The IUPAC names. The IUPAC system of nomenclature is based on a fundamental principle that an aliphatic compound, in general, is considered to be a derivative of a hydrocarbon comprising of the longest continuous carbon chain (the parent chain) in the molecule, and the branches (side-chains) of the parent chain are considered as the substituents. In the case of alkanes, the parent hydrocarbons are also alkanes, but the side-chains are alkane fragments which are generally known as *alkyl groups*.

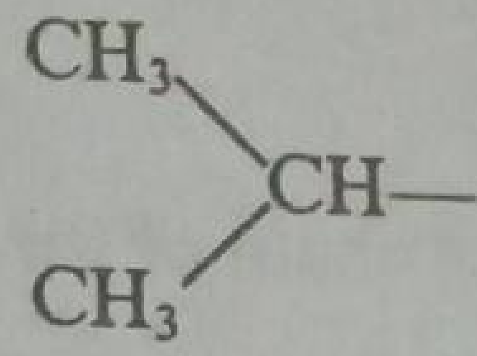
An **alkyl group** is obtained by removing a hydrogen atom of an alkane, and is expressed by the general formula C_nH_{2n+1}. The name of the alkyl group is derived by replacing the ending *-ane* of the corresponding alkane by *-yl*, e.g., methyl (CH_3—) from methane (CH_4) and ethyl (CH_3CH_2—) from ethane (CH_3CH_3). A general symbol *R* is commonly used to represent any alkyl group. For example, *R* may be methyl, ethyl or any other alkyl group. Although there is only one propane, two different alkyl groups (*n*-propyl and isopropyl) are derived from it, depending on whether the hydrogen atom is removed from the terminal or the middle carbon of propane. Similarly, two alkyl groups are derived from each of *n*-butane and isobutane. Some of the common alkyl groups are given below:

Scanned by TapScanner

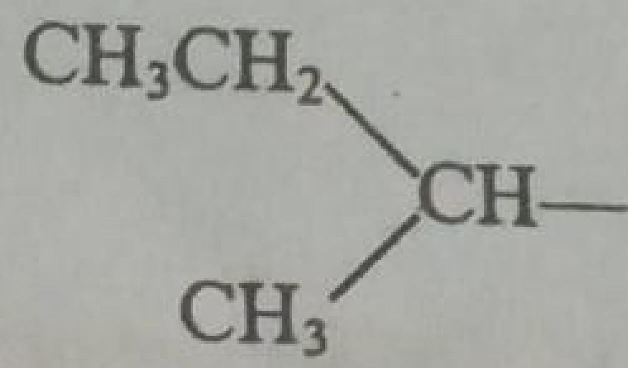
Methyl $CH_3—$

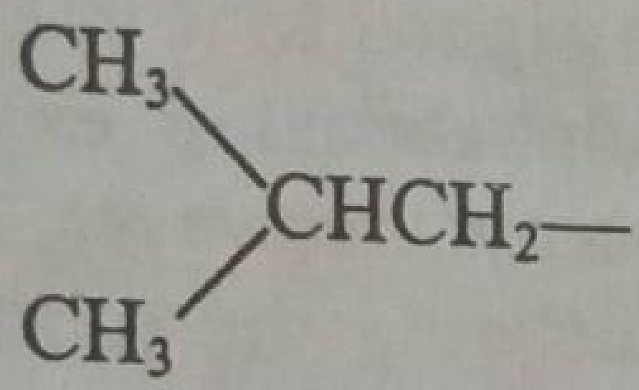
Ethyl $CH_3CH_2—$

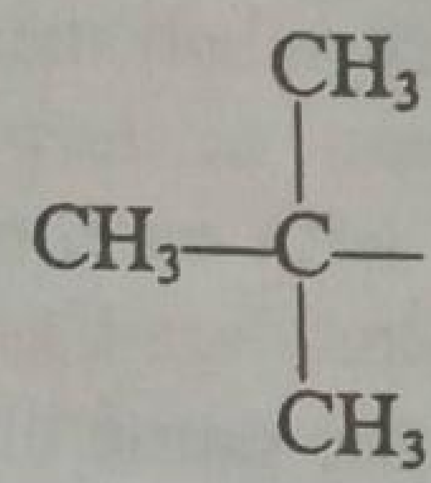
n-Propyl $CH_3CH_2CH_2—$

Isopropyl 

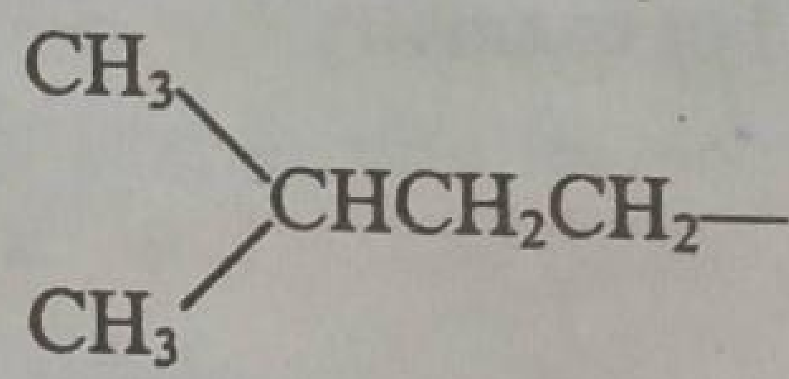
n-Butyl $CH_3CH_2CH_2CH_2—$

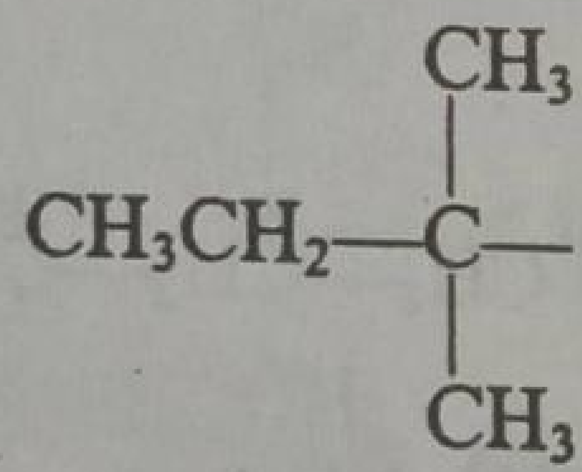
sec-Butyl 

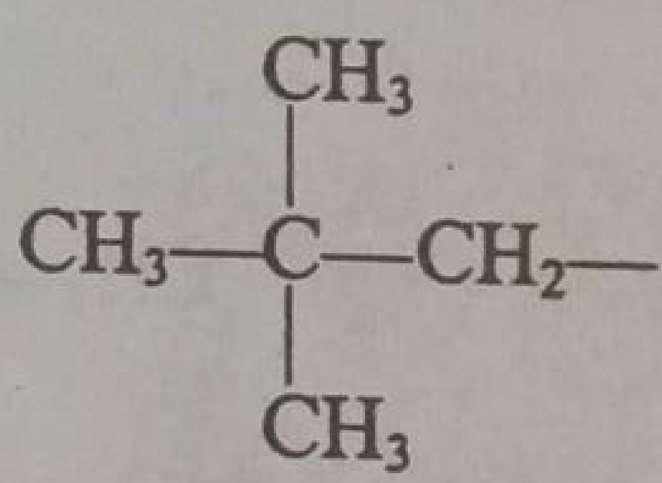
Isobutyl 

tert-Butyl 

n-Pentyl $CH_3CH_2CH_2CH_2CH_2—$

Isopentyl 

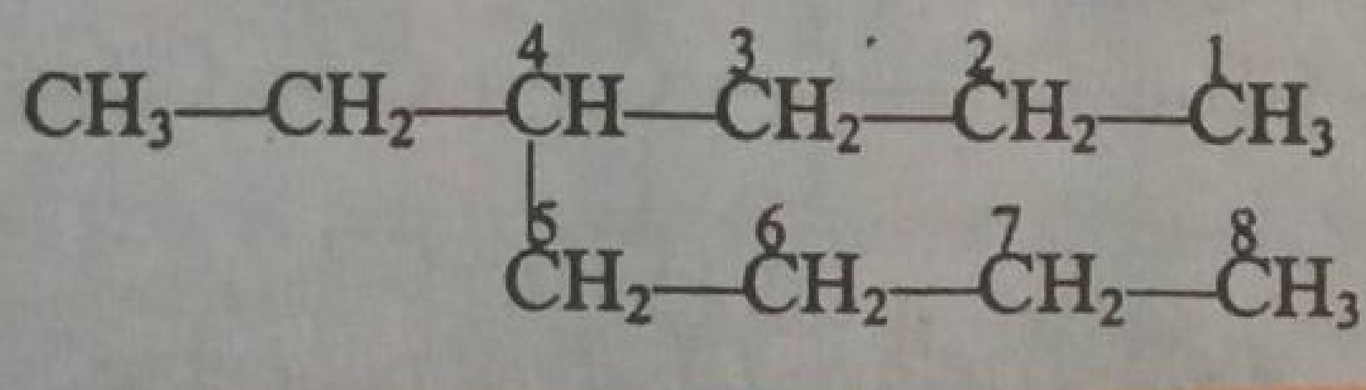
tert-Pentyl 

Neopentyl 

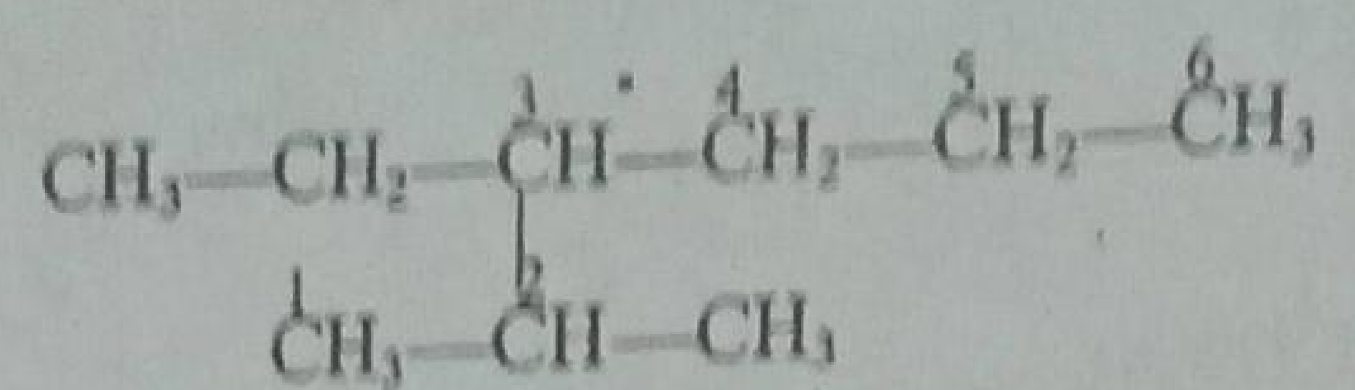
An alkyl group is known as **primary** if its carbon of attachment is bonded to only one other carbon