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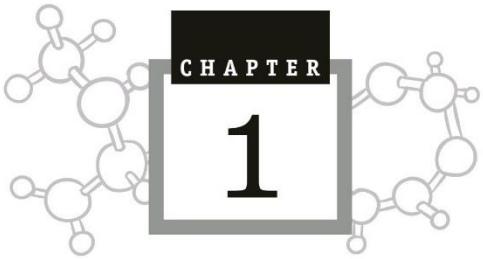
This set contains solutions for the important Organic Chemistry Topic-Wise Theory With Important Reagents & Name Reactions For Mains & Advanced/NEET. Topic-wise questions with solutions will help aspirants to clear their concepts and score more in the IIT JEE/NEET examination. Also, students will be able to easily refer to the past questions asked in the JEE Main.

ORGANIC CHEMISTRY VOLUME 01



Introduction

WHAT IS ORGANIC CHEMISTRY

What is organic chemistry, and why should you study it (other then scoring good marks in exams)☺ The answers to these questions are all around you. Every living organism is made of organic chemicals. The proteins that make up your hair, skin, and muscles; the DNA that controls your genetic heritage; the foods that nourish you; and the medicines that heal you are all organic chemicals. Anyone with a curiosity about life and living things, and anyone who wants to be a part of the remarkable advances now occurring in medicine and the biological sciences, must first understand organic chemistry.

Organic chemistry, then, is the study of carbon compounds.

But why is carbon special? Why, of the more than 50 million presently known chemical compounds, do most of them contain carbon?

From the simple methane, with one carbon atom, to the staggeringly complex DNA, which can have more than 100 million carbons.

At the time of writing there were about 16.5 million organic compounds known. How many more are possible? There is no limit. Imagine you've just made the longest hydrocarbon ever made—you just have to add another carbon atom and you've made another.

The Wohler synthesis is the conversion of ammonium cynate into urea. This chemical reaction was discovered in 1828 by Friedrich Wohler in an attempt to synthesize ammonium cyanate.

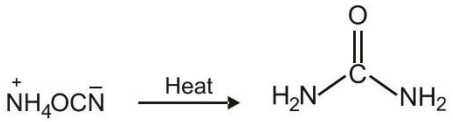
Ammonium cyanate decomposes to ammonia and cyanic acid which in turn react to produce urea in a nucleophilic addition followed by tautomeric isomerization :

The **Wohler synthesis** is of great historical significance because for the first time an organic compound was produced from inorganic reactants. This finding went against the mainstream theory of that time called vitalism which stated that organic

matter possessed a special force or vital force inherent to all things living. For this reason a sharp boundary existed between organic and inorganic compounds. Urea was discovered in 1799 and could until then only be obtained from biological sources such as urine Wohler reported to his teacher Berzelius

"I cannot, so to say, hold my chemical water and must tell you that I can make urea without thereby needing to have kidneys, or anyhow, an animal, be it human or dog".

Little more than a decade later, the vitalistic theory suffered still further when Friedrich Wöhler discovered in 1828 that it was possible to convert the "inorganic" salt ammonium cyanate into the "organic" substance urea, which had previously been found in human urine.

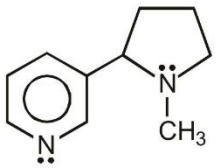


Ammonium cyanate Urea

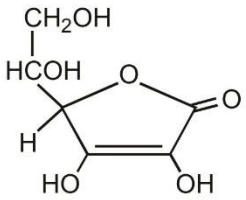
ORGANIC CHEMISTRY AND DRUGS

Four examples of organic compound in living organisms.

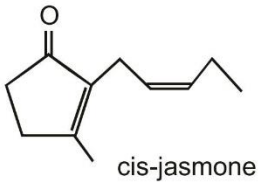
Nicotine



Tobacco contains nicotine, an addictive alkaloid.



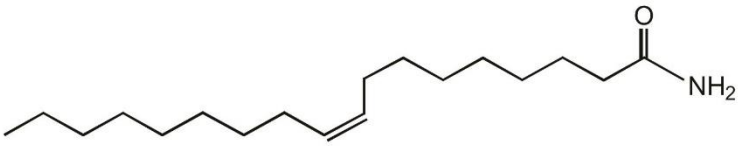
Vitamin C (ascorbic acid) Rose hips contain vitamin C, essential for preventing scurvy.



cis-jasmone

cis-jasmone an example of a perfume distilled from jasmine flowers.

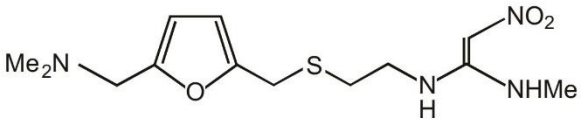
Again, let's not forget other creatures. Cats seem to be able to go to sleep at any time and recently a compound was isolated from the cerebrospinal fluid of cats that makes them, or rats, or humans go off to sleep quickly. It is a surprisingly simple compound.



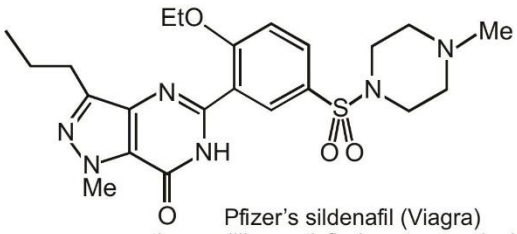
a sleep-inducing fatty acid derivative
cis-9,10-octadecenoamide

The pharmaceutical businesses produce drugs and medicinal products of many kinds. One of the great revolutions of modern life has been the expectation that humans will survive diseases because of a treatment designed to deal specifically with that disease. The most successful drug ever is ranitidine (Zantac), the Glaxo–Wellcome ulcer treatment, and one of the fastest-growing is Pfizer's sildenafil (Viagra). 'Success' refers both to human health and to profit!

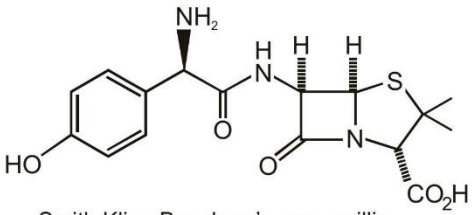
One of the most successful of these is Smith Kline Beecham's amoxycillin. The four-membered ring at the heart of the molecule is the 'β-lactam'.



Glaxo-Wellcome's ranitidine
the most successful drug to date
world wide sales peaked >£1,000,000,000 per annum



Pfizer's sildenafil (Viagra)
three million satisfied customers in 1998

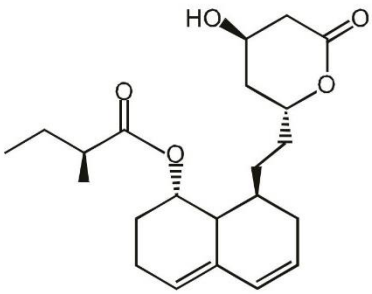


Smith Kline Beecham's amoxycillin
β-lactam antibiotic
for treatment of bacterial infections

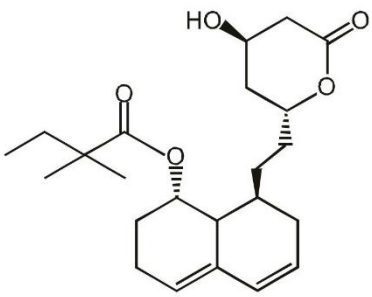
☑ SPECIAL TOPIC

HOW HIGH CHOLESTEROL IS TREATED CLINICALLY

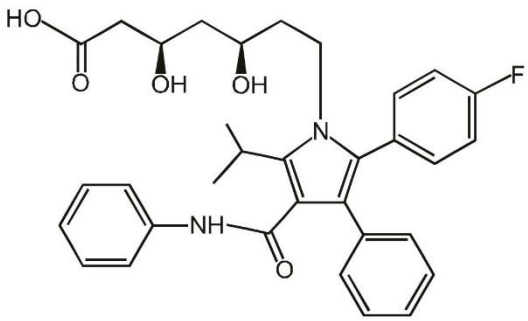
Statins are drugs that reduce serum cholesterol levels by inhibiting the enzyme that catalyzes the formation of a compound needed for the synthesis of cholesterol. As a consequence of diminished cholesterol synthesis in the liver, the liver forms more LDL receptors—the receptors that help clear LDL (the so-called "bad" cholesterol) from the bloodstream. Studies show that for every 10% that cholesterol is reduced, deaths from coronary heart disease are reduced by 15% and total death risk is reduced by 11%.☺



lovastatin
Mevacor



simvastatin
Zocor



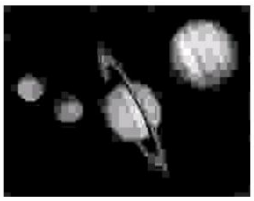
atorvastatin
Lipitor

Lovastatin and simvastatin are natural statins used clinically under the trade names Mevacor and Zocor. Atorvastatin (Lipitor), a synthetic statin, is the most popular statin. It has greater potency and lasts longer in the body than natural statins because the products of its breakdown are as active as the parent drug in reducing cholesterol levels. Therefore, smaller doses of the drug may be administered.

In addition, Lipitor is less polar than lovastatin and simvastatin, so it persists longer in liver cells, where it is needed. Lipitor has been one of the most widely prescribed drugs in the United States for the past several years.

☑ SPECIAL TOPIC

ORGANIC CHEMISTRY AND COLOURS



The blue colors of Uranus and Neptune are caused by the presence of methane, a colorless and odorless gas, in their atmospheres. Natural gas—called a fossil fuel because it is formed from the decomposition of plant and animal material in the Earth's crust—is approximately 75% methane. The methane in Uranus' upper atmosphere absorbs the red light from the Sun but reflects the blue light from the Sun back into space. This is why Uranus appears blue.

ORGANIC FOODS

Contrary to what you may hear in supermarkets or on television, all foods are organic—that is, complex mixtures of organic molecules. Even so, when applied to food, the word organic has come to mean an absence of synthetic chemicals, typically pesticides, antibiotics, and preservatives. How concerned should we be about traces of pesticides in the food we eat? Or toxins in the water we drink? Or pollutants in the air we breathe?☹

Life is not risk-free—we all take many risks each day without even thinking about it. We decide to ride a bike rather than drive, even though there is a ten times greater likelihood per mile of dying in a bicycling accident than in a car. Some of us decide to smoke cigarettes, even though it increases our chance of getting cancer by 50%. But what about risks from chemicals like pesticides?

One thing is certain: without pesticides, whether they target weeds (herbicides), insects (insecticides), or molds and fungi (fungicides), crop production would drop significantly, food prices would increase, and famines would occur in less developed parts of the world. Take the herbicide atrazine, for instance. In the United States alone, approximately 100 million pounds of atrazine are used each year to kill weeds in corn, sorghum, and sugarcane fields, greatly improving the yields of these crops. The results obtained in animal tests are then distilled into a single number called an LD_{50}, the amount of substance per kilogram body weight that is a lethal dose for 50% of the test animals. For atrazine, the LD_{50} value is between 1 and 4 g/kg depending on the animal species. Aspirin, for comparison, has an LD_{50} of 1.1 g/kg, and ethanol (ethyl alcohol) has an LD_{50} of 10.6 g/kg.

Table-1 : lists values for some other familiar substances. The lower the value, the more toxic the substance. Note, though, that LD_{50} values tell only about the effects of heavy exposure for a relatively short time.

Table - 1 : Some LD_{50} Values

Substance	LD_{50}(g/kg)	Substance	LD_{50}(g/kg)
Strychnine	0.005	Chloroform	1.2
Arsenic trioxide	0.015	Iron (II) sulfate	1.5
DDT	0.115	Ethyl alcohol	10.6
Aspirin	1.1	Sodium cyclamate	17

They say nothing about the risks of long-term exposure, such as whether the substance can cause cancer or interfere with development in the unborn.

So, should we still use atrazine? All decisions involve tradeoffs, and the answer is rarely obvious. Does the benefit of increased food production outweigh possible health risks of a pesticide? Do the beneficial effects of a new drug outweigh a potentially dangerous side effect in a small number of users? Different people will have different opinions, but an honest evaluation of facts is surely the best way to start. At present, atrazine is approved for continued use in the United States because the EPA believes that the benefits of increased food production outweigh possible health risks. At the same time, though, the use of atrazine is being phased out in Europe.

❑❑❑

CHAPTER

2

Representation of Organic Compounds

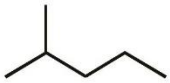
BOND-LINE DRAWINGS

To do well in organic chemistry, you must first learn to interpret the drawings that organic chemists use. When you see a drawing of a molecule, it is absolutely critical that you can read all of the information contained in that drawing. Without this skill, it will be impossible to master even the most basic reactions and concepts.

