11. Organic Chemistry

Many areas rely on organic chemistry

biology
petroleum industry
polymers
genetic engineering
agriculture
pharmacology
consumer products

Organic Chemistry

Organic: overused word

Organic
can be biological or chemical term

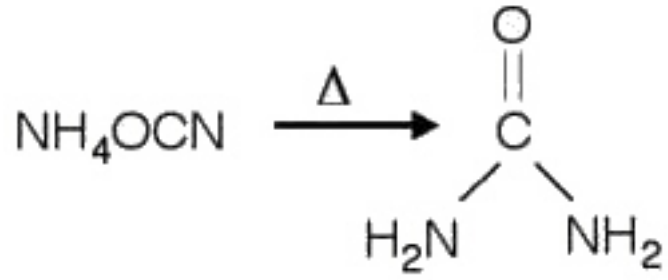
Biology:
anything living or has lived

Chemistry:
most substances containing carbon

Originally the study of chemicals extracted from living systems

Today, organic chemistry is the study of compounds containing carbon

Synthesis of urea from ammonium cyanate



Wohler, 1928

IMPORTANCE OF CARBON

basis for all life

stable covalent bonds **catenation**

forms C–C C=C C≡C

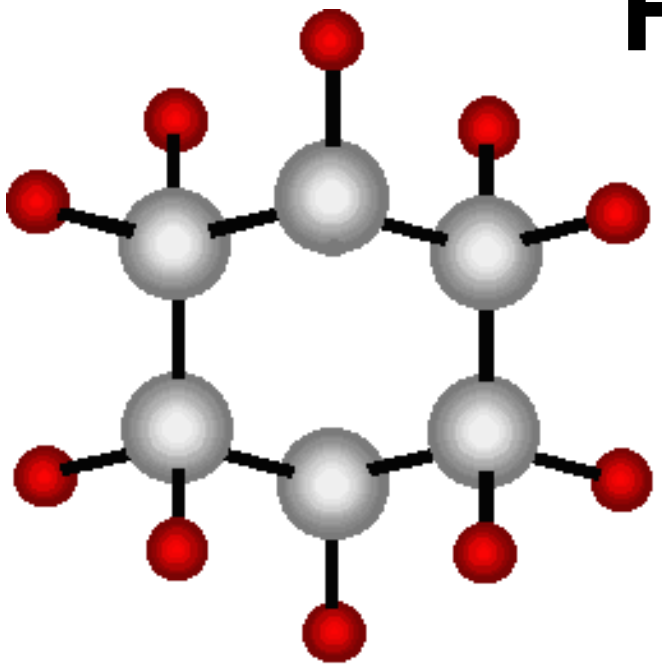
forms long chain molecules

C–C–C–C–C–C–C–C–C–C–C–C

bonds with most elements

infinite number of compounds possible

Rings



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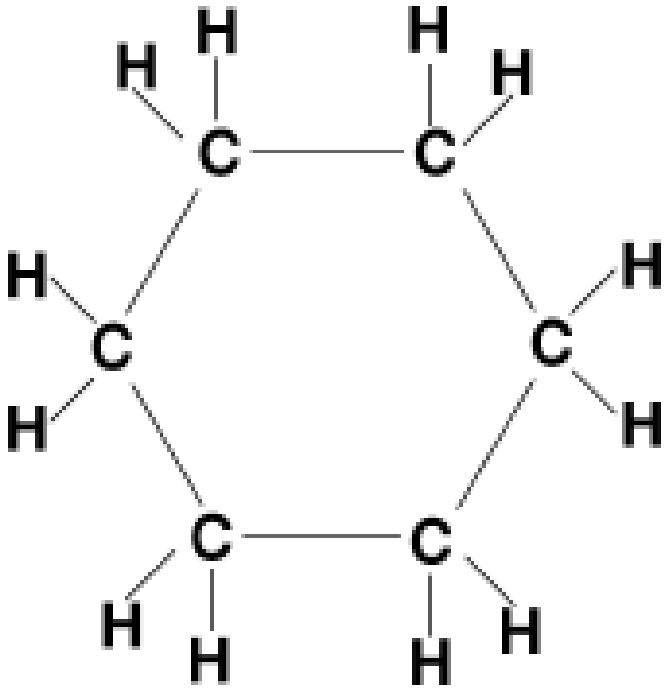
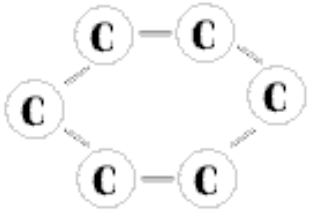


