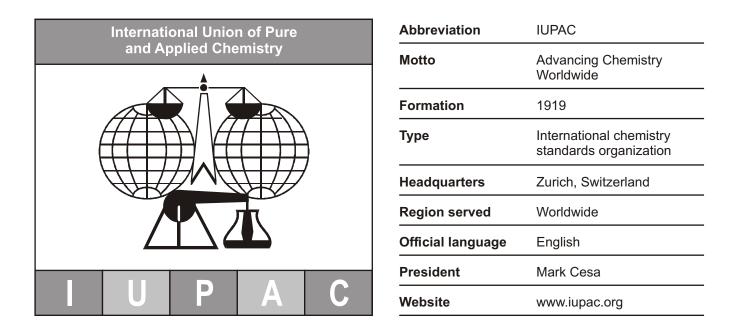


# **Nomenclature of Alkanes**



The International Union of Pure and Applied Chemistry (IUPAC), is an international federation of National Adhering Organizations that represents chemists in individual countries. It is a member of the International Council for Science (ICSU). The international headquarters of IUPAC is in Zurich, Switzerland. The administrative office, known as the "IUPAC Secretariat". Is in Research Triangle Park, North Carolina, United States. This administrative office is headed by the IUPAC executive director, currently Lynn Soby.

#### **Creation and history**

The need for an international standard for chemistry was first addressed in 1860 by a committee headed by German scientist Friedrich August Kekule von Stradonitz. This committee was the first international conference to create an international conference to create an international naming system for organic compounds. The ideas that were formulated in that conference evolved into the official IUPAC nomenclature of organic chemistry. The IUPAC stands as a legacy of this meeting, making it one of the most important historical international collaborations of chemistry societies. Since this time, IUPAC has been the official organization held with the responsibility of updating and maintaining official organic nomenclature. IUPAC as such was established in 1919. One notable country excluded from this early IUPAC was Germany. Germany's exclusion was a result of prejudice towards Germans by the allied powers after World War I. Germany was finally admitted into IUPAC during World War II.



During World war II, IUPAC was affiliated with the Allied powers, but had little involvement during the war effort itself. After the war, West Germany was allowed

Friedrich August Kekule von Stradonitz

back into IUPAC. Since World War II, IUPAC has been focused on standardizing nomenclature and methods in science without interruption.

# ALKANES

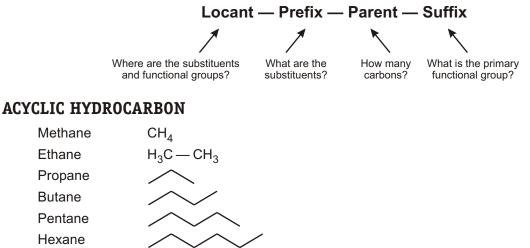
In organic chemistry, an **alkane**, or **paraffin** (a historical name that also has other meanings), is a saturated hydrocarbon. Alkanes consist only of hydrogen and carbon atoms and all bonds are single bonds. Alkanes (technically, always acyclic or open-chain compounds) have the general chemical formula  $C_n H_{2n \ 2}$ . For example, Methane is  $CH_4$ , in which n = 1 (n being the number of carbon atoms).

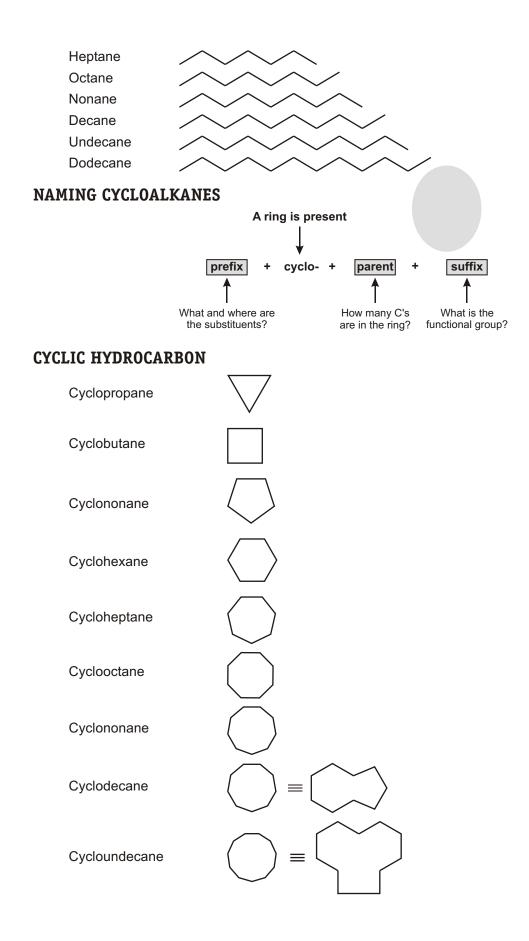
# SPECIAL TOPIC

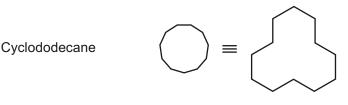
# WHY ARE ALKANES CALLED PARRAFINS?