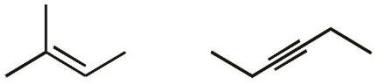
HOW TO READ BOND-LINE DRAWINGS

For example, the following compounds has 6 carbon atoms:

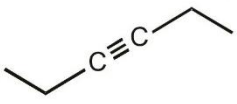
It is a common mistake to forget that the ends of lines represent carbon atoms as well. For example, the following molecule has six carbon atoms (Make sure you can count them)



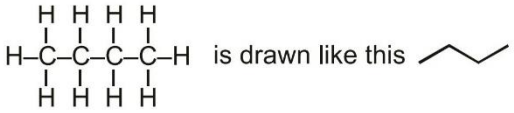
Double bonds are shown with two lines, and triple bonds are shown with three lines :



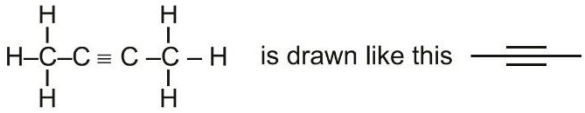
When drawings triple bonds, be sure to draw them in a straight line rather than zigzag, because triple bonds are linear (There will be more about this in the chapter on geometry). This can be quite confusing at first, because it can get hard to see just how many carbon atoms are in a triple bond, so let's make it clear:

 is the same as  so this compound has 6 carbon atoms

Don't let triple bonds confuse you. The two carbon atoms of the triple bond and the two carbons connected to them are drawn in a straight line. All other bonds are drawn as a zigzag:

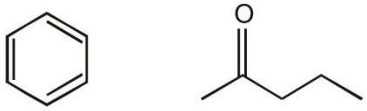


But



Solved Example

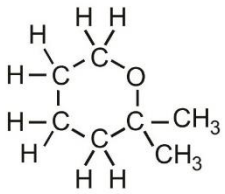
- Count the number of carbon atoms in each of the following drawings:



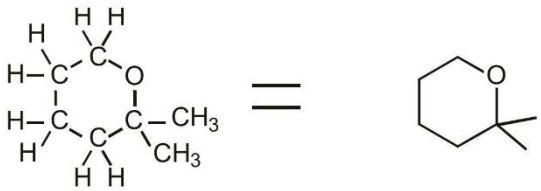
Ans. The first compound has six carbon atoms, and the second compound has five carbon atoms.

HOW TO DRAW BOND-LINE DRAWINGS

Now that we know how to read these drawings, we need to learn how to draw them. Take the following molecule as an example:

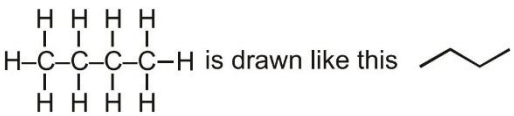


To draw this as a bond-line drawing, we focus on the carbon skeleton, making sure to draw any atoms other than C and H. All atoms other than carbon and hydrogen must be drawn. So the example above would look like this:

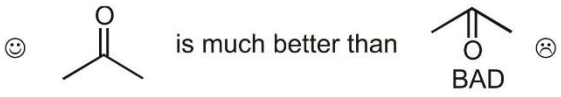


Points to Remember

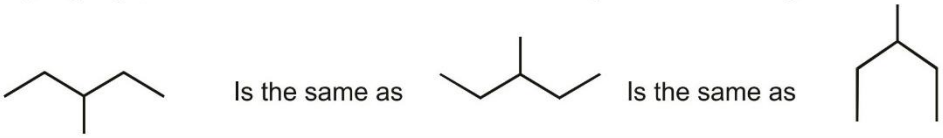
1. Don't forget that carbon atoms in a straight chain are drawn in a zigzag format:



2. When drawing double bonds, try to draw the other bonds as far away from the double bond as possible:

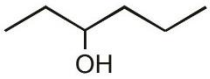
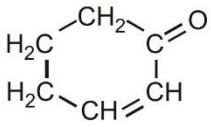
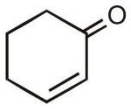
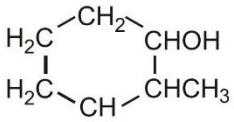
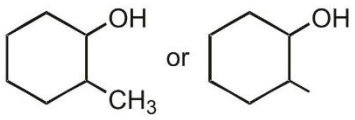
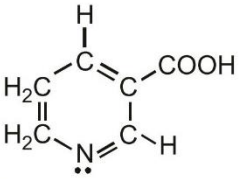
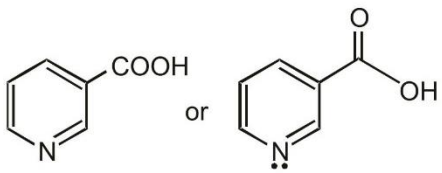


3. When drawing zigzags, it does not matter in which direction you start drawing:



LINE-ANGLE FORMULAS

Another kind of shorthand used for organic structures is the line-angle formula, sometimes called a skeletal structure or a stick figure. Line-angle formulas are often used for cyclic compounds and occasionally for noncyclic ones. In a stick figure, bonds are represented by lines, and carbon atoms are assumed to be present wherever two lines meet or a line begins or ends. Nitrogen, oxygen, and halogen atoms are shown, but hydrogen atoms are not usually drawn unless they are bonded to an atom that is drawn. Each carbon atom is assumed to have enough hydrogen atoms to give it a total of four bonds. Nonbonding electrons are rarely shown.\

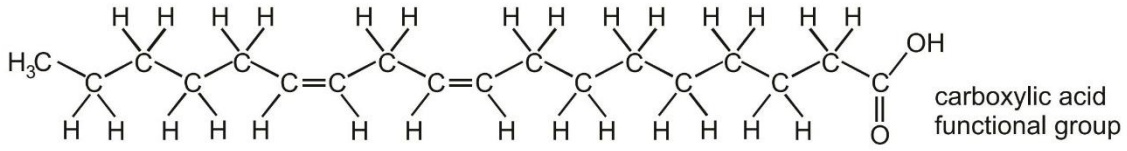
Compound	Condensed Structure	Line-angle Formula
hexane	$CH_3(CH_2)_4CH_3$	
hex-2-ene	$CH_3CH = CHCH_2CH_2CH_3$	
hexan-3-ol	$CH_3CH_2CH(OH)CH_2CH_2CH_3$	
cyclohex-2-en-1-one		
2-methylcyclohexan-1-ol		
nicotinic acid (a vitamin,also called niacin)		

❑ **NOTE:** IUPAC names will be discussed in next chapter.

DRAWING MOLECULES

Be realistic

Below is another organic structure—again, you may be familiar with the molecule it represents; it is a fatty acid commonly called linoleic acid.



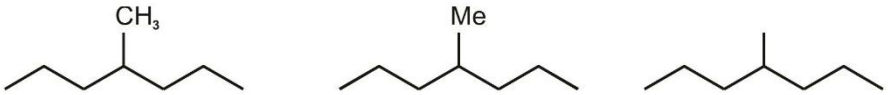
linoleic acid

We could also depict linoleic acid as

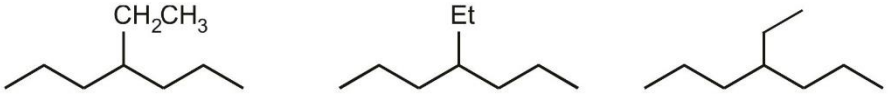
$CH_3CH_2CH_2CH_2CH=CHCH_2CH=CHCH_2CH_2CH_2CH_2CH_2CH_2CO_2H$

(Condensed formula)

Methyl groups can be shown in a numbers of ways, and all of them are acceptable :

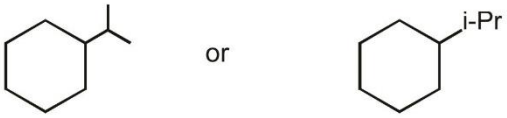


Ethyl groups can also be shown in a number of ways:



Propyl groups are usually just drawn, but sometimes you will see the term Pr (which stands for propyl):

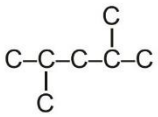
Look at the propyl group above and you will notice that it is a small chain of 3 carbon atoms that is attached to the parent chain by the first carbon of the small chain. But what if it is attached by the middle carbon? Then it is not called propyl anymore :



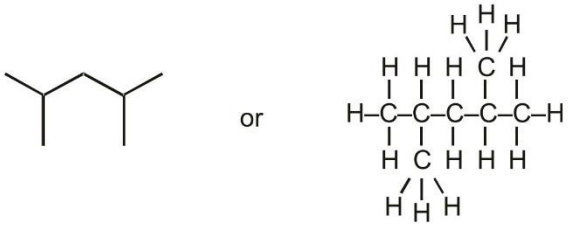
It is called as iso-Propyl or i-Pr.

MISTAKES TO AVOID

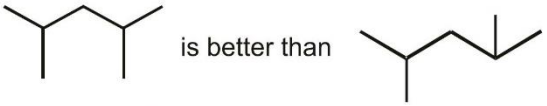
Drawing where the C's and H's are not drawn. You cannot draw the C's without also drawing the H's:



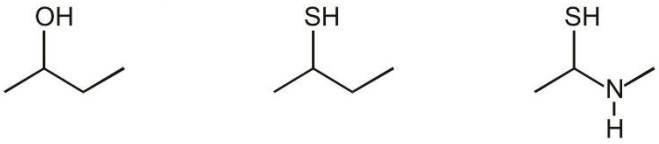
This drawing is no good. Either leave out the C's (which is preferable) or put in the H's:



When drawing each carbon atom in a zigzag, try to draw all of the bonds as far apart as possible:

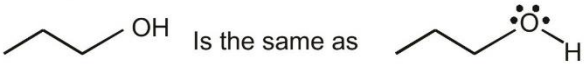


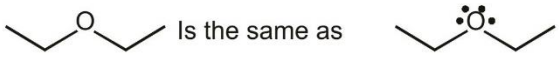
In bond-line drawings, we do draw any H's that are connected to atoms other than carbon. For example,

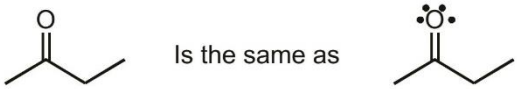


FINDING LONE PAIRS THAT ARE NOT DRAWN

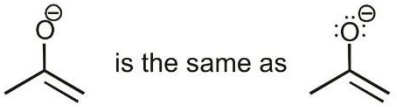
When oxygen has no formal charge, it will have two bonds and two lone pairs:



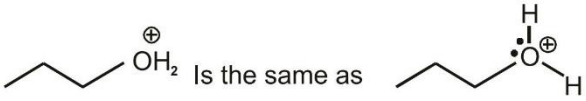


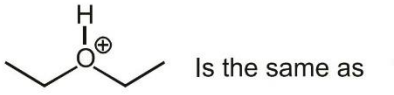


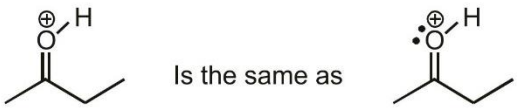
If oxygen has a negative formal charge, then it must have one bond and three lone pairs:



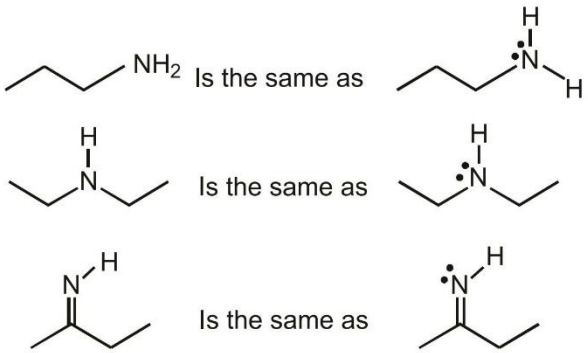
If oxygen has a positive charge, then it must have three bonds and one lone pair:



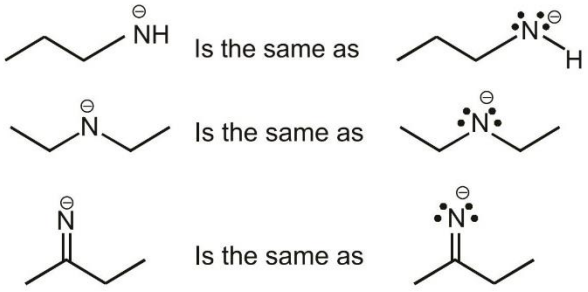




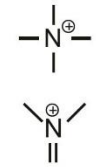
Now let's look at the common situations for nitrogen atoms. When nitrogen has no formal charge, it will have three bonds and one lone pair:



If nitrogen has a negative formal charge, then it must have two bonds and two lone pairs:



If nitrogen has a positive charge, then it must have four bonds and no lone pairs:

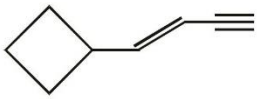

has no lone pairs

has no lone pairs


has no lone pairs

Solved Example

- The number of hydrogen atoms associated with the molecule shown below is ?

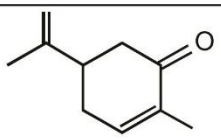


Ans. 10 hydrogens

INTERPRETING A BOND-LINE STRUCTURE

Solved Example

- Carvone, a substance responsible for the odor of spearmint, spearmint, has the following structure. Tell how many hydrogens are bonded to each carbon, and give the molecular formula of carvone.

