

Lecture Outline 2: ALKANES

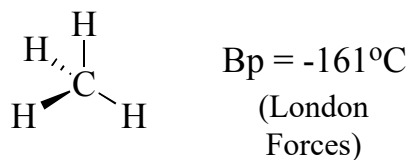
Hydrocarbons – Compounds that contain only C and H

- Alkanes contain only single bonds (C-H, C-C), sp^3
- Alkenes = contains C=C and has sp^2 hybridization (e.g. olefins)
- Alkynes = contains C $\equiv$ C and has sp hybridization (acetylenes)

Alkanes

- All carbons are sp^3 hybridized (optimal bond angle of 109°)
- Single bonds (σ bonds).
- Tetrahedral geometry at every carbon
- Held together by London (dispersion) forces

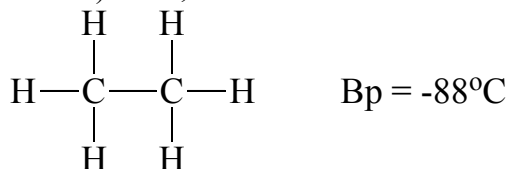
Ex #1) CH₄, methane



BP = -164°C

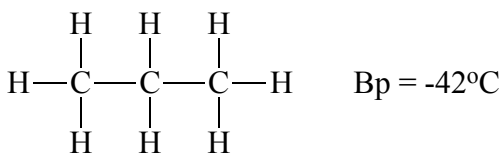
CH₄ H₄C CH₃-H

Ex #2) C₂H₆, ethane



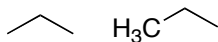
C₂H₆ CH₃-CH₃ BP = -88°C
H₃C-CH₃

Ex #3) C₃H₈, propane



C₃H₈

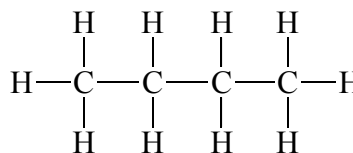
CH₃CH₂CH₃



H₃C

BP = -42°C

Ex #4) C₄H₁₀, butane

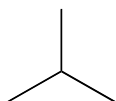
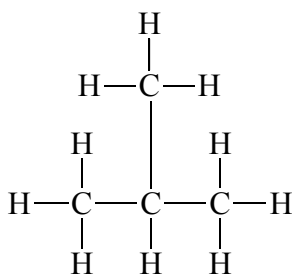


C₄H₁₀, CH₃CH₂CH₂CH₃

n-Butane: normal straight chain butane

NOTE: Propane has a boiling point of -42°C , which is higher than methane because its chain-like structure allows for more surface area for London dispersion forces to take effect.

Ex #5) C_4H_{10} , isobutane or i-Butane



structural isomer = constitutional isomer

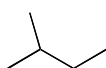
- Isomers are different compounds that have the same molecular formula and different structure. They have different physical properties (e.g. mp, bp, odour, biological effects)

- iso - meros
same - parts

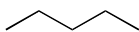
one type: structural (same as constitutional)

second type: stereoisomers (diastereomers and enantiomers) – will talk about more

Ex #6) Pentane C_5H_{12}



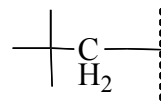
(isopentane or
2-methylbutane)



n - pentane



Neopentane

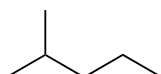


Neo Group

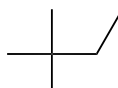
Ex #7) Hexane C_6H_{14}



n-hexane



Isohexane

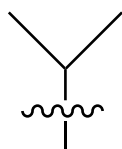


neohexane

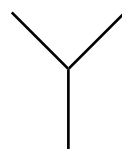
Systematic (IUPAC) Nomenclature

RULES:

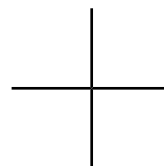
1. Find the longest straight chain
2. Number from end of the chain, so that the 1st branch point has the lowest number
3. Name the chain, then add prefixes (for the groups attached) with number and name the groups attached
4. Separate numbers and names by dash



Common name: isopropyl
 Systematic name:



isobutane
 2-methylpropane



neopentane
 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)

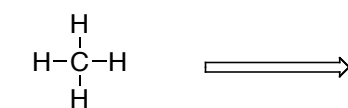
Prefixes for naming:

Di (2), Tri (3), Tetra (4), Penta (5), Hexa (6) etc.