Paraffins is a latin word meaning (parum = little + affinis = reactivity). Alkanes are called paraffins because they have a little affinity towards a general reagent. In other words, alkanes are inert substances. They undergo reactions under drastic conditions.

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







# **IUPAC SYSTEM OF NAMING COMPOUNDS**

The IUPAC name of any organic compound essentially consists of three parts:

1. Word root2. Suffix3. Prefix

# WORD ROOT

*Word root* is the basic unit of the name denoting the number of C atoms present in the principal chain (longest possible continuous chain of C atoms including the functional group and multiple bonds).

For  $C_1$  to  $C_4$ , the normal common root based on names like meth, -eth-, and prop- are used. For  $C_5$  or more carbon atoms chain, an extra letter (a) is used only if the primary suffix to be added to word root begins with a consonant.

Straight-chain alkanes take the suffix "-ane" and are prefixed depending on the number of carbon atoms in the chain, following standard rules. The first few are :

Number of carbons	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	20	30	40	50
Prefix	meth	eth	Prop	But	Pent	Hex	Hept	Oct	Non	Dec	Undec	Dodec	Tridec	Tetradec	Pentadec	Eicos	Triacont	Tetracont	Pentacont

# SUFFIX

Suffix are of two types.

(i) **Primary Suffix :** is always added to word root to indicate whether the carbon chain is saturated or unsaturated. For saturated the primary suffix is 'ane'. For unsaturated (one double bond) it is -'ene' and for unsaturated (one triple bond) it is - 'yne'. If the number of double bonds is two or three, then the primary suffix is 'diene' or 'triene'. If there are two triple bonds then it is 'diyne'.

#### Example:

HC CH ethyne;  $CH_3 - CH$   $CH_2$  propene ;  $CH_2$  CH - CH  $CH_2$  Butadiene

('a' has been added to word root since primary suffix starts with a consonant 'd'.)

HC C – C CH Butadiyne

(ii) Secondary Suffix: is added to primary suffix to indicate the nature of the functional group present in an organic compound.

For alcohol (-OH), -ol is added; for aldehydes (-CHO), -al is added.

For ketones (>C = O), -one is added; for acids (-COOH) -oic acid is added.

While adding the secondary suffix (to represent the functional group), the terminal 'e' of primary suffix is dropped. For example,  $CH_3CH_2OH$  is ethanol (e-dropped) and  $CH_2$  = CHCHO is prop-2-en-1-al (e-dropped). However, it is not always dropped. For example,  $CH_3CH_2CN$  is propanenitrile (e-not dropped)

It should also be noted that locants are to be placed immediately before the part of the name to which they 3 2 1

relate. For example,  $HC^{3}$   $C^{2}$   $C^{1}$  COOH is prop-2-yn-1-oic acid (working name 2-propynoic acid)

**IUPAC** Name

 $CICH_2 CH_2OH$  is 2-chloroethan-1-ol (working name 2-chloroethanol)

# PREFIX

These are also of two types.

(i) Primary Prefix: It distinguishes between a cyclic and an acyclic compound. In a cyclic compound, the  $\wedge$ 

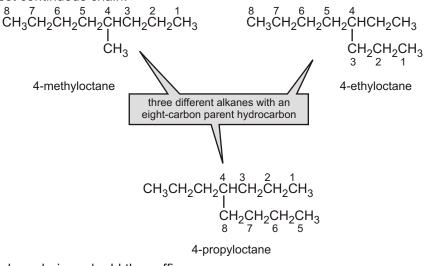
word 'cyclo' is used before the word root, for example,  $\bigtriangleup$  is cyclopropane. If the prefix is not used, one can take the compound to be of open chain.

(ii) Secondary Prefix: Sometimes, certain groups are not considered functional groups. These are treated as substituents and added before the word root in an alphabetical order. For example,  $C_2H_5 - O - C_2H_5$  is ethoxy ethane. In this, the secondary prefix is 'ethoxy', the word root is 'eth', and the primary suffix is 'ane'.

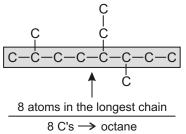
### THE NOMENCLATURE OF ALKANES

The systematic name of an alkane is obtained using the following rules:

Determine the number of carbons in the longest continuous carbon chain. This chain is called the parent hydrocarbon. The longest continuous chain is not always in a straight line; sometimes you have to "turn a corner" to obtain the longest continuous chain.

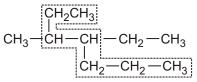


Find the parent carbon chain and add the suffix.



#### Rule 1:

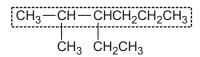
**Longest chain rule :** Select the longest continuous chain of carbon atoms. This is called the parent chain while all other carbon atoms which are not included in the parent chain are called branch chains or side chains or substituents.