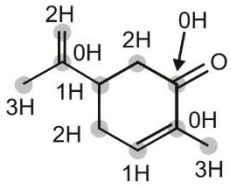


Carvone

Strategy

The end of a line represents a carbon atom with 3 hydrogens, CH_3; a two-way intersection is a carbon atom with 2 hydrogens, CH_2; a three-way intersection is a carbon atom with 1 hydrogen, CH; and a four-way intersection is a carbon atom with no attached hydrogens.

Sol.

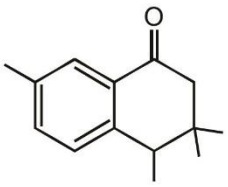


Carvone ($C_{10}H_{14}O$)

COUNTING THE NUMBER OF HYDROGEN ATOMS

Now that we know to count carbon atoms, we must learn how to count the hydrogen atoms in a bond-line drawing of a molecule. The hydrogen atoms are not shown, and this is why it is so easy and fast to draw bond-line drawings. Neutral carbon atoms always have a total of four bonds.

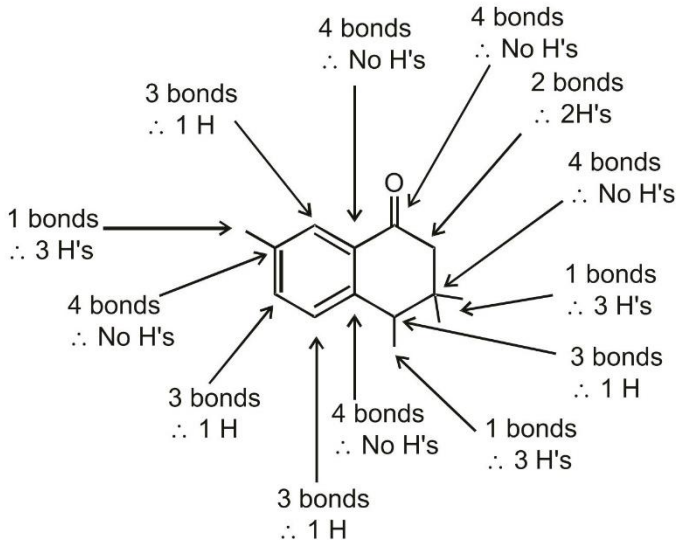
So you only need to count the number that you can see on a carbon atom, and then you know that there should be enough hydrogen atoms to give a total of four bonds to the carbon atom.



Solved Example

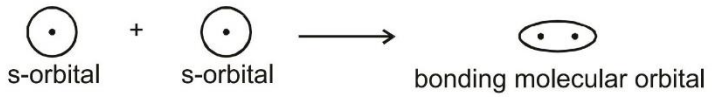
- The following molecule has 14 carbon atoms. Count the number of hydrogen atoms connected to each carbon atom

Ans.

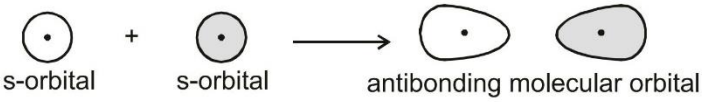


SIGMA (σ–) AND PI (π–) BONDS

The electrons shared in a covalent bond result from overlap of atomic orbitals to give a new molecular orbital. Electrons in 1s and 2s orbitals combine to give sigma (σ–) bonds. When two 1s orbitals combine in phase, this produces a bonding molecular orbital.

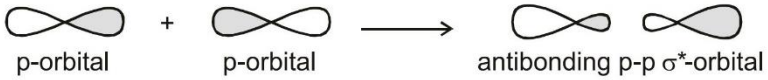


When two 1s orbitals combine out-of-phase, this produces an antibonding molecular orbital.

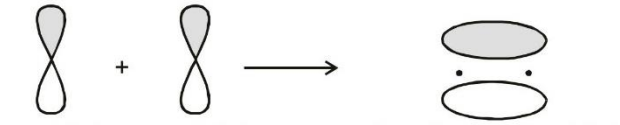


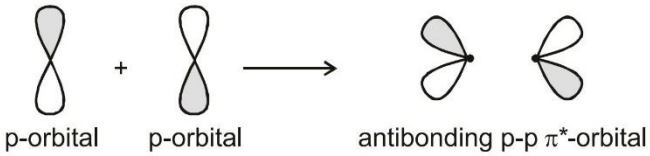
Electrons in p orbitals can combine to give sigma (σ) or pi (π) bonds.

- Sigma (σ-) bonds are strong bonds formed by head-on overlap of two atomic orbitals.



- Pi(π–) bonds are weaker bonds formed by side-on overlap of two π-orbitals.



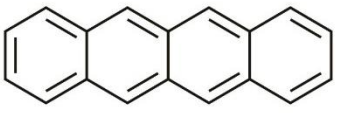


Only σ- or π-bonds are present in organic compounds. All single bonds are s-bonds while all multiple (double or triple) bonds are composed of one s-bond and one or two p-bonds.

EXERCISE

SINGLE CHOICE QUESTIONS

1. Number of p-bonds present in given compound are:



(A) 8 (B) 9 (C) 10 (D) 12

2. How many Hydrogens does an alkane with 17 carbons have?

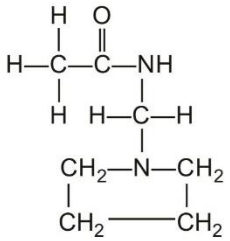
(A) 32 (B) 34 (C) 36 (D) 38

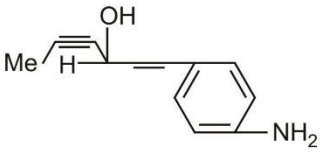
3. How many carbons does an alkane with 34 hydrogens have?

(A) 16 (B) 14 (C) 15 (D) 17

SUBJECTIVE TYPE QUESTIONS

1. What is wrong with these structures ? Suggest better ways of representing these molecules.



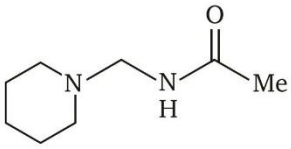


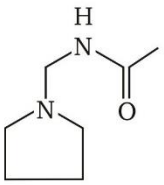
Purpose of the Problem

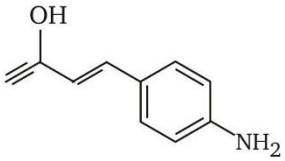
To shock you with two dreadful structure and to try and convince you that well drawn realistic structures are more attractive to the eye as well as easier to understand.

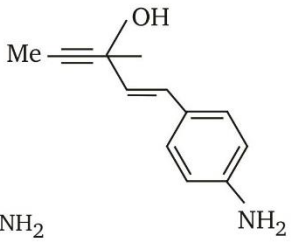
Suggested solution

The bond angles are grotesque with square planar saturated carbon, alkynes at 120°, alkenes at 180°, bonds coming off benzene rings at the wrong angle, and so on, The left-hand structure would be clear if most of the hydrogens were omitted. Hence there are two possible better structure for each molecule. There are many other correct possibilities.









Answers

Single Choice Questions

1. (B) **2.** (C) **3.** (A)

❑❑❑

CHAPTER 3

Degree of Carbon & Hydrogen, Alcohol & Amine

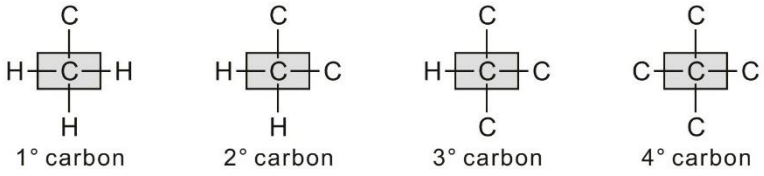
DEGREE OF CARBON AND HYDROGEN IN HYDROCARBON

DEGREE OF CARBON

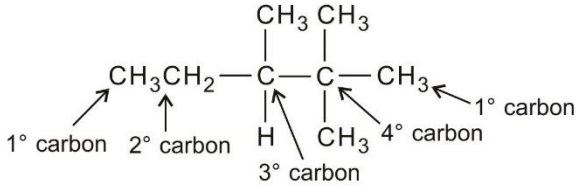
Carbon atoms in alkanes and other organic compounds are classified by the number of other carbons directly bonded to them.

1º or Primary
2º or Secondary
3º or Tertiary
4º or Quaternary

CLASSIFICATION OF CARBON ATOMS

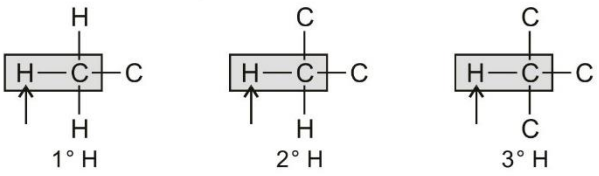


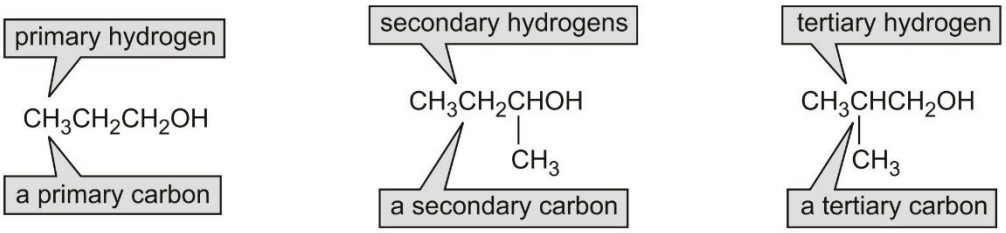
Solved Example



CLASSIFICATION OF HYDROGEN ATOMS

Like the carbons, the hydrogens in a molecule are also referred to as primary, secondary, and tertiary. **Primary hydrogens** are attached to a primary carbon, **secondary hydrogens** are attached to a secondary carbon, and **tertiary hydrogens** are attached to a tertiary carbon.

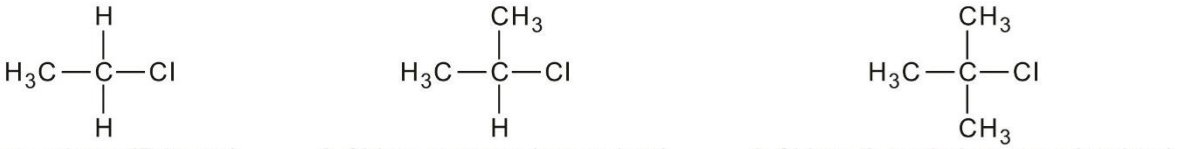




DEGREE OF CARBON IN ALKYLHALIDE

Alkyl halides are classified as primary, secondary and tertiary alkyl halides depending on whether the halogen atom is attached to a primary, secondary or tertiary carbon atom respectively.

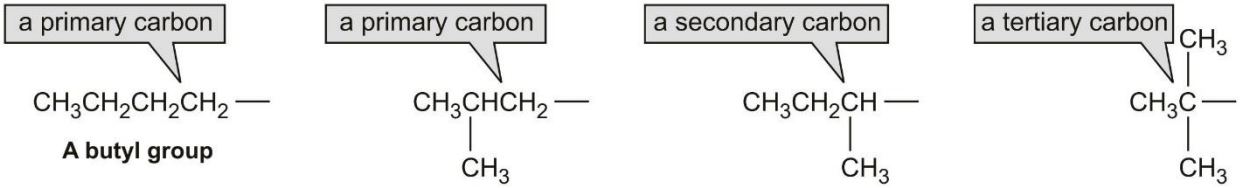
For example



Chloro ethane (Primary) | 2-Chloro propane (secondary) | 2-Chloro-2-methyl propane (tertiary)

Aromatic halogen compounds or halo arenes are the halogen compounds which contain atleast one aromatic ring.

There are four alkyl groups that have four carbons. Two of them, the butyl and isobutyl groups, have a hydrogen removed from a primary carbon. A *sec* -butyl group has a hydrogen removed from a secondary carbon (*sec*- , sometimes abbreviated *s*- , stands for secondary), and a *tert* -butyl group has a hydrogen removed from a tertiary carbon (*tert*-, often abbreviated *t*- , stands for tertiary). **A tertiary carbon** is a carbon that is bonded to three other carbons. Notice that the isobutyl group is the only one with an iso structural unit.