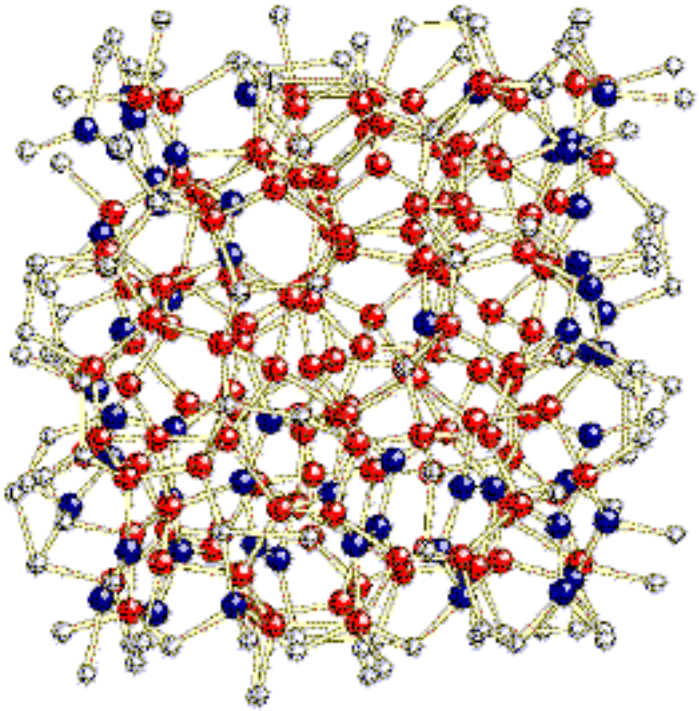


cyclohexane

Carbon: the element

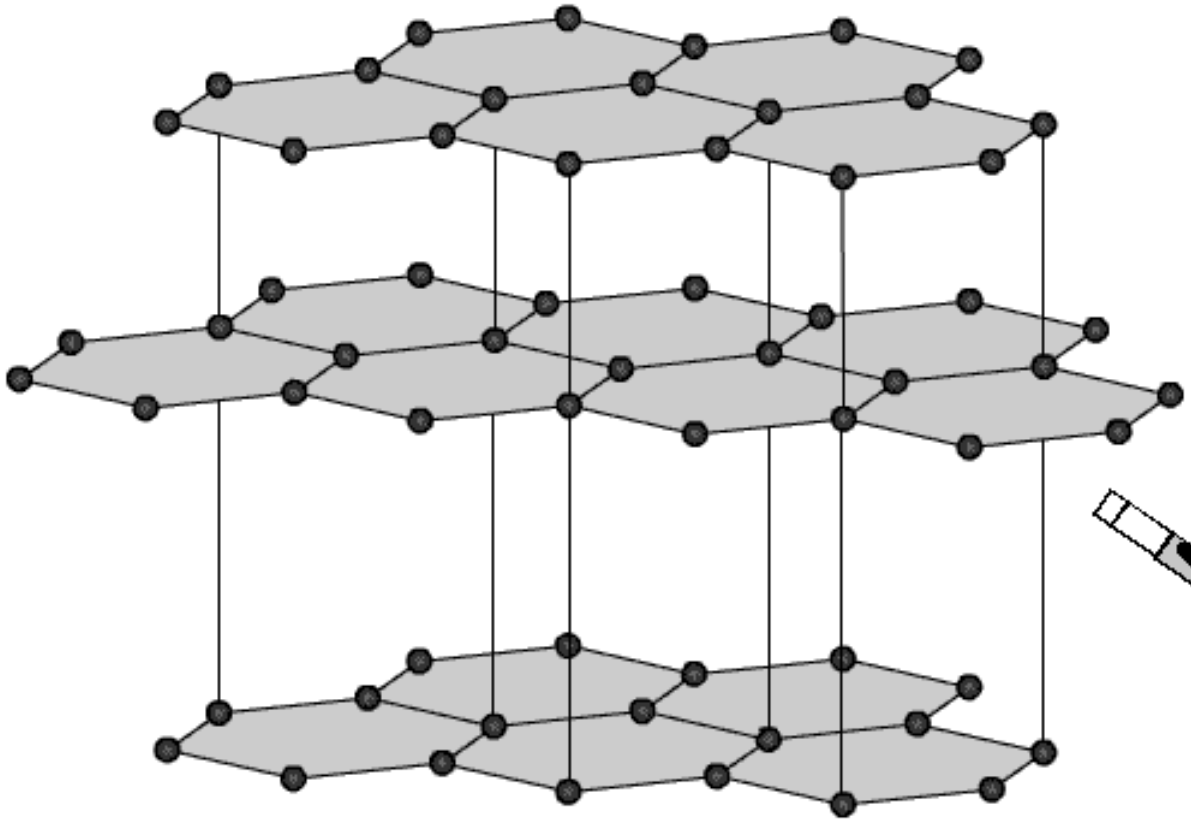
Exists in 4 allotropic forms:

1. **Amorphous**

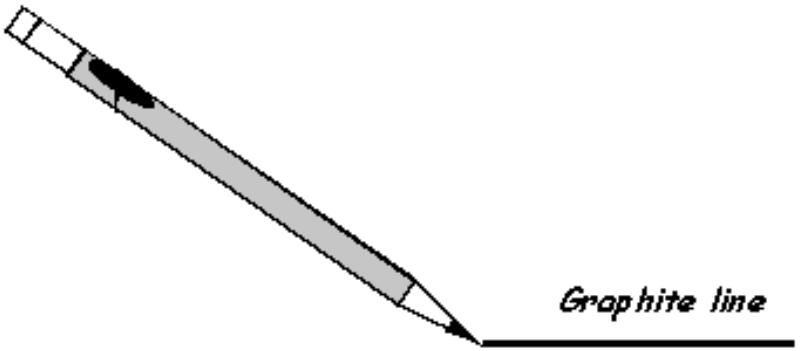


Soot

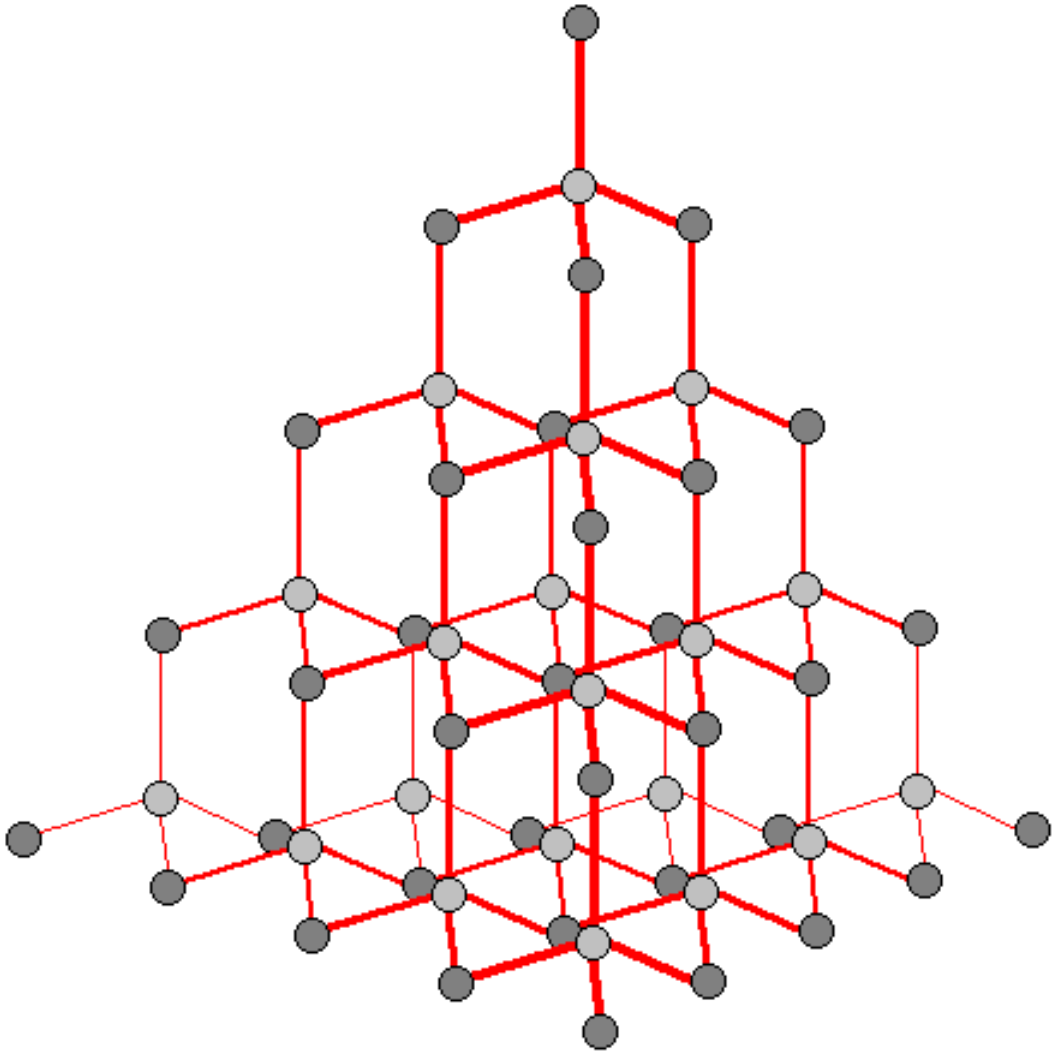
2. Graphite



Sheets of rings which can slip over each other



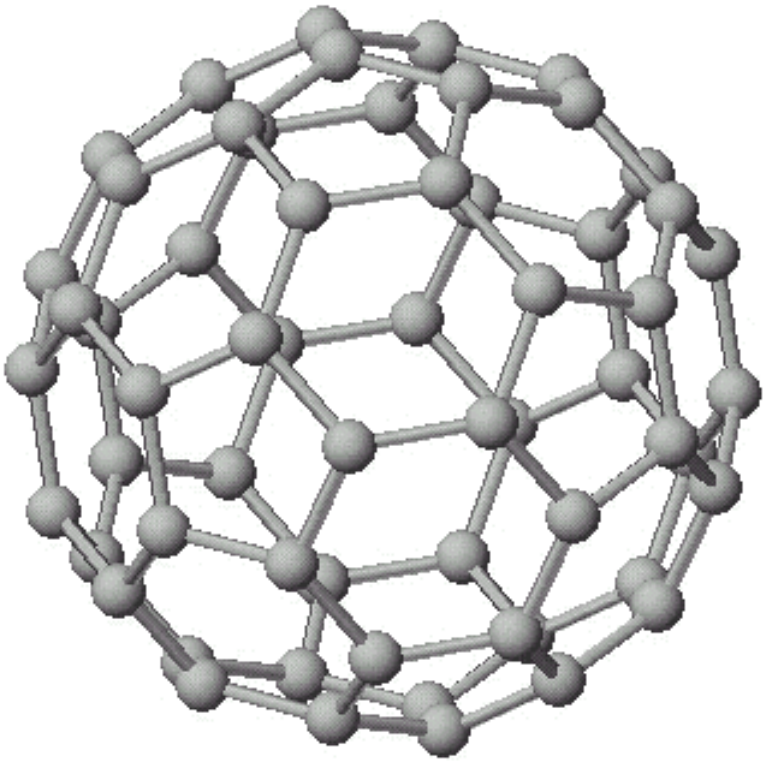
3. Diamond



Tetrahedral arrangement of atoms

Hard

4. Spherical Composed of rings



CLASSES OF COMPOUNDS

CLASSES OF COMPOUNDS

Classify by how carbon atoms are arranged & what groups attached

Simplest: hydrocarbons

Divided into 2 classes: aliphatic and aromatic

Methane: CH_4

ORGANIC COMPOUNDS

classify by functional group:
specific combinations of atoms

hydrocarbons C & H contain only

alcohols	**R–OH**
acids	**R–COOH**
amines	**R–NH_2**
ketones	**R(C=O)R**
aldehydes	**R–CHO**

How do we write formulas, draw structures and name organic compounds?

ORGANIC COMPOUNDS CAN BE COMPLEX

Need a system that shows structure
Must be easy to read

LINE REPRESENTATIONS

Write all atoms in single line

Use subscripts, (), and lines

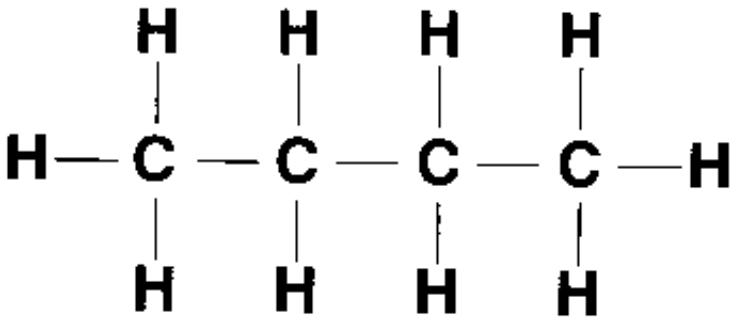
Show special bonds and branches

Drawing Structures

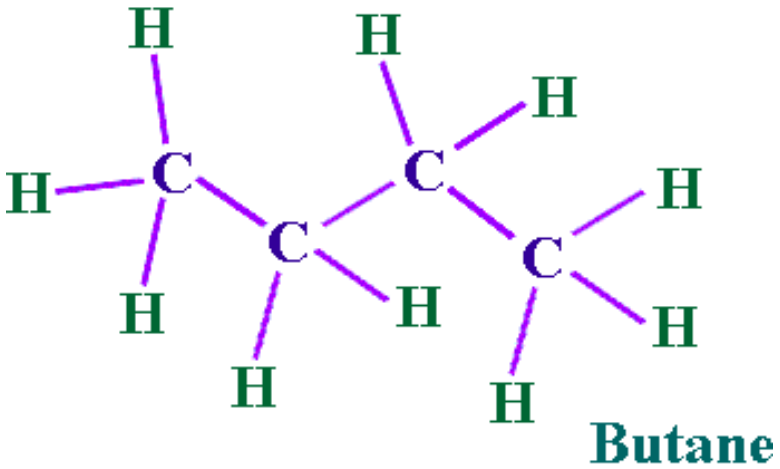
Molecular formula: C_4H_{10}

Line representation: $CH_3CH_2CH_2CH_3$

Condensed formula



Butane



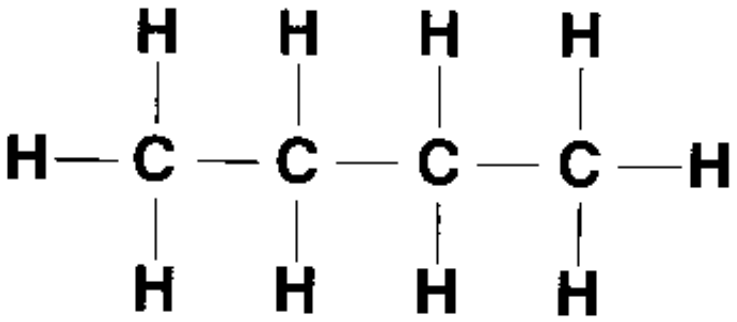
Butane

Drawing Structures

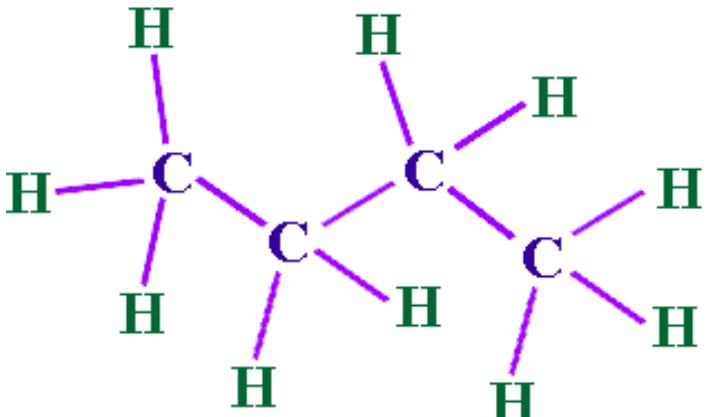
Molecular formula: C_4H_{10}

Line representation:

