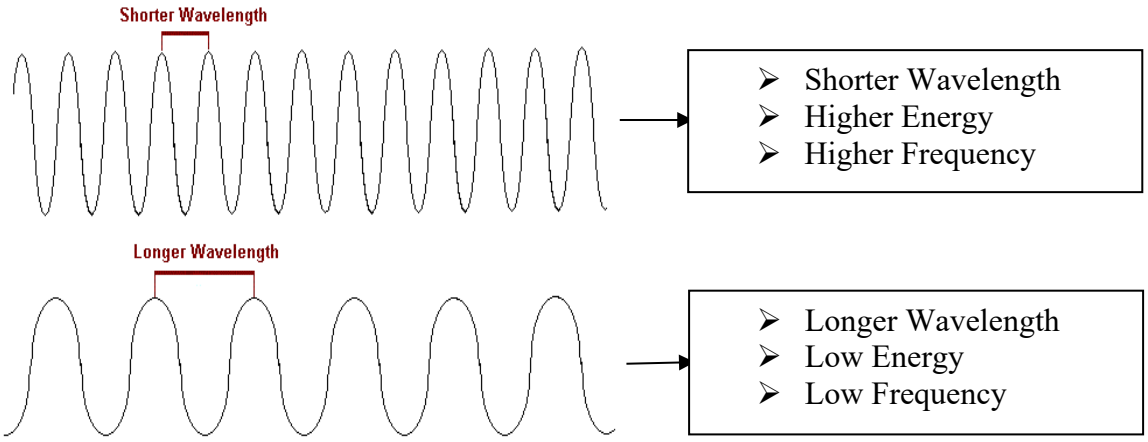
CHEM 261 January 24, 2023

Electromagnetic Radiation:

Infrared (IR) Spectroscopy – Background only:

$E = hc/\lambda = h\nu$, energy is quantized

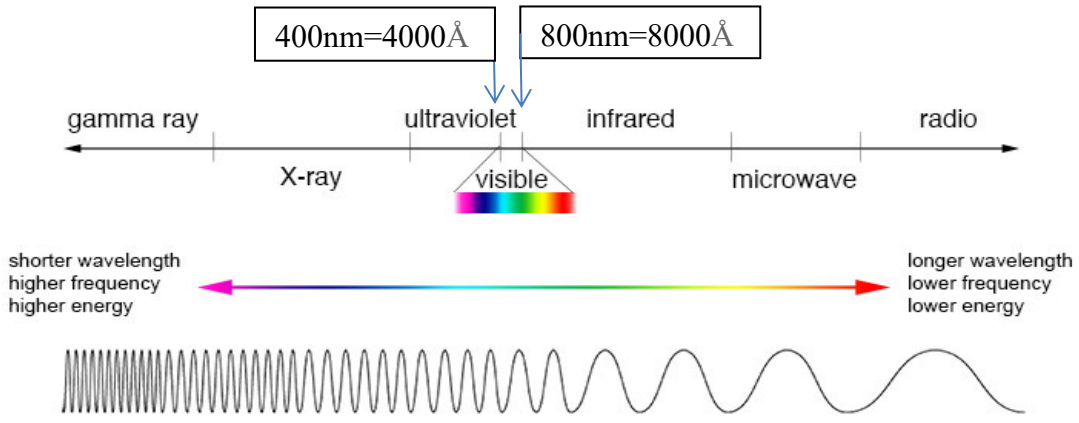
E = Energy
h = Planck's Constant= 6.6×10^{-34} joules/sec
ν = Frequency
λ = Wavelength
c = Speed of light = 3.0×10^{10} cm/sec



NB: There is an inverse relationship between wavelength and frequency.