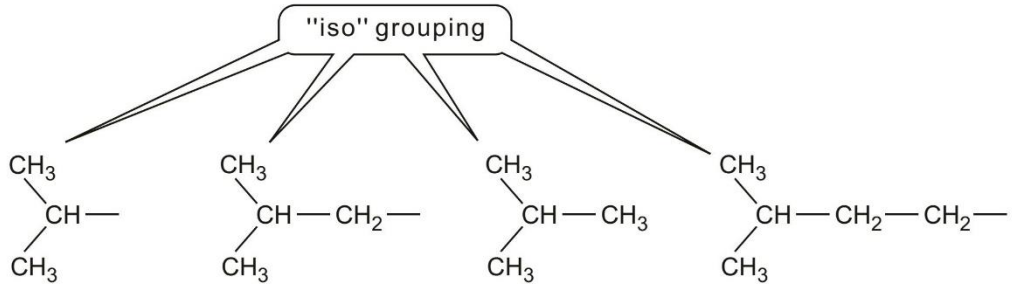


A chemical name must specify one compound only. The prefix "*sec*, " therefore, can be used only for *sec* -butyl compounds. **The name "*sec*-pentyl" cannot be used because pentane has two different secondary carbons.** Thus, removing a hydrogen from a secondary carbon of pentane produces one of two different alkyl groups, depending on which hydrogen is removed. As a result, *sec*-pentyl chloride would specify two different alkyl chlorides, so it is *not* a correct name.

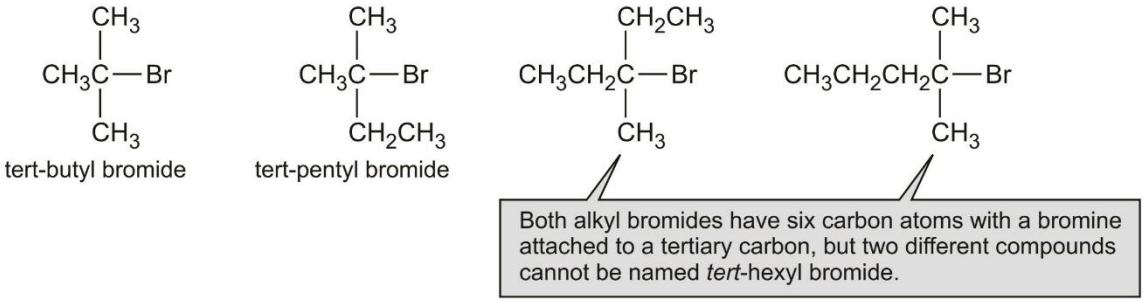
Both alkyl halides have five carbon atoms with a chlorine attached to a secondary carbon, but two compounds cannot be named *sec*-pentyl chloride.

PROBLEM-SOLVING HINT

When looking for the longest continuous chain (to give the base name), look to find all the different chains of that length, Often, the longest chain with the most substituents is not obvious.



isopropyl group | **isobutyl group** | **isobutane** | **isopentyl group (isoamyl group)**



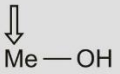
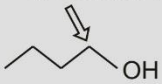
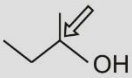
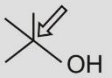
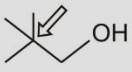
tert-butyl bromide | tert-pentyl bromide

Both alkyl bromides have six carbon atoms with a bromine attached to a tertiary carbon, but two different compounds cannot be named *tert*-hexyl bromide.

DEGREE OF ALCOHOL

- **Primary, secondary, and tertiary**

  The prefixes *sec* and *tert* are really short for secondary and tertiary, terms that refer to the carbon atom that attaches these groups to the rest of the molecular structure.

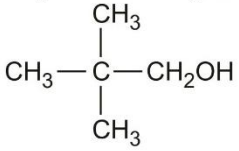
methyl (no attached C)	primary (1 attached C)	secondary (2 attached C)	tertiary (3 attached C)	quaternary (4 attached C)
				
methanol	(1°-alcohol) butan-1-ol *n*-butanol	(2°-alcohol) butan-2-ol sec-butanol	(3°-alcohol) 2-methypropan-2-ol tert-butanol	(1°-alcohol) 2, 2-dimethylpropan-1-ol

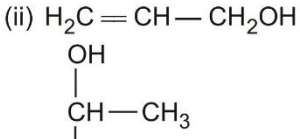
A primary carbon atom is attached to only one other C atom, a secondary to two other C atoms, and so on. This means there are five types of carbon atom.

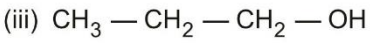
These names for bits of hydrocarbon framework are more than just useful ways of writing or talking about chemistry. They tell us something fundamental about the molecule and we shall use them when we describe reactions.

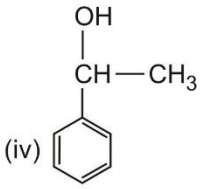
Solved Example

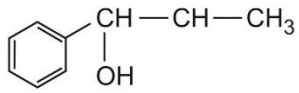
- Classify the following as primary, secondary and tertiary alcohols :

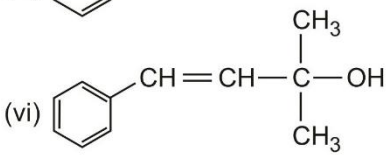
(i) 

(ii) 

(iii) 

(iv) 

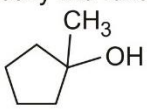
(v) 

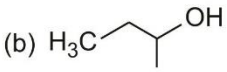
(vi) 

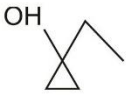
Ans. Primary alcohol (i), (ii) and (iii), Secondary alcohol (iv) and (v), Tertiary alcohol (vi)

Solved Example

- Classify the following into primary, secondary and tertiary alcohols :

(a) 

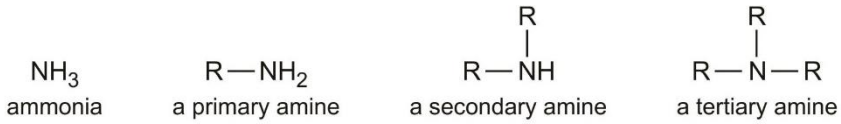
(b) 

(c) 

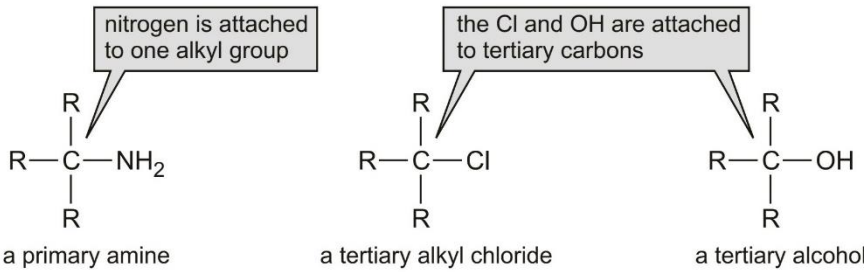
Ans. (a) Tertiary (b) Secondary (c) Tertiary

DEGREE OF AMINE

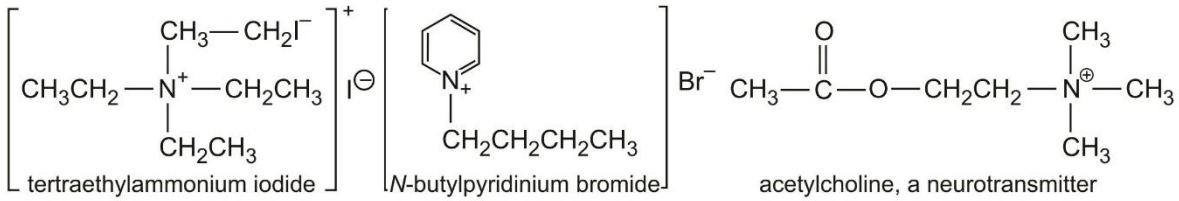
An amine is a compound in which one or more hydrogens of ammonia have been replaced by alkyl groups. Amines are classified as **primary**, **secondary**, and **tertiary**, depending on how many alkyl groups are attached to the nitrogen. Primary amines have one alkyl group attached to the nitrogen, secondary amines have two, and tertiary amines have three.



Be sure to note that the number of alkyl groups attached to the nitrogen determines whether an amine is primary, secondary,

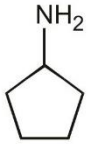


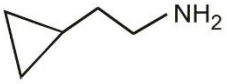
Quaternary ammonium salts have four alkyl or aryl bonds to a nitrogen atom. The nitrogen atom bears a positive charge, just as it does in simple ammonium salts such as ammonium chloride. The following are examples of quaternary (4°) ammonium salts:

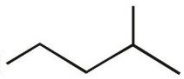


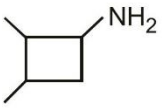
Solved Example

- Which among the following compound(s) is a primary amine with the molecular formula $C_5H_{11}N$?

(A) 

(B) 

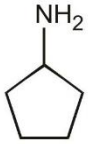
(C) 

(D) 

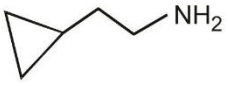
Ans. (A, B)

Sol. $C_5H_{11}N$; D.B.E. $= (5+1) - \frac{(11-1)}{2} = 1$

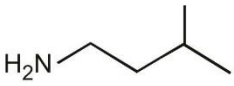
Thus, amine either be a cyclic or having double bond



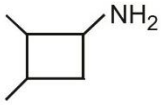
$C_5H_{11}N$ ✓



$C_5H_{11}N$ ✓



$C_5H_{13}N$ ×

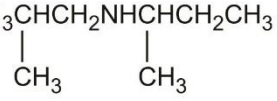


$C_6H_{13}N$ ×

Solved Example

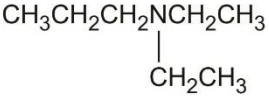
- Give a systematic name and a common name (if it has one) for each of the following amines and indicate whether each is a primary, secondary, or tertiary amine :

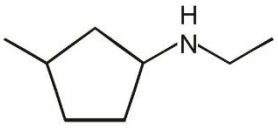
(a) $CH_3CH_2CH_2CH_2CH_2CH_2NH_2$

(b) 

(c) $(CH_3CH_2)_2NCH_3$

(d) $CH_3CH_2CH_2NHCH_2CH_2CH_2CH_3$

(e) 

(f) 

Sol. (a) Hexan-1-amine (1°)

(b) N-(2-methylpropyl)butan-2-amine (2°)

(c) N-ethyl-N-methylethan-1-amine (3°)

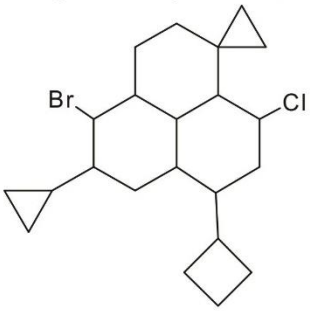
(d) N-propylbutanamine (2°)

(e) N,N-diethylpropan-1-amine (3°)

(f) N-ethyl-3-methylcyclopentanamine (2°)

Solved Example

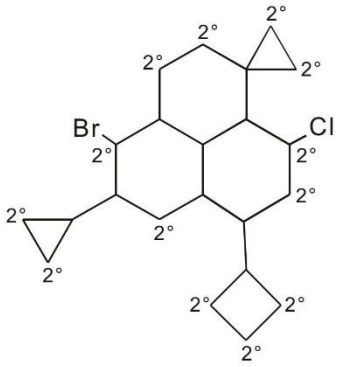
- Total number of 2° carbon present in given compound is , so the value of



is :

Ans. 13

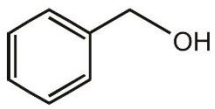
Sol.

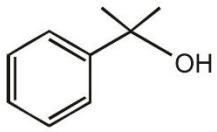


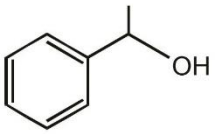
2º carbons are present = 13

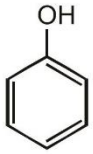
Solved Example

- Which of the following compounds is a secondary alcohol?

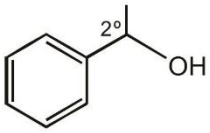
(A) 

(B) 

(C) 

(D) 

Ans. (C)

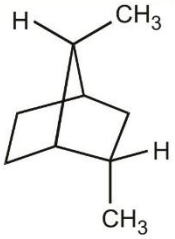
Sol. 

❑ **NOTE:** (Phenol is not alcohol).

Solved Example

- How many secondary hydrogens are present in the hydrocarbon below?

(A) 2
(B) 6
(C) 7
(D) 8
(E) 16

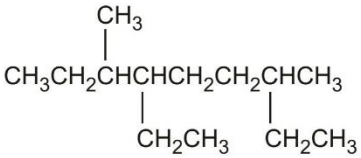
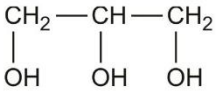
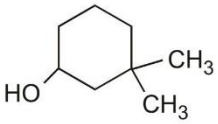
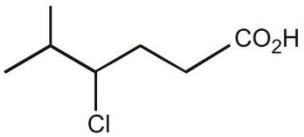
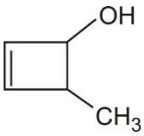
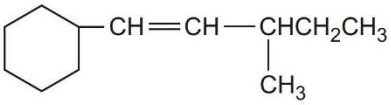
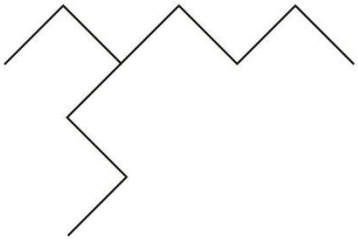
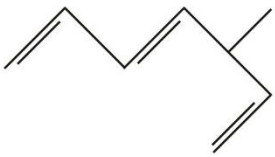
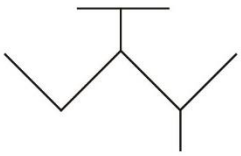


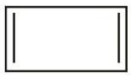
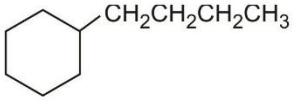
Ans. (B)

EXERCISE

WORK SHEET - 1

Count the number of primary, secondary, tertiary, quarternary carbon as well as hydrogen in given compound :

S.No.	Compound	1°C	2°C	3°C	4°C	1°H	2°H	3°H
1.								
2.								
3.								
4.								
5.								
6.								
7.								
8.								
9.								