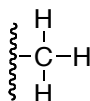
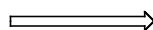
Groups (part of an alkane structure)

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

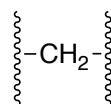
(i) Methyl group – CH_3



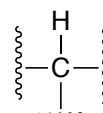
methane



methyl group

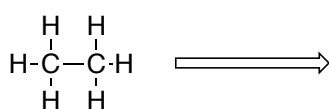


methylene

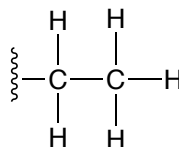
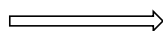


methine

(ii) Ethyl group – CH_2CH_3

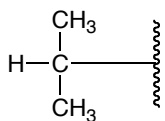
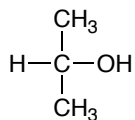
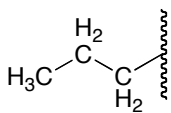
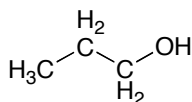
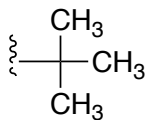
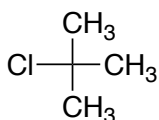


ethane

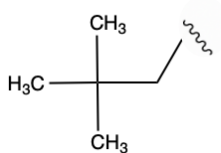


ethyl

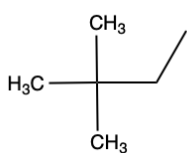
(iii) Isopropyl group

iso-propyl
groupiso-propyl
alcohol(iv) *n*-Propyl group*n*-propyl chain*n*-propyl alcohol(v) *tert*-Butyl group (t-butyl)*tert*-Butyl chain*tert*-Butyl chloride

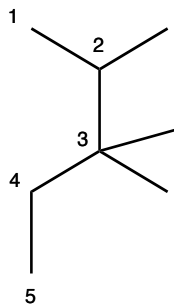
(vi) neo group



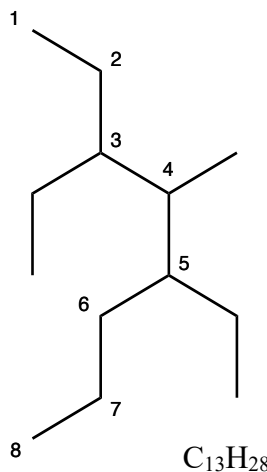
neo chain



2,2-dimethylbutane

Naming Examples:

2,3,3-trimethylpentane



3,5-diethyl-4-methyloctane

Cycloalkanes:**General Molecular Formula of Alkanes**

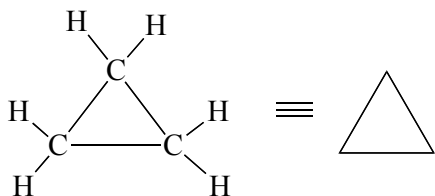
- Linear alkanes: general formula is C_NH_{2N+2}
- Each **degree of unsaturation** “removes” 2 hydrogens from the C_NH_{2N+2} formula
- (if there are no nitrogens in the molecule, there will always be an even # of hydrogens)
- Cycloalkanes always have at least 1 degree of unsaturation

e.g.

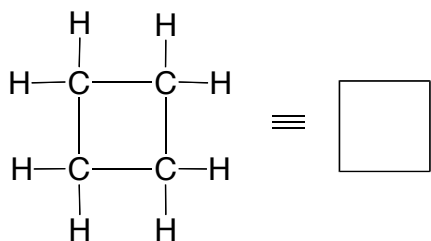
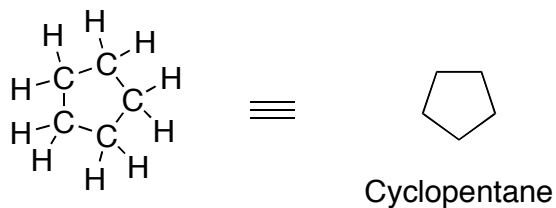
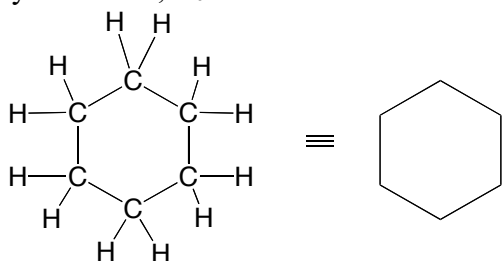
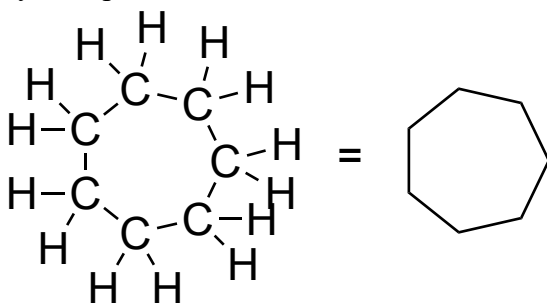
- o 1 Degree of unsaturation: C_NH_{2N} Alkanes with one ring or double bond
- o 2 Degrees of unsaturation: C_NH_{2N-2} Alkanes with two rings or double bonds, or one each

