BASIC IUPAC RULES

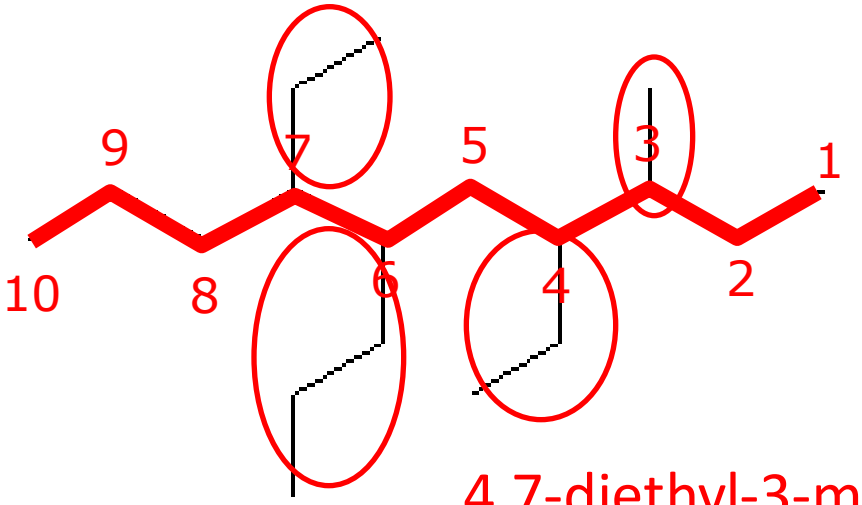
BASIC IUPAC RULES

The **IUPAC** name of an organic compound can be constructed based on a series of steps and rules:

1) Identification of the **principle functional group** and **substituents**

2) Identification of the **longest continuous chain** containing the principal functional group.

3) Assign **locants** (*i.e.* numbering) to the **principle functional group** and **substituents**.



