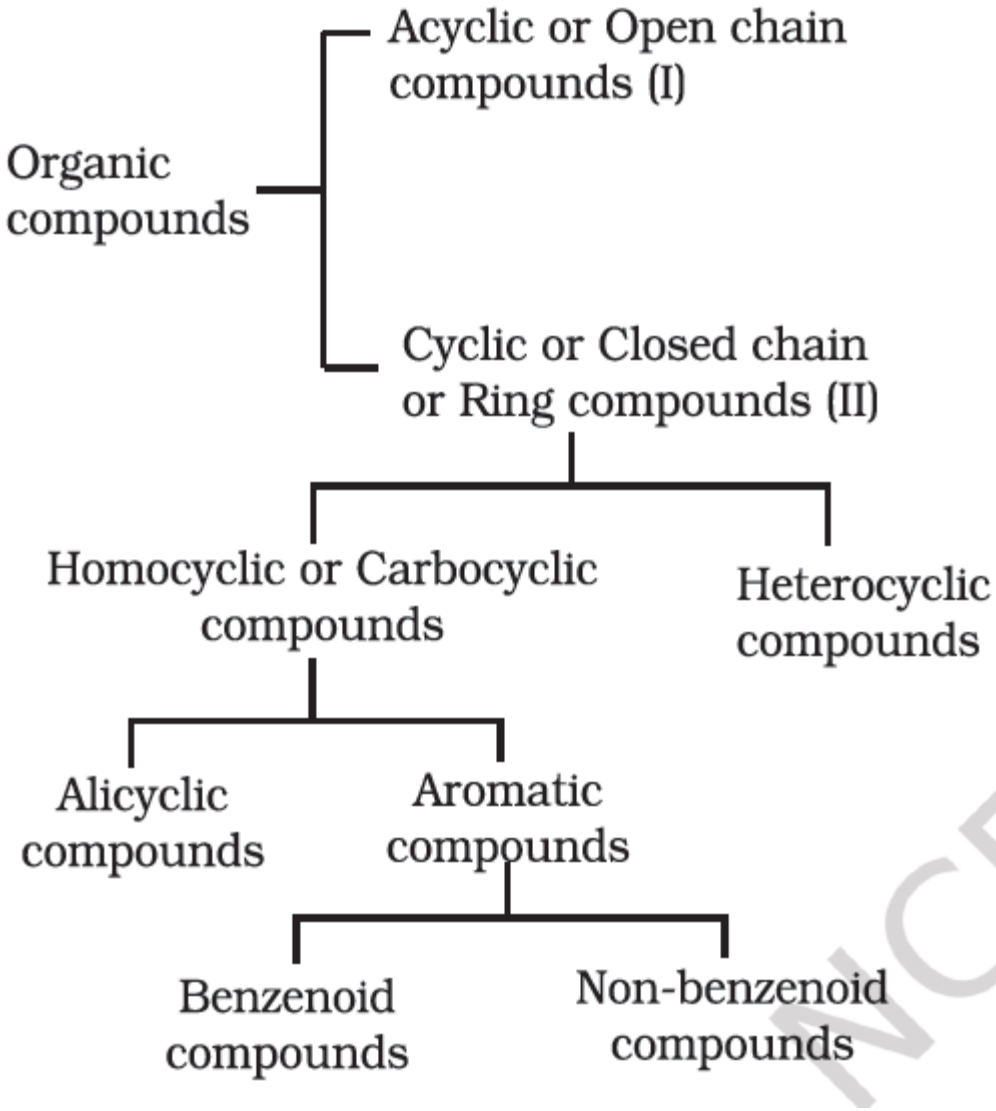
**Generic names** in the United States is the U.S. Adopted Names (USAN) Council, a private organization.

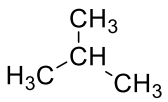
**International Proprietary Names** (INN) are generic names as designated by the World Health Organization.



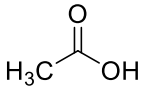



# Classification

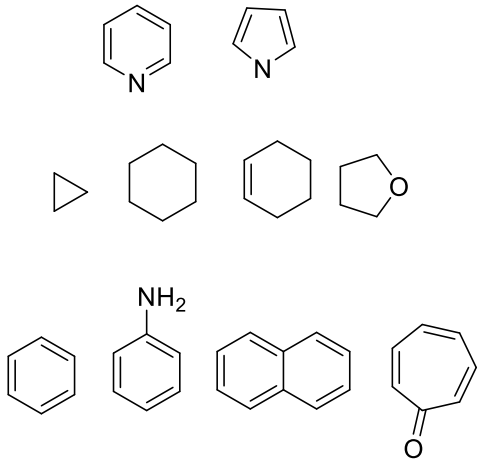


isobutane



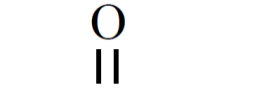
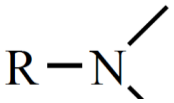
acetic acid



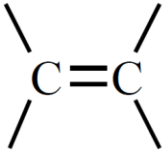
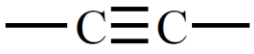
# *Nomenclature of Organic Compounds*

- IUPAC System: International Standard: Unique and Unambiguous
- Fundamental Principle: Longest Chain of Carbons Connected by Single Bond.
- Alkanes and Cycloalkanes: Linear/Acyclic, Rings (Cyclic or alicyclic): The names of alkanes and cycloalkanes are the root names of organic compounds.
- Substituents and Functional Group: All deviations, either multiple bonds or atoms other than carbon and hydrogen, are indicated by prefixes or suffixes according to a specific set of priorities/rules.