atom, **secondary** if bonded to two other carbon atoms and **tertiary** if bonded to three other carbon atoms. Thus, isopropyl group is a secondary alkyl group but isobutyl group is a primary alkyl group.

The assignment of a correct name to an alkane by the IUPAC system depends on the choice of the parent name, and the proper application of the following rules:

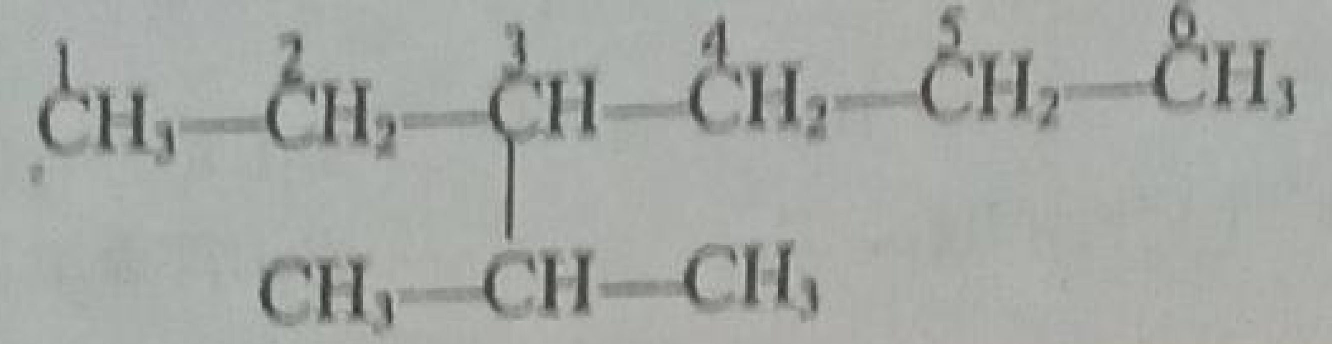
1. The longest continuous carbon chain in the molecule is located, according to which the parent name of the compound is determined. The parent name of the following compound is octane, and not hexane or heptane. Note that the prefix *n*- is not part of the IUPAC system.