$CH_3CH_2CH_2CH_3$ $CH_3(CH_2)_2CH_3$

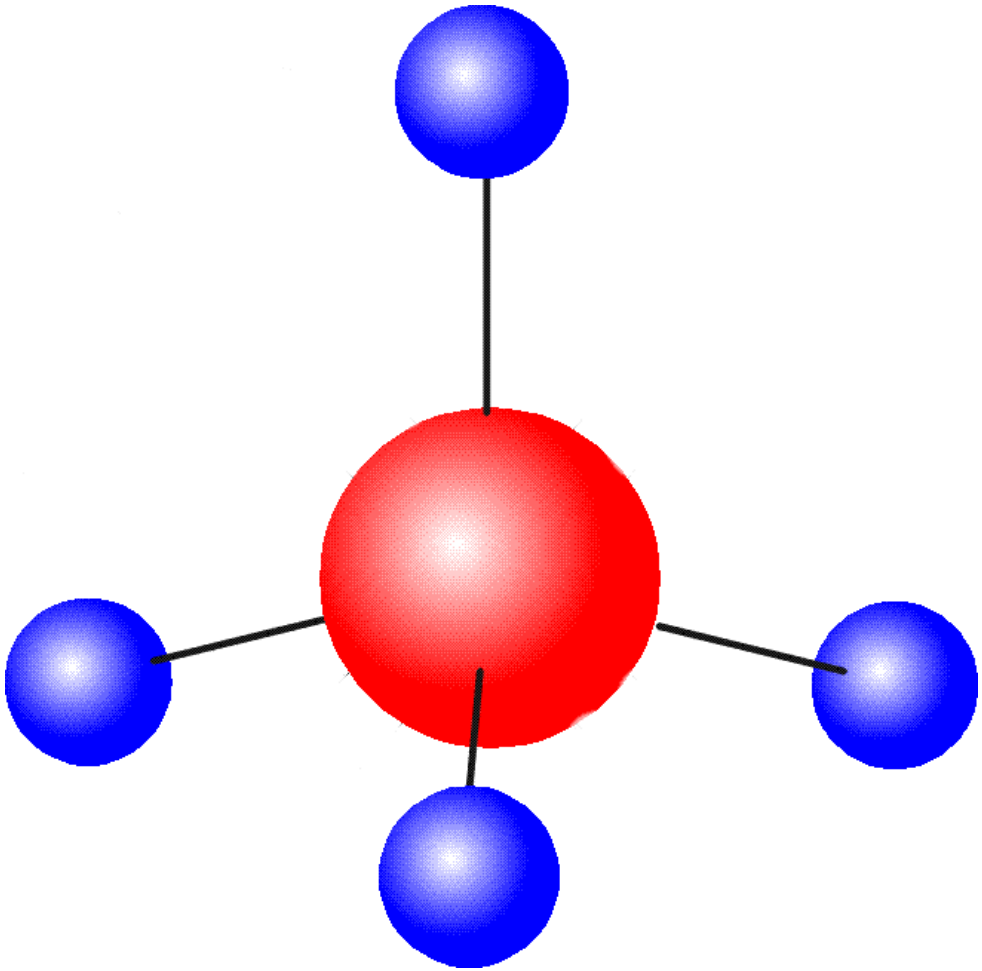


Butane

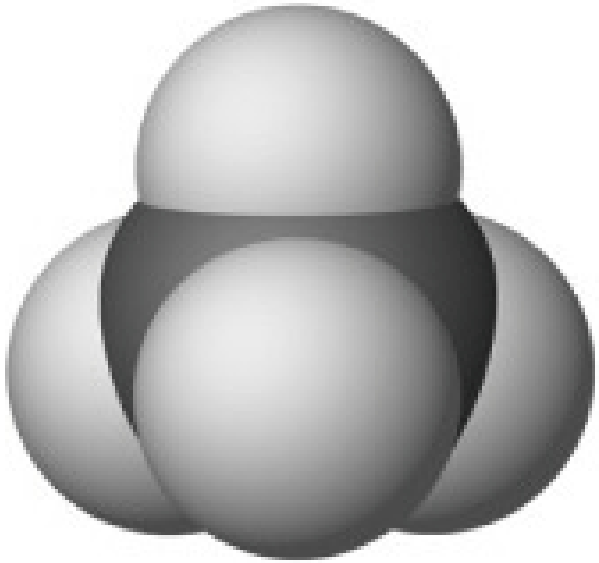


Butane

Ball and stick model



Space filling model



Simplest Aliphatic Hydrocarbons

Series of similar C & H compounds

CH_4	methane
C_2H_6	ethane
C_3H_8	propane
C_4H_{10}	butane
C_5H_{12}	pentane
C_6H_{14}	hexane

C_nH_{2n+2}

Alkanes

BASE NAMES

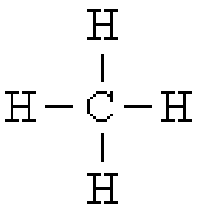
Prefix	No. Carbons
Meth	**1**
Eth	**2**
Prop	**3**
But	**4**
Pent	5
Hex	6
Hept	7
Oct	8
Non	9
Dec	10

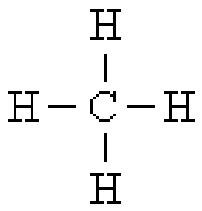
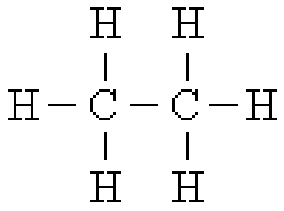
Alkanes

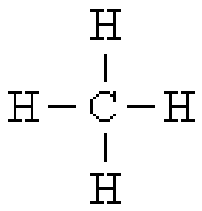
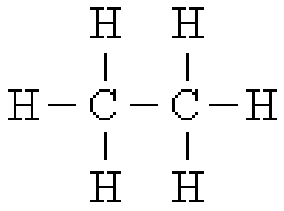
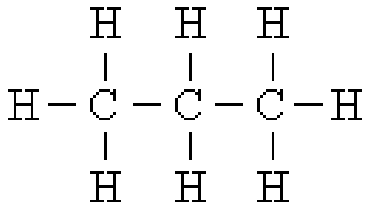
Formula and name for 8 carbons ?

