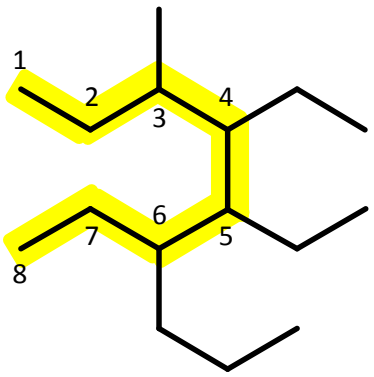
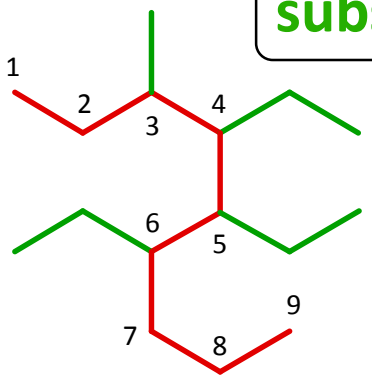
Naming Alkanes – Parent Chain

Root + ending "-ane"

substituents + parent + ane



Identify longest chain →

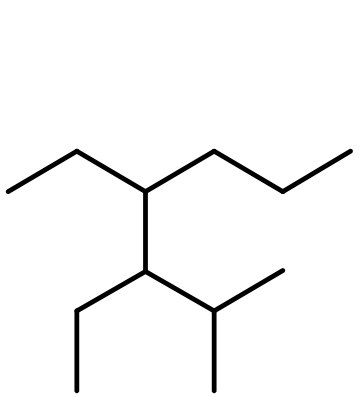


Parent chain has 9 carbons →

Nonane

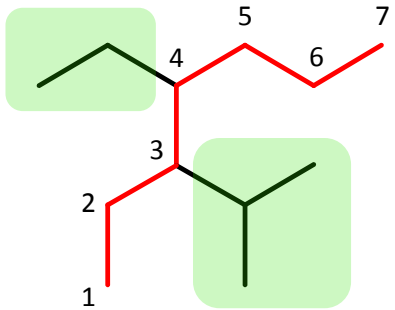
# of C	Root
1	meth
2	eth
3	prop
4	but
5	pent
6	hex
7	hept
8	oct
9	**non**
10	dec
11	undec
12	dodec

If two or more longest chains exist, choose the one with **the greater number of substituents**.



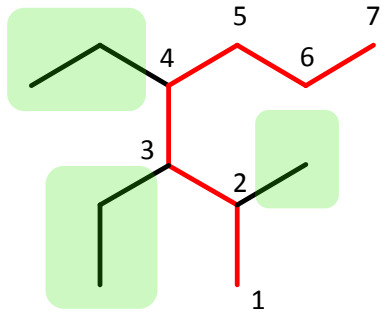
→

✗



Heptane

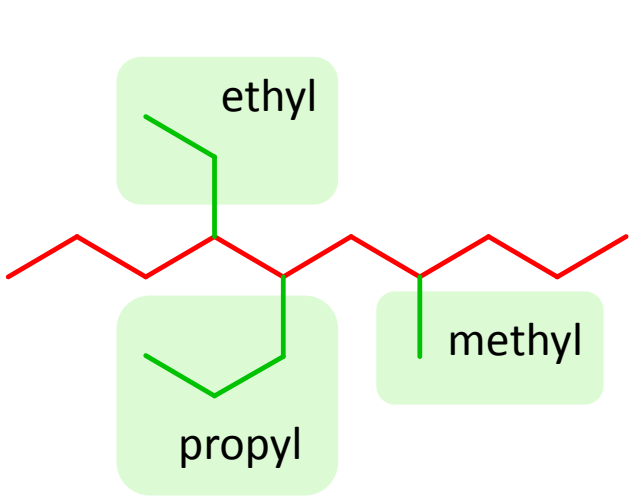
✓



Heptane

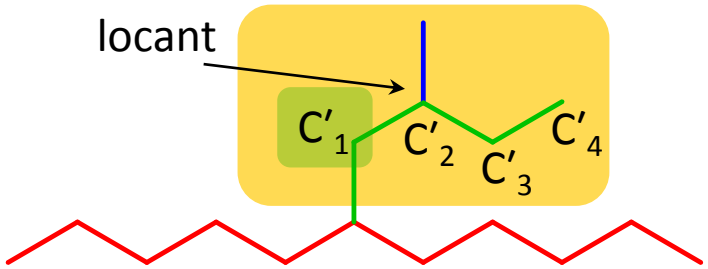
Naming Alkanes – Substituents

Root + ending "-yl"



alkyl group

# of C	Name
1	meth
2	eth
3	prop
4	but
5	pent
6	hex
7	hept
8	oct
9	non
10	dec
11	undec
12	dodec



parent chain (**undecane**)