10.							
11.							

Answers

Work Sheet-1

S.No.	1°C	2°C	3°C	4°C	1°H	2°H	3°H
1.	5	5	3	0	15	10	3
2.	2	1	0	0	4	1	0
3.	2	5	0	1	6	9	0
4.	3	3	1	0	6	5	1
5.	1	3	1	0	3	3	1
6.	2	8	2	0	6	14	2
7.	3	6	1	0	9	12	1
8.	3	4	1	0	7	4	1
9.	5	1	3	0	15	2	3
10.	0	4	0	0	0	4	0
11.	1	8	1	0	3	16	1

❑❑❑

CHAPTER 4

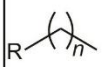
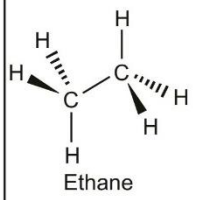
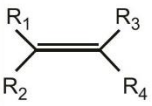
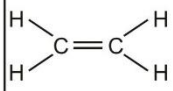
Functional Groups

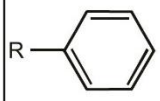
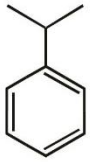
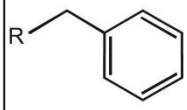
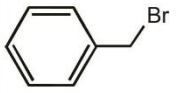
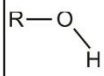
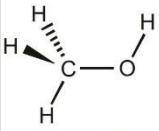
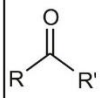
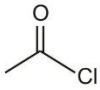
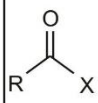
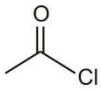
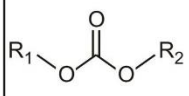
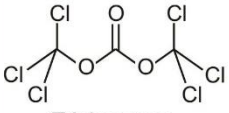
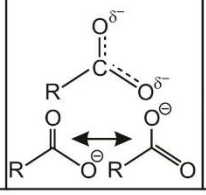
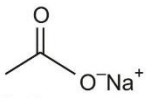
FUNCTIONAL GROUPS

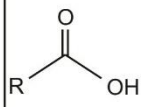
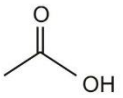
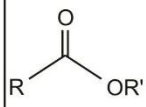
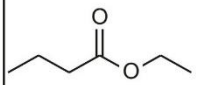
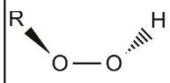
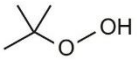
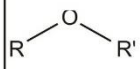
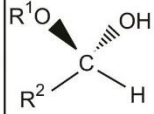
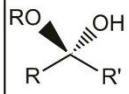
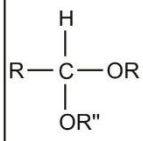
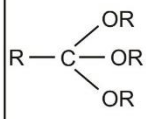
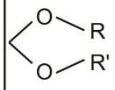
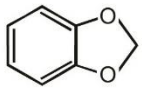
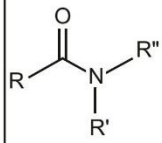
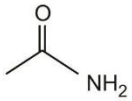
In organic chemistry, functional groups are specific groups of atoms or bonds within molecules that are responsible for the characteristic chemical reactions of those molecules. The same functional group will undergo the same or similar chemical reaction(s) regardless of the size of the molecule it is a part of.

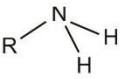
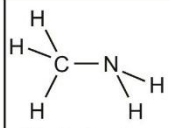
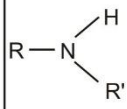
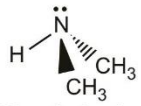
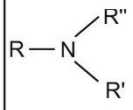
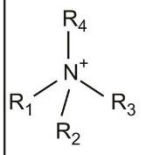
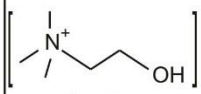
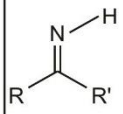
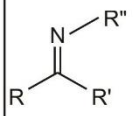
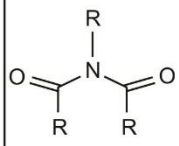
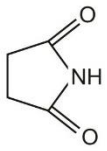
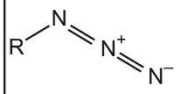
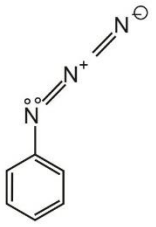
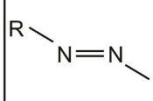
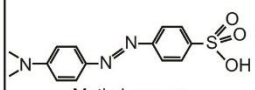
Combining the names of functional groups with the names of the parent alkanes generates a powerful systematic nomenclature for naming organic compounds.

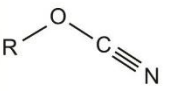
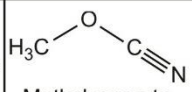
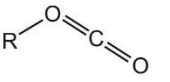
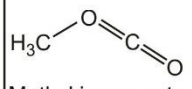
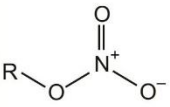
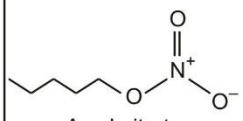
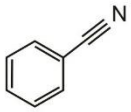
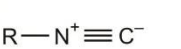
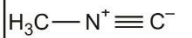
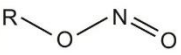
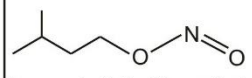
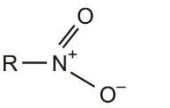
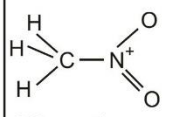
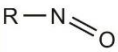
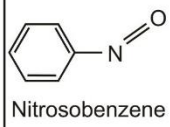
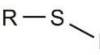
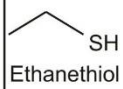
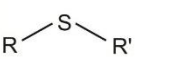
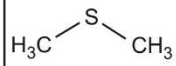
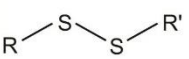
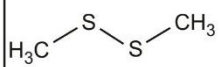
TABLE OF COMMON FUNCTIONAL GROUPS

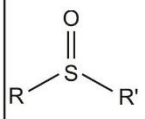
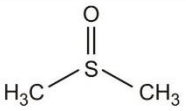
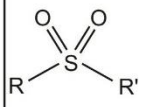
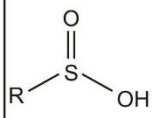
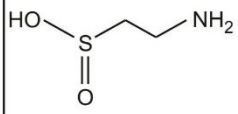
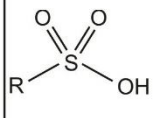
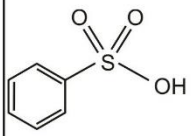
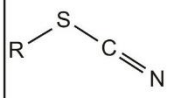
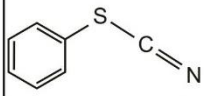
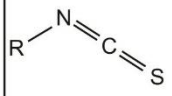
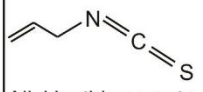
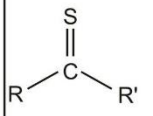
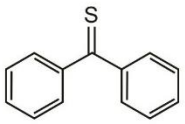
S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
1.	Alkane	Alkyl	$R(CH_2)_nH$		alkyl	-ane	 Ethane
2.	alkene	alkenyl	$R_2C=CR_2$		alkenyl-	-ene	
3.	Alkyne	Alkynyl	$RC\equiv CR'$	$R-C\equiv C-R'$	alkynyl-	-yne	$H-C\equiv C-H$ Acetylene (Ethyne)

S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
4.	Benzene derivative	Phenyl	RC_6H_5(RPh)		phenyl-	-benzene	 Cumene (2-phenylpropane)
5.	Toluene derivative	Benzyl	$RCH_2C_6H_5$ (R—Ph)		benzyl-	1-(substituent) toluene	 Benzyl bromide (α-Bromotoluene)
6.	haloalkane	halo	RX		halo-	alkyl halide	 Chloroethane (Ethylchloride)
7.	Alcohol	Hydroxyl	ROH		hydroxy-	-ol	 Methanol
8.	Ketone	Carbonyl	RCOR′		-oyl-(-COR′) or OXO or keto	-one	 Acetyl chloride (Ethanoyl chloride)
9.	Aldehyde	Aldehyde	RCHO		formyl-(—COH)	-al	 Acetaldehyde
10.	Acyl halide	Haloformyl	RCOX		carbonofluoridoyl- carbonochloridoyl- carbonobromidoyl- carbonoiodidoyl-	-oyl **halide**	 Acyl chloride (Ethanoyl chloride)
11.	Carbonate	Carbonate ester	ROCOOR		(alkoxycarbonyl) oxy-	alkyl **carbonate**	 Triphosgene (bis(trichloromethyl) carbonate)
12.	Carboxylate	Carboxylate	$RCOO^-$		carboxy-	-oate	 Sodium acetate (Sodium ethanoate)

S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
13.	Carboxylic acid	Carboxyl	RCOOH		carboxy-	-oic **acid**	 Acetic acid (*Ethanoic acid*)
14.	Ester	Ester	RCOOR′		alkanoyloxy- or alkoxycarbonyl	alkyl alkanoate	 Ethyl butyrate (*Ethyl butanoate*)
15.	Hydroperoxide	Hydroperoxy	ROOH		hydroperoxy-	alkyl **hydroperoxide**	 tert-Butyl hydroperoxide
16.	Ether	Ether	ROR′		alkoxy-	alkyl **ether**	 Diethyl ether (Ethoxyethane)
17.	Hemiacetal	Hemiacetal	RCH(OR′) (OH)		alkoxy-ol	-one alkyl **hemiacetal**	
18.	Hemiketal	Hemiketal	RC(OR″)(OH)R′		alkoxy-ol	-one alkyl **hemiketal**	
19.	Acetal	Acetal	RCH(OR′)(OR″)		dialkoxy-	-al dialkyl **acetal**	
20.	Orthoester	Orthoester	RC(OR′)(OR″)(OR‴)		trialkoxy-		
21.	Heterocycle	Methylenedioxy	ROCOR′		methylene- dioxy-	-dioxole	 1,2-Methylenedioxy-benzene (1,3-Benzodioxole)
22.	Amide	Carboxamide	$RCONR_2$		Carboxamido- or carbamoyl-	-amide	 Acetamide (*Ethanamide*)

S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
23.	Amines	Primary amine	RNH_2		amino-	-amine	 Methylamine (*Methanamine*)
24.	Amines	Secondary amine	R_2NH		amino-	-amine	 Dimethylamine
25.	Amines	Tertiary amine	R_3N		amino-	-amine	 Trimethylamine
26.	Amines	4° ammonium ion	R_4N^+		ammonio-	-ammonium	 Choline
27.	Imine	Primary ketimine	RC(=NH) R′				
28.	Imine	Secondary ketimine	RC(=NR)R′				
29.	Imide	Imide	$(RCO)_2NR'$		imido-	imide	 Succinimide (Pyrrolidine-2,5-dione)
30.	Azide	Azide	RN_3		azido-	alkyl **azide**	 Phenyl azide (Azidobenzene)
31.	Azo compound	Azo (Diimide)	RN_2R		azo-	-diazene	 Methyl orange (*p*-dimethylamino-azobenzenesulfonic acid)

S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
32.	Cyanates	Cyanate	ROCN		Cyanato-	alkyl **cyanate**	 Methyl cyanate
33.	Cyanates	Isocyanate	RNCO		isocyanato-	alkyl **isocyanate**	 Methyl isocyanate
34.	Nitrate	Nitrate	$RONO_2$		nitrooxy-, nitroxy-	alkyl **nitrate**	 Amyl nitrate (1-nitroxypentane)
35.	Nitrile	Nitrile	RCN		cyano-	alkanenitrile alkyl **cyanide**	 Benzonitrile (Phenyl cyanide)
36.	Isonitrile	Isonitrile	RNC		isocyano-	alkaneisonitrile alkyl **isocyanide**	 Methyl isocyanide
37.	Nitrite	Nitroxooxy	RONO		nitrosooxy-	alkyl **nitrite**	 Isoamyl nitrite (3-*methyl*-1- *nitrosoxybutane*)
38.	Nitro compound	Nitro	RNO_2		nitro-		 Nitromethane
39.	Nitroso	RNO		nitroso-(Nitrosyl-)			 Nitrosobenzene
40.	Thiol	Sulfhydryl	RSH		sulfanyl-(-SH)	**-thiol**	 Ethanethiol
41.	Sulfide (Thioether)	Sulfide	RSR′		*substituent* sulfanyl- (-SSR′)	di(substituent) **sulfide**	 (Methylsulfanyl) methane (prefix) or Dimethyl sulfide (sulfix)
42.	Disulfide	Disulfide	RSSR′		*substituent* disulfanyl- (-SSR′)	di(substituent) **dissulfide**	 (Methyldisulfanyl) methane (prefix) or Dimethyl disulfide (sulfix)