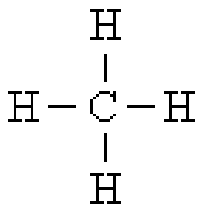
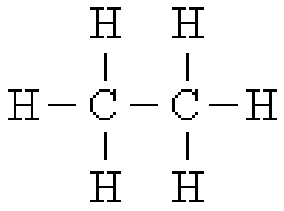
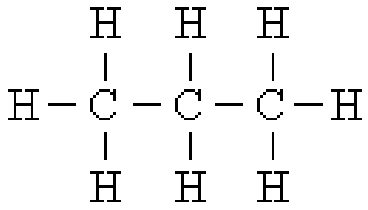
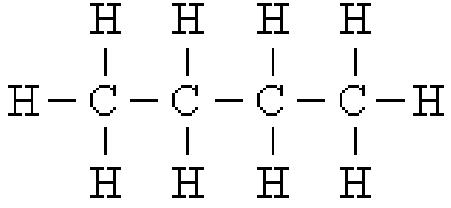
use standard prefixes and -ane ending

C_8H_{18} octane

formula	structure	condensed
CH_4		CH_4

formula	structure	condensed
CH_4		CH_4
C_2H_6		CH_3CH_3

formula	structure	condensed
CH_4		CH_4
C_2H_6		CH_3CH_3
C_3H_8		$CH_3CH_2CH_3$

formula	structure	condensed
CH_4		CH_4
C_2H_6		CH_3CH_3
C_3H_8		$CH_3CH_2CH_3$
C_4H_{10}		$CH_3CH_2CH_2CH_3$

Alkanes

PHYSICAL PROPERTIES

Non-polar molecules

Not water soluble

Low density

Low melting point

Low boiling point

PHYSICAL PROPERTIES

Non-polar molecules

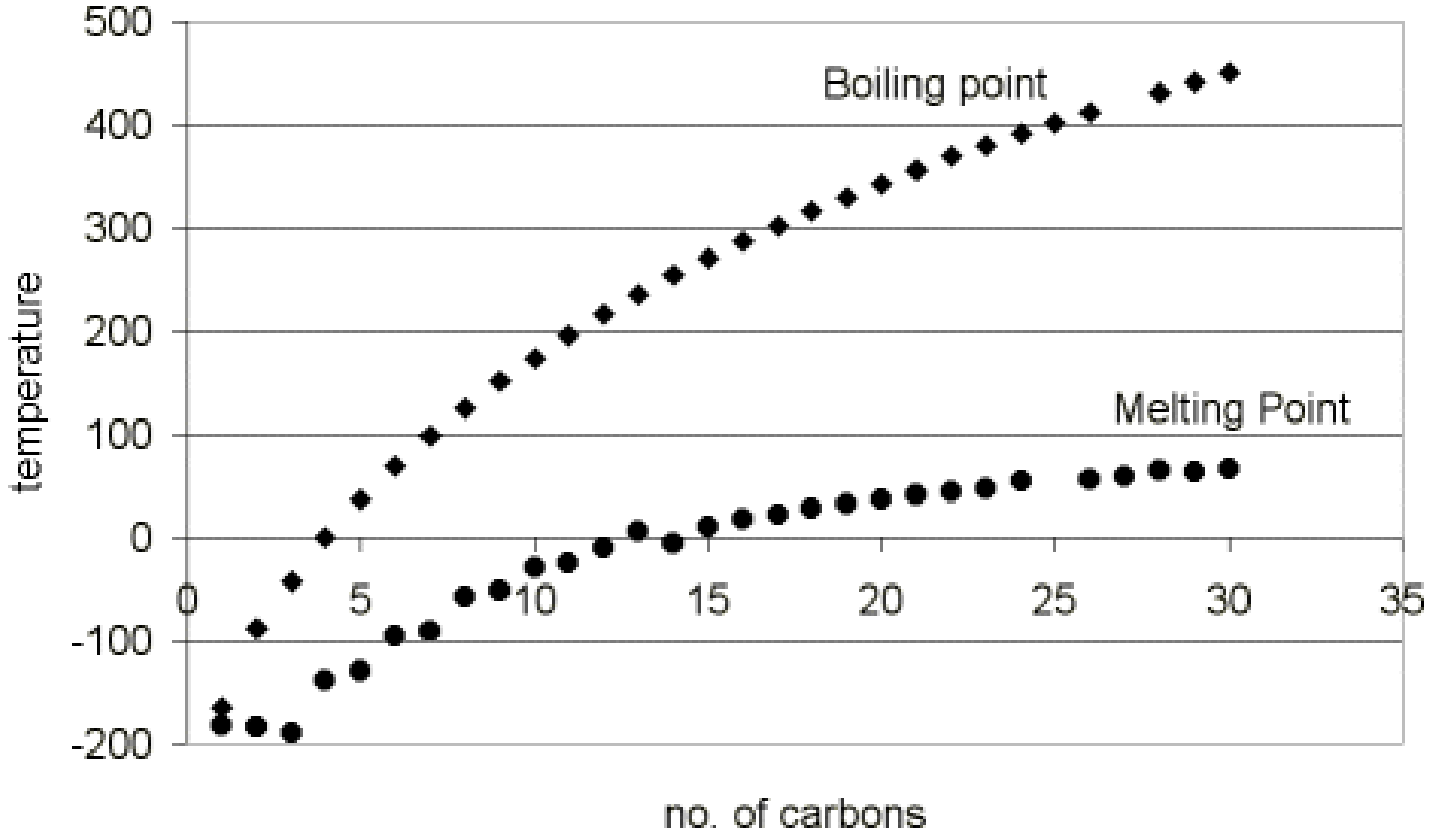
Not water soluble

Low density

Low melting point

Low boiling point

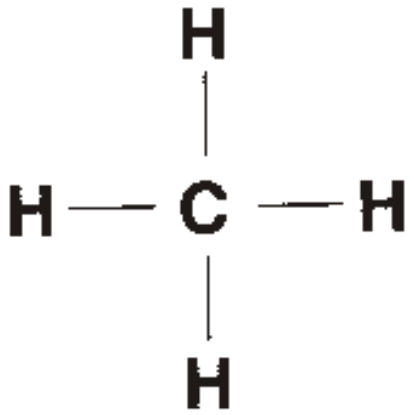
Increase as the number of C atoms increase



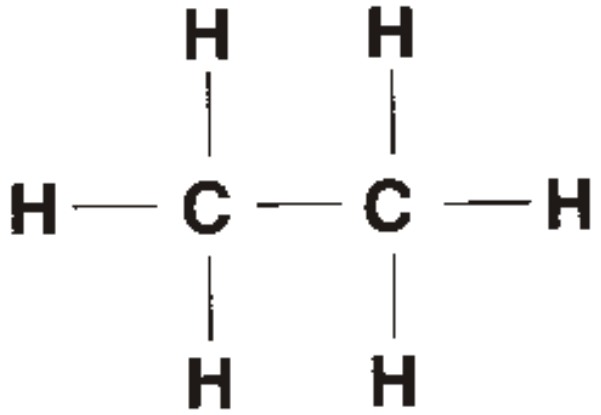
See Table 11.1

SOURCES

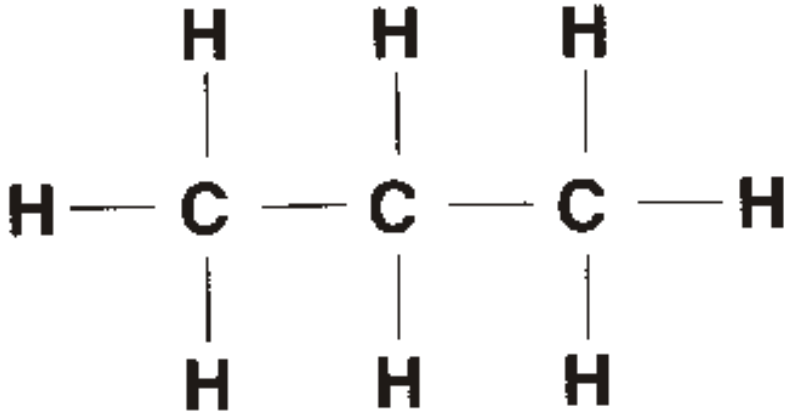
Hydrogenation of:
petroleum
shale oil
coal