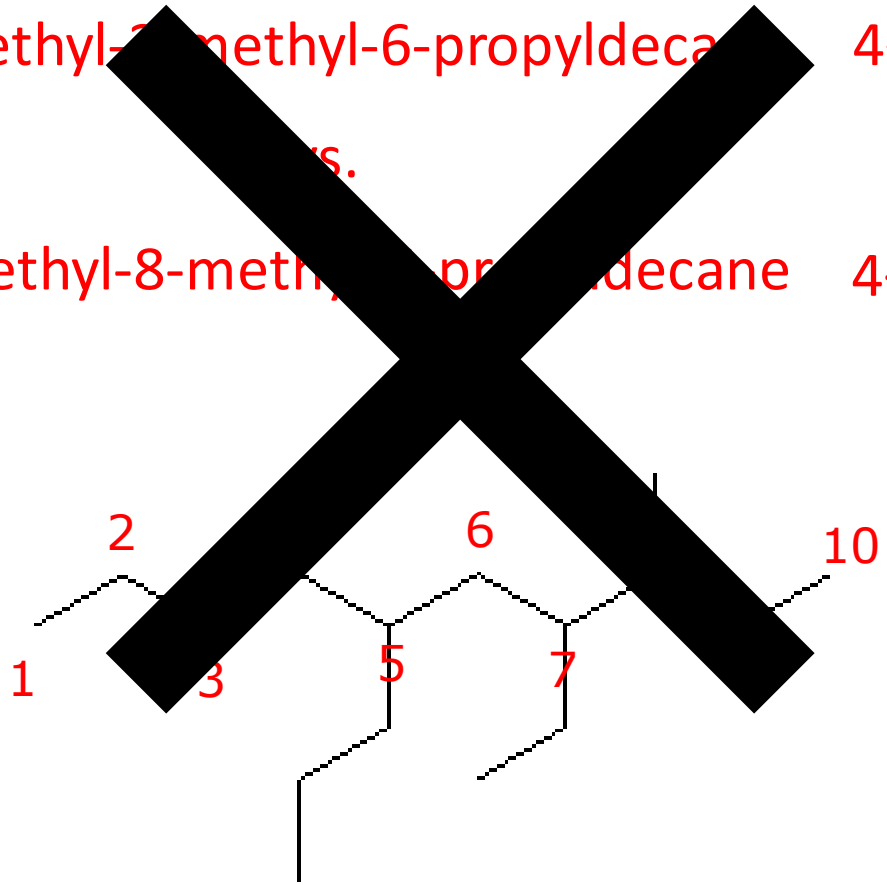
4,7-diethyl-3-methyl-6-propyldecane

BASIC IUPAC RULES

Misconception Alert!
When assigning the numbers (*i.e.* the locants) while naming an organic compound there is **NO rule** based on summing the numbers.

4,7-diethyl-3-methyl-6-propyldecane 4+7+3+6 = 20

4,7-diethyl-8-methyl-5-propyldecane 4+7+8+5 = 24



BASIC IUPAC RULES

The steps and rules are *summarized* below, more details are provided as the cases are encountered.

Principal Functional group	•The **principal functional group** is used to define the class the compound belongs to *e.g.* an alcohol, ROH •The **principal functional group** is the **highest priority functional group**. Functional group priority is discussed later. •The **principal functional group** is usually given the **lowest locant possible**.
Longest chain	•The **longest continuous chain** containing the **principal functional group** defines the **root name**. •Other groups attached to this chain are called **substituents**. •If there are two chains of equal length, then the choice that gives the simplest **substituents** is chosen.
Numbering (*i.e.* assigning locants)	•The numbers that define the positions of the principal functional group and substituents are called **locants**. •Compounds are numbered from one end of the **longest continuous chain**. •The locants are assigned such that the **principal functional group** gets the **lowest possible locant**. •If this results in a "tie" then the **first point of difference rule** is applied so that the first time a difference in numbering occurs, then the method that gives the lower number at this first difference is used. •In the event that there is no first point of difference then **alphabetisation** is used.

FIRST POINT OF DIFFERENCE RULE

The factors that influence the numbering according to the first point of difference rule are:

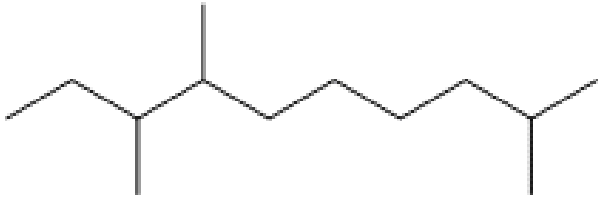
1) the principle functional group is given the lowest possible locant

2) substituents are then assigned locants based on this numbering scheme in such a way as to give the lowest locant number at the first time there is a difference

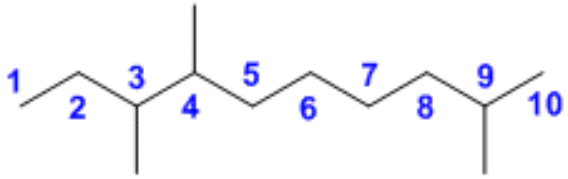
3) in the event that there is no first point of difference in the locants, substituents are numbered based on alphabetisation giving the first substituent the lowest possible locant number

FIRST POINT OF DIFFERENCE RULE

Example:

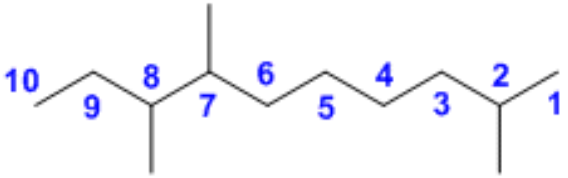


First, look at numbering the longest chain from left to right



Locants would be 3,4,9

Second, look at numbering the longest chain from right to left



Locants would be 2,7,8

Identifying the first point of difference:

1) List out the locant set for each scenario with the locants in numerical order
2) Compare the lists looking for the first time the numbers are different
3) Pick the scenario with the lower number at the first difference (here 2 is less than 3)