S.N.	Chemical class	Group	Formula	Structural Formula	Prefix	Suffix	Example
43.	Sulfoxide	Sulfinyl	RSOR′		-sulfinyl-(-SOR′)	di(substituent) **sulfoxide**	 (Methanesulfinyl) methane (prefix) or Dimethyl sulfoxide (suffix)
44.	Sulfone	Sulfonyl	RSO_2R'		-sulfonyl- ($-SO_2R'$)	di(substituent) **sulfone**	 (Methanesulfonyl) methane (prefix) or Dimethyl sulfone (suffix)
45.	Sulfinic acid	Sulfino	RSO_2H		sulfino- ($-SO_2H$)	**-sulfinic acid**	 2-Aminoethane sulfinic acid
46.	Sulfonic acid	Sulfo	RSO_3H		sulfo- ($-SO_3H$)	**-sulfonic acid**	 Benzenesulfonic acid
47.	Thiocyanate	Thiocyanate	RSCN		thiocyanato- (-SCN)	*substituent* **thiocyanate**	 Phenyl thiocyanate
48.	Isothio-cyanate	Isothiocyanate	RNCS		isothiocyanato- (-NCS)	*substituent* ***isothiocyanate***	 Allyl isothiocyanate
49.	Thione	Carbonothioyl	RCSR′		-thioyl- (-CSR′) or sulfanylidene- (=S)	-thione	 Diphenylmethanethione (Thiobenzophenone)

IDENTIFY FUNCTIONAL GROUPS

Solved Example

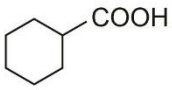
- Classify each of the following compounds. the possible classifications are as follows :

  alcohol ketone carboxylic acid ether

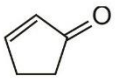
  aldehyde alkene

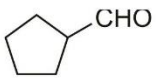
  (a) CH_2CH_2CHO **(b)** $CH_3CH_2CH(OH)CH_3$

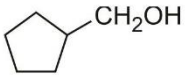
  (c) $CH_3COCH_2CH_3$ **(d)** $CH_3 — CH_2OCH_2CH_6$

(e) 

(f) 

(g) 

(h) 

(i) 

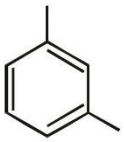
Sol. (a) aldehyde (b) alcohol (c) ketone (d) ether
(e) carboxylic acid (f) ether, alkene (g) ketone, alkene (h) aldehyde
(i) alcohol

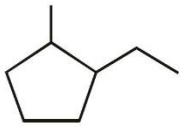
Solved Example

- For each molecule circle and name the functional group. If the functional group is an alcohol identify it as a primary (1°), secondary (2°), or tertiary (3°) alcohol. Some molecules will have more than one functional group; in those case circle and name all functional groups present. Functional groups: Alkane, alkene, alkyne, cyclic, aromatic, alcohol, ether.

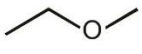
(a) 

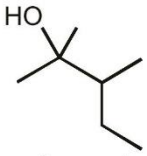
(b) 

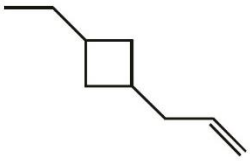
(c) 

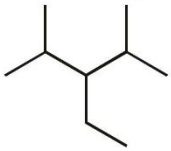
(d) 

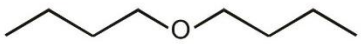
(e) CH_3CH_2OH

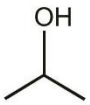
(f) 

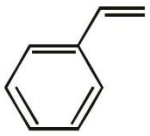
(g) 

(h) 

(i) 

(j) 

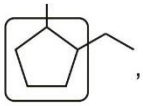
(k) 

(l) 

Ans. (a)  , alkene

(b)  , alkyne

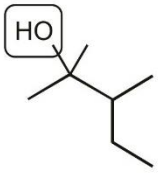
(c)  , aromatic

(d)  , cyclic

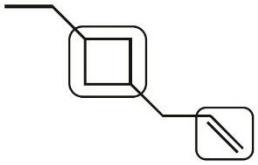
(e) $CH_3\boxed{CH_2OH}$ or $H_3C-\boxed{CH_2-OH}$, 1° Alcohol

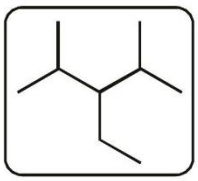
(f) 

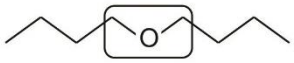
, ether

(g) 

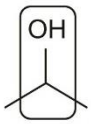
, 3°alcohol

(h) 
,cyclic and alkene

(i) 
, alkane

(j) 

, ether

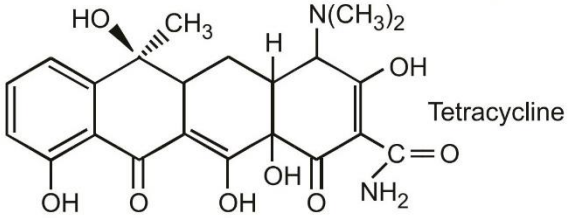
(k) 

, 2° alcohol

(l) 
,aromatic and alkene

Solved Example

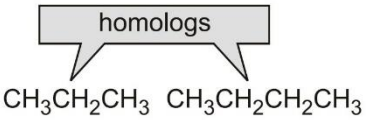
- The discovery of penicillin in 1928 marked the beginning of what has been called the "golden age of chemotherapy," in which previously life-threatening bacterial infections were transformed into little more than a source of discomfort. For those who are allergic to penicillin, a variety of antibiotics, including tetracycline, are available. Identify the numerous functional groups in the tetracycline molecule.

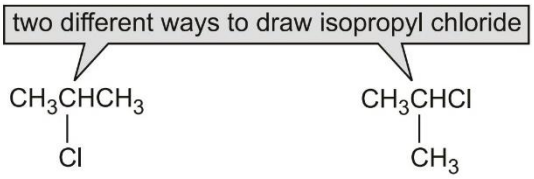


Sol. The compound contains an aromatic ring fused to three six-membered rings. It is also an alcohol and phenol (with five — OH groups), a ketone (with C = O groups at the bottom of the second and fourth rings), an amine [the — $N(CH_3)_2$ substituent at the top of the fourth ring], and an amide (the — $CONH_2$ group at the bottom right-hand corner of the fourth ring.)

HOMOLOGS

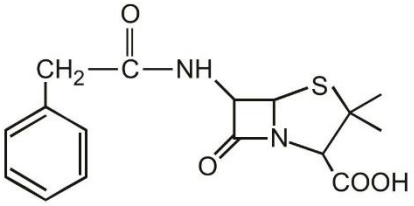
The family of alkanes shown in the table is an example of a homologous series. A **homologous series** (homos is Greek for "the same as") is a family of compounds in which each member differs from the one before it in the series by **one methylene (CH_2) group**. The members of a homologous series are called **homologs**



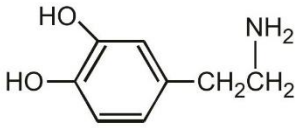


Solved Example

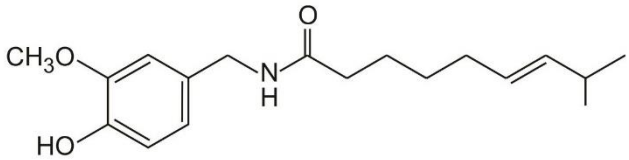
- Many naturally occurring compounds contain more than one functional group. Identify the functional groups in the following compounds:
  (a) Penicillin G is a naturally occurring antibiotic.
  (b) Dopamine is the neurotransmitter that is deficient in Parkinson's disease.
  (c) Capsaicin gives the fiery taste to chili peppers.
  (d) Thyroxine is the principal thyroid hormone.
  (e) Testosterone is a male sex hormone.



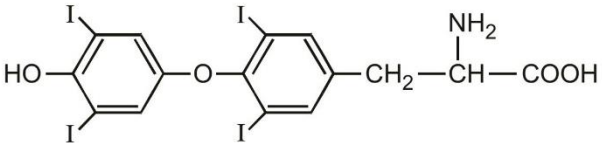
penicillin G



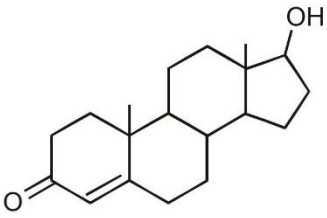
dopamine



capsaicin



thyroxine-T_4



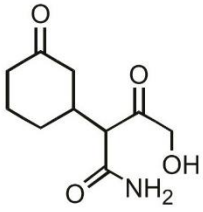
testosterone

Sol. **(a)** Penicillin-G: Carboxylic acid, thioether, amide
(b) Dopamine: Amine, aromatic alcohol (Phenol)
(c) Capsaicin: Phenol, ether, amide, alkene
(d) Thyroxine: Aryl iodide, phenol, ether, amine, carboxylic acid
(e) Testosterone: Alcohol, ketone, alkene

EXERCISE

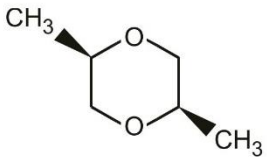
SINGLE CHOICE QUESTIONS

1. Functional group not present in given compound is/are?



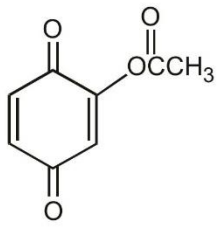
(A) Alcohol (B) Ketone (C) Carboxylic acid (D) Amide

2. Present functional group is :



(A) ketone (B) ester (C) ether (D) alcohol

3. Present functional group is/ are :



(A) ketone (B) ester (C) ether (D) A and B both

4. What is the lowest molecular weight possible for Ester?

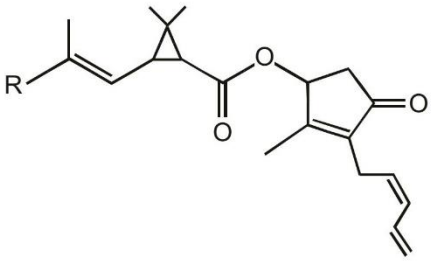
(A) 30 (B) 46 (C) 56 (D) 60

5. Which of the following compounds belong to the same homologous series ?

(1) 1-chloropropene (2) 1-chloropropane (3) 2-chlorobutane

(A) (1) and (2) only (B) (1) and (3) only (C) (2) and (3) only (D) (1), (2) and (3)

6. Pyrethrum flowers contain a natural insecticide called pyrethrin. Pyrethrin has the following structure:



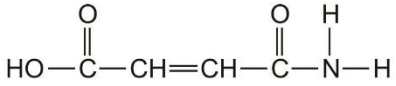
Which of the following functional groups are present in pyrethrin?

(1) Carbon-carbon double bond (2) Ester group

(3) Ketone group

(A) (1) and (2) only (B) (1) and (3) only (C) (2) and (3) only (D) (1), (2) and (3)

7. Consider the following compound :



Which of the following functional groups does it contain?

(1) Carboxyl group (2) Carbonyl group (3) Amide group

(A) (1) and (2) only (B) (1) and (3) only (C) (2) and (3) only (D) (1), (2) and (3)

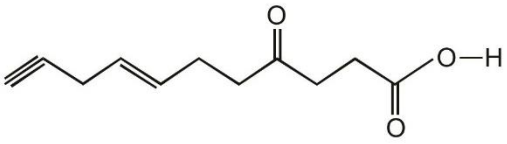
8. Which of the following statements is/are correct?

(1) Two organic compounds with the same general formula must belong to the same homologous series.

(2) Two organic compounds with main functional groups the same must belong to the same homologous series.

(3) Two organic compounds with the molecular mass differing by 14 must belong to the same homologous series.

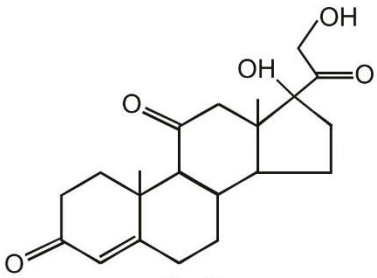
(A) (1) only (B) (2) only (C) (1) and (3) only (D) (2) and (3) only

9. 