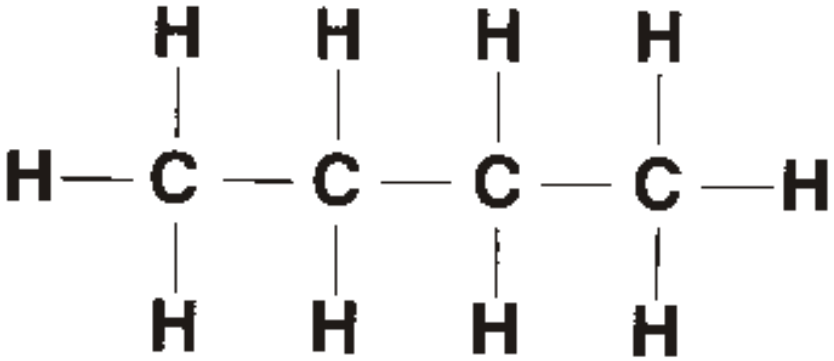
Methane



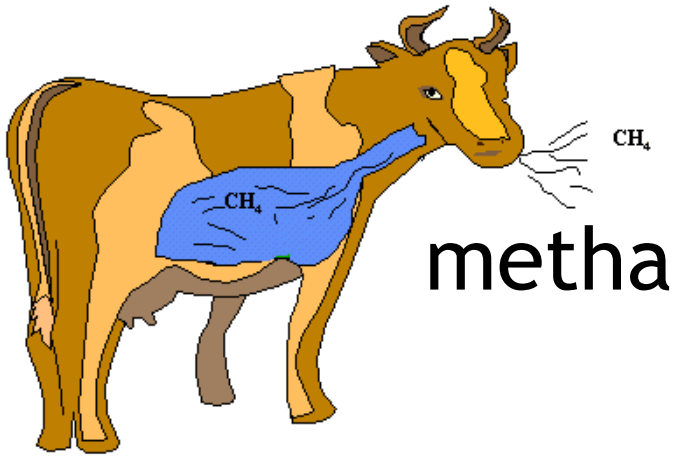
Ethane



Propane



Butane



methane

butane

ORGANIC NOMENCLATURE

Naming system must show:

Number of carbons in longest chain

Location of any branches

Where functional groups are (if any)

IUPAC RULES

1. Find longest carbon chain.
   Use as base name ending - ane

2. Locate any branches on chain.
   Use base names with yl ending

3. For muliple branch of same
   type, add di, tri, tetra....

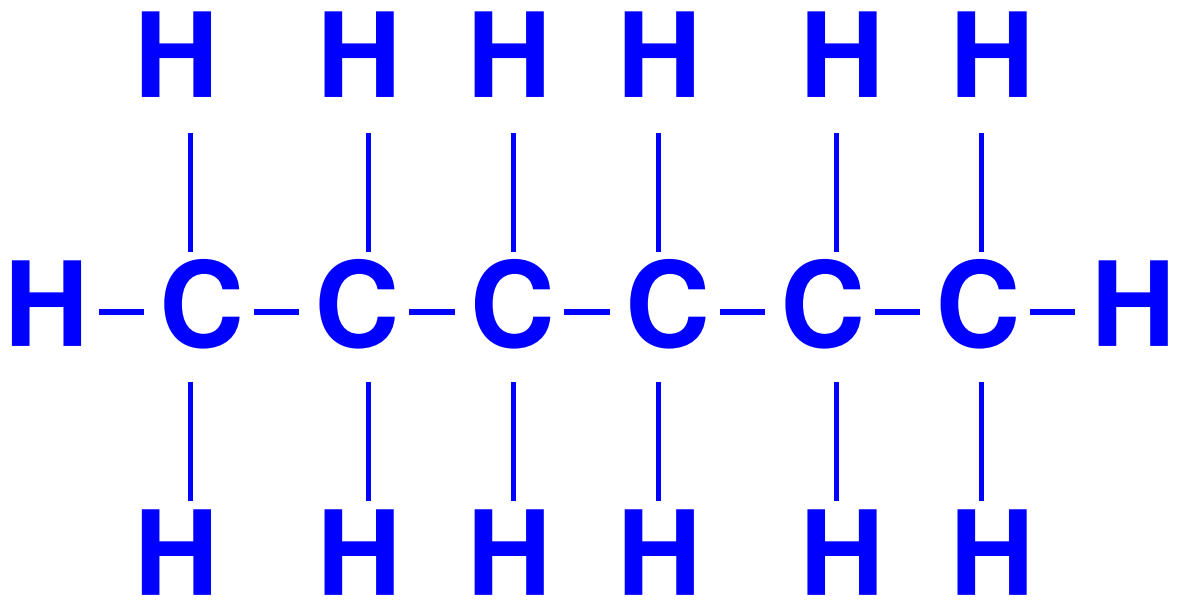
IUPAC RULES

Naming system must show:

4. Show location of each branch with numbers
5. List multiple branches alphabetically
   - the di, tri, tetra don't count

