Lecture Outline 2: ALKANES

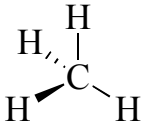
Hydrocarbons – Compounds that contain only C and H

- 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≡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) CH_4, methane

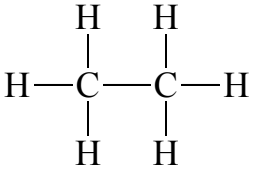


Bp = -161°C
(London Forces)

BP = -164 °C

CH_4 H_4C CH_3-H

Ex #2) C_2H_6, ethane

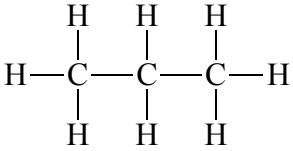


Bp = -88°C

BP = -88 °C

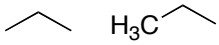
C_2H_6 CH_3-CH_3 H_3C-CH_3

Ex #3) C_3H_8, propane



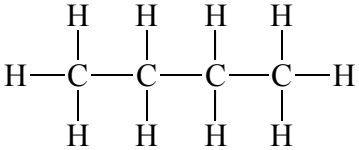
Bp = -42°C

C_3H_8 $CH_3CH_2CH_3$



BP = -42 °C

Ex #4) C_4H_{10}, butane

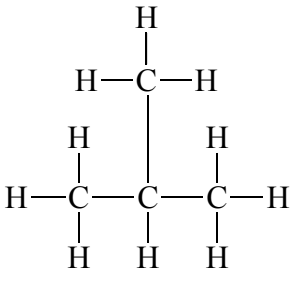


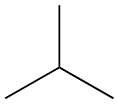
C_4H_{10}, $CH_3CH_2CH_2CH_3$

n-Butane: normal straight chain butane

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

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



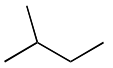


structural isomer = constitutional isomer

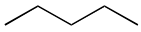
- Isomers are different compounds that have the same molecular formula and different structure. They have different physical properties (e.g. mp, bp, odour, biological effects)
- iso - meros
  same - parts

one type: structural (same as constitutional)
second type: stereoisomers (diastereomers and enantiomers) – will talk about more

Ex #6) Pentane C_5H_{12}

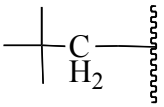


(isopentane or 2-methylbutane)



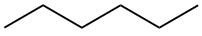
n - pentane

Neopentane

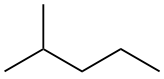


Neo Group

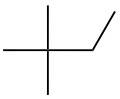
Ex #7) Hexane C_6H_{14}



n-hexane



Isohexane



neohexane

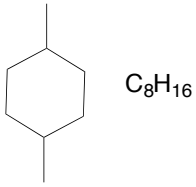
ISOMERS

Structural (Constitutional) Isomers

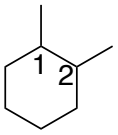
- Share the same molecular formula but have the atomic bonds in different places