# Functional Groups Indicated By Prefix Or Suffix

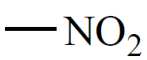
| Family of Compound | Structure | Prefix | Suffix |
|---|---|---|---|
| Carboxylic Acid |  | carboxy- | -oic acid (-carboxylic acid) |
| Aldehyde |  | oxo- (formyl) | -al (carbaldehyde) |
| Ketone |  | oxo- | -one |
| Alcohol |  | hydroxy- | -ol |
| Amine |  | amino- | -amine |

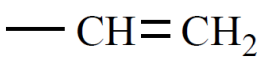
# Functional Groups Indicated By Suffix Only

| Family of Compound | Structure | Prefix | Suffix |
|---|---|---|---|
| Alkene |  | -------- | -ene |
| Alkyne |  | -------- | -yne |

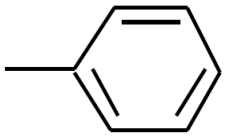
# Functional Groups Indicated By Prefix Only

| Substituent | Structure | Prefix | Suffix |
|---|---|---|---|
| Alkyl (see list below) | R— | alkyl- | ---------- |
| Alkoxy | R— O — | alkoxy- | ---------- |
| Halogen | F —<br>Cl —<br>Br —<br>I — | fluoro-<br>chloro-<br>bromo-<br>iodo- | ----------<br>----------<br>----------<br>---------- |


nitro

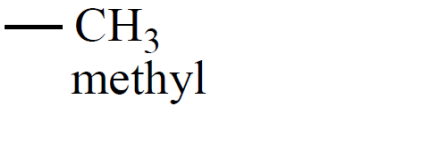

vinyl


allyl

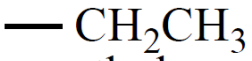

phenyl

# Common Alkyl Groups:

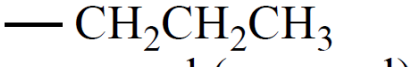
## replace "ane" ending of alkane name with "yl". Alternate names for complex substituents are given in brackets



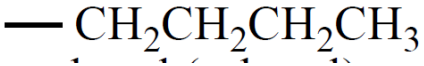

methyl

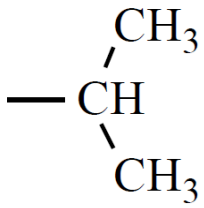



ethyl

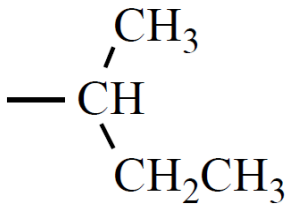



propyl (*n*-propyl)

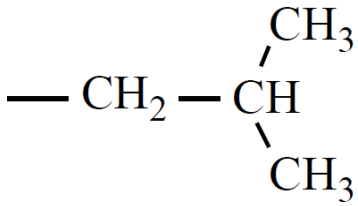


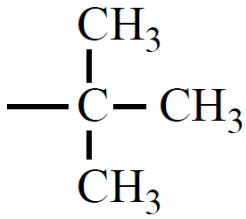

isopropyl
[1-methylethyl]




*sec*-butyl
[1-methylpropyl]



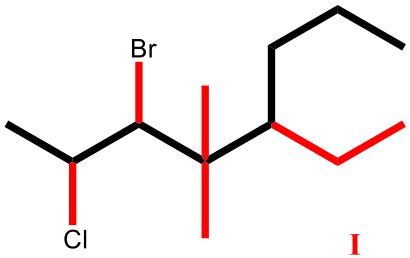

isobutyl
[2-methylpropyl]




*tert*-butyl or *t*-butyl
[1,1-dimethylethyl]

# NOMENCLATURE: PRACTICE

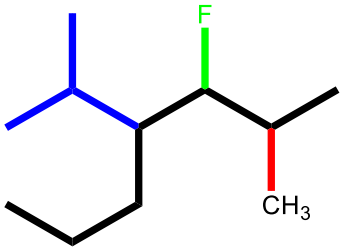
3-bromo-2-chloro-5-ethyl-4,4-dimethyloctane




