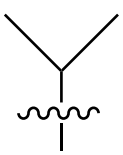
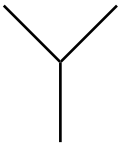
CHEM 261 September 21, 2023

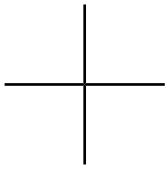
Systematic (IUPAC) Nomenclature

RULES:

1. Find the longest straight chain
2. Number from end of the chain, so that the 1st branch point has the lowest number
3. Name the chain, then add prefixes (for the groups attached) with number and name the groups attached
4. Separate numbers and names by dash







Common name:	isopropyl	isobutane	neopentane
Systematic name:		2-methylpropane	2,2-dimethylpropane

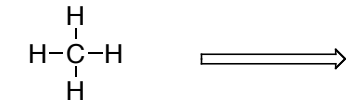
Note: iso = second-to-last carbon of the chain is disubstituted (2 methyl groups)
neo = second-to-last carbon of the chain is trisubstituted (3 methyl groups)

Prefixes for naming:
Di (2), Tri (3), Tetra (4), Penta (5), Hexa (6) etc.

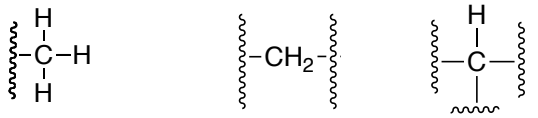
Groups (part of an alkane structure)

- In naming the particular group, drop the "ane" part and add "yl" to the name
- For example, methane → methyl

(i) Methyl group – CH_3

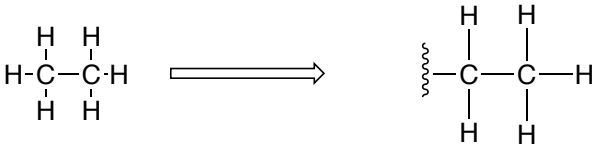


methane



methyl group methylene methine

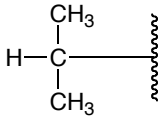
(ii) Ethyl group – CH_2CH_3



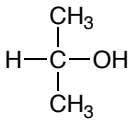
ethane

ethyl

(iii) Isopropyl group

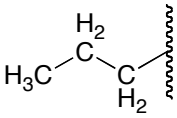


iso-propyl group

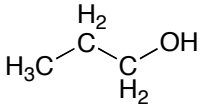


iso-propyl alcohol

(iv) *n*-Propyl group

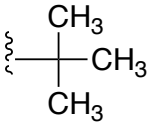


n-propyl chain

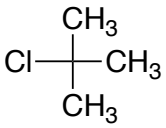


n-propyl alcohol

(v) *tert*-Butyl group (t-butyl)

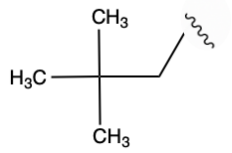


tert-Butyl chain

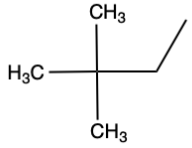


tert-Butyl chloride

(vi) neo group

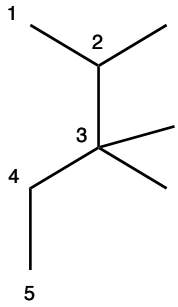


neo chain

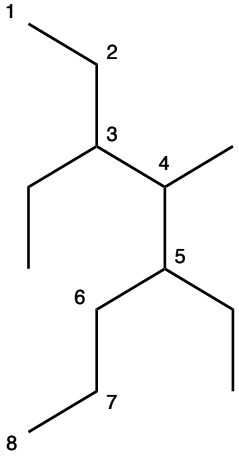


2,2-dimethylbutane

Naming Examples:



2,3,3-trimethylpentane



3,5-diethyl-4-methyloctane

<u>Cycloalkanes</u>:

General Molecular Formula of Alkanes

- Linear alkanes: general formula is C_NH_{2N} + 2
- Each **degree of unsaturation** "removes" 2 hydrogens from the C_NH_{2N} +2 formula
- (if there are no nitrogens in the molecule, there will always be an even # of hydrogens)
- Cylcoalkanes always have at least 1 degree of unsaturation

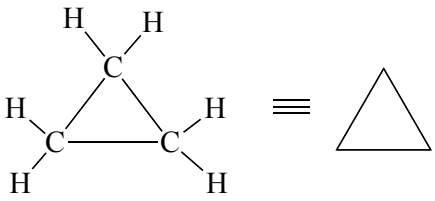
  e.g.
  - 1 Degree of unsaturation : C_NH_{2N} Alkanes with one ring or double bond
  - 2 Degrees of unsaturation : C_NH_{2N-2} Alkanes with two rings or double bonds, or one each