Example 1

1,1-dimethylcyclohexane



1,4-dimethylcyclohexane

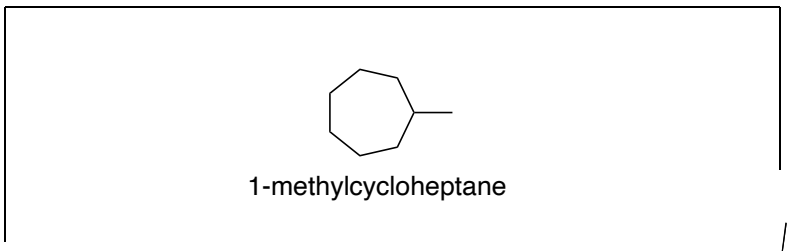


1,2-dimethylcyclohexane

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

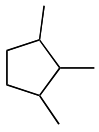
Example 2

Structural or constitutional isomers



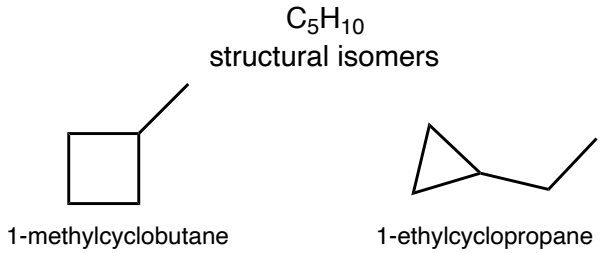
1-methylcycloheptane

1,1,3-trimethylcyclopentane 1,1,2-trimethylcyclopentane

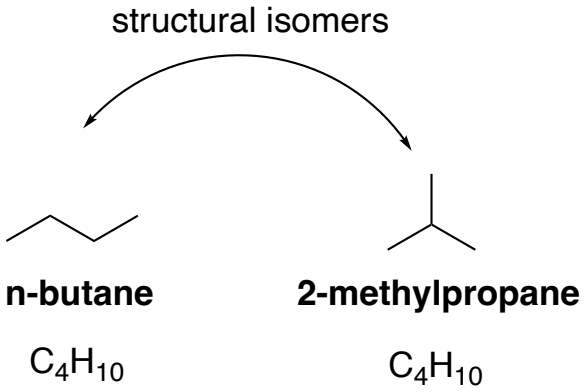


1,2,3-trimethylcyclopentae

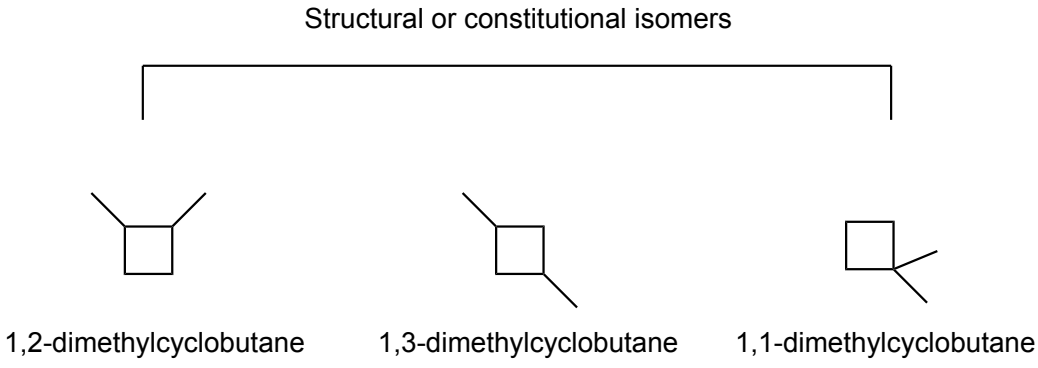
Example 3



Example 4



Example 5



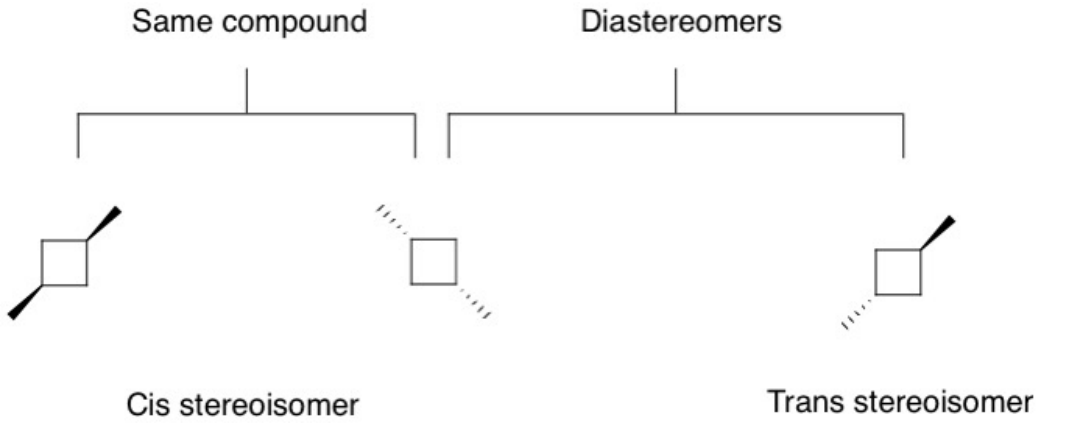
Stereoisomers

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



cis-1,3-dimethylcyclobutane trans-1,3-dimethylcyclobutane