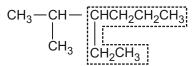


Longest chain contains seven carbon atoms and hence is named as a derivative of heptane

#### Rule 2:

**Rule for larger number of side chains :** If two chains of equal lengths are possible, select the one with the larger number of side chains. For example,

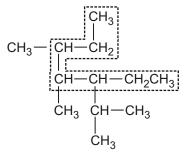




Named as hexane with two alkyl substituents (Correct)

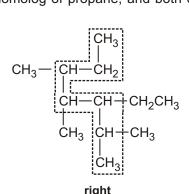
Named as hexane with one alkyl substituent (Wrong)

The series are called homologs. For example, butane is a homolog of propane, and both of these are homologs of hexane and decane.



wrong

seven-carbon chain, but only three substituents



right seven-carbon chain, four substituents

#### Rule 3 :

The name of any alkyl substituent that hangs off the parent hydrocarbon is placed in front of the name of the parent hydrocarbon, together with a number to designate the carbon to which the alkyl substituent is attached. The carbons in the parent chain are numbered in the direction that gives the substituent as low a number as possible. The substituents name and the name of the parent hydrocarbon are joined into one word. preceded by a hyphen that connects the substituent's number with its name.

$ \begin{array}{cccccccccccccccccccccccccccccccccccc$	$\stackrel{6}{\text{CH}_3}\stackrel{5}{\text{CH}_2}\stackrel{4}{\text{CH}_2}\stackrel{3}{\text{CH}_2}\stackrel{2}{\text{CH}_2}\stackrel{1}{\text{CH}_2}\stackrel{1}{\text{CH}_2}\stackrel{1}{\text{CH}_3}$	$^{1}_{CH_{3}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{2}CH_{3}}$
2-methylpentane	3-ethylhexane	4-propyloctane
not	not	not
4-methylpentane	4-ethylhexane	5-propyloctane

Only systematic names have numbers; common names never contain numbers

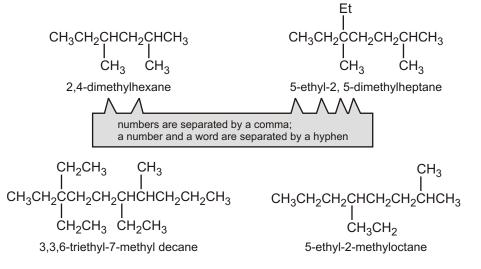
$$\begin{array}{c} \mathsf{CH}_3\\ \mathsf{I}\\ \mathsf{CH}_3\mathsf{CHCH}_2\mathsf{CH}_2\mathsf{CH}_2\mathsf{CH}_3\end{array}$$

common name : isohexane systematic names : 2-methypentane

If more than one substituent is attached to the parent hydrocarbon, the chain is numbered in the direction that will produce a name containing the lowest of the possible numbers.

$$\begin{array}{c} \mathsf{CH}_3\mathsf{CH}_2\mathsf{CH}\mathsf{CH}_2\mathsf{CH}_2\mathsf{CH}_2\mathsf{CH}_2\mathsf{CH}_3\\ | & |\\ \mathsf{CH}_3 & \mathsf{CH}_2\mathsf{CH}_3\\ 3\text{-ethyl-5-methyloctane}\\ & \text{not}\\ 4\text{-ethyl-6-methyloctane}\\ & \text{because } 3 < 4\end{array}$$

If two or more substituents are the same, the prefixes "di," "tri," and "tetra" are used to indicate how many identical substituents the compound has. The numbers indicating the locations of the identical substituents are listed together, separated by commas. There are no spaces on either side of a comma. There must be as many numbers in a name as there are substituents. The prefixes "di," "tri," "tetra," "sec," and "tert" are ignored in alphabetizing substituents.



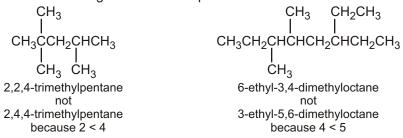
### **MISTAKES TO AVOID**

#### Adding of punctuation:

- 1. Commas are put between numbers (2, 5, 5 becomes 255)
- 2. Hyphens are put between a number and a letter (2,5,5 trimethylheptane becomes 2,5,5-trimethylheptane).
- 3. Successive words are merged into one word (trimethyl heptane becomes trimethylheptane) **NOTE**: IUPAC uses one-word names throughout. This is why all parts are connected.
- 4. When assigning the numbers (*i.e.*, the locants) while naming an organic compound there is NO rule based on summing the numbers.

#### Rule 4:

1. When numbering in either direction leads to the same lowest number for one of the substituents, the chain is numbered in the direction that gives the lowest possible number to one of the remaining substituents.