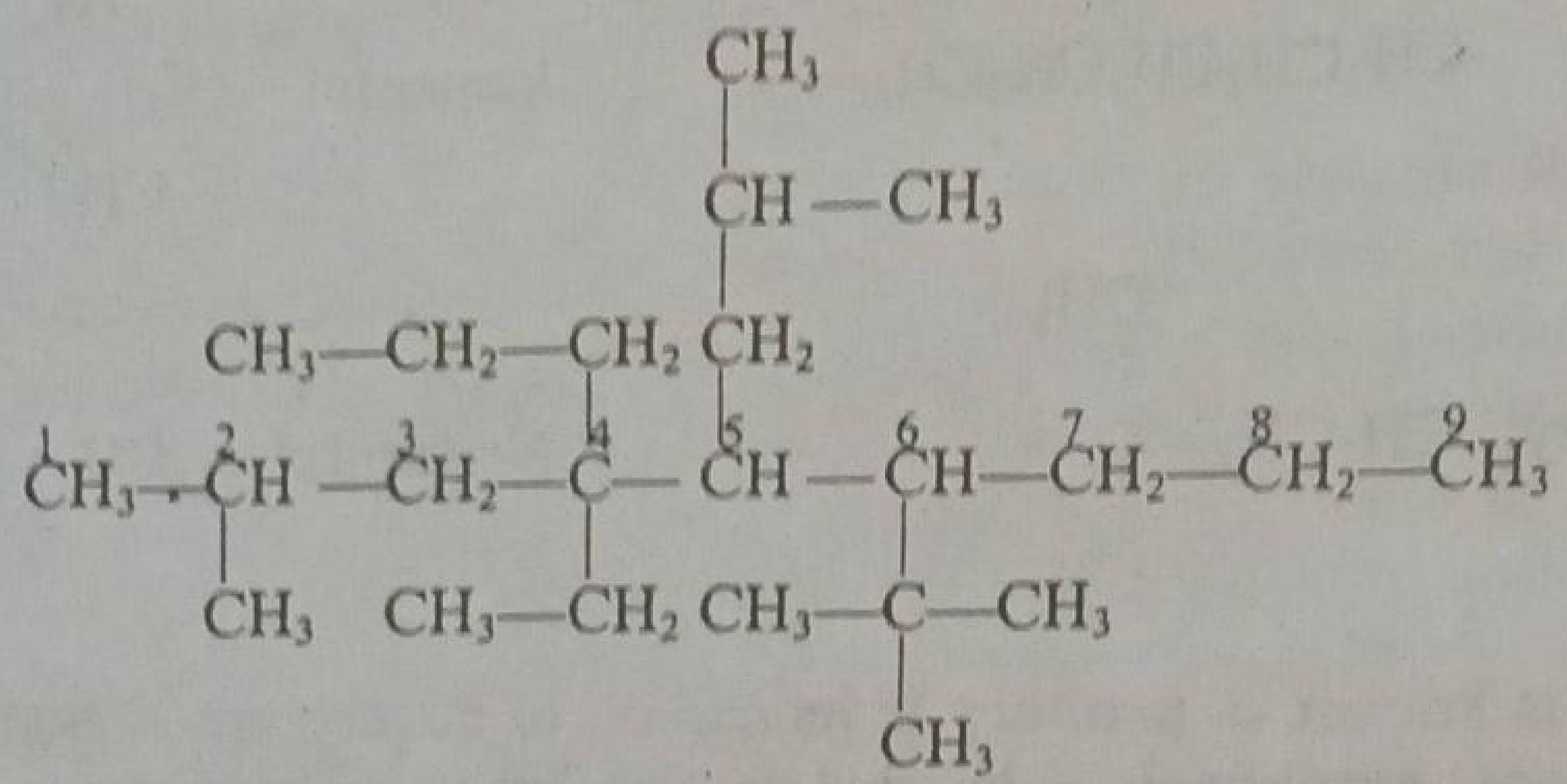
2. The carbon atoms of the parent chain are numbered consecutively starting from the end that gives the lowest number to the substituents at the first point of branching. The numbering sequence that begins at the other end of the chain in the above structure will be incorrect because it will have the substituent (ethyl) at C-5. When chains of equal length compete for selection as the parent chain, the choice is made in favour of the chain with greatest number of substituents. For example,