Number of Functional group in above compound is

(A) 3 (B) 4 (C) 5 (D) 6

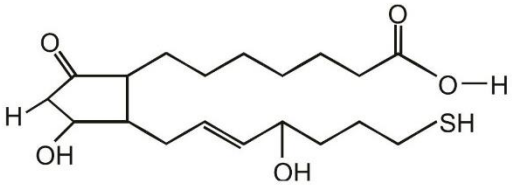
10. The functional groups in Cortisone are :



Cortisone

(A) Ether, alkene, alcohol (B) Alcohol, ketone, alkene

(C) Alcohol, ketone, amine (D) Ether, amine ketone

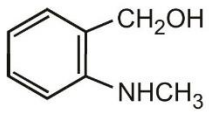
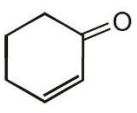
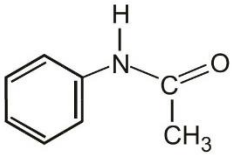
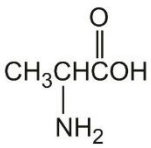
11. 

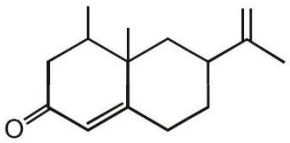
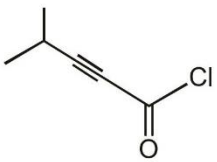
How many types of functional groups are present in given compound.

(A) 6 (B) 5 (C) 4 (D) 7

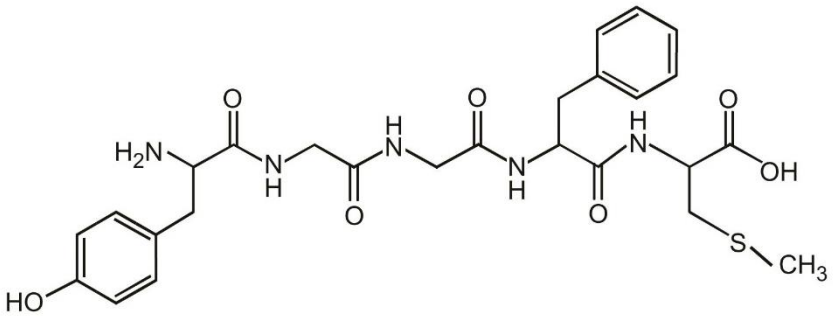
UNSOLVED EXAMPLE

1. Locate and identify the functional groups in the following molecules.

(a)  **(b)**  **(c)**  **(d)** 

(e)  **(f)** 

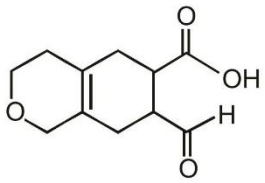
2. Met-enkephalin, an endorphin, serves as natural pain reliever that changes or removes the perception of nerve signals. Label all of the functional groups present in Met-enkephalin.



3. x = Types of functional group

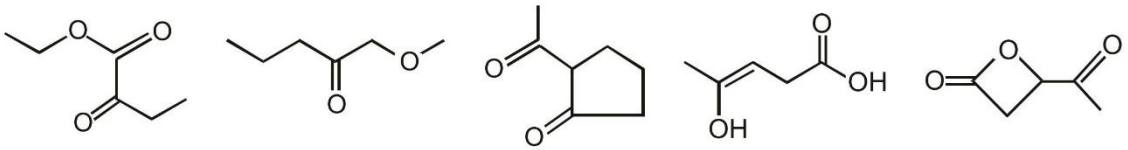
   y = Double bond equivalent

   Value of $(x + y)$ in given compound is :



(A) 7 (B) 8 (C) 9 (D) 10

4. Which compound can be classified as an ester as well as a Ketone?

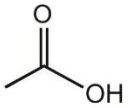


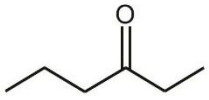
(A) (B) (C) (D) (E)

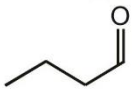
(A) A, B, E (B) E, B, C (C) A, E (D) C, E

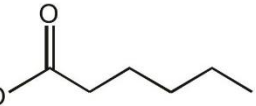
WORK SHEET

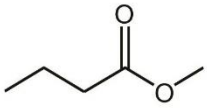
1. For each molecule circle and name the functional group. If the functional group is an amine identify it as a primary (1°), secondary (2°), or tertiary (3°) amine. some molecules will have more than one functional group; in those case circle and name all functional groups present. functional groups: Aldehyde, ketone, carboxylic acid, ester, amide, amine.

(a) 

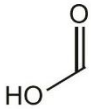
(b) 

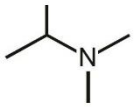
(c) 

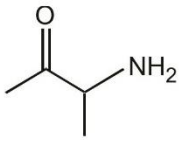
(d) HO 

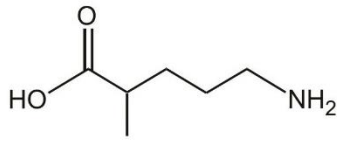
(e) 

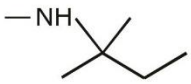
(f) CH_3COOH

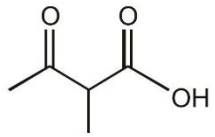
(g) HO 

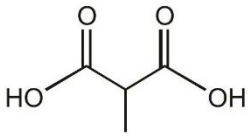
(h) 

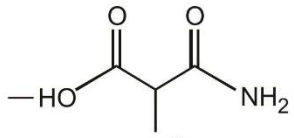
(i) 

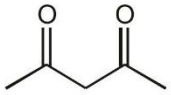
(j) 

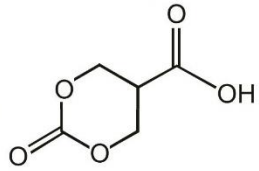
(k) 

(l) 

(m) 

(n) 

(o) 

(p) 

(q) HCHO

(r) HCOOH

(s) $CH_3(CO)CH_3$

SUBJECTIVE TYPE QUESTIONS

1. Suggest at least six different structures that would fit the formula C_4H_7NO. Make good realistic diagrams of each one and identify which functional groups(s) are present.

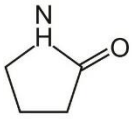
Purpose of the Problem

The identification and naming of functional groups is more important than the naming of compounds. This was your chance to experiment with different functional groups as well as different carbon skeletons.

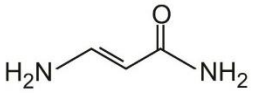
Suggested solution

You will have found the carbonyl and amino groups very useful, but did you also use alkenes and alkynes, rings, ethers, alcohols, and cyanides? Here are twelve possibilities but there are many more. The functional group names in brackets are alternatives. Some you will not have known. You need not to have classify the alcohols and amines.

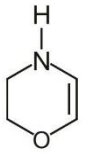
alkyne, primary alcohol, primary amine



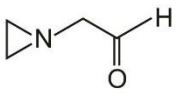
cyclic amide



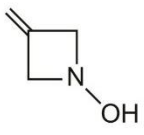
Amide, alkene, primary amine (enamine)



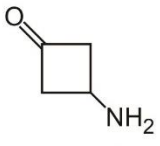
Ether, alkene, secondary amine



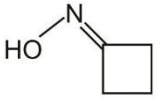
cyclic tertary amine, aldehyde



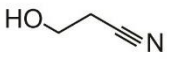
alkene, secondary amine, alcohol (cyclic hydroxylamine)



cyclic ketone, primary amine

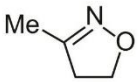


oxime, imine + alcohol

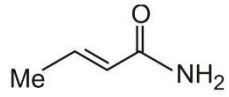


alcohol, nitrile (cyanide)

primary alcohol, nitrile (cyanide)



imine, ether (isoxazoine)



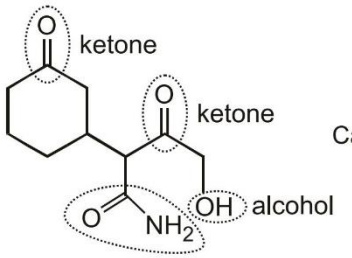
alkene, primary amide

Answers

Single Choice Questions

1. (C) **2.** (C) **3.** (D) **4.** (D) **5.** (C) **6.** (D) **7.** (B) **8.** (B)
9. (B) **10.** (B) **11.** (B)

1.

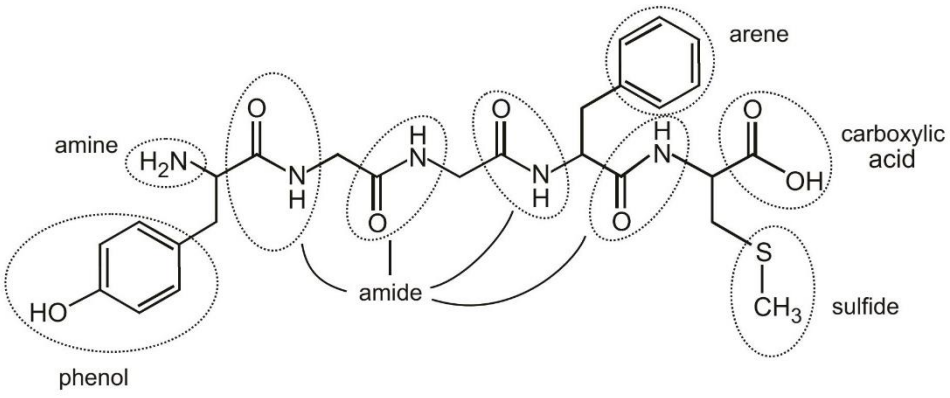


Carboxylic acid is not present

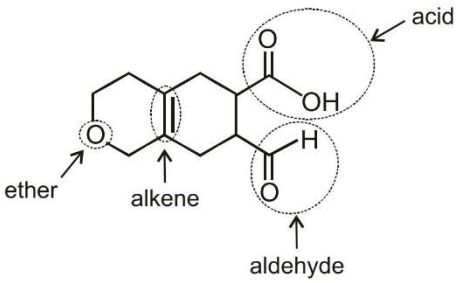
Unsolved Example

1. **(a)** alcohol, amine **(b)** ketone, alkene **(c)** amide
(d) carboxylic acid, amine **(e)** ketone,alkene **(f)** acyl halide, alkyne

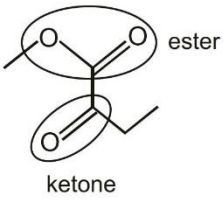
2.

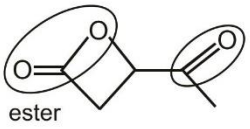


3.

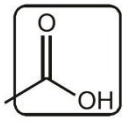


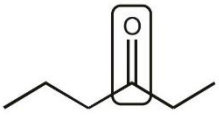
4.

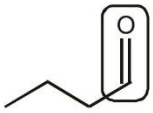


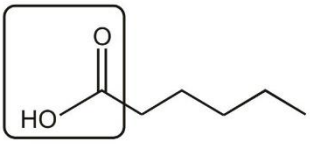


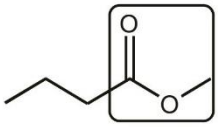
Work Sheet

1. (a)  , carboxylic acid

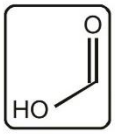
(b)  , ketone

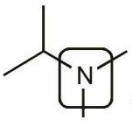
(c)  , aldehyde

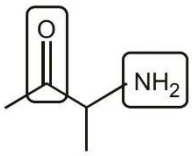
(d)  , carboxylic acid

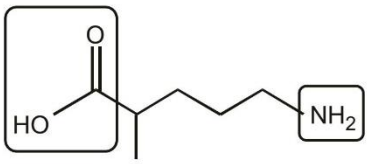
(e)  , ester

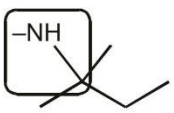
(f) CH_3 COOH or H_3C — C — OH , carboxylic acid

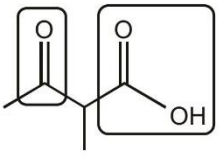
(g)  , carboxylic acid

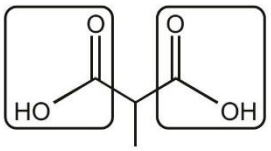
(h)  , 3° amine

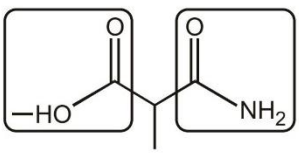
(i)  , ketone and 1° amine

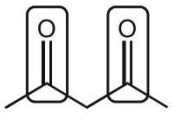
(j)  , carboxylic acid and 1°amine

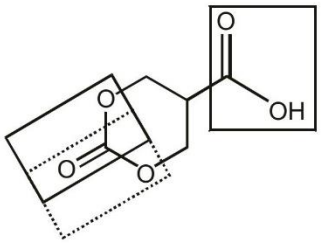
(k)  , 2° amine

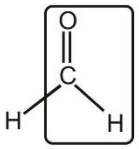
(l)  , ketone and carboxylic acid

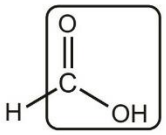
(m)  , 2 carboxylic acids

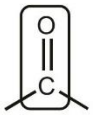
(n)  Carboxylic acid , and amide

(o)  , 2 ketones

(p)  , 2 esters and 1 carboxylic acid

(q)  , aldehyde

(r)  or , H  , carboxylic acid

(s)  , ketone

❑❑❑

CHAPTER 5

Double Bond Equivalent

DOUBLE BOND EQUIVALENTS (DBE) OR HYDROGEN DEFICIENCY INDEX OR DEGREES OF UNSATURATION

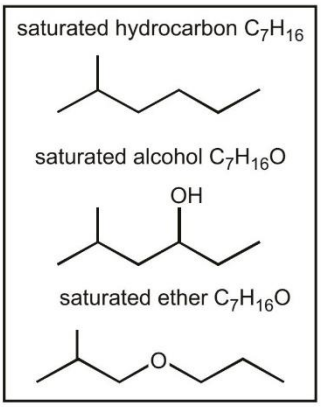
DBE help in the search for a structure

HOW TO CALCULATE DBE

Hello students! Have problems with calculating DBE ? No worries! Here is the tutorial which will help you step by step. Hopefully after reading this tutorial, you can calculate DBE faster and more accurately.