I

**3-fluoro-4-isopropyl-2-methylheptane**

II

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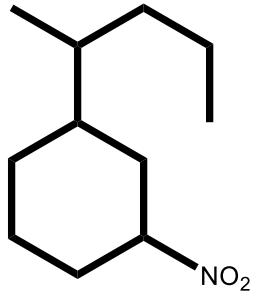
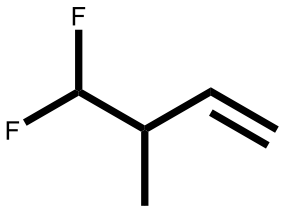
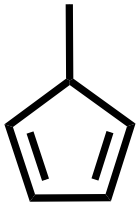


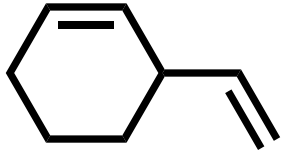

IV



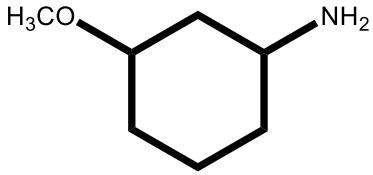

V



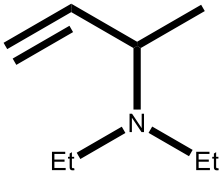
VI



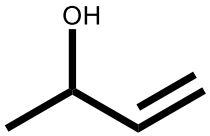
VII



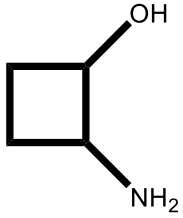

VIII



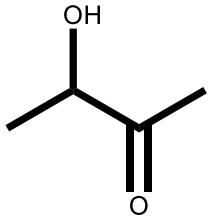

IX



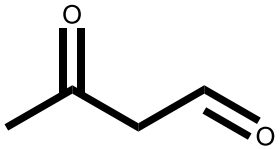

X



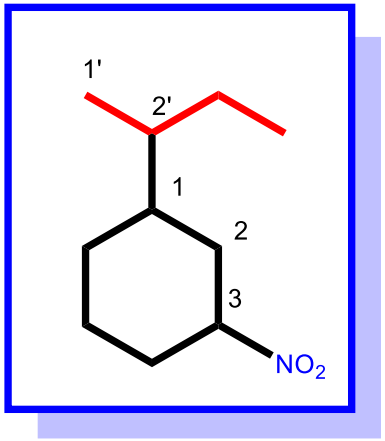

XI



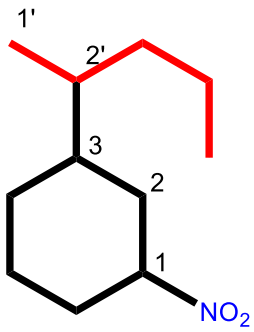

XII



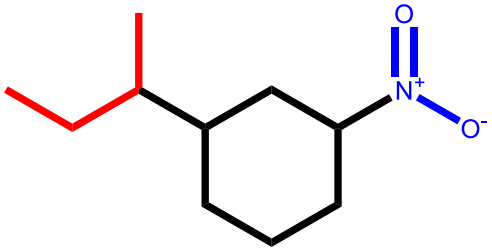
**1-(*sec*-butyl)-3-nitrocyclohexane**




III

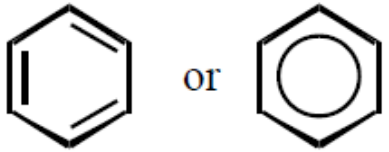



1-nitro-3-(pentan-2-yl)cyclohexane

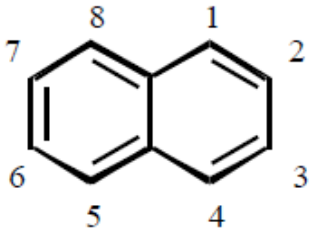



**1-NITRO-3-(BUTAN-2-YL)CYCLOHEXANE**

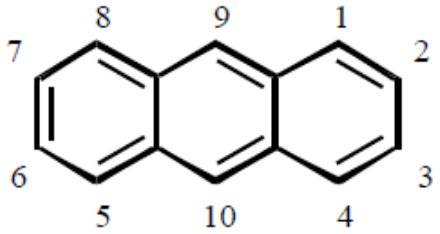
# Common Parent Ring Systems



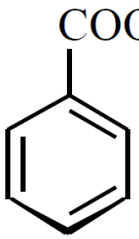

benzene



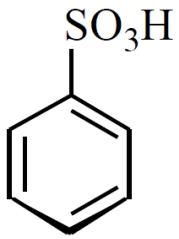

naphthalene



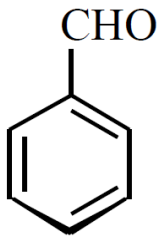

anthracene



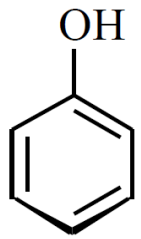

benzoic acid



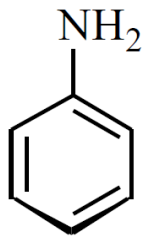

benzene-sulfonic acid




benzaldehyde




phenol

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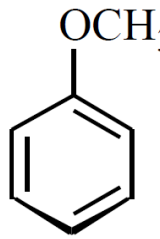
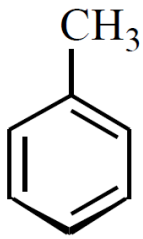
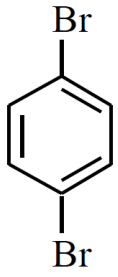