Note: Ring Structure Naming

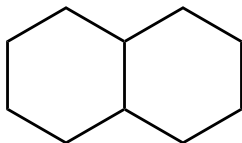
- Parent ring is the largest one
- Prefix with “cyclo”
- Start with numbering at point of maximum branching/most important functional group
- Number so as to give next branch/functional group lowest number

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°)

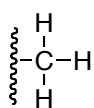
Cyclobutane, C_4H_8 Cyclopentane, C_5H_{10} Cyclohexane, C_6H_{12} Cycloheptane, C_7H_{14} **The degree of Unsaturation:**

It is commonly referred to as the number of double bonds (π -bonds) or a ring. Each pi-bond or ring is an additional degree of unsaturation. This is because each installation of an olefin, or ring removes two hydrogens from the organic structure.

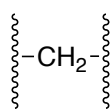
Decalin structure, $C_{10}H_{18}$ 

(two fused cyclohexenes) C_nH_{2n-4n}

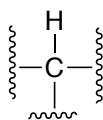
(4_n comes from the degree of unsaturation, two rings = two degrees of unsaturation. One degree of unsaturation = $-2H$. Therefore, decalin is $-4H$)



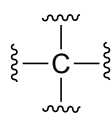
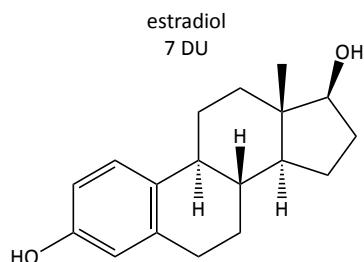
methyl group



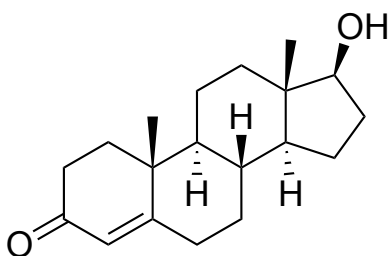
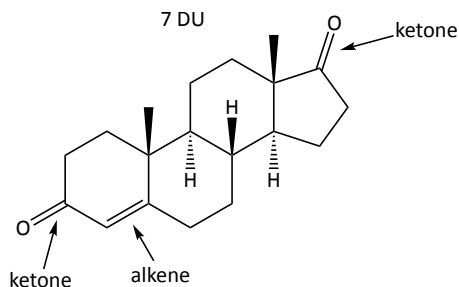
methylene



methine

quaternary
carbon**Example: steroids**

androstenedione

**Testosterone**

Molecular formula?

Functional groups?

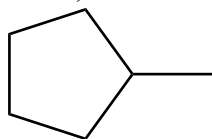
Degrees of Unsaturation?

How many methyls?

How many methylenes?

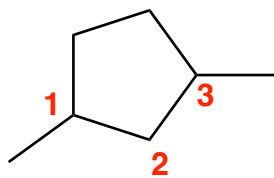
How many methines?