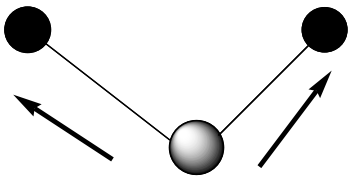
Electromagnetic Spectrum:

NB: 1nm = 10 angstrom

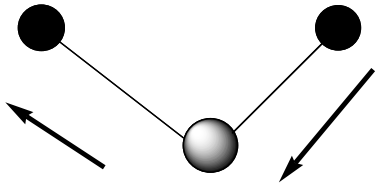


UV and visible light: conjugated double bond systems
e.g. C=C bonds absorb UV light and some visible light

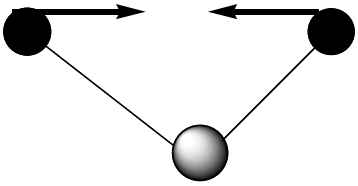
Infrared Radiation: bond stretching and bending modes
-Measured in wavenumbers (cm^{-1})
- Defined as cycles/second
e.g. O-H bond can be seen around ~3400cm^{-1} in an IR spectrum



SYMMETRIC STRETCHING

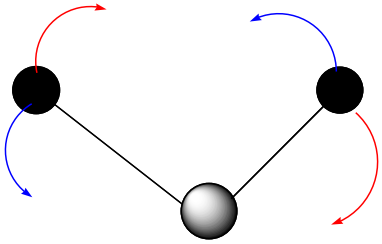


ASYMMETRIC STRETCHING



IN PLANE BENDING

(SCISSORING)



OUT OF PLANE BENDING

(TWISTING)

IR is Background Only - NOT on Midterm for Lecture Part

NEXT SECTION: Lecture Outline 2: ALKANES

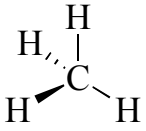
<u>Hydrocarbons</u> – Compounds that contain only C and H

- Alkanes contain only single bonds (C-H, C-C), sp^3
- Alkenes = Olefins (C=C), sp^2
- Alkynes =Acetylenes (C≡C), sp

<u>Alkanes</u>

- 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



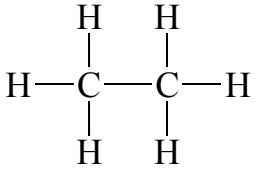
Bp = -161°C

(London Forces)

BP = -161.5 °C

CH_4 H_4C CH_3-H

Ex #2) C_2H_6, ethane

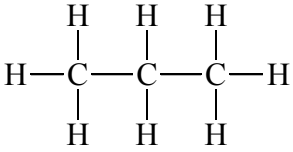


Bp = -88°C

BP = -88 °C

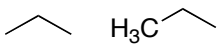
C_2H_6 CH_3-CH_3 H_3C-CH_3

Ex #3) C_3H_8, propane



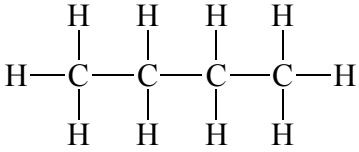
Bp = -42°C

C_3H_8 $CH_3CH_2CH_3$



BP = -42 °C

Ex #4) C_4H_{10}, butane

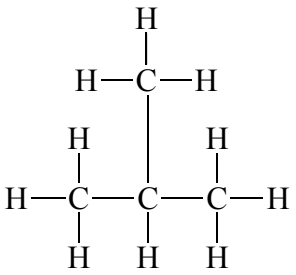


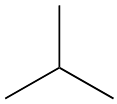
C_4H_{10}, $CH_3CH_2CH_2CH_3$

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



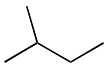


structural isomer = constitutional isomer

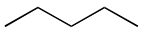
- Isomers are different compounds that have the same molecular formula and different structure. They have different physical properties (e.g. mp, bp, odour, biological effects)
- iso - meros
  same - parts

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

Ex #6) Pentane C_5H_{12}

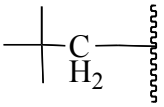


(isopentane or 2-methylbutane)



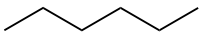
n - pentane

Neopentane

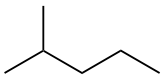


Neo Group

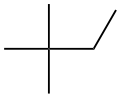
Ex #7) Hexane C_6H_{14}



n-hexane



Isohexane

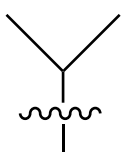


neohexane

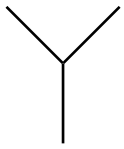
<u>Systematic (IUPAC) Nomenclature</u>

RULES:

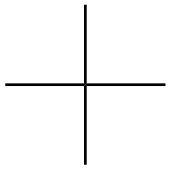
1. Find the longest straight chain
2. Number from end of the chain, so that the 1st branch point has the lowest number
3. Name the chain, then add prefixes (for the groups attached) with number and name the groups attached
4. Separate numbers and names by dash



isopropyl



isobutane
2-methylpropane



neopentane
2,2-dimethylpropane

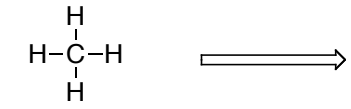
Note: iso = second-to-last carbon of the chain is disubstituted (2 methyl groups)
neo = second-to-last carbon of the chain is trisubstituted (3 methyl groups)

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

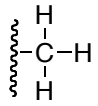
Groups (part of an alkane structure)

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

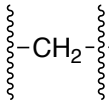
(i) Methyl group – CH_3



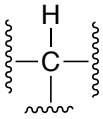
methane



methyl group

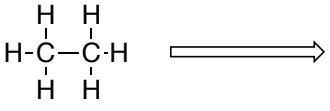


methylene

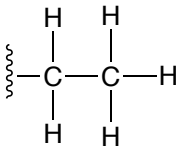


methine

(ii) Ethyl group – CH_2CH_3

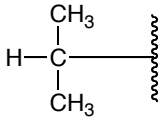


ethane

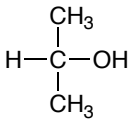


ethyl

(iii) Isopropyl group

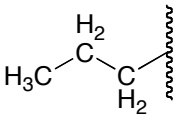


iso-propyl group

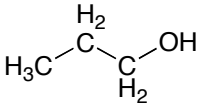


iso-propyl alcohol

(iv) *n*-Propyl group

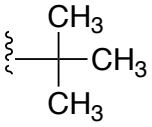


n-propyl chain

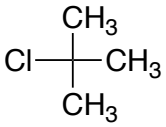


n-propyl alcohol

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

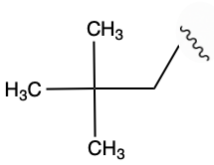


tert-Butyl chain

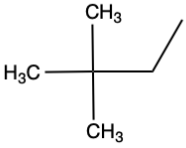


tert-Butyl chloride

(vi) neo group

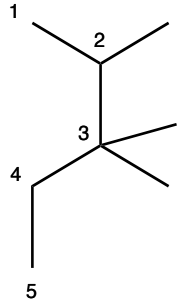


neo chain

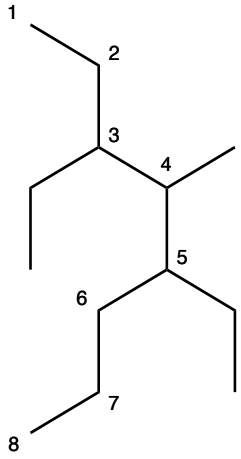


2,2-dimethylbutane

Naming Examples:



2,3,3-trimethylpentane



3,5-diethyl-4-methyloctane

<u>Cycloalkanes</u>:

General Molecular Formula of Alkanes

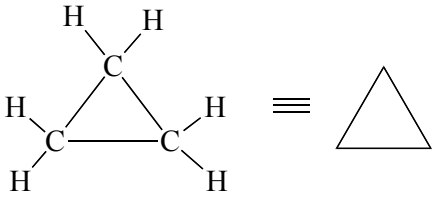
- Linear alkanes: general formula is $C_NH_{2N}+2$
- Each **degree of unsaturation** "removes" 2 hydrogens from the $C_NH_{2N}+2$ formula
- (if there are no nitrogens in the molecule, there will always be an even # of hydrogens)
- Cylcoalkanes always have at least 1 degree of unsaturation

  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

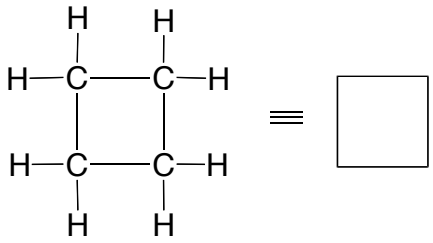
- Parent ring is the largest one
- Prefix with "cyclo"
- Start with numbering at point of maximum branching/most important functional group
- Number so as to give next branch/functional group lowest number