Note: Ring Structure Naming

- Parent ring is the largest one
- Prefix with "cyclo"

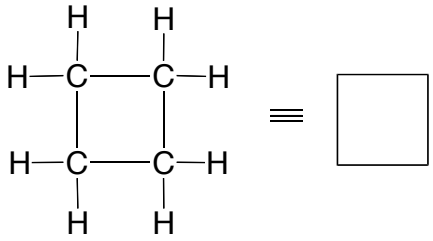
- Start with numbering at point of maximum branching/most important functional group
- Number so as to give next branch/functional group lowest number

Cyclopropane, C_3H_6

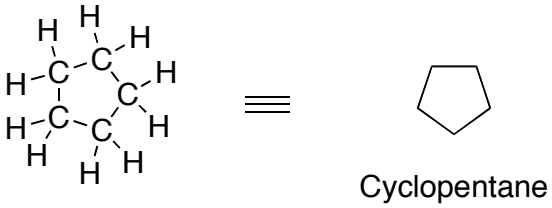


- One degree of unsaturation (*n*-propane is C_3H_8)
  - Not a structural isomer (different molecular formula)
- C-C-C bond angle (60°)
- Highly reactive due to ring strain (sp^3 carbons prefer to be 109°)

Cyclobutane, C_4H_8

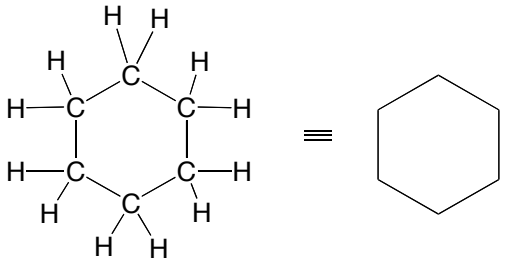


Cyclopentane, C_5H_{10}



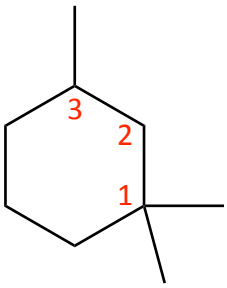
Cyclopentane

Cyclohexane, C_6H_{12}



Examples of Naming Cycloalkanes:

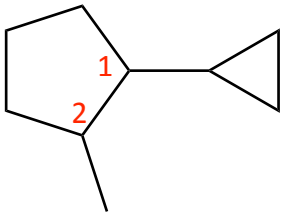
Ex #1) C_9H_{18}



1,1,3-trimethylcyclohexane

Degree of Unsaturation= 1

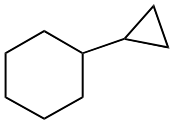
Ex #2) C_9H_{16}



1-cyclopropyl-2-methylcyclopentane

Degree of Unsaturation= 2

Ex #3) C_9H_{16}

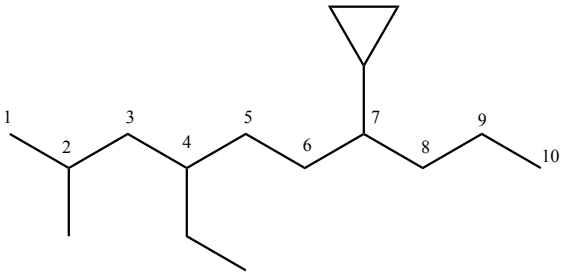


Degree of Unsaturation= 2

1-Cyclopropylcyclohexane

Example 2 and 3 both have the formula C_9H_{16} so they are structural isomers

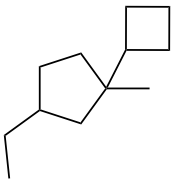
Ex #4) $C_{16}H_{32}$



Degree of Unsaturation= 1

7-cyclopropyl-4-ethyl-2-methyldecane

Ex #5) $C_{12}H_{22}$



Degree of Unsaturation= 2

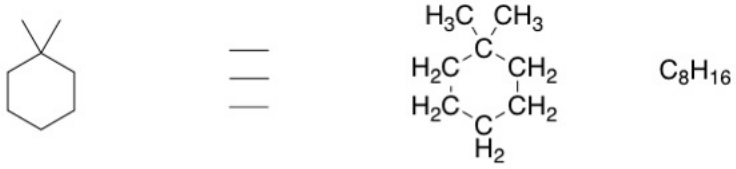
1-Cyclobutyl-3-ethyl-1-methylcyclopentane