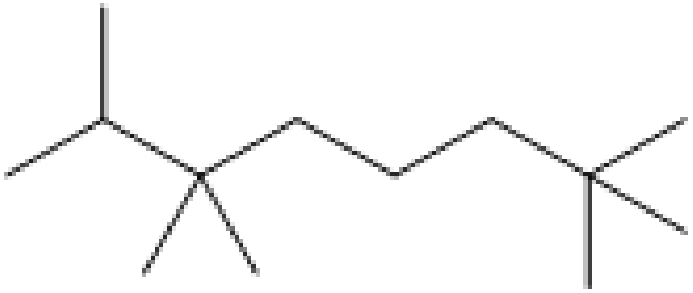
3 4 9

2 7 8

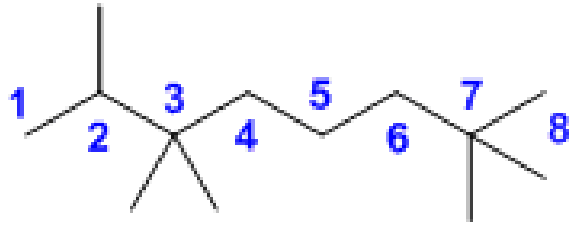
Correct name: 2,7,8-trimethyldecane

FIRST POINT OF DIFFERENCE RULE

Example:

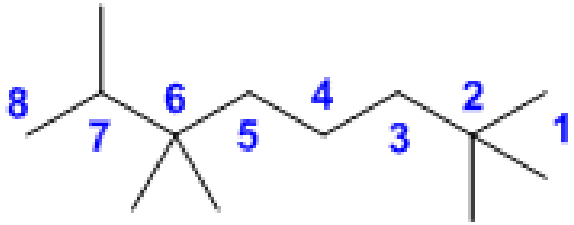


First, look at numbering the longest chain from left to right



Locants would be 2,3,3,7,7

Second, look at numbering the longest chain from right to left



Locants would be 2,2,6,6,7

Identifying the first point of difference:

1) List out the locant set for each scenario with the locants in numerical order
2) Compare the lists looking for the first time the numbers are different
3) Pick the scenario with the lower number at the first difference (here 2 is less than 3)

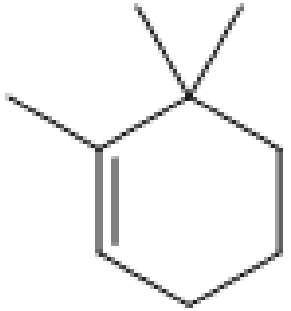
2 3 3 7 7

2 2 6 6 7

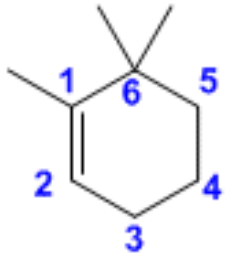
Correct name: 2,2,6,6,7-pentamethyloctane

FIRST POINT OF DIFFERENCE RULE

Example:

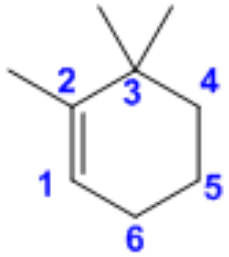


First, look at numbering counter clockwise from the top alkene C



Locants would be 1,6,6

Second, look at numbering clockwise from the bottom alkene C



Locants would be 2,3,3

Identifying the first point of difference:

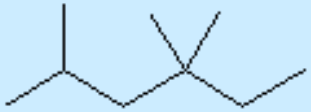
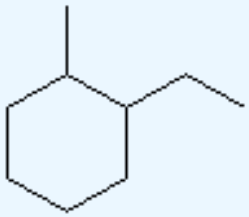
1) List out the locant set for each scenario with the locants in numerical order
2) Compare the lists looking for the first time the numbers are different
3) Pick the scenario with the lower number at the first difference (here 1 is less than 2)