Cyclopropane, C_3H_6

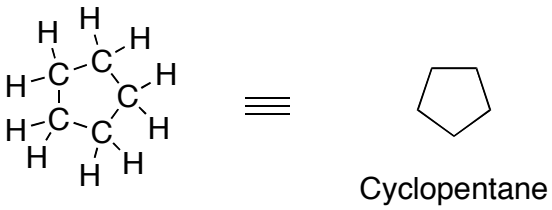


- One degree of unsaturation (*n*-propane is C_3H_8)
  - Not a structural isomer (different molecular formula)
- C-C-C bond angle (60°)
- Highly reactive due to ring strain (sp^3 carbons prefer to be 109°)

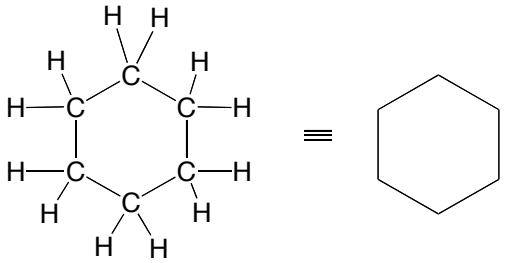
Cyclobutane, C_4H_8



Cyclopentane, C_5H_{10}

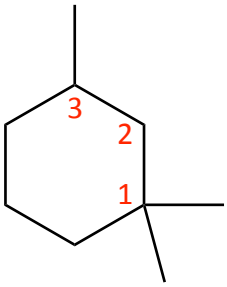


Cyclohexane, C_6H_{12}



Examples of Naming Cycloalkanes:

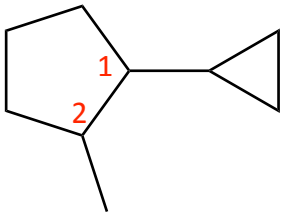
Ex #1) C_9H_{18}



1,1,3-trimethylcyclohexane

Degree of Unsaturation= 1

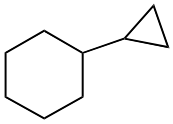
Ex #2) C_9H_{16}



1-cyclopropyl-2-methylcyclopentane

Degree of Unsaturation= 2

Ex #3) C_9H_{16}

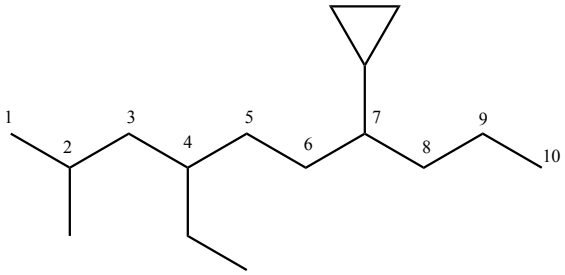


Degree of Unsaturation= 2

1-Cyclopropylcyclohexane

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

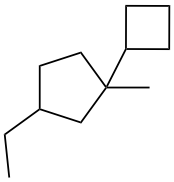
Ex #4) $C_{16}H_{32}$



Degree of Unsaturation= 1

7-cyclopropyl-4-ethyl-2-methyldecane

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



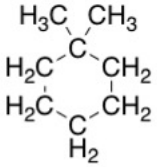
Degree of Unsaturation= 2

1-Cyclobutyl-3-ethyl-1-methylcyclopentane

ISOMERS

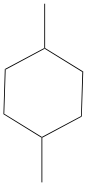
Structural (Constitutional) Isomers

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



C_8H_{16}