TEST YOURSELF

Examples of Naming Cycloalkanes:Ex #1) C_6H_{12} 

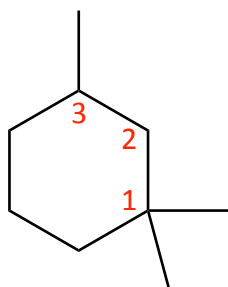
Degree of Unsaturation= 1

1-methylcyclopentane (structural isomer of hexane)

Ex #2) C_7H_{14} 

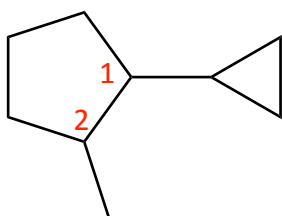
1,3-dimethylcyclopentane

Degree of Unsaturation= 1

Ex #3) C_9H_{18} 

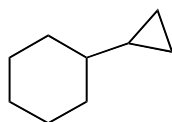
1,1,3-trimethylcyclohexane

Degree of Unsaturation= 1

Ex #4) C_9H_{16} 

1-cyclopropyl-2-methylcyclopentane

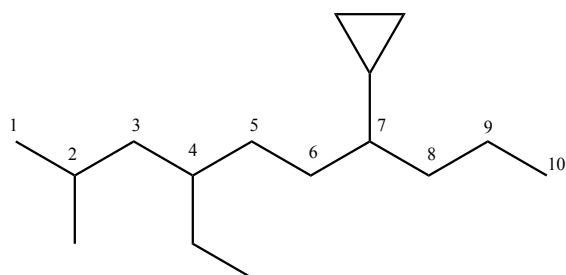
Degree of Unsaturation= 2

Ex #5) C_9H_{16} 

1-Cyclopropylcyclohexane

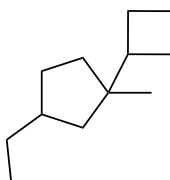
Degree of Unsaturation= 2

Example 3 and 4 both have the formula C_9H_{16} so they are structural isomersEx #6) $C_{16}H_{32}$



7-cyclopropyl-4-ethyl-2-methyldecane

Degree of Unsaturation= 1

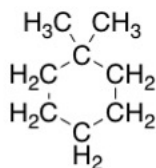
Ex #7) $C_{12}H_{22}$ 

Degree of Unsaturation= 2

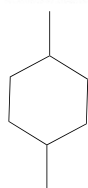
1-Cyclobutyl-3-ethyl-1-methylcyclopentane

ISOMERS**Structural (Constitutional) Isomers**

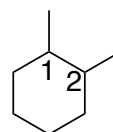
- Share the same molecular formula but have the atomic bonds in different places

Example 1 C_8H_{16}

1,1-dimethylcyclohexane

 C_8H_{16}

1,4-dimethylcyclohexane

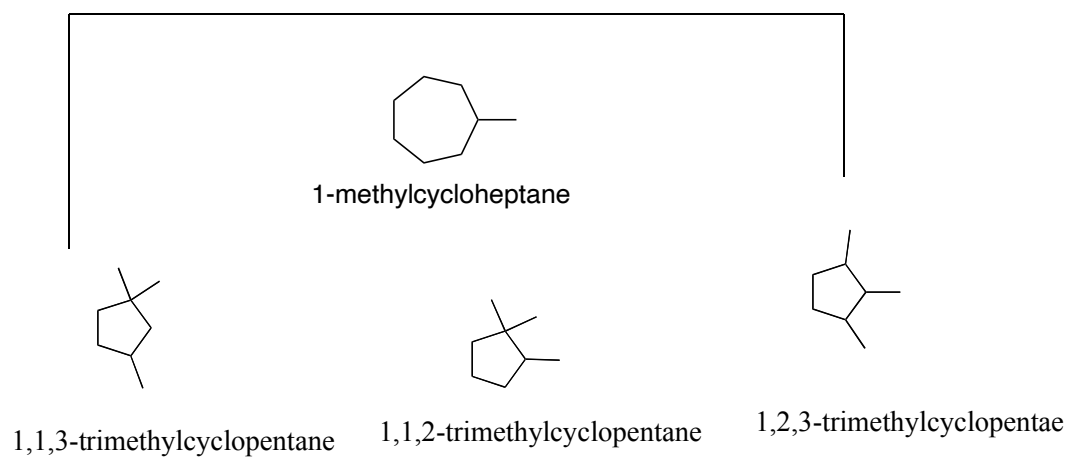
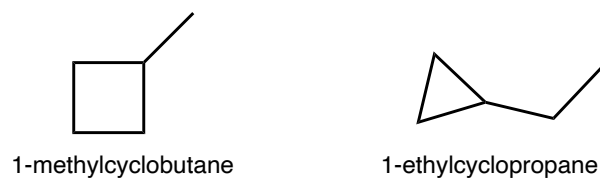