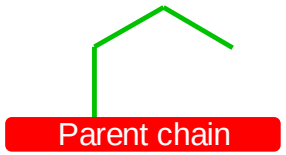
substituent (a **butyl** chain)

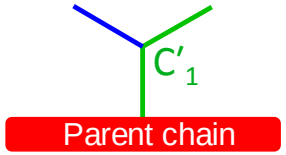
substituent of the substituent (a **methyl on C′2**)

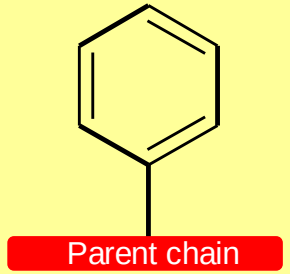
The name of the **overall substituent** is (2-methylbutyl). Names of branched alkyl groups should be given in brackets.

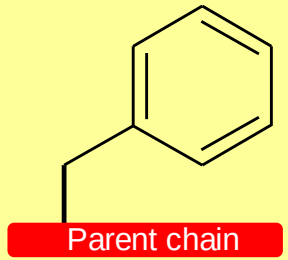
Common names of recurring substituents (allowed by IUPAC)

3 C



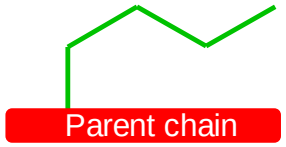


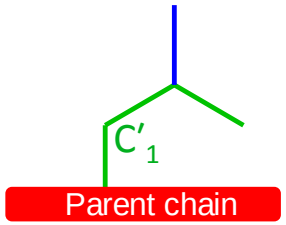


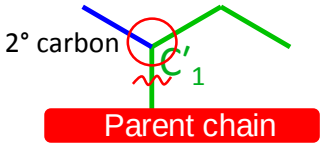


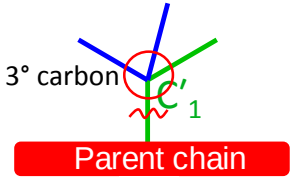
Common nomenclature	propyl	isopropyl	phenyl	benzyl
IUPAC nomenclature		(1-methylethyl)		

4 C









Common nomenclature	butyl	isobutyl	*sec*-butyl	*tert*-butyl
IUPAC nomenclature		(2-methylpropyl)	(1-methylpropyl)	(1,1-dimethylethyl)

To help you remember

An iso alkyl group is branched into two methyl groups at the end of the chain

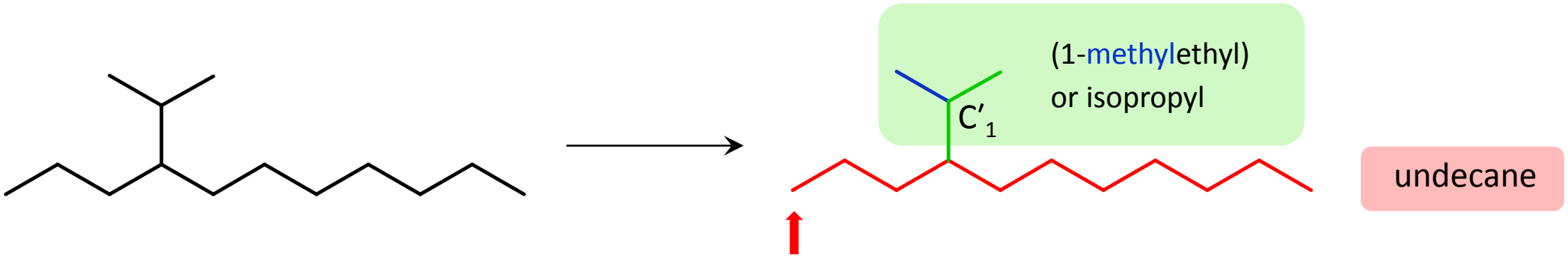
A *sec*- alkyl group is branched at C'_1 and C'_1 is a *sec*ondary carbon

A *tert*- alkyl group is branched at C'_1 and C'_1 is a *tert*iary carbon

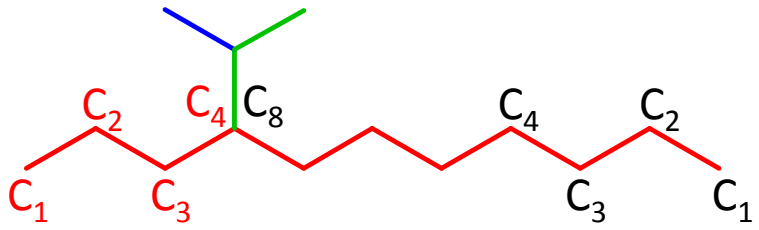
Assembling the systematic name of an alkane

locant + substituents + parent

Determine:
- the name of the **parent chain**
- the name of the **substituents**
- the correct numbering of the parent chain



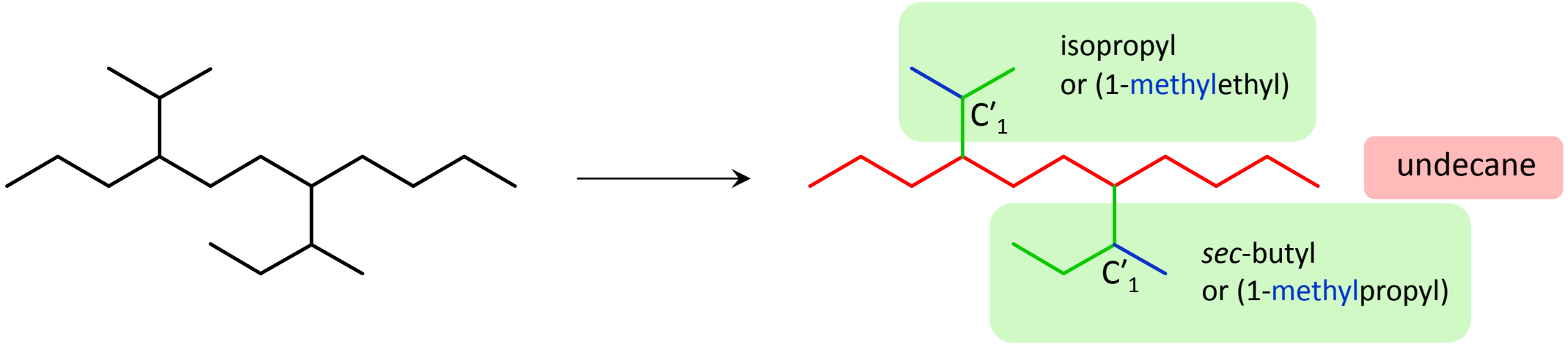
The **parent chain** is numbered in a way that the **substituent** is associated with the lowest possible **locant**.



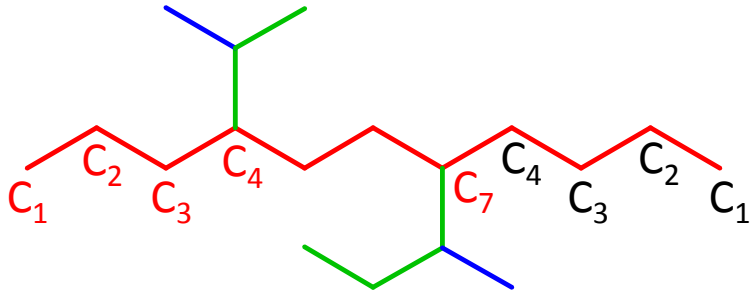
4-(1-methylethyl)undecane ✓
or 4-isopropylundecane

8-(1-methylethyl)undecane ✗

If two or more substituents are present on the parent chain,



start counting from both ends of the parent chain at the same time and adopt the numbering that finds a substitutent first.



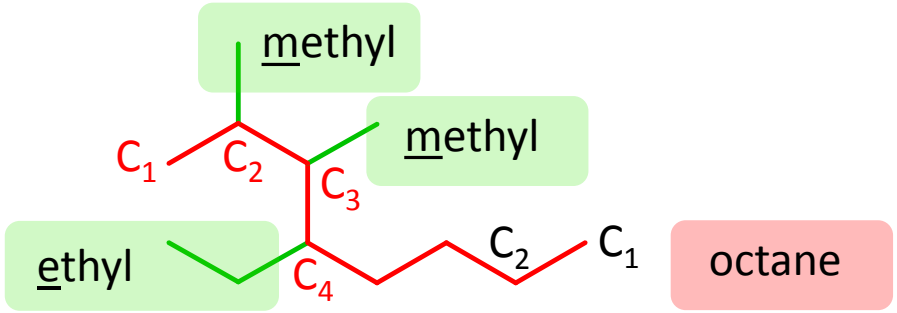
7-*sec*-butyl-4-isopropylundecane

or 4-(1-methylethyl)-7-(1-methylpropyl)undecane

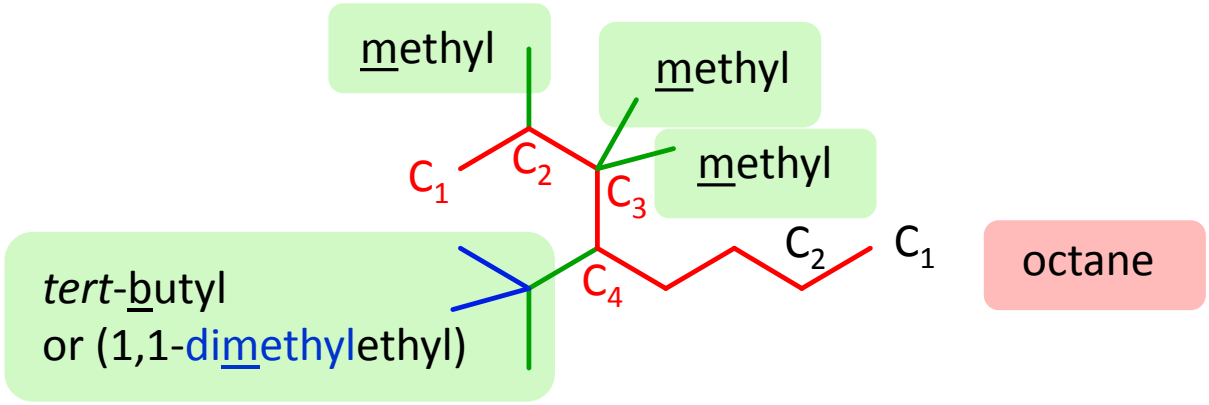
Note: the order of the substitution has changed

- Substituents are listed in **alphabetical order**.
- The prefixes "*sec*" and "*tert*" are neglected when alphabetizing the substituents.
  (unlike "iso", "*sec*" and "*tert*" are followed by a hyphen and are written in italics)

If the **parent chain** bears two or more identical **substituents**, their locants are **all** listed, but their names are listed only once, preceded by the prefixes **di, tri, tetra** etc. depending on the number of times they appear on the parent chain.



4-ethyl-2,3-dimethyloctane



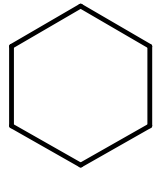
4-*tert*-butyl-2,3,3-trimethyloctane

or 2,3,3-trimethyl-4-(1,1-dimethylethyl)octane

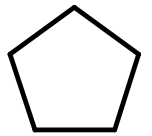
Note: The prefixes “di”, “tri”, “tetra” etc. are always neglected when alphabetizing the substituents.
If two identical substituents have the same locant, the latter is repeat (as in 2,3,3-trimethyl).

Syntax:
- Commas appear **only** between locants that refer to the same substituent.
  In all other cases, numbers are separated byhyphens.
- No space appears in the names of alkanes.