ISOMERS

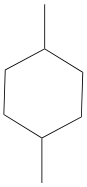
Structural (Constitutional) Isomers

- Share the same molecular formula but have the atomic bonds in different places

Example 1



1,1-dimethylcyclohexane



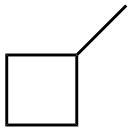
C_8H_{16}

1,4-dimethylcyclohexane

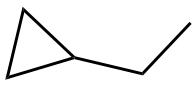
The above two compounds are structural (also known as constitutional) isomers

Example 2

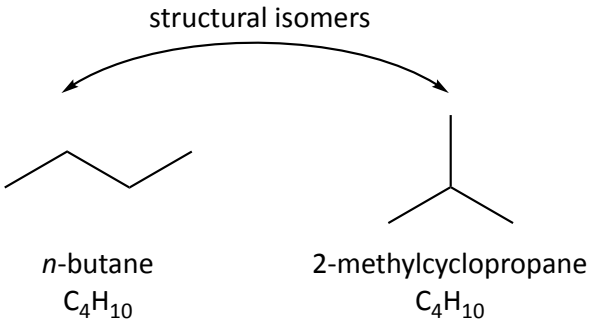
C_5H_{10}
structural isomers



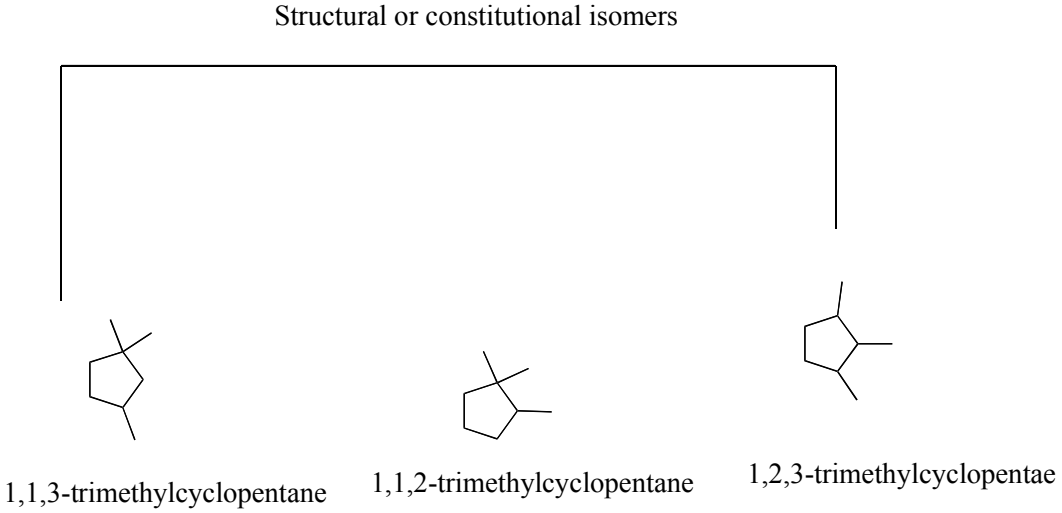
1-methylcyclobutane



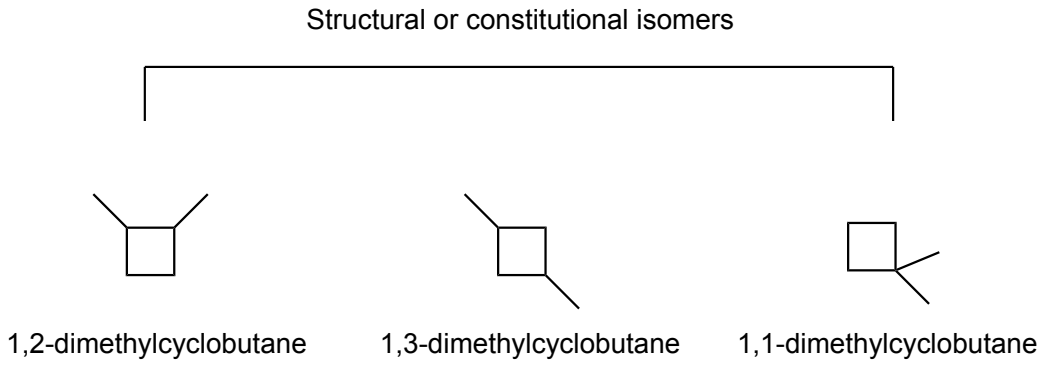
1-ethylcyclopropane



Example 3



Example 4