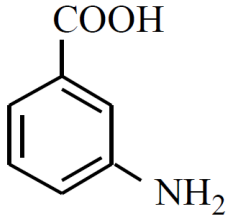

anisole



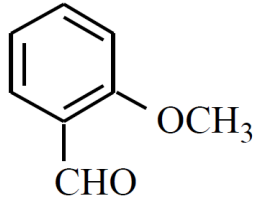

toluene



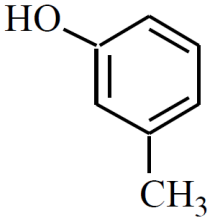

1,4-dibromobenzene




3-aminobenzoic acid

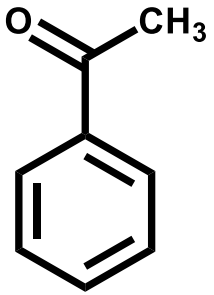


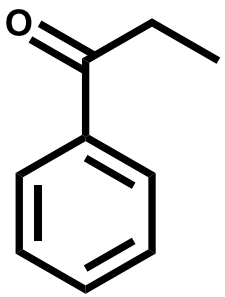

2-methoxybenzaldehyde

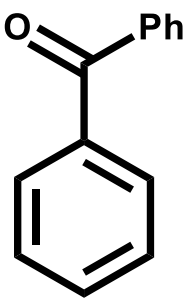


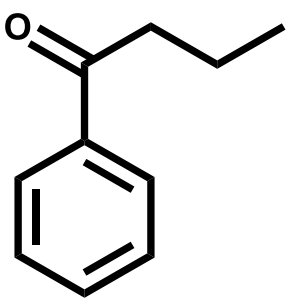

3-methylphenol

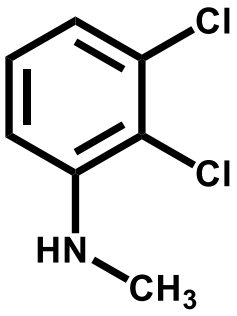
# Common Parent Ring Systems

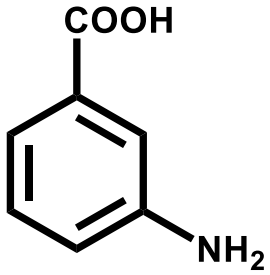


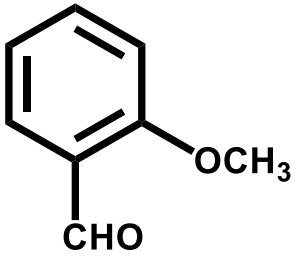



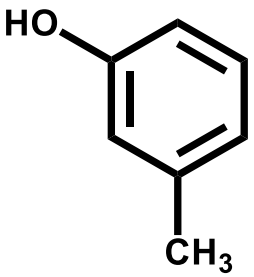



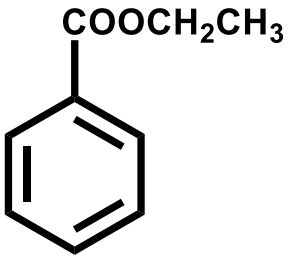



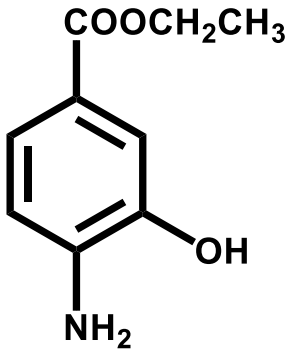



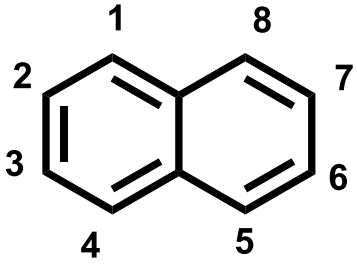



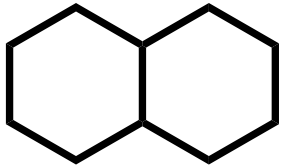



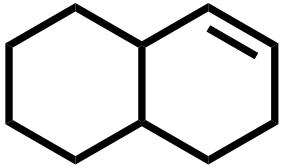



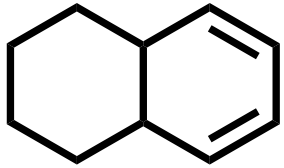



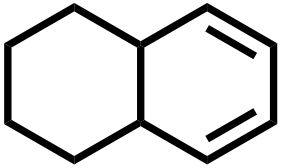
# *Parent Ring Systems Based Naming*

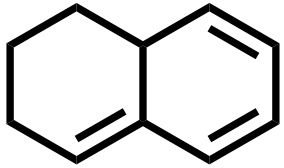


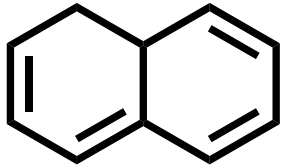



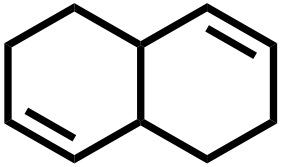


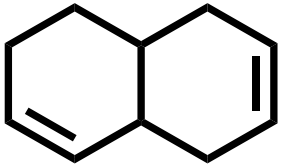


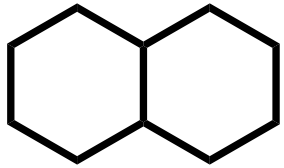








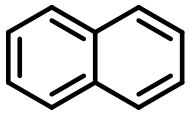




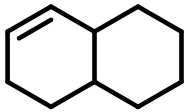
**decahydronaphthalene**

**BICYCLO[4,4,0]DECANE**

# *Fused System Nomenclature*

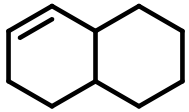


naphthalene



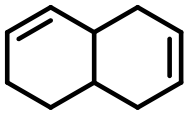
1,2,3,4,4a,5,6,8a-octahydronaphthalene

bicyclo[4,4,0]dec-2-ene

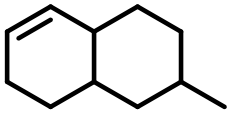


(E)-bicyclo[4,4,0]dec-2-ene

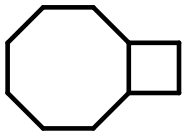
Caution: Stereochemical terms discarded: e