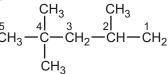


2. Lowest set of locants rule : When two or more substituents are present, the lowest set of locants rule is applied. According to this rule when two or more different sets of locants containing the same number of terms is possible, then that set of locants is the lowest which when compared term by term with other sets, each in order of increasing magnitude, has the lowest term at the first point of difference.

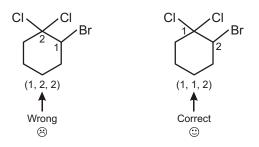
That is why this rule is also sometimes called as first point of difference rule.



Set of locants = 2, 2, 4 (correct)

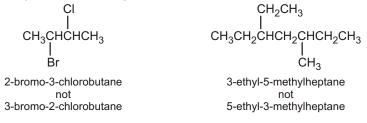


Set of locants = 2, 4, 4 (wrong)



#### Rule 5 :

If the same substituent numbers are obtained in both directions, the first group listed receives the lower number (according to alphabetical order).



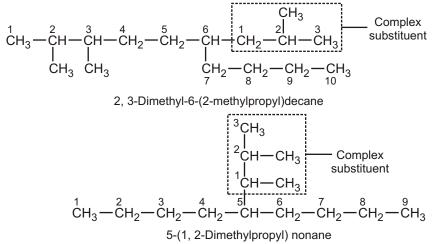
#### Rule 6 :

# NAMING OF COMPLEX SUBSTITUENT

Alkyl group, R-	Common name	Complex name (if different)
CH <sub>3</sub> -	methyl-	
CH <sub>3</sub> CH <sub>2</sub> -	ethyl-	
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -	propyl-	
(CH <sub>3</sub> ) <sub>2</sub> CH-	isopropyl-	(1-methylethyl)-
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -	butyl-	
$CH_3 - CH_2 CH - CH_3$	sec-butyl- or s-butyl	(1-methylpropyl)-
(CH <sub>3</sub> ) <sub>2</sub> CHCH <sub>2</sub> -	isobutyl	(2-methylpropyl)-
(CH <sub>3</sub> ) <sub>3</sub> C-	tert-butyl or t-butyl	(1,1-dimethylethyl)-

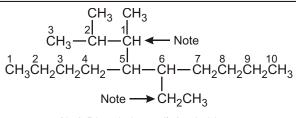
#### NUMBERING THE COMPLEX SUBSTITUENT

(a) In case the substituent on the parent chain is complex (*i.e.*, it has branched chain), it is named as a substituted alkyl group by numbering the carbon atom of this group attached to the parent chain as 1. The name of such a substituent is always enclosed in brackets to avoid confusion with the numbers of the parent chain. For example,



(b) While deciding the alphabetical order of the various substituents, the name of the complex substituent is considered to begin with the first letter of the complete name, eventhough di, tri, iso, neo.

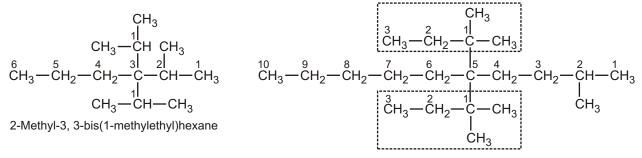
#### Solved Example



5-(1, 2-Dimethylpropyl)-6-ethyldecane

It may be noted here that the complete name of the complex substituent is dimethylbutyl. Since d of dimethylbutyl group comes first than e of the ethyl group in the alphabetical order, therefore, locant 5 is given to the complex substituent and 6 to the ethyl group.

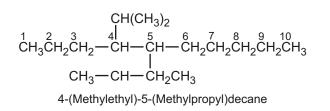
(c) If the same complex substituent occurs more than once on the parent chain, prefixes bis (for two), tris (for three), tetrakis (for four), pentakis (for five) etc. are used before the name of the complex substituent. For example,

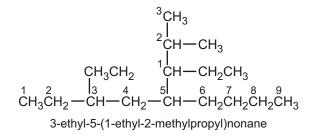


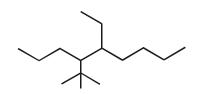
5, 5-Bis (1, 1-dimethylpropyl)-2-methyldecane

Note that while deciding the alphabetical order of the various alkyl groups, prefixes iso and neo are considered to be part of the fundamental name of the alkyl group while the prefixes sec, tert, di, tri are not.

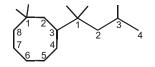
Solved Example





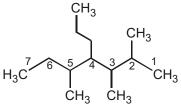


4-(1,1-dimethylethyl)-5-ethylnonane not 5-ethyl-4-(1,1-dimethylethyl) nonane



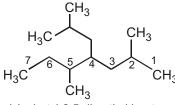
1,1 dimethyl-3-(1, 1,3-trimethylbutyl)cycloctane

If Chains of equal length are competing for selection as main chain in a saturated branched acyclic hydrocarbon, then the choice goes in series to : (a) The chain which has the greatest number of side chains.