The other chain of the same length in this structure will have only one substituent.

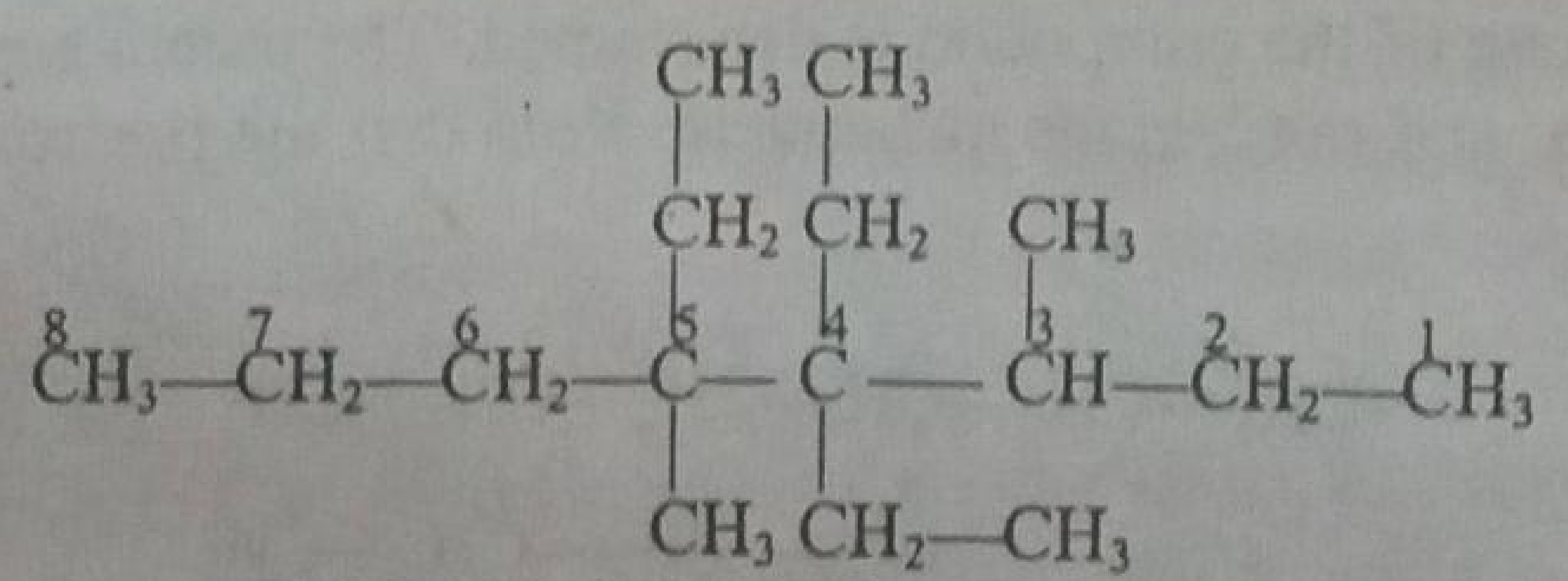


3. The names of the substituents are written in alphabetical order before the parent name. Each substituent is prefixed by the number assigned to it in the parent chain. The prefixes *sec-* or *tert-* are not considered when alphabetizing except when they are compared with each other; *sec*-butyl precedes *tert*-butyl. However, the prefixes *iso* and *neo* are considered as part of the name for alphabetizing the substituents. The parent name and the name of the substituent immediately preceding it are written as one word. For example,