1	6	6
2	3	3

Correct name: 1,6,6-trimethylcyclohexene

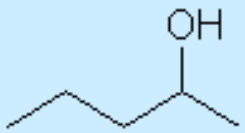
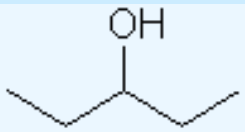
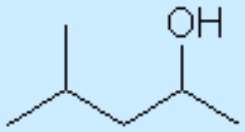
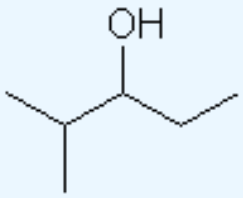
FIRST POINT OF DIFFERENCE RULE

Examples:

2-methylpentane *not* 4-methylpentane.		Here the methyl group is given the lowest number by numbering as shown (2- rather than 4-).
2,2,4-trimethylpentane *not* 2,4,4-trimethylpentane		The first difference is at the *second* locant - by numbering as shown this is kept lower (2- rather than 4-).
2,4,4-trimethylhexane *not* 3,3,5-trimethylhexane		The first difference is at the *first* locant - by numbering as shown this is kept lower (2- rather than 3-).
1-ethyl-2-methylcyclohexane *not* 2-ethyl-1-methylcyclohexane *or* 1-ethyl-6-methylcyclohexane		The first difference is at the *second* locant (2- rather than 6-) which means 1,2- is preferred over 1,6-. The application of this numbering is then dictated by the alphabetisation : **ethyl** preceeds **methyl** so ethyl gets the lower number.

FIRST POINT OF DIFFERENCE RULE

Examples:

pentan-2-ol *not* pentan-4-ol		Here the principle functional group, the alcohol -OH is give the lowest locant by numbering as shown (2- rather than 4-).
pentan-3-ol *no choice !*		No matter which way this is numbered, the -OH is at C3.
4-methylpentan-2-ol *not* 2-methylpentan-4-ol		The first difference is in the -OH locant - by numbering as shown this is kept lower (2- rather than 4-).
2-methylpentan-3-ol *not* 4-methylpentan-3-ol		The first difference is in the methyl locant - since the -OH must be at C3 either way, but by numbering as shown the methyl locant kept lower (2- rather than 4-).

ALPHABETIZATION

In constructing the name, **substituents** are cited in alphabetical order, *e.g.* an **e**thyl group proceeds a **m**ethyl group.

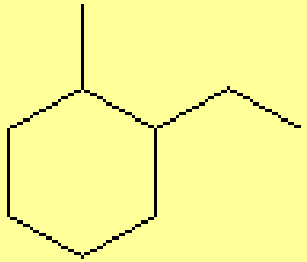
Only in the event that the **first point of difference rule** doesn't give a result is alphabetization used to define the numbering

-multiplier prefixes (di-, tri- tetra- etc.) are ignored

-prefixes such as neo-, sec-, tert- (or their abbreviations) are ignored

-the prefixes iso- and cyclo- **are** included (*note* they are are used without hyphens and are part of the substituent name)

1-ethyl-2-methylcyclohexane
not
2-ethyl-1-methylcyclohexane
or
1-ethyl-6-methylcyclohexane



The numbering is determined by the alphabetisation: **ethyl** preceeds **methyl** so ethyl gets the lower number. But then we number counter-clockwise to give the methyl the lower number (2- vs 6-)

ALPHABETIZATION

For systems named with **complex substituents**, the following additional guideline applies:

-in alphabetizing complex substituents, any terms used in the brackets are included.

-for example (1,1-dimethylethyl)- is alphabetized as "**d**"

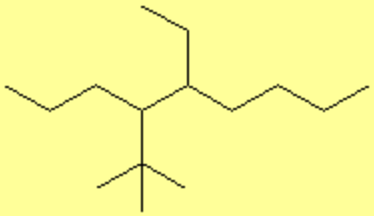
-this is because the term in brackets is the name of the whole complex substituent and not several individual substituents.

4-(1,1-dimethylethyl)-5-ethylnonane

not

5-ethyl-4-(1,1-dimethylethyl)nonane

(the naming of complex substituents is covered later)



The order is determined by the alphabetisation: the **dimethyl** of the complex substituent preceeds the simple**ethyl** substituent.