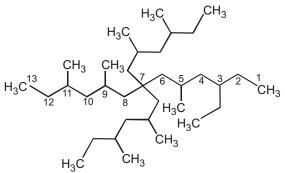
2,3,5-Trimethyl-4-propylheptane

(b) The chain whose side chains have the lowest-numbered locants.



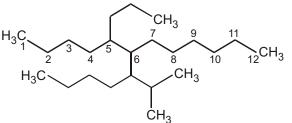
4-IsobutyI-2,5-dimethyl heptane

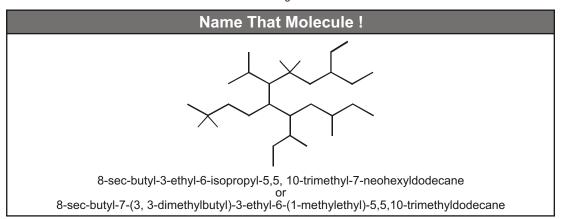
(c) The chain having the greatest number of carbon atoms in the smaller side chains.



7,7,Bis(2,4-dimethylhexyl)-3-ethyl 5, 9, 11-trimethyl tridecane

(d) The chain having the least branched side chains.





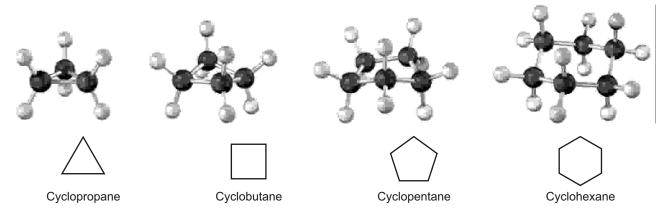
# **COMMON NAMES AND STRUCTURAL ABBREVIATIONS**

<b>Group</b> Alkyl	<b>Abbreviation</b> R	Structure
Aryl	Ar	
Methyl	Me	–CH <sub>3</sub>
Ethyl	Et	–CH <sub>2</sub> CH <sub>3</sub>
Propyl	Pr or n-Pr	-CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
Butyl	Bu or n-Bu	-CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>
-		,CH <sub>3</sub>
Isopropyl	i-Pr or <sup>i</sup> Pr	CH
торгоруг	I-FI OI FI	$\mathbf{i}$
		СН <sub>3</sub>
		CH <sub>3</sub>
Isobutyl	i-Bu or <sup>i</sup> Bu	−CH <sub>2</sub> ĆH
		CH <sub>3</sub>
		CH <sub>2</sub> CH <sub>3</sub>
sec-Butyl	s-Bu or <sup>s</sup> Bu	—CH
ooo Dutyi		$\mathbf{i}$
		Сн₃ ,⊂Н₃
tout Dutul	t-Bu or <sup>t</sup> Bu	
tert-Butyl	I-BU OF BU	-C-CH <sub>3</sub>
		СН <sub>3</sub>
Phenyl	Ph	
		-CH <sub>2</sub>
Benzyl	Bn	
Donley	2	« »
Acetyl	Ac	
		ĊH <sub>3</sub>
		Н
Vinyl		-c,
		CH <sub>2</sub>
Allyl		CH <sub>2</sub> -CH <sub>2</sub> C=CH <sub>2</sub>
-		/ - ́ Н
Halide	Х	–F –Cl –Br

# NOMENCLATURE OF CYCLIC ALKANE

Saturated cyclic hydrocarbons are called cycloalkanes, or alicyclic compounds (aliphatic cyclic). Because cycloalkanes consist of rings of  $-CH_2$ -units, they have the general formula  $(CH_2)_n$ , or  $C_nH_{2n}$ , and can be represented by polygons in skeletal drawings.

-l

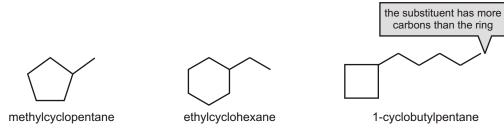


#### Find the parent.

Count the number of carbon atoms in the ring and the number in the largest substituent. If the number of carbon atoms in the ring is equal to or greater than the number in the substituent, the compound is named as an alkyl-substituted cycloalkane. If the number of carbon atoms in the largest substituent is greater than the number in the ring, the compound is named as a cycloalkyl-substituted alkane. For example:

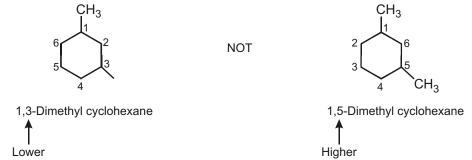


In a cycloalkane with an attached alkyl substituent, the ring is the parent hydrocarbon unless the substituent has more carbons than the ring. In that case, the substituent is the parent hydrocarbon and the ring is named as a substituent. There is no need to number the position of a single substituent on a ring.

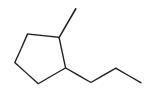


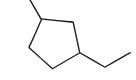
Number the substituents, and write the name.