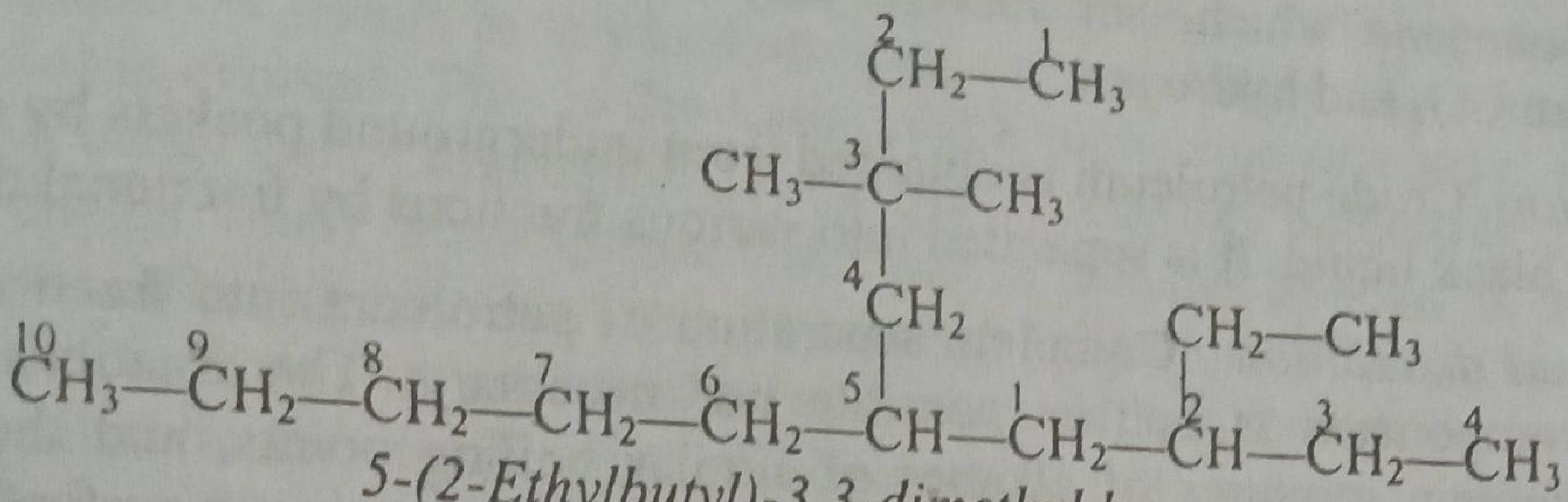
6-tert-Butyl-4-ethyl-5-isobutyl-2-methyl-4-propylnonane

4. If two or more substituents are identical, their name is written only once. Their multiplicity is indicated by the prefix *di-* for two, *tri-* for three, *tetra-* for four, *penta-* for five, etc., and the numbers assigned to them are grouped together with commas in between them and separated from the word by hyphen. The multiplying prefixes do not affect the alphabetical order of the substituents. For example,