NAMING ALKANES

Omit hydrogens



NAMING ALKANES

Omit hydrogens

C–C–C–C–C–C

1. 6 carbon chain: hex
2. Use -ane ending
3. Name: hexane

NAMING ALKANES

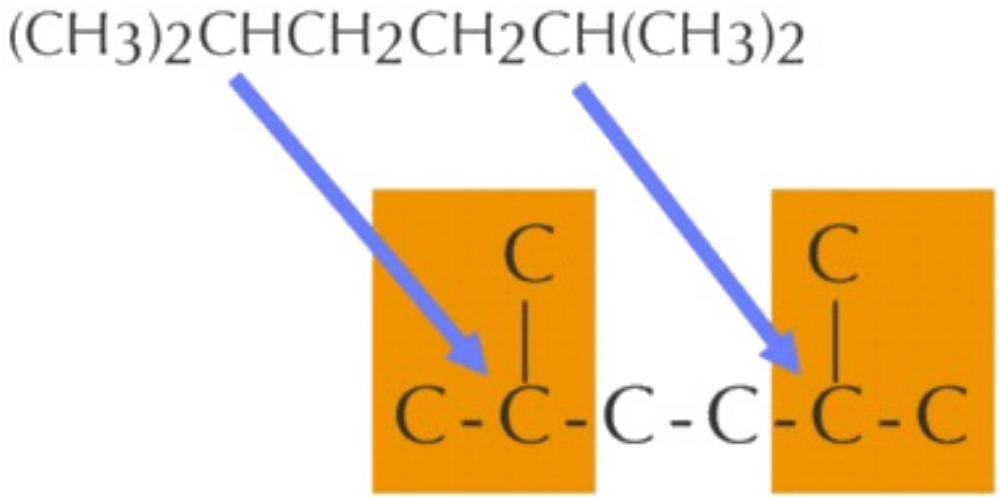
$(CH_3)_2CHCH_2CH_2CH(CH_3)_2$

Convert from condensed structural formula to simple carbon skeleton

NAMING ALKANES

$(CH_3)_2CHCH_2CH_2CH(CH_3)_2$

Convert from condensed structural formula to simple carbon skeleton



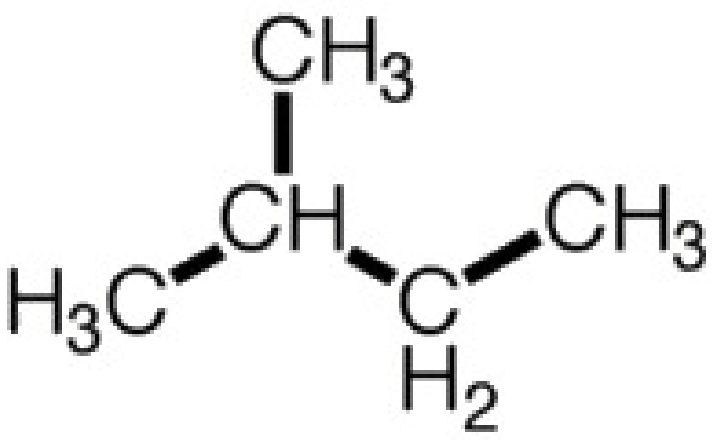
NAMING ALKANES

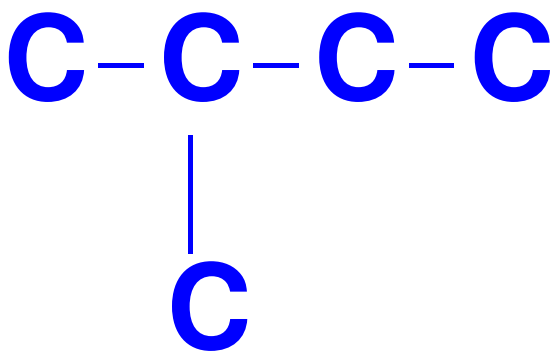
$(CH_3)_2CHCH_2CH_2CH(CH_3)_2$

Convert from condensed structural formula to simple carbon skeleton

1.
2. Two methyl groups - dimethyl
3. 2,5-dimethylhexane

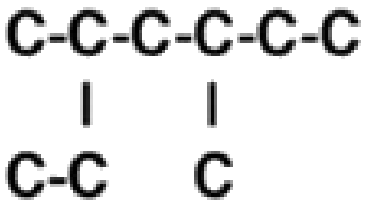
NAMING ALKANES



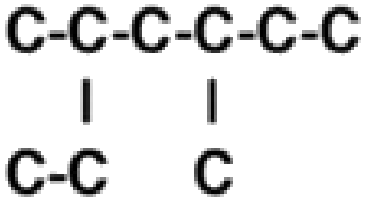


1. 4 carbon chain: but
2. Use -ane ending
3. Methyl group on second C
4. Name: 2-methylbutane