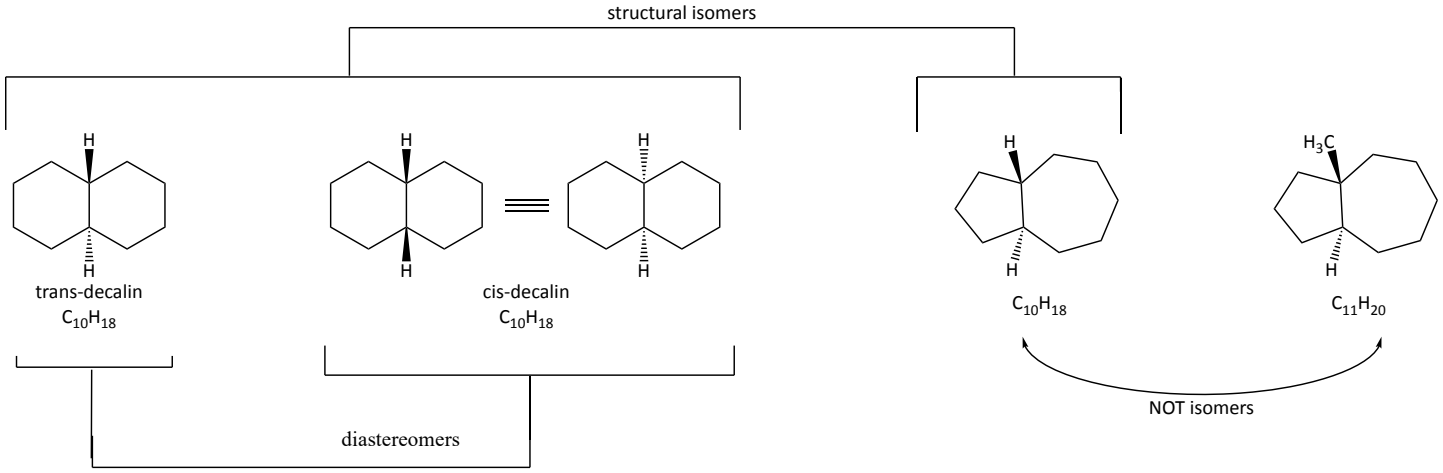
Structural Isomers:

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.

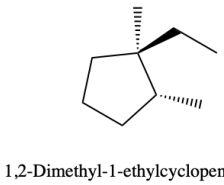
Cis - the substituents are on the same side of the ring

Trans - the substituents are on opposite sides of the ring

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

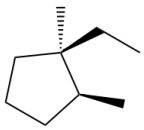


Example: steroisomers

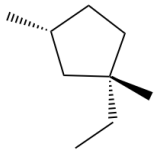


1,2-Dimethyl-1-ethylcyclopentane

Stereoisomers

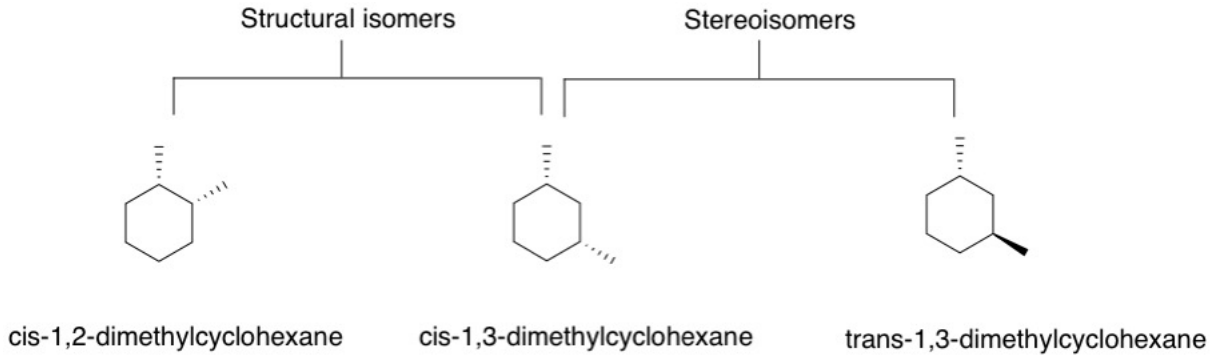


Structural isomers



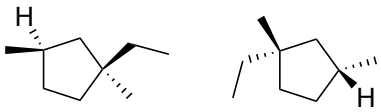
1,3-Dimethyl-1-ethylcyclopentane

Example: 1,2-dimethylcyclohexane and 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 isomer of each other?