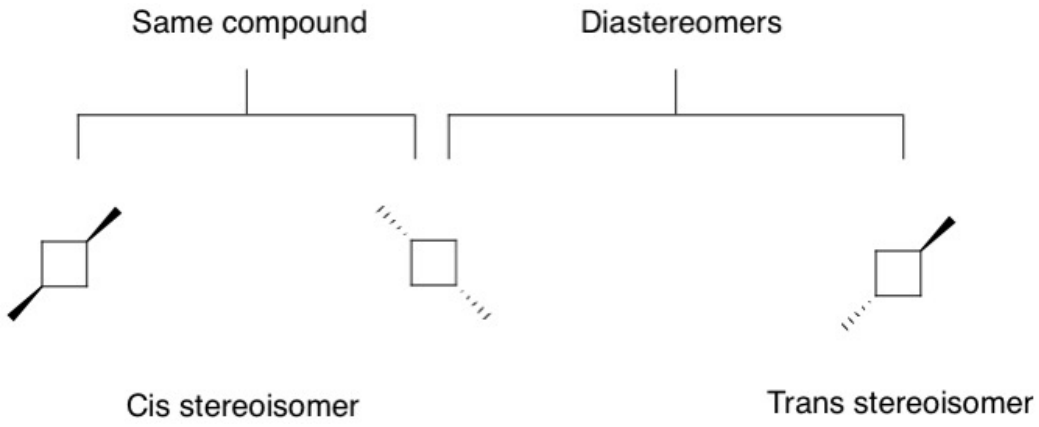
Stereoisomers

Compounds with the same molecular formula, same order of connection (base name) but connection of atoms that differ in 3D geometry

Two Types:

1. Diastereomers - stereoisomers that are not mirror images (all stereoisomers that are not enantiomers)
2. Enantiomers - stereoisomers that are non-superimposable mirror images of each other

Example: 1,3-dimethylcyclobutane

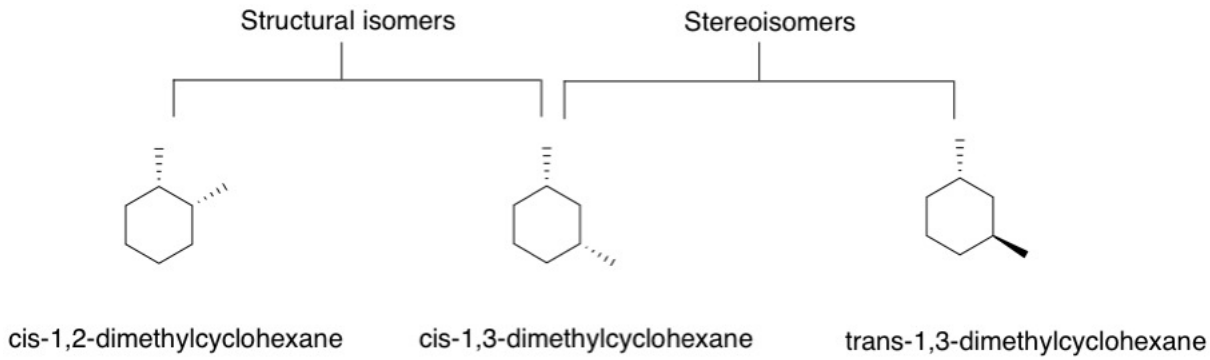


The first and second compounds are the same compound rotated in 3D space. The third compound has different geometry at one center, making it a stereoisomer, specifically a diastereomer.