For an alkyl- or halo-substituted cycloalkane, choose a point of attachment as carbon 1 and number the substituents on the ring so that the second substituent has as low a number as possible. If ambiguity still exists, number so that the third or fourth substituent has as low a number as possible, until a point of difference is found.



If the ring has two different substituents, they are listed in alphabetical order and the number-1 position is given to the substituent listed first.







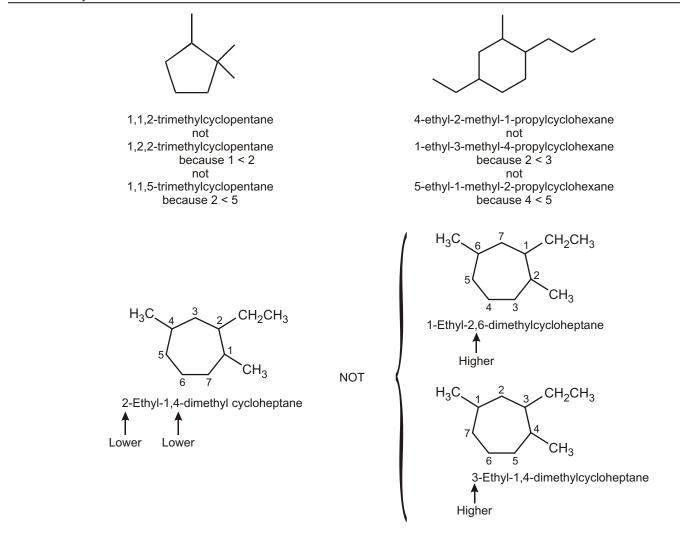
1-methyl-2-propylcyclopentane

1-ethyl-3-methylcyclopentane

1,3-dimethylcyclohexane

If there are more than two substituents on the ring, they are listed in alphabetical order, and the substituent given the number-1 position is the one that results in a second substituent getting as low a number as possible. If two substituents have the same low numbers, the ring is numbered—either clockwise or counterclockwise—in the direction that gives the third substituent the lowest possible number.

Solved Example



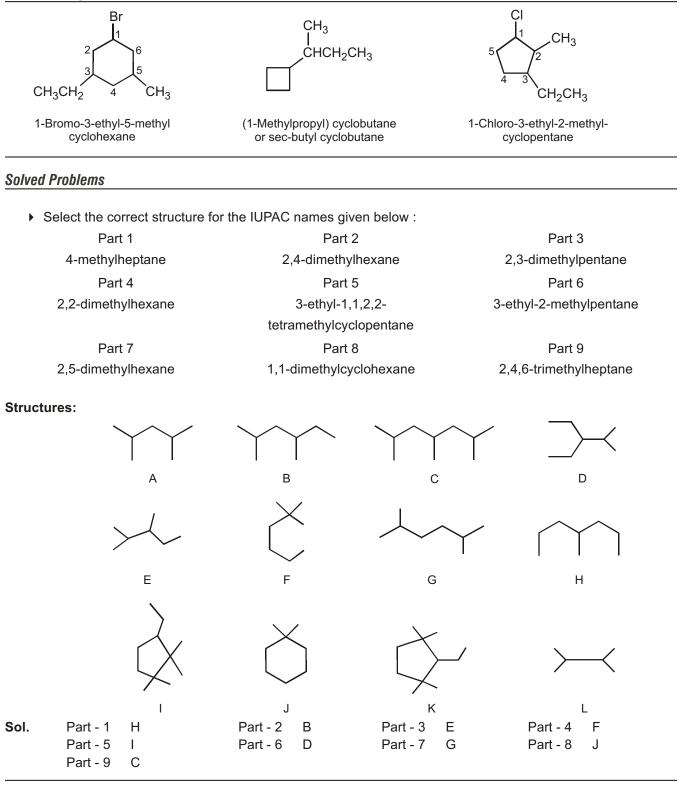
If more than one alicyclic ring is attached to a single chain, the compound is named as a derivative of alkane irrespective of the number of carbon atoms in the ring or the chain. For example,