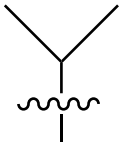
C_4H_8 C_4H_{10}

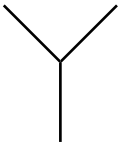
These compounds are not structural isomers of each other because they have different molecular formulas

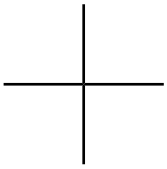
Systematic (IUPAC) Nomenclature

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

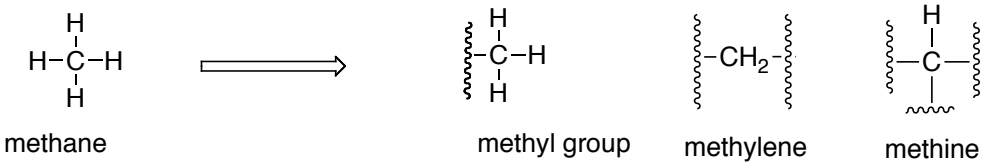
Note: iso = second-to-last carbon of the chain is disubstituted (2 methyl groups)
neo = second-to-last carbon of the chain is trisubstituted (3 methyl groups)

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

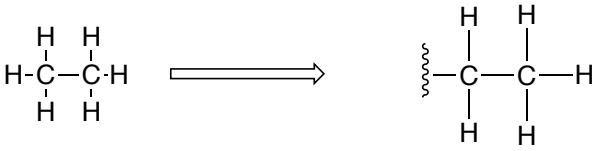
Groups (part of an alkane structure)

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

(i) Methyl group – CH_3

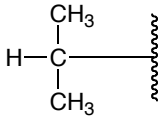


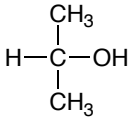
(ii) Ethyl group – CH_2CH_3



ethane ethyl

(iii) Isopropyl group

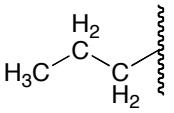


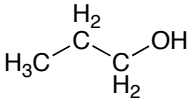


iso-propyl group

iso-propyl alcohol

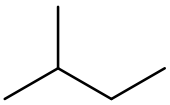
(iv) *n*-Propyl group





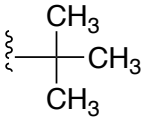
n-propyl chain n-propyl alcohol

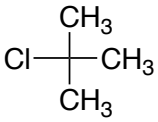
v) Isopentane



Isopentane

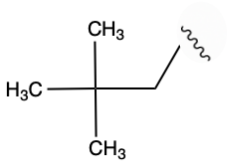
(vi) *tert*-Butyl group (t-butyl)



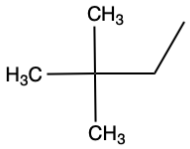


tert-Butyl chain *tert*-Butyl chloride

(vii) neo group

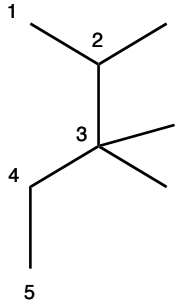


neo chain



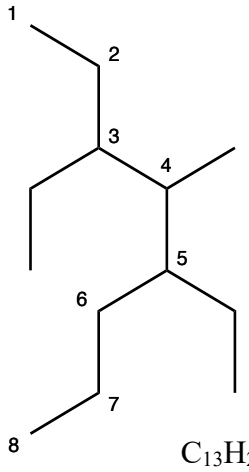
2,2-dimethylbutane

Naming Examples:



2,3,3-trimethylpentane

C_8H_{18}



$C_{13}H_{28}$

3,5-diethyl-4-methyloctane

Degree of unsaturation C_nH_{2n+2}: Each double bond or ring is 1 degree of unsaturation, removes 2 hydrogens.