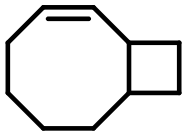
1,2,4a,5,8,8a-hexahydronaphthalene



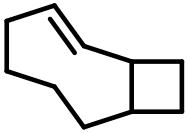
3-methyl-1,2,3,4,4a,5,6,8a-octahydronaphthalene



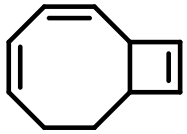
bicyclo[6.2.0]decane



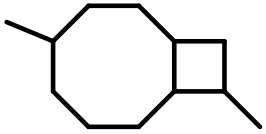
(*Z*)-bicyclo[6.2.0]dec-2-ene



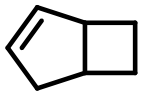
(E)-bicyclo[6,2,0]dec-2-ene



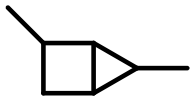
(2*Z*,4*Z*)-bicyclo[6.2.0]deca-2,4,9-triene



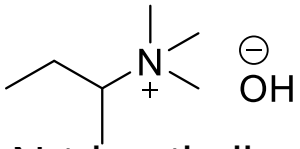
4,9-dimethylbicyclo[6.2.0]decane



bicyclo[3.2.0]hept-2-ene

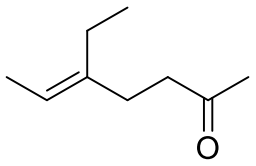


2,5-dimethylbicyclo[2.1.0]pentane



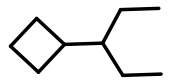

N,N,N-trimethylbutan-2-aminium

SEC-BUTYLTRIMETHYLAMMONIUM HYDROXIDE

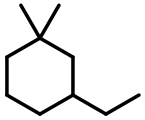



(E)-5-ethylhept-5-en-2-one

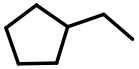
# Ques-Ans: Morrison& Boyd: 7th Ed. P:11.



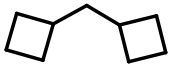
pentan-3-ylcyclobutane
3-cyclobutyl pentane



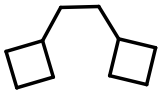
3-ethyl-1,1-dimethylcyclohexane



ethylcyclopentane
1-cyclopentylethane



dicyclobutyl methane



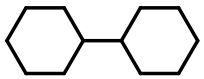
1,2-dicyclobutylethane

bicyclo[2.2.0]hexane

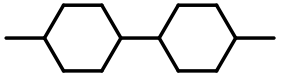
bicyclo[3.1.0]hexane

bicyclo[2.2.1]heptane

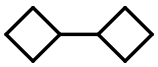
bicyclo[2.2.2]octane



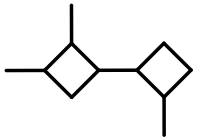
1,1'-bi(cyclohexane)



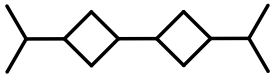
4,4'-dimethyl-1,1'-bi(cyclohexane)



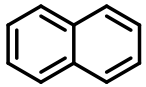
1,1'-bi(cyclobutane)



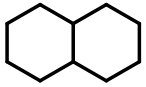
2,2',3-trimethyl-1,1'-bi(cyclobutane)