 $CH_2$ 

dicyclopropylmethane

1,3-dicyclohexylpropane

#### Solved Example



#### Solved Example

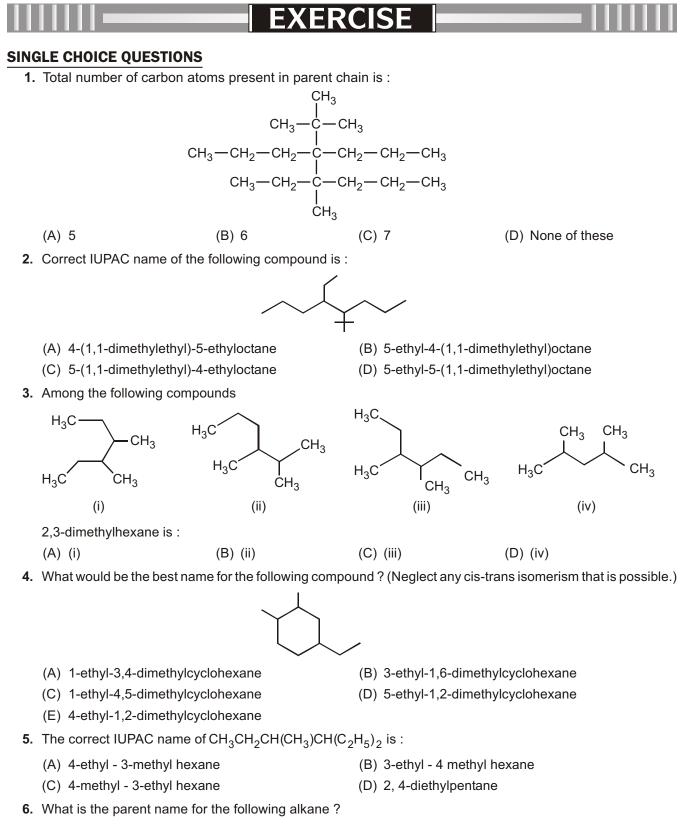
Deduce structural formul not among the nine ?	as and give IUPAC names for the nine isomers of	fC <sub>7</sub> H <sub>16</sub> . (b) Why is 2-ethylpentane
(a) seven-C chain	1. $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$	Heptane
	СН <sub>3</sub>	
six-C chain	2. $CH_3CHCH_2CH_2CH_2CH_3$	2-Methylhexane
	СН <sub>3</sub>	
	$CH_3$ I 3. CH <sub>3</sub> CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	3-Methylhexane
	CH <sub>3</sub>	
five-C chain	4. CH <sub>3</sub> CHCHCH <sub>2</sub> CH <sub>3</sub>	2,3-Dimethylpentane
	CH3 CH3	
	CH <sub>3</sub> CH <sub>3</sub> I I 5. CH <sub>3</sub> CHCH <sub>2</sub> CHCH <sub>3</sub> z	2,4-Dimethylpentane
	ĊН <sub>3</sub>	
	6. $CH_3CCH_2CH_2CH_3$	2,2-Dimethylpentane
	CH <sub>3</sub> I 6. CH <sub>3</sub> CCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> I CH <sub>3</sub>	
SPECIAL 1	TOPIC	

# **OCTANE NUMBER**

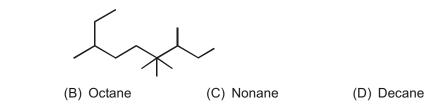
In addition to being volatile, gasoline must resist the potentially damaging explosive combustion known as knocking. The antiknock properties of gasoline are rated by an octane number that is assigned by comparing the gasoline to a mixture of *n*-heptane (which knocks badly) and isooctane (2,2,4-trimethylpentane, which is not prone to knocking). The gasoline being tested is used in a test engine with a variable compression ratio. Higher compression ratios induce knocking, so the compression ratio is increased until knocking begins. Tables are available that show the percentage of isooctane in an isooctane/heptane blend that begins to knock at any given compression ratio. The octane number assigned to the gasoline is simply the percentage of isooctane in an isooctane/heptane mixture that begins to knock at that same compression ratio.

$$\begin{array}{c} \mathsf{CH}_{3} & \mathsf{CH}_{3} \\ \mathsf{H}_{3} \\ \mathsf{CH}_{3} \\ \mathsf{CH}_{2} \\ \mathsf{CH}_{3} \\$$

The octane number of a gasoline is determined by comparing its knocking with the knocking of mixtures of heptane and 2,2,4-trimethylpentane. The octane number given to the gasoline corresponds to the percent of 2,2,4-trimethylpentane in the matching mixture. Thus, a gasoline with an octane rating of 91 has the same "knocking" property as a mixture of 91% 2,2,4-trimethylpentane and 9% heptane. The term octane number originated from the fact that 2,2,4-trimethylpentane contains eight carbons. Because slightly different methods are used to determine the octane number, gasoline in Canada and the United States will have an octane number that is 4 to 5 points less than the same gasoline in Europe and Australia.