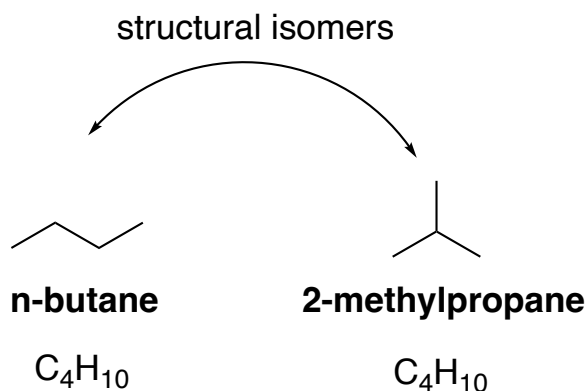
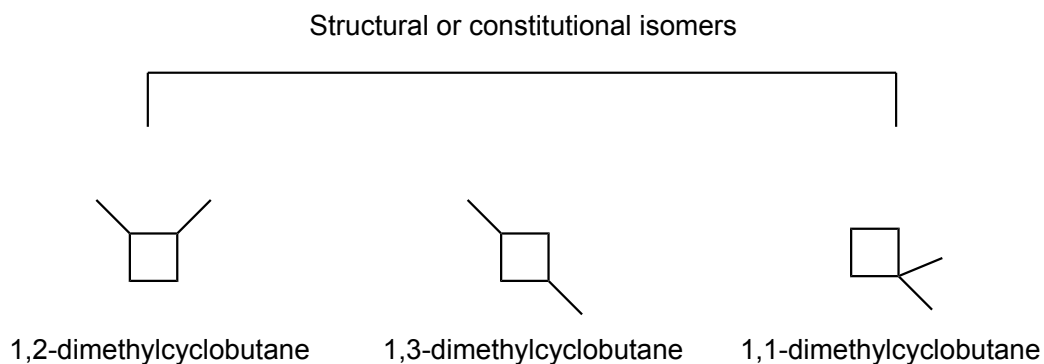
1,2-dimethylcyclohexane

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

Example 2

Structural or constitutional isomers

Example 3 C_5H_{10}
structural isomersExample 4

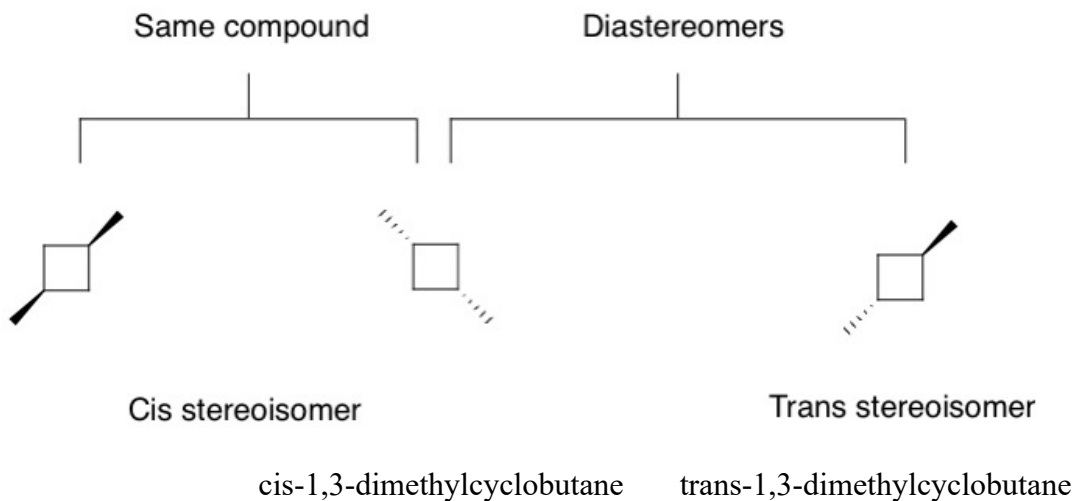
Example 5**Stereoisomers**

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



Structural Isomers:

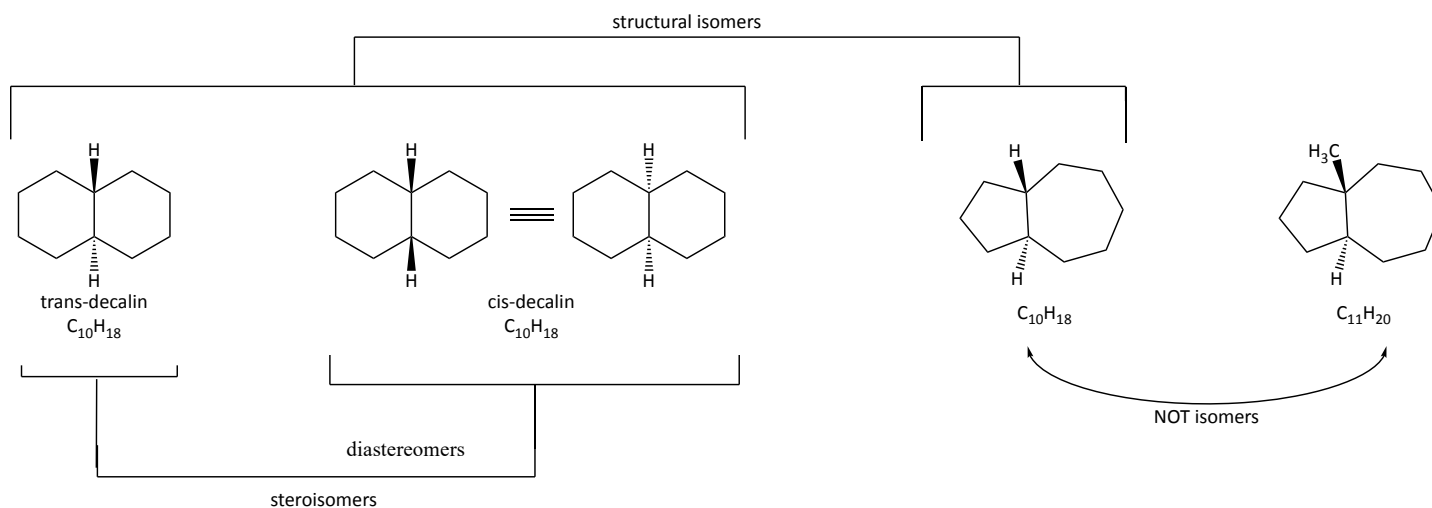


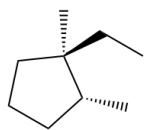
The first and second compounds are the same compound rotated in 3D space. The third compound has different geometry at one center, making it a stereoisomer, specifically a diastereomer.

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

Trans - the substituents are on opposite sides of the ring

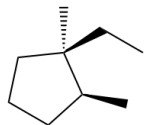
Example: decalin - $C_{10}H_{18}$



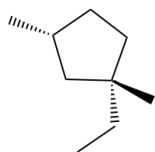
Example:

1,2-Dimethyl-1-ethylcyclopentane

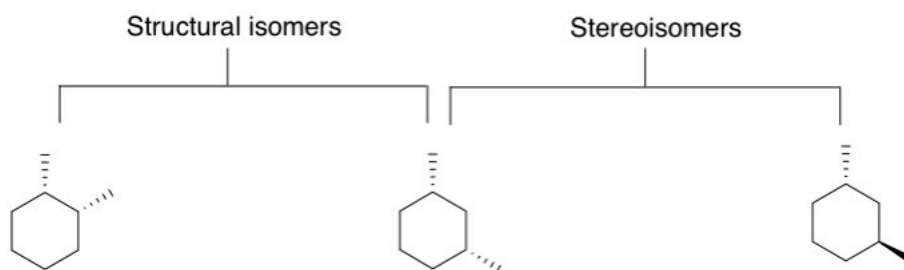
Stereoisomers



Structural isomers



1,3-Dimethyl-1-ethylcyclopentane

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

cis-1,2-dimethylcyclohexane

cis-1,3-dimethylcyclohexane

trans-1,3-dimethylcyclohexane

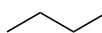
The second two compounds are diastereomers of each other.

Example: 1,3-dimethyl-3-ethylcyclohexane



Enantiomers
(Non-superimposable mirror images of each other)

Example: Are these compounds structural isomers of each other?



These compounds are not structural isomers of each other because they have different molecular formulas