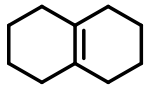
3,3'-diisopropyl-1,1'-
bi(cyclobutane)



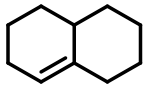
naphthalene



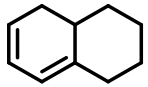
decahydronaphthalene
bicyclo[4,4,0]decane



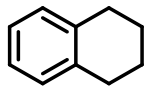
1,2,3,4,5,6,7,8-octahydronaphthalene



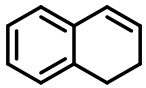
1,2,3,4,4a,5,6,7-octahydronaphthalene



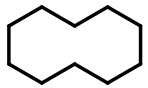
1,2,3,4,4a,5-hexahydronaphthalene



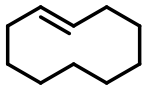
1,2,3,4-tetrahydronaphthalene



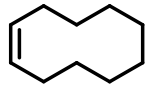
1,2-dihydronaphthalene



cyclodecane

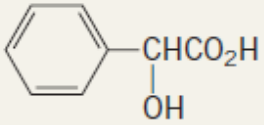
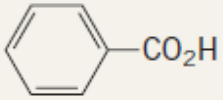
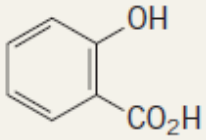
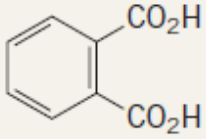


(*E*)-cyclodecene

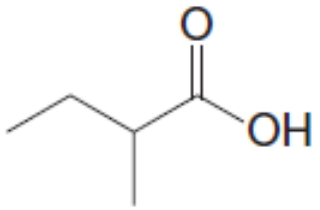


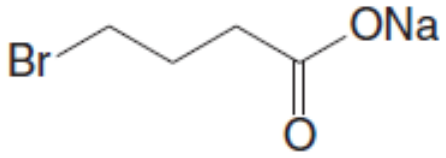
(*Z*)-cyclodecene

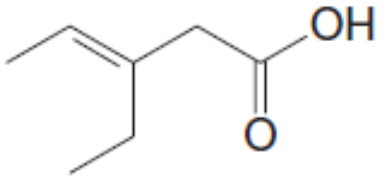
# Nomenclature: Carboxylic Acid

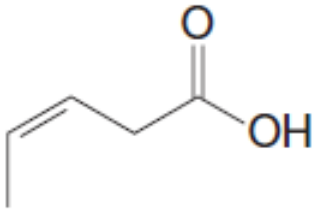
| | Structural formula | Systematic name | Common name* |
|---|---|---|---|
| 1. | $HCO_2H$ | Methanoic acid | Formic acid |
| 2. | $CH_3CO_2H$ | Ethanoic acid | Acetic acid |
| 3. | $CH_3(CH_2)_{16}CO_2H$ | Octadecanoic acid | Stearic acid |
| 4. | $CH_3CHCO_2H$ (OH) | 2-Hydroxypropanoic acid | Lactic acid |
| 5. |  | 2-Hydroxy-2-phenylethanoic acid | Mandelic acid |
| 6. | $H_2C{=}CHCO_2H$ | Propenoic acid | Acrylic acid |
| 7. | $CH_3(CH_2)_7$, $(CH_2)_7CO_2H$, C=C, H, H | (*Z*)-9-Octadecenoic acid or (*Z*)-9-Octadec-9-enoic acid | Oleic acid |
| 8. |  | Benzenecarboxylic acid | Benzoic acid |
| 9. |  | *o*-Hydroxybenzenecarboxylic acid | Salicylic acid |
| 10. | $HO_2CCH_2CO_2H$ | Propanedioic acid | Malonic acid |
| 11. | $HO_2CCH_2CH_2CO_2H$ | Butanedioic acid | Succinic acid |
| 12. |  | 1,2-Benzenedicarboxylic acid | Phthalic acid |

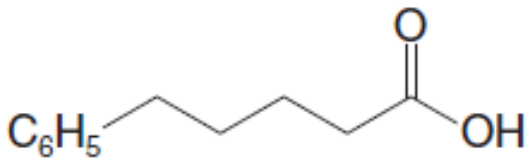
# Questions

(a) 

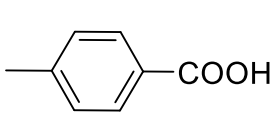

(c) 


(e) 

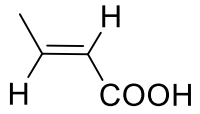

(b) 


(d) 

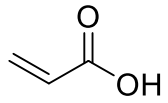

(a) 2-Methylbutanoic acid
(b) (*Z*)-3-Pentenoic acid or (*Z*)-pent-3-enoic acid
(c) Sodium 4-bromobutanoate
(d) 5-Phenylpentanoic acid
(e) (*E*)-3-Ethyl-3-pentenoic acid or (*E*)-3-Ethylpent-3-enoic acid