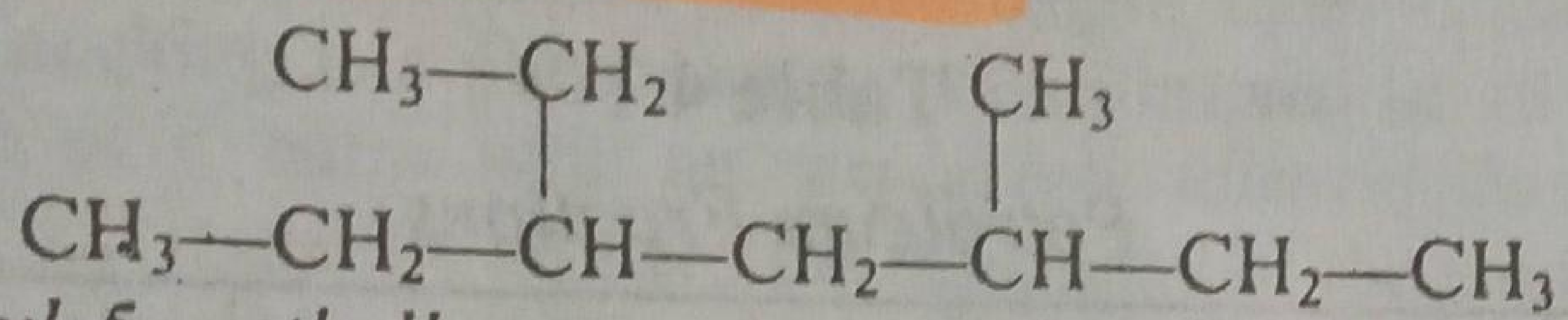
4,4,5-Triethyl-3,5-dimethyloctane

5. Although it is possible to assign common names to most of the alkyl substituents, complex alkyl groups (side chains having additional side chains of their own) are better named systematically making use of the foregoing rules. The positions of the additional side chains are indicated by numbering the main side chain, starting from the carbon atom attached to the parent chain. The name of the complex alkyl group is enclosed in parentheses to avoid confusion.



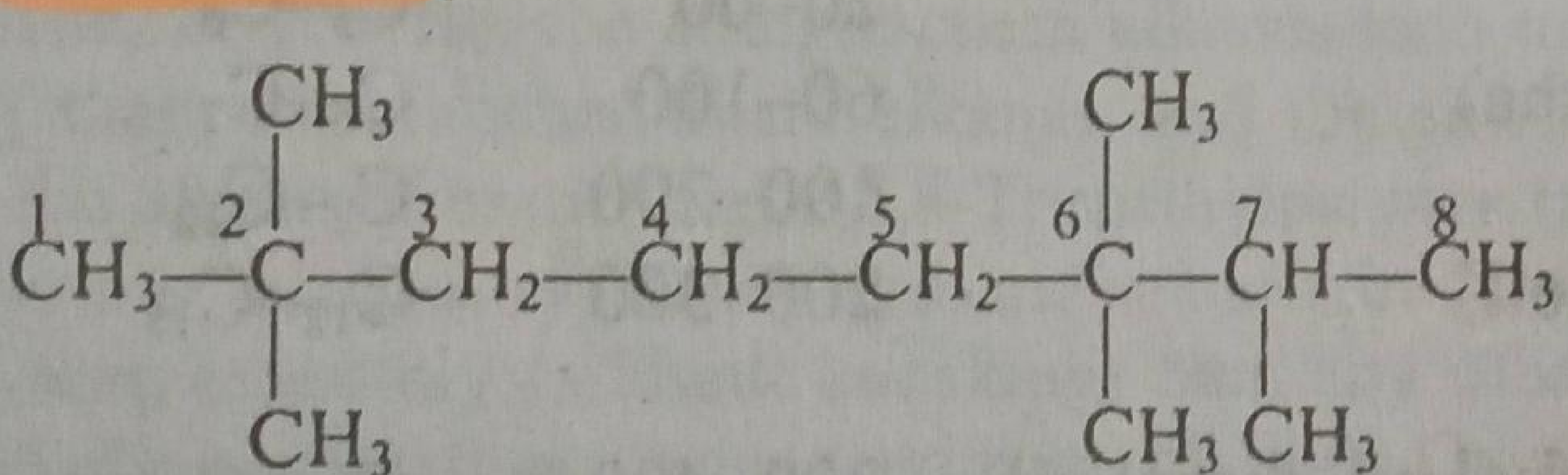
5-(2-Ethylbutyl)-3,3-dimethyldecane

6. When two or more substituents are in equivalent positions, the lower number is assigned to the one that appears first in the name



3-Ethyl-5-methylheptane (not 5-Ethyl-3-methylheptane)

When alternative directions of numbering produce different sets of numbers to designate location of substituents, the alternative sets are compared one to one in the ascending order of numbers. The set with the lower individual number at the 'first point of difference' is chosen. For example,



2,2,6,6,7-Pentamethyloctane

(2,2,6,6,7 is lower than 2,3,3,7,7 at the first point of difference)