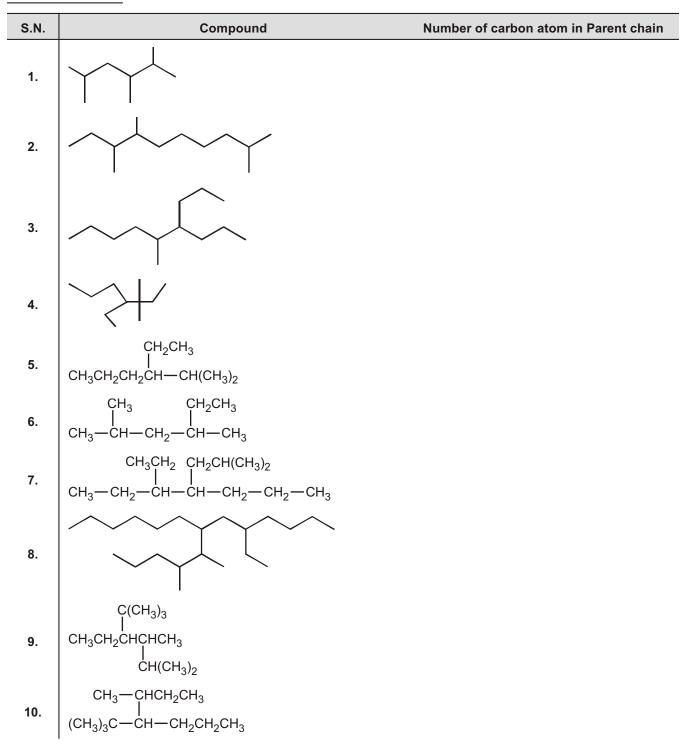


(Note : The parent name corresponds to the longest continuous chain of carbon atoms.)



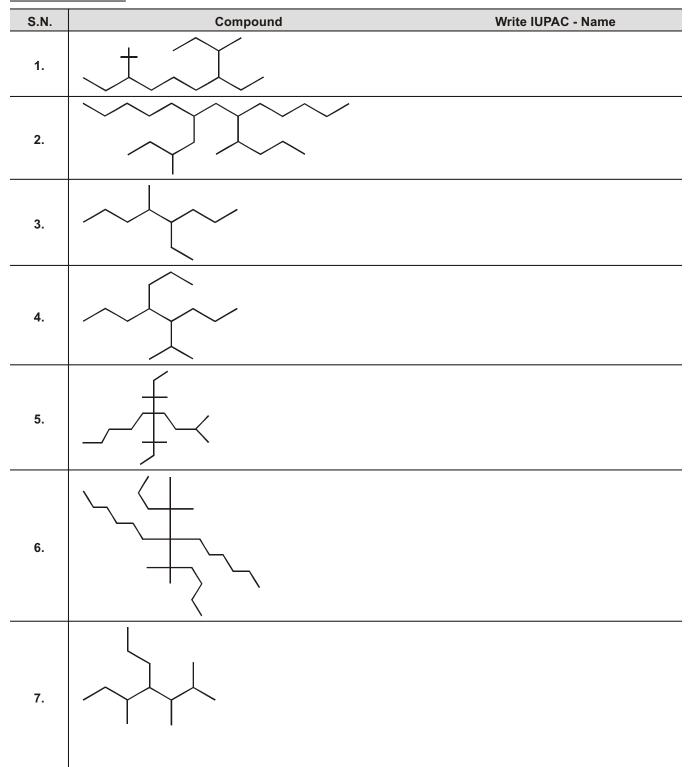
### WORK SHEET - 1

(A) Heptane



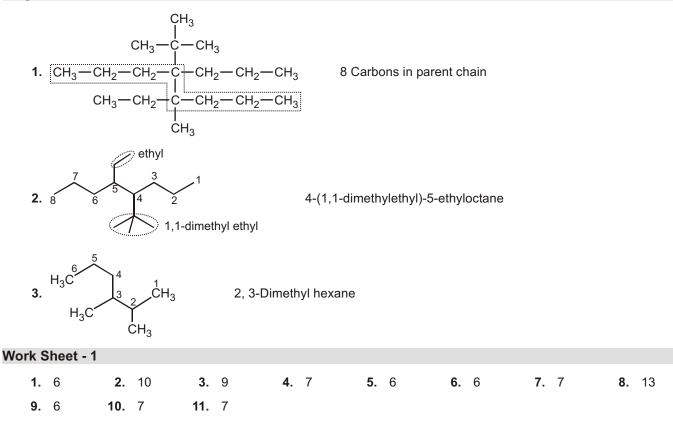
# **11.** CH<sub>3</sub>C(CH<sub>3</sub>)<sub>2</sub>CH(CH<sub>2</sub>CH<sub>3</sub>)CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH(CH<sub>3</sub>)<sub>2</sub>

# WORK SHEET - 2



#### **1.** (D) **2.** (A) **3.** (B) **4.** (E) **5.** (B) **6.** (C)

Single Choice Questions



#### Work Sheet - 2

- 1. 3, 7-Diethyl 2, 2,8-trimethyl decane
- 2. 6-(1-methylbutyl) 8-(2-methylbutyl) tridecane
- 3. 4-ethyl 5 methyl octane
- 4. 4-(1-methyl ethyl) 5-propyl octane or 4-isopropyl-5-propyl octane
- 5. 5, 5-Bis (1, 1-dimethyl propyl)-2-methyl- decane
- 6. 7-(1,1-dimethyl butyl)-7-(1,1-dimethyl pentyl) tridecane
- 7. 2, 3, 5-trimethyl 4-propyl heptane