Cis - the substituents are on the same side of the ring

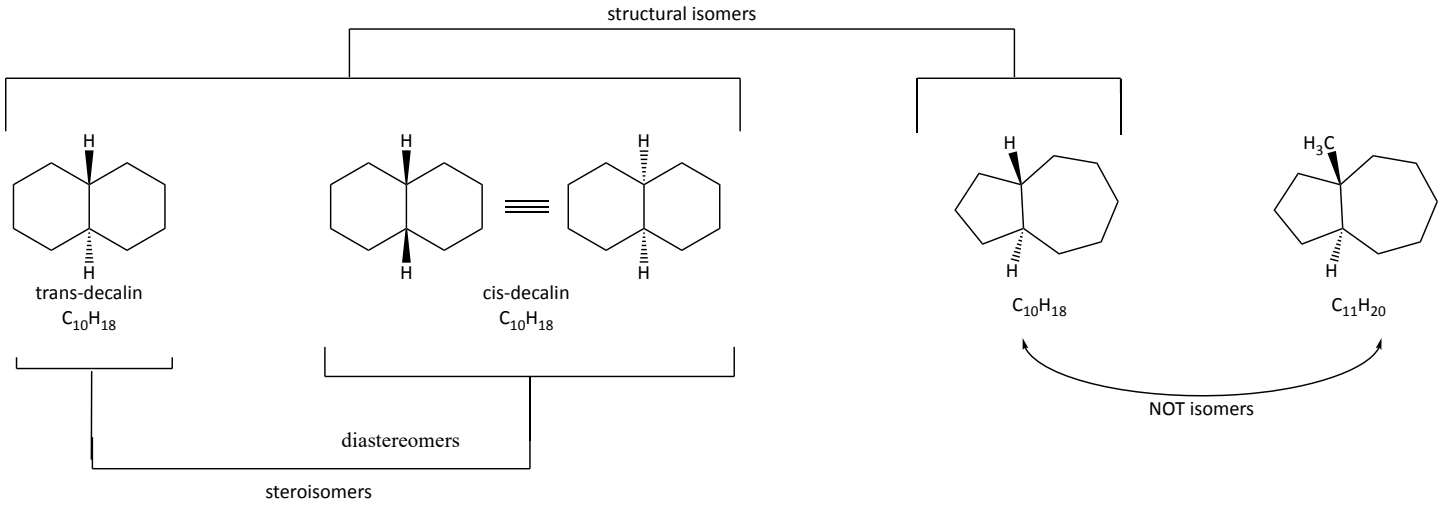
Trans - the substituents are on opposite sides of the ring

Example: 1,2-dimethylcyclohexane and 1,3-dimethylcyclohexane



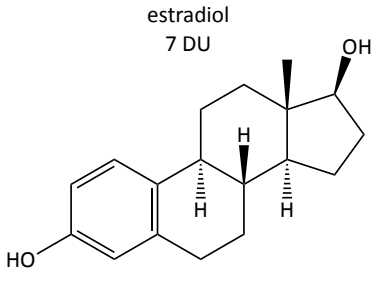
The second two compounds are diastereomers of each other.