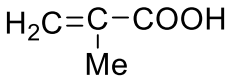

4-methylbenzoic acid
Toluic Acid



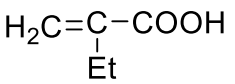

(*E*)-but-2-enoic acid
Crotonic Acid




Prop-2-enoic acid
acrylic acid




2-Methyl prop-2-enoic acid
methacrylic acid

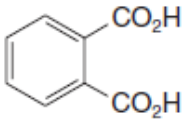
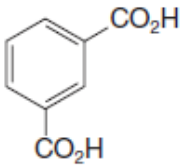
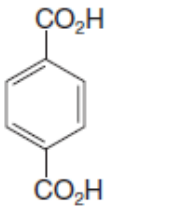



2-methylenebutanoic acid

# *Dicarboxylic Acids*

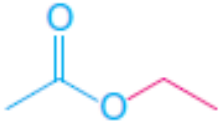
- Dicarboxylic acids are named as **alkanedioic acids** in the IUPAC systematic or substitutive system. Most simple dicarboxylic acids have common names

ethanedioic acid
1,3-propanedioic acid

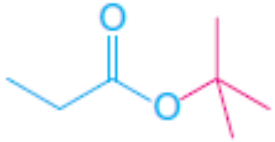
| Structure | Common Name | mp (°C) | p$K_a$ (at 25 °C) p$K_{a1}$ | p$K_{a2}$ |
|---|---|---|---|---|
| $HO_2C-CO_2H$ | Oxalic acid | 189 dec | 1.2 | 4.2 |
| $HO_2CCH_2CO_2H$ | Malonic acid | 136 | 2.9 | 5.7 |
| $HO_2C(CH_2)_2CO_2H$ | Succinic acid | 187 | 4.2 | 5.6 |
| $HO_2C(CH_2)_3CO_2H$ | Glutaric acid | 98 | 4.3 | 5.4 |
| $HO_2C(CH_2)_4CO_2H$ | Adipic acid | 153 | 4.4 | 5.6 |
| *cis*-$HO_2C-CH=CH-CO_2H$ | Maleic acid | 131 | 1.9 | 6.1 |
| *trans*-$HO_2C-CH=CH-CO_2H$ | Fumaric acid | 287 | 3.0 | 4.4 |
|  | Phthalic acid | 206–208 dec | 2.9 | 5.4 |
|  | Isophthalic acid | 345–348 | 3.5 | 4.6 |
|  | Terephthalic acid | Sublimes | 3.5 | 4.8 |

# Esters

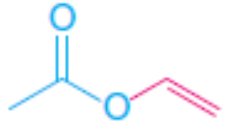
The names of esters are derived from the names of the alcohol (with the ending -**yl**) and the acid (with the ending -**ate** or -**oate**). The portion of the name derived from the alcohol comes first



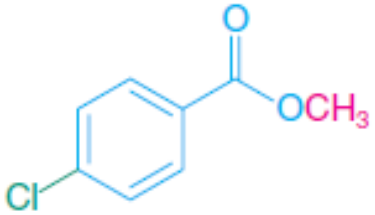
Ethyl acetate or
ethyl ethanoate



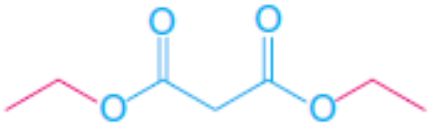
*tert*-Butyl propanoate



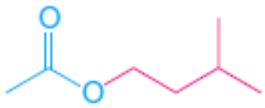
Vinyl acetate or
ethenyl ethanoate



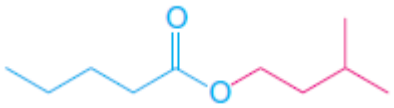

Methyl *p*-chlorobenzoate



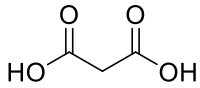
Diethyl malonate



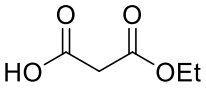
Isopentyl acetate
(used in synthetic banana flavor)



Isopentyl pentanoate
(used in synthetic apple flavor)

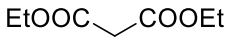



PROPANEDIOIC ACID
Malonic Acid

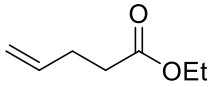



3-ethoxy-3-oxopropanoic acid

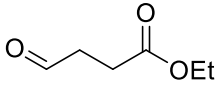
diethyl malonate




Diethyl propanedioate

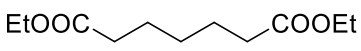


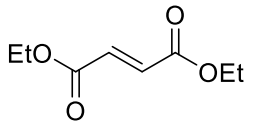

ethyl pent-4-enoate



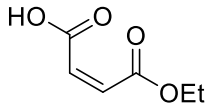

ethyl 4-oxobutanoate

diethyl heptanedioate

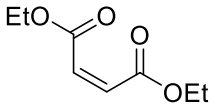


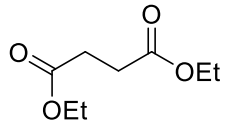

diethyl fumarate




(*Z*)-4-ethoxy-4-oxobut-2-enoic acid

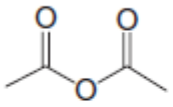



diethyl maleate

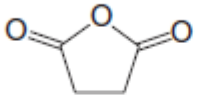



diethyl succinate

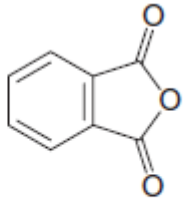
# Acid Derivatives



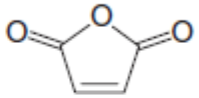
Acetic anhydride
(ethanoic anhydride)
mp –73 °C