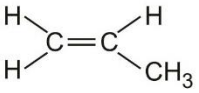
If DBE = 0

1. Ethylene, C_2H_6 is a saturated acyclic alkane and it does not have any π bond or ring, so DBE = 0.



If DBE = 1

2. Propylene, C_3H_6 , contains a pi bond, so DBE = 1.



Propylene
DBE = 1

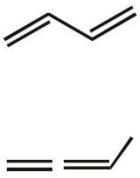
Cyclohexane
DBE = 1

$C_7H_{15}NO_2$ = one DBE

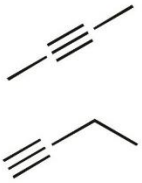
If DBE = 2

3. Propylene, C_4H_6 DBE = 2. There are several ways for a compound to possess two degrees of unsaturation : two double bonds, or two rings, or one double bond and one ring, or one triple bond. Let's explore all of these possibilities for C_4H_6 :

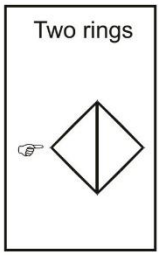
Two double bonds



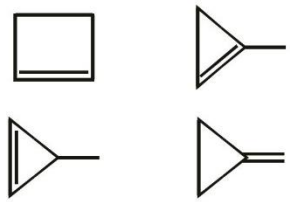
One triple bond



Two rings

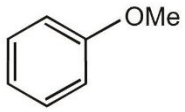


One ring and one double bond

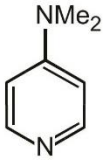


These are all of the possible constitutional isomers for C_6H_6. With this in mind, let's expand our skills set. Let's explore how to calculate the DBE when other elements are present in the molecular formula.

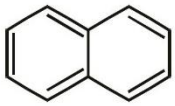
A benzene ring contains four DBE.



C_6H_8O = four DBE



$C_7H_{10}N_2$ = four DBE



only count two rings in this structure 5 pi bonds + 2 rings = > DBE = 5 + 2 = 7

HOW TO CALCULATE THE DBE IF WE DO NOT KNOW THE STRUCTURE OF THE CHEMICALS?

All the problems we have ever met talk about the organic chemicals which only contain carbon, oxygen, hydrogen, nitrogen, and halogens. Therefore, people summarized a DBE formula for our convenience.

$$\boxed{DBE = C - \frac{H}{2} + \frac{N}{2} + 1}$$

In this formula, C means the number of carbon. H means the number of hydrogen and X is number of halogen. N means the number of the nitrogen.

Let's apply the formula to the chemicals that we mentioned before.

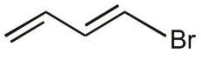
Ethylene (C_2H_6) : $DBE = C - \frac{H}{2} + \frac{N}{2} + 1 = 2 - \left(\frac{6}{2}\right) + \left(\frac{0}{2}\right) + 1 = 0$

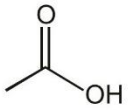
Propylene (C_3H_6) : $DBE = C - \frac{H}{2} + \frac{N}{2} + 1 = 3 - \left(\frac{6}{2}\right) + \left(\frac{0}{2}\right) + 1 = 1$

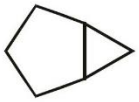
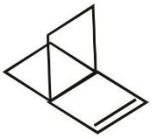
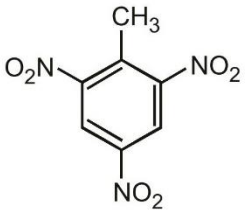
Cyclohexane (C_6H_{12}) : $DBE = C - \frac{H}{2} + \frac{N}{2} + 1 = 6 - \left(\frac{12}{2}\right) + \left(\frac{0}{2}\right) + 1 = 1$

Solved Example

- Look at the chemical structure below and calculate the DBE.

(1) 
(2) 

(3) 

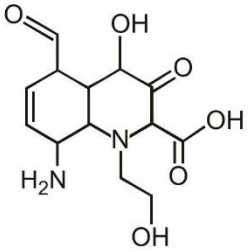
(4) 
(5) 
(6) 

Ans. (1) One pi bond. DBE = 1
(2) Two pi bond. DBE = 2
(3) One pi bond. DBE = 1
(4) Two rings. DBE = 2
(5) One pi bonds and three rings. DBE = 4
(6) Three pi bonds and one ring in the middle and three pi bonds on substituents. DBE = 7 exercise

EXERCISE

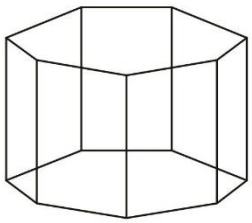
SINGLE CHOICE QUESTIONS

1. Find the sum of total number of different Functional groups and Double bond equivalent (DBE) value.



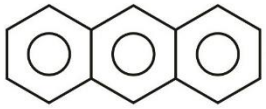
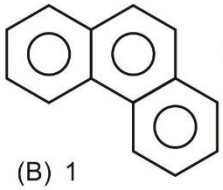
(A) 12 (B) 13 (C) 14 (D) 15

2. What is the Index of Hydrogen Deficiency (I.H.D) or Double Bond Equivalant (D.B.E.) for the following compound?



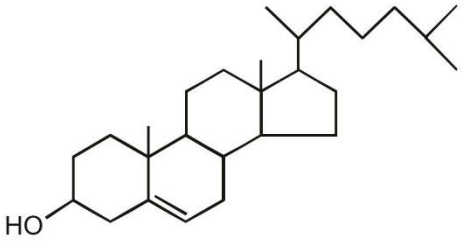
(A) 6 (B) 7 (C) 8 (D) 9

3. The difference in Double Bond Equivalent (DBE) value between

 and  is :

(A) 0 (B) 1 (C) 2 (D) 3

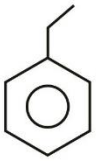
4. What is the correct molecular formula of following compound :

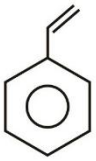


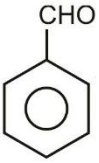
(Cholesterol)

(A) $C_{27}H_{46}O$ (B) $C_{25}H_{42}O$ (C) $C_{28}H_{46}O$ (D) $C_{23}H_{40}O$

5. Which of following compound. has D.B.E is 5 :

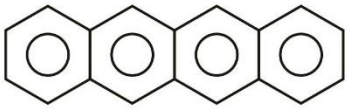
(A) 

(B) 

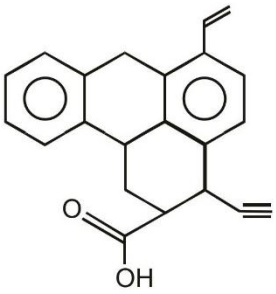
(C) 

(D) Both (B) & (C)

6. Number of p-bond present in given compound is



(A) 8 (B) 9 (C) 10 (D) 12

7. 

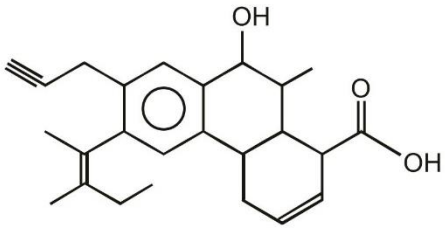
D.B. E of above compound is :

(A) 12 (B) 13 (C) 14 (D) 15

8. D.B.E of $(C_7H_5O_2)$ is :

(A) 3 (B) 5 (C) 5.5 (D) 4.5

9. How many degrees of unsaturation are there the following compound?



(A) 6 (B) 7 (C) 10 (D) 11

10. How many elements of unsaturation are implied by the molecular formula C_6H_{12}?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

11. How many elements of unsaturation are implied by the molecular formula C_5H_8O?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

12. How many elements of unsaturation are implied by the molecular formula $C_7H_{11}Cl$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

13. How many elements of unsaturation are implied by the molecular formula $C_5H_5NO_2$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

14. How many elements of unsaturation are implied by the molecular formula $C_8H_{11}N$?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

15. Consider molecules with the formula $C_{10}H_{16}$. Which of the following structural features are not possible within this set of molecules?

(A) 2 triple bonds
(B) 1 ring and 1 triple bond
(C) 2 rings and 1 double bond
(D) 2 double bonds and 1 ring
(E) 3 double bonds

16. A newly isolated natural product was found to have the molecular formula $C_{15}H_{28}O_2$. By hydrogenating a sample of the compound, it was determined to possess one π-bond. How many rings are present in the compound?

(A) 0 (B) 1 (C) 2 (D) 3
(E) 4

17. Which of the following molecular formulas corresponds to a monocyclic saturated compound?

(A) C_6H_6 (B) C_3H_7Br (C) C_3H_7N (D) C_3H_8O
(E) C_3H_8O

MULTIPLE CHOICE QUESTIONS

1. Which of the following statements applies to $C_{10}H_{14}O_2$ compound?

(A) It may have 2 double bonds and 2 rings.
(B) It may have 3 double bond and Oxygen ring.
(C) It may have 1 triple bond and 2 rings.
(D) It may have zero double bond and 3 rings

UNSOLVED EXAMPLE

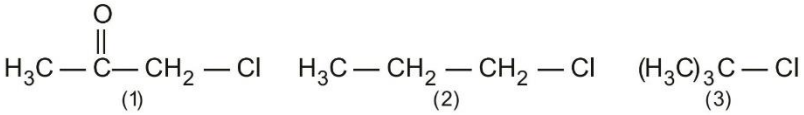
1. How many hydrogens does each of the following compounds have?

(a) $C_8H_?O_2$, has two rings and one double bond
(b) $C_7H_?N$, has two double bonds
(c) $C_9H_?NO$, has one ring and three double bonds

2. Calculate the degree of unsaturation in each of the following formulas :
   (a) Cholesterol, $C_{27}H_{46}O$
   (b) DDT, $C_{14}H_9Cl_5$
   (c) Prostaglandin E_1, $C_{20}H_{34}O_5$
   (d) Caffeine, $C_8H_{10}N_4O_2$
   (e) Cortisone, $C_{21}H_{28}O_5$
   (f) Atropine, $C_{17}H_{23}NO_3$

SUBJECTIVE TYPE QUESTIONS

1. The order of S_N1 reactivity in aqueous acetic acid solution for the compounds :



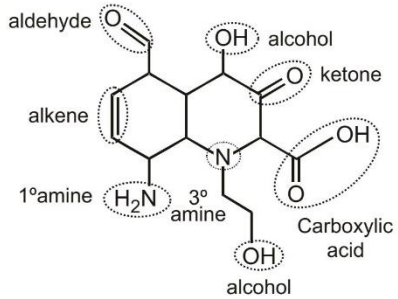
(a) 1 > 2 > 3 (b) 1 > 3 > 2 (c) 3 > 2 > 1 (d) 3 > 1 > 2

Answer

Single Choice Questions

1.	(B)	**2.**	(C)	**3.**	(A)	**4.**	(A)	**5.**	(D)	**6.**	(B)	**7.**	(C)	**8.**	(C)
9.	(D)	**10.**	(B)	**11.**	(C)	**12.**	(C)	**13.**	(E)	**14.**	(E)	**15.**	(A)	**16.**	(B)
17.	(C)														

1. D.B.E. value = 6



Different functional group = 7

2. The molecular formula of the compound shown is $C_{14}H_{14} \Rightarrow$ D.B.E. value $= (14 + 1) - (14 / 2) = 8$
3. D.B.E. of both anthracene & phenanthrene is 10.
4. Calculate DBE value of given compound $\Rightarrow$ DBE value of given compound is 5

Multiple Choice Questions

1. (A,B, C)

   $C_{10}H_{14}O_2$, DBE $= (C + 1) - \left(\frac{H + X - N}{2}\right)$

   DBE (4) means = 2 double bonds + 2 rings
   = 1 triple bond + 2 rings

Unsolved Example

1.	(a) 12	(b) 13	(c) 13				
2.	(a) 5	(b) 8	(c) 4	(d) 6	(e) 8	(f) 7	

Subjective Type Questions

1. (c)

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