NAMING ALKANES

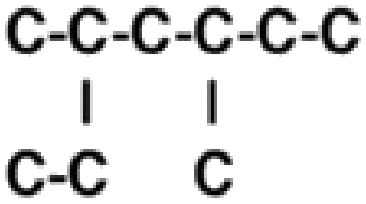


NAMING ALKANES

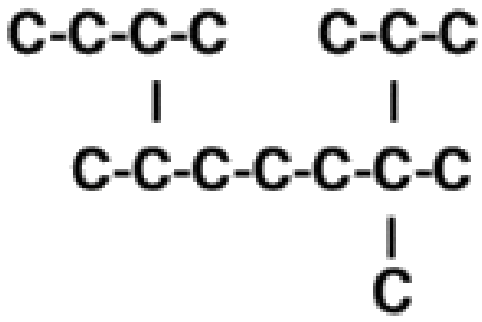


3,5-dimethyl heptane

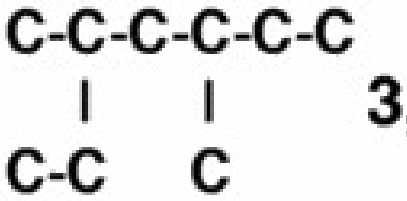
NAMING ALKANES



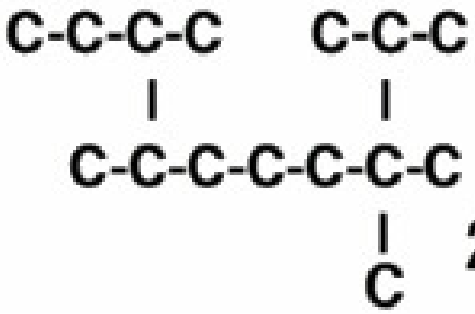
3,5-dimethyl heptane



NAMING ALKANES



3,5-dimethyl heptane



2,3,3,7,8-pentamethyldecane

DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane

Start with base, draw C skeleton

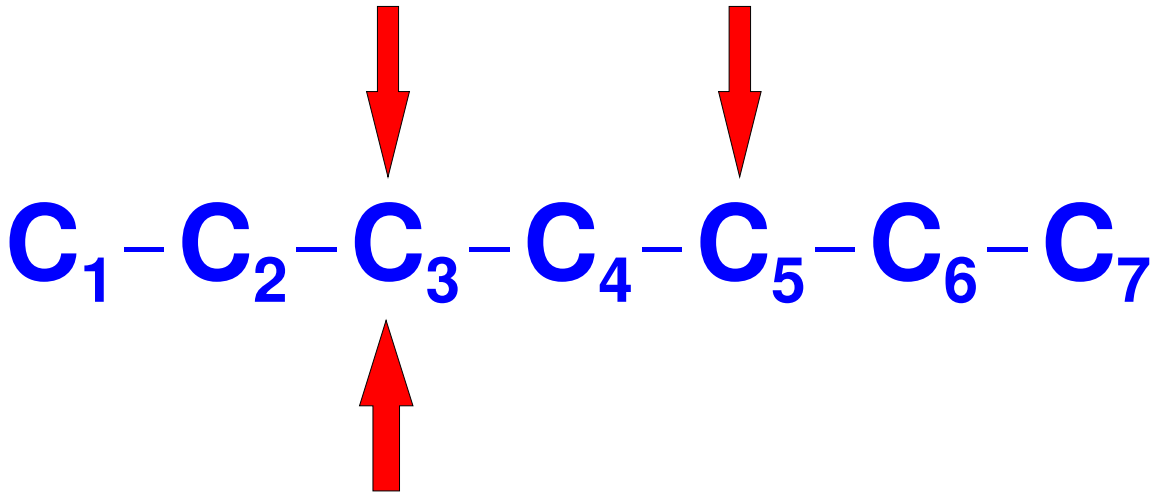
3,5,5-trimethylheptane

C–C–C–C–C–C–C

Number carbon atoms

DRAWING STRUCTURES FROM NAMES

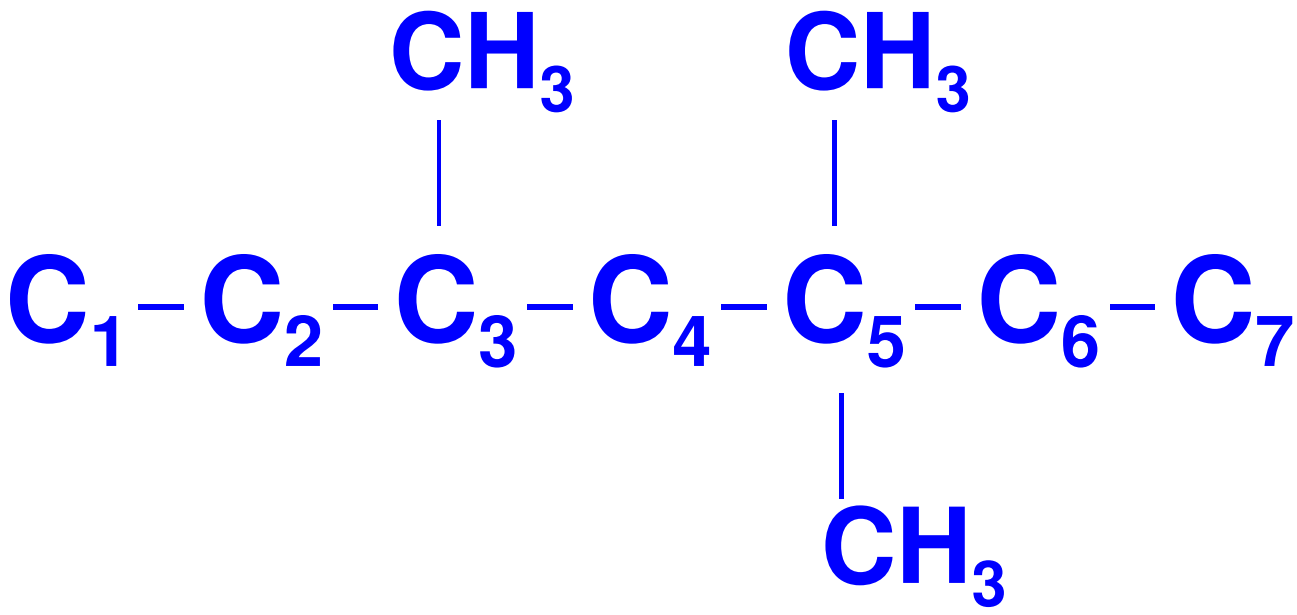
3,3,5-trimethylheptane



Where do the 3 methyl groups go?

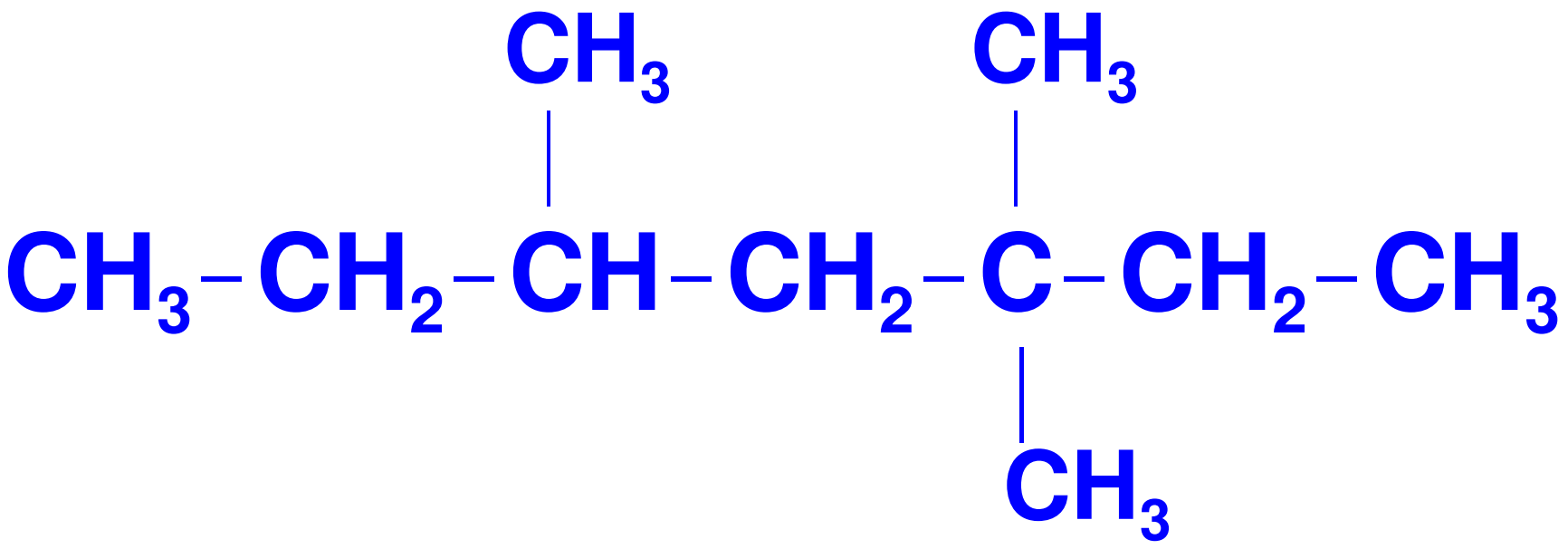
DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane



DRAWING STRUCTURES FROM NAMES

3,5,5-trimethylheptane

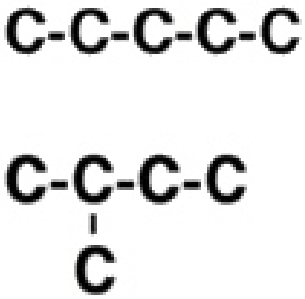


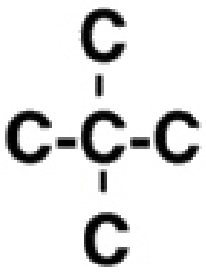
All carbons have 4 bonds

STRUCTURAL ISOMERS

All have same formula, but different structures and properties

Example
C_5H_{12}