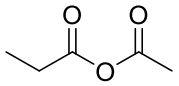
Succinic anhydride
mp 121 °C



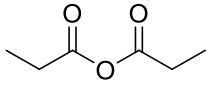
Phthalic anhydride
mp 131 °C



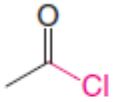
Maleic anhydride
mp 53 °C



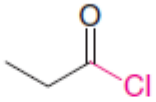
acetic propionic anhydride



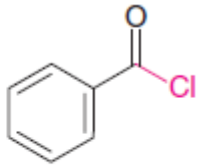
propionic anhydride



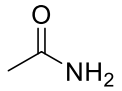
Acetyl chloride
(ethanoyl chloride)
mp –112 °C; bp 51 °C



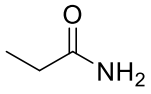
Propanoyl chloride
mp –94 °C; bp 80 °C



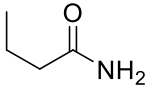
Benzoyl chloride
mp –1 °C; bp 197 °C



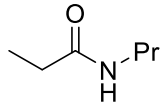
Ethanamide
acetamide



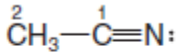
propionamide



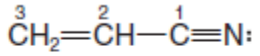
butyramide



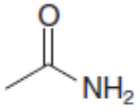
*N*-propylpropionamide



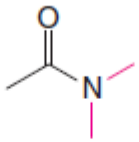
Ethanenitrile
(acetonitrile)



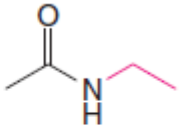
Propenenitrile
(acrylonitrile)



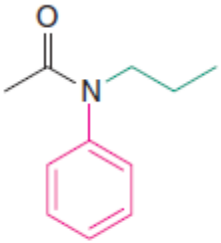
Acetamide
(ethanamide)
mp 82 °C; bp 221 °C



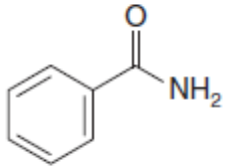
*N*,*N*-Dimethylacetamide
mp –20 °C; bp 166 °C



*N*-Ethylacetamide
bp 205 °C



*N*-Phenyl-*N*-propylacetamide
mp 49 °C; bp 266 °C at 712 torr



Benzamide
mp 130 °C; bp 290 °C

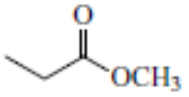
# *Questions*

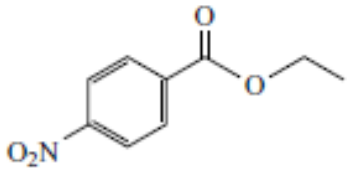
Write structural formulas for the following:

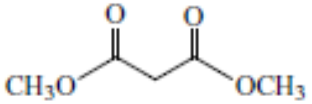
**(a)** Methyl propanoate
**(b)** Ethyl *p*-nitrobenzoate
**(c)** Dimethyl malonate
**(d)** *N*,*N*-Dimethylbenzamide
**(e)** Pentanenitrile
**(f)** Dimethyl phthalate
**(g)** Dipropyl maleate
**(h)** *N*,*N*-Dimethylformamide
**(i)** 2-Bromopropanoyl bromide
**(j)** Diethyl succinate

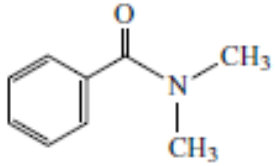
*N*,*N*-Diethyl-3-methylbenzamide:
(also called *N*,*N*-diethyl-***m*-toluamide**, or DEET): Insect Repellant

# Answers

(a) 

(b) 

(c) 

(d) 

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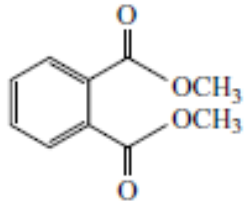
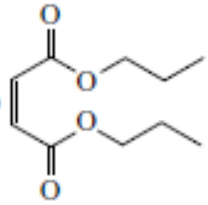
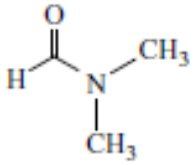
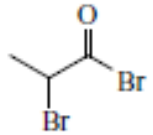
(f) 

(g) 

(h) 

(i) 

(j)