<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.

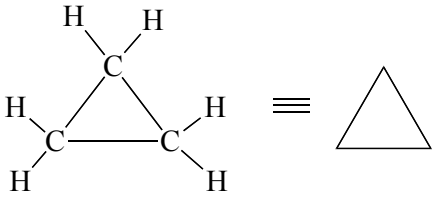
  - 1 Degree of unsaturation : C_NH_{2N} Alkanes with one ring or double bond

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

Note: Ring Structure Naming

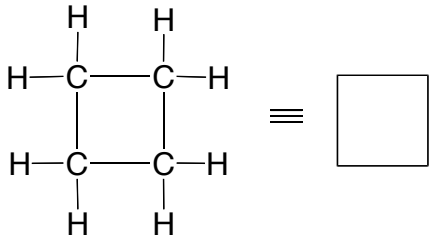
- Parent ring is the largest one
- Prefix with "cyclo"
- Start with numbering at point of maximum branching/most important functional group
- Number so as to give next branch/functional group lowest number

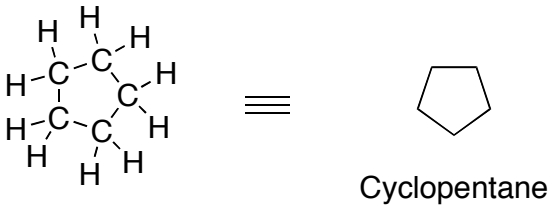
Cyclopropane, C_3H_6



- 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°)
- Reactive with O2 → explosive

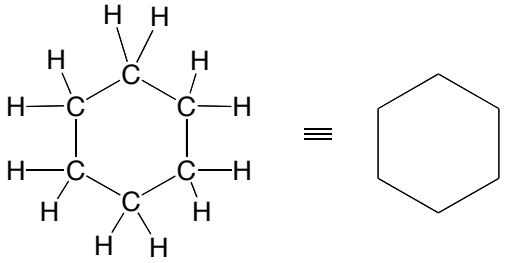
Cyclobutane, C_4H_8





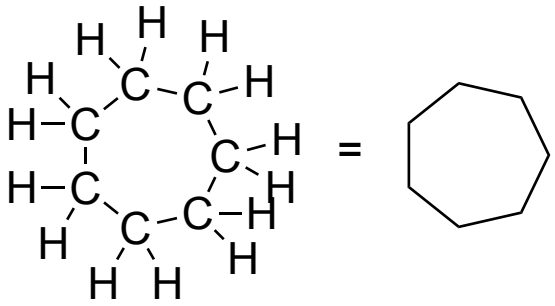
Cyclopentane

Cyclohexane, C_6H_{12}



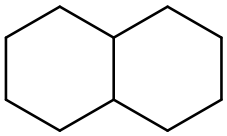
Cyclopentane, C_5H_{10}

Cycloheptane, C_7H_{14}

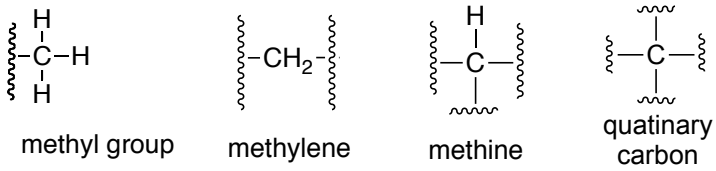


The degree of Unsaturation:
It is commonly referred to as the number of double bonds (π-bonds) or a ring. Each pi-bond or ring is an additional degree of unsaturation. This is because each installation of an olefin, or ring removes two hydrogens from the organic structure.