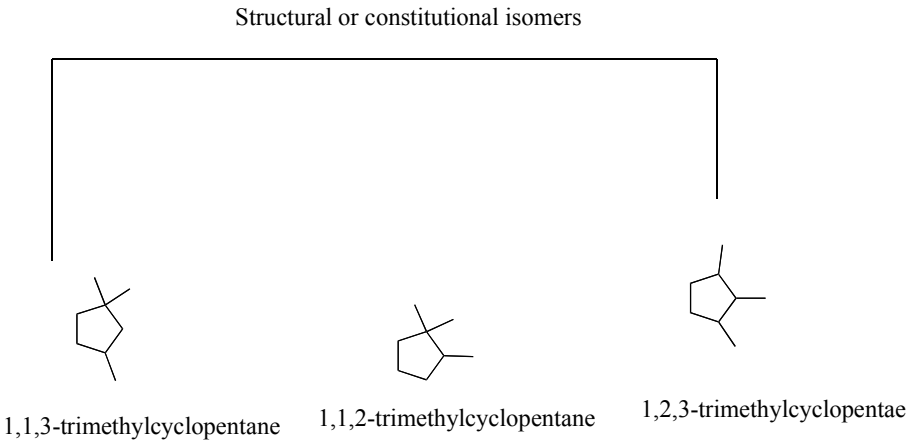
1,1-dimethylcyclohexane

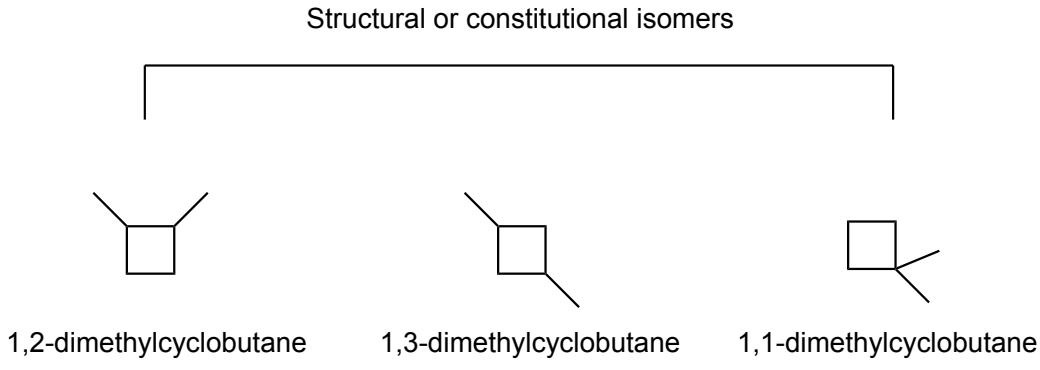


C_8H_{16}

1,4-dimethylcyclohexane

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





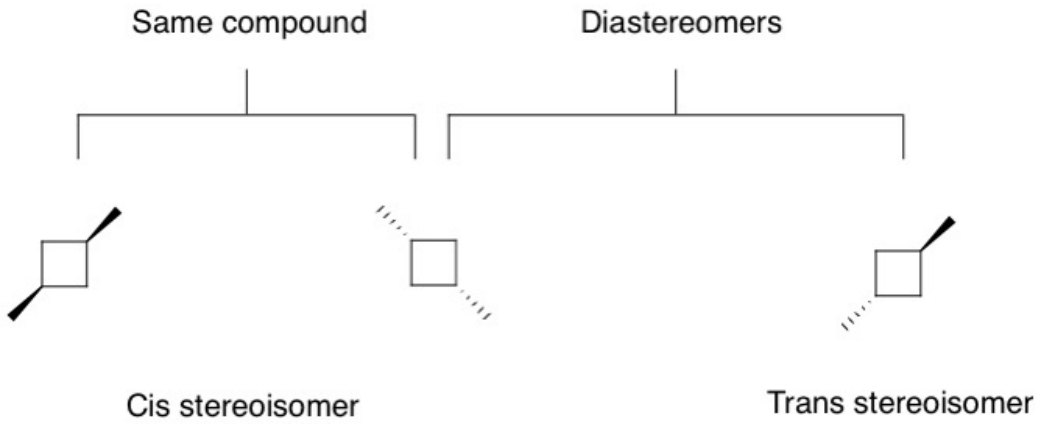
Stereoisomers

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

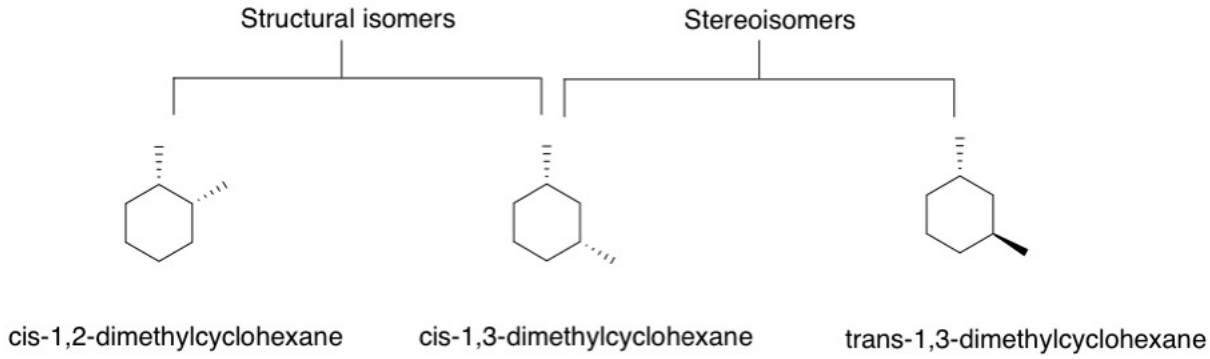


The first and second compounds are the same compound rotated in 3D space. The third compound has different geometry at one center, making it a stereoisomer, specifically a diastereomer.

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

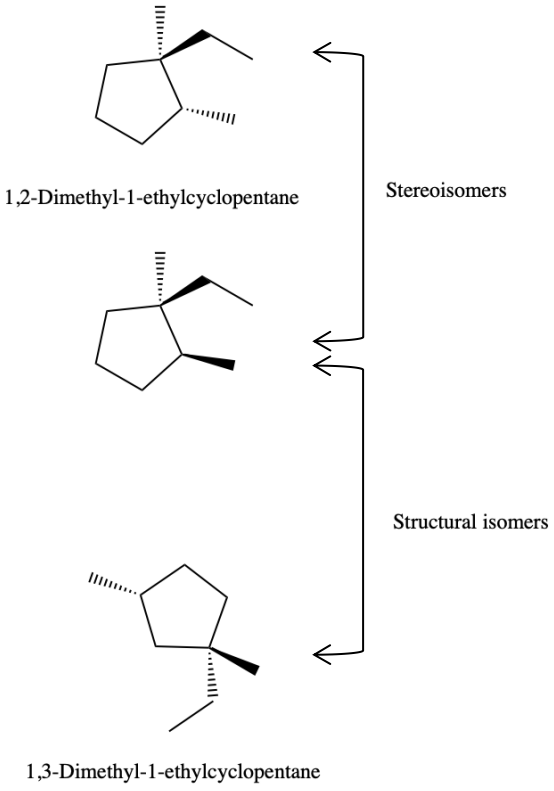
Trans - the substituents are on opposite sides of the ring

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

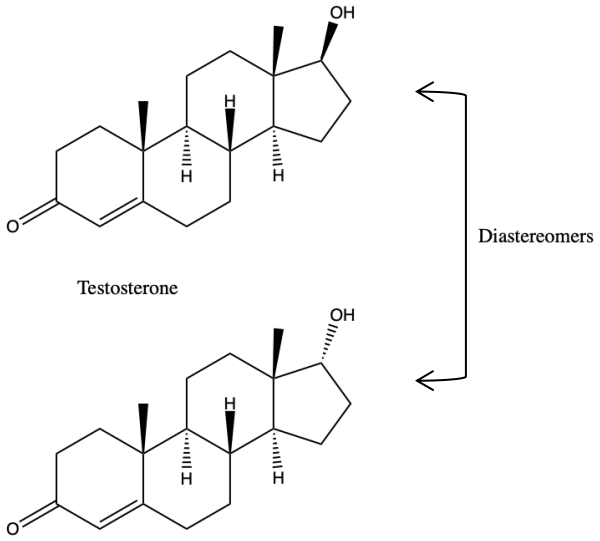


The second two compounds are diastereomers of each other.

Example:



Example:



Testosterone