Nomenclature of cycloalkanes



Cyclohexane

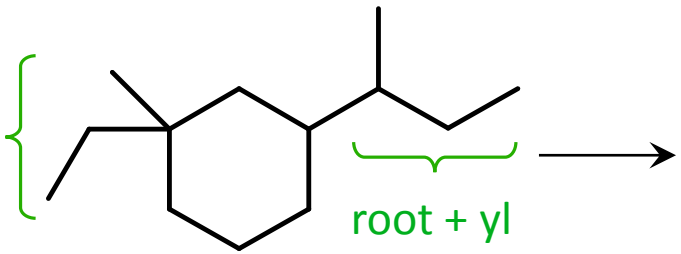


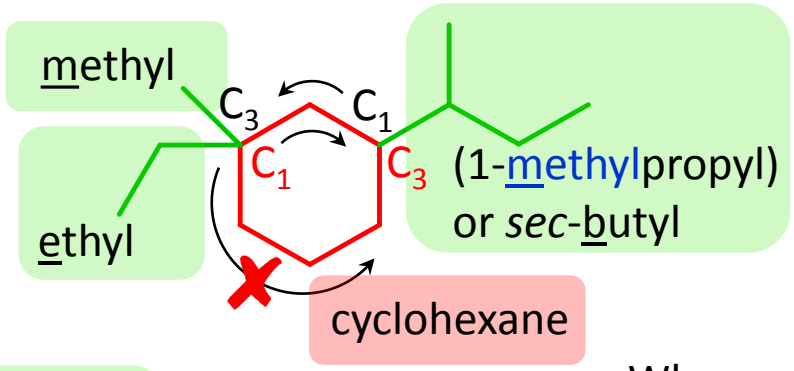
Cyclopentane

Cyclobutane

The same rules apply.

- The names of cyclic alkanes is preceded by "**cyclo**".
- If a ring contains a number of carbons higher than that in each substituent, it is used as the parent chain and named with the ending **–ane**. Otherwise, it is considered a substituent and named with the ending **–yl**.
- When a ring is the parent chain, there are not two ends to start the numbering from. By trial and error, choose the numbering that yields the **lowest sum of the locants**.

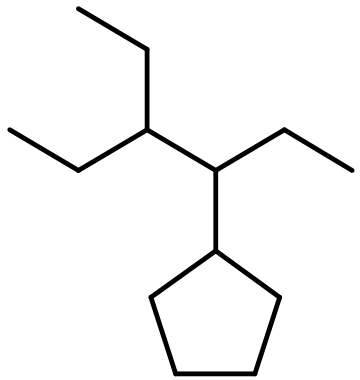


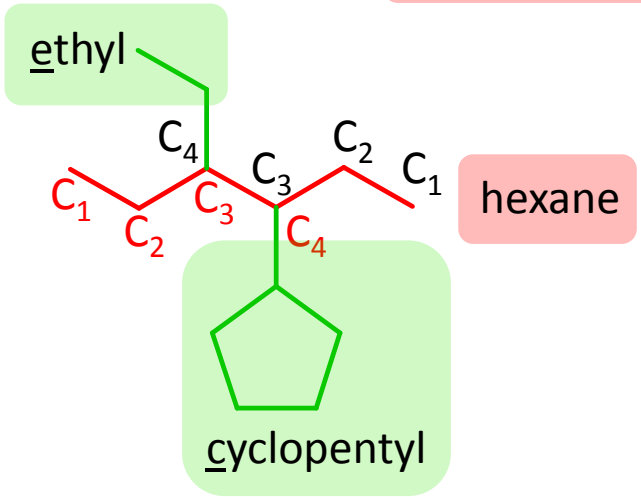


1,3,3
Σ locants = 7 ✗

1,1,3
Σ locants = 5 ✓

1-ethyl-1-methyl-3-(1-methylpropyl)cyclohexane
or 3-*sec*-butyl-1-ethyl-1-methylcyclohexane





When two numberings intercepts substituents at the same positions, list the substituents in order of increasing locant as well as in alphabetical order.

4-cyclopentyl-3-ethylhexane ✗ alphabetical order

3-cyclopentyl-4-ethylhexane ✓ alphabetical order + increasing locant

We have seen:

- How to combine the name of parent chain and substituents to obtain the full name of an alkane
- How to select the correct numbering of the parent chain when more than one substituent is present
- How to use the locants and the prefixes “di”, “tri” and “tetra” to indicate the presence of the same substituent on the same or on different locations on the parent chain
- How to select the correct numbering among two that give the same set of locants (alphabetical order + increasing number of locant)
- How to name cycloalkanes when the ring is the longest chain and when it is simply a substituent
- How to correctly number cycloalkanes based on the lowest sum of locants
- How to write a chemical name using the correct syntax (no spaces, commas only between locants, hyphens for all other cases)

Determine:

- the name of the **parent chain**
- the name of the **substituents**
- the correct numbering of the parent chain