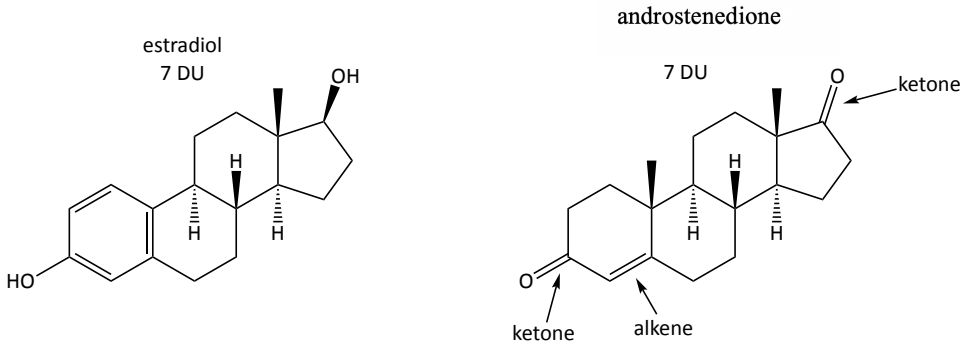
Decalin structure, $C_{10}H_{18}$

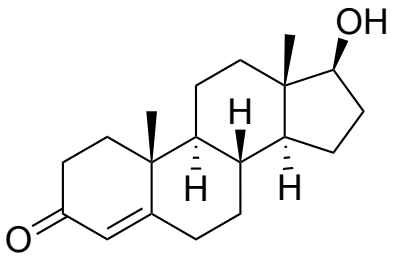


(two fused cyclohexenes) C_nH_{2n}-4_n
(4_n comes from the degree of unsaturation, two rings = two degrees of unsaturation. One degree of unsaturation = -2H. Therefore, decalin is -4H)



Example: steroids





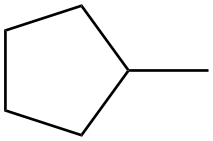
Testosterone
Molecular formula?
Functional groups?
Degrees of Unsaturation?
How many methyls?
How many methylenes?
How many methines?

TEST YOURSELF

Examples of Naming Cycloalkanes:

1. Start the number at point of max branching
2. Count so as to give next branch the lowest number

Ex #1) C_6H_{12}



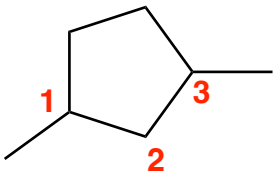
Degree of Unsaturation= 1

1-methylcyclopentane

1')  Degree of Unsaturation = 1

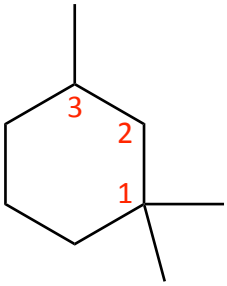
→ 1 and 1' are structural isomers.

Ex #2) C_7H_{14}



1,3-dimethylcyclopentane Degree of Unsaturation= 1

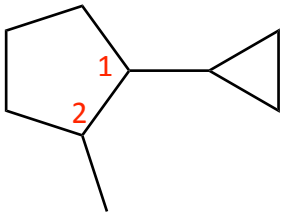
Ex #3) C_9H_{18}



1,1,3-trimethylcyclohexane

Degree of Unsaturation= 1

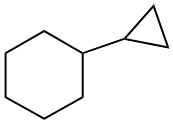
Ex #4) C_9H_{16}



1-cyclopropyl-2-methylcyclopentane

Degree of Unsaturation= 2

Ex #5) C_9H_{16}

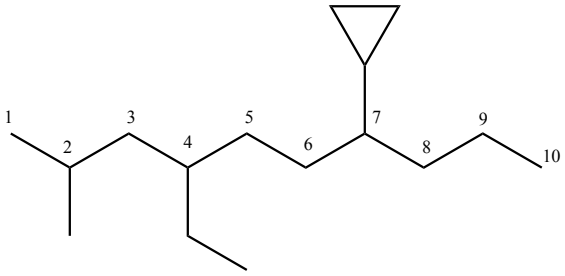


1-Cyclopropylcyclohexane

Degree of Unsaturation= 2

Example 3 and 4 both have the formula C_9H_{16} so they are structural isomers

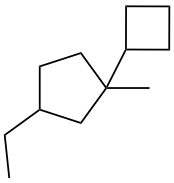
Ex #6) $C_{16}H_{32}$



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