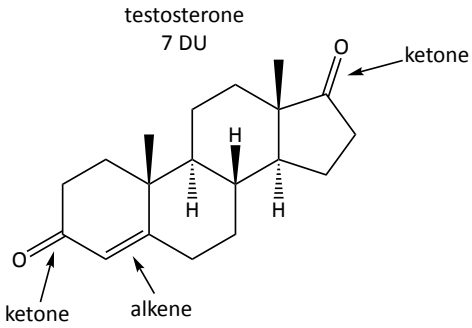
Example: decalin - $C_{10}H_{18}$

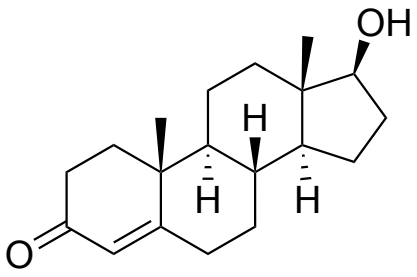


Example: steroids

androstenedione



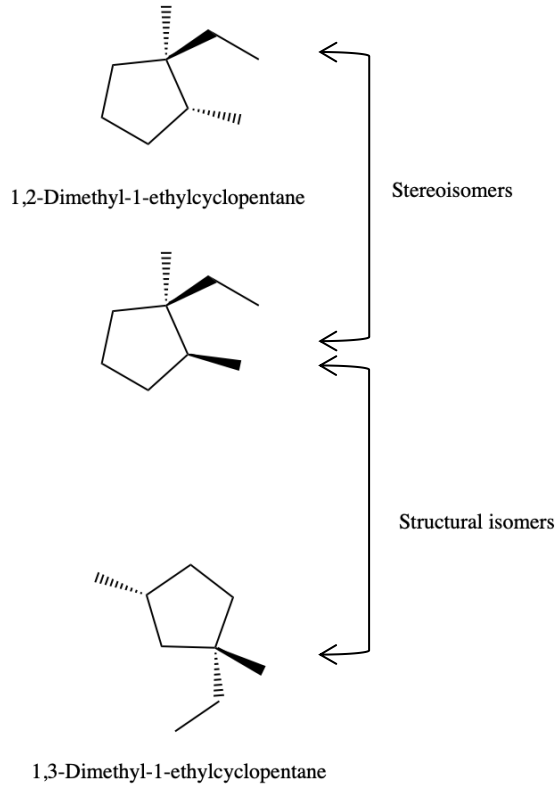




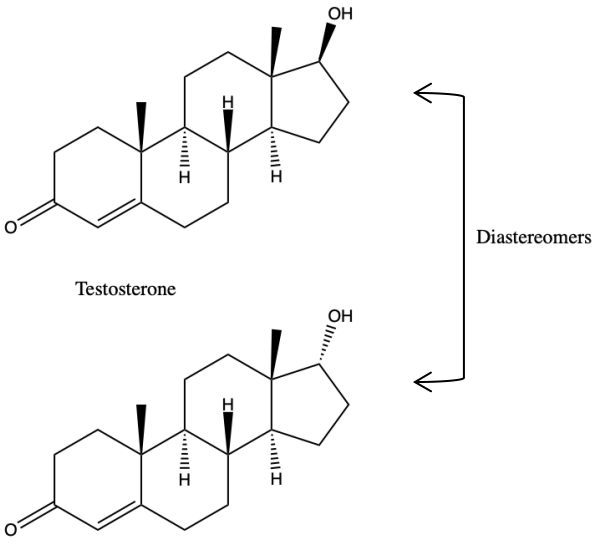
Testosterone
Molecular formula?
Functional groups?
Degrees of Unsaturation?
How many methyls?
How many methylenes?
How many methines?

TEST YOURSELF

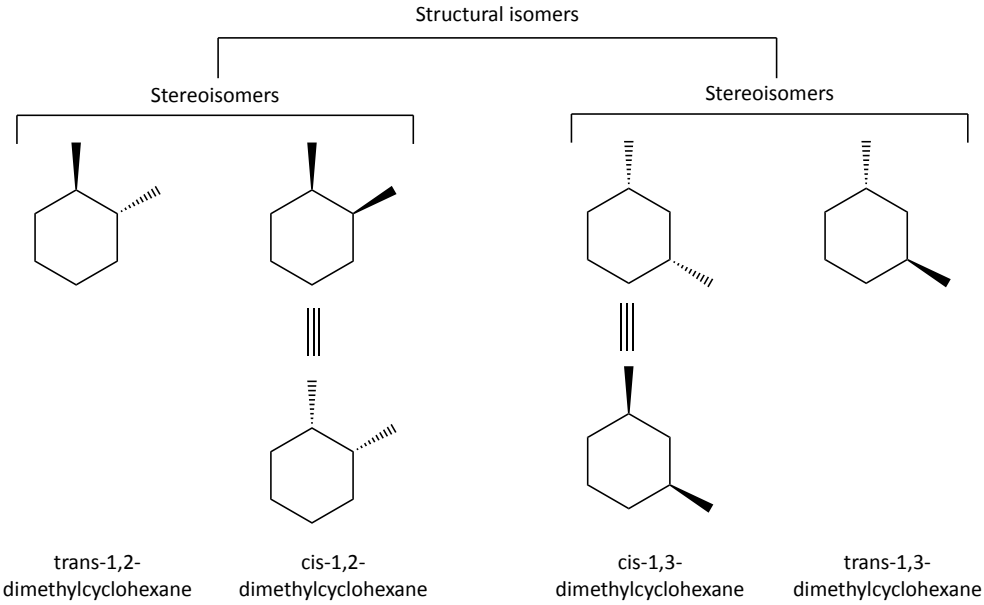
Example:



Example of diastereomers:

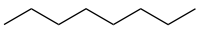


More on differentiating structural and stereoisomers

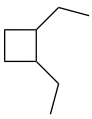


Example:

cyclooctane
C_8H_{16}
DOU = 1



n-octane
C_8H_{18}
DOU = 0

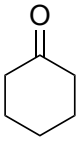


1,2-diethylcyclobutane
C_8H_{16}
DOU = 1

1,1-diethylcyclobutane
C_8H_{16}
DOU = 1

Cyclooctane and 1,2-diethylcyclobutane and 1,1-diethylcyclobutane are structural (constitutional) isomers – they all have the same molecular formula

n-octane is not a structural isomer of the others, it has a different molecular formula



Degrees of Unsaturation = 2
(1 ring and 1 double bond)
$C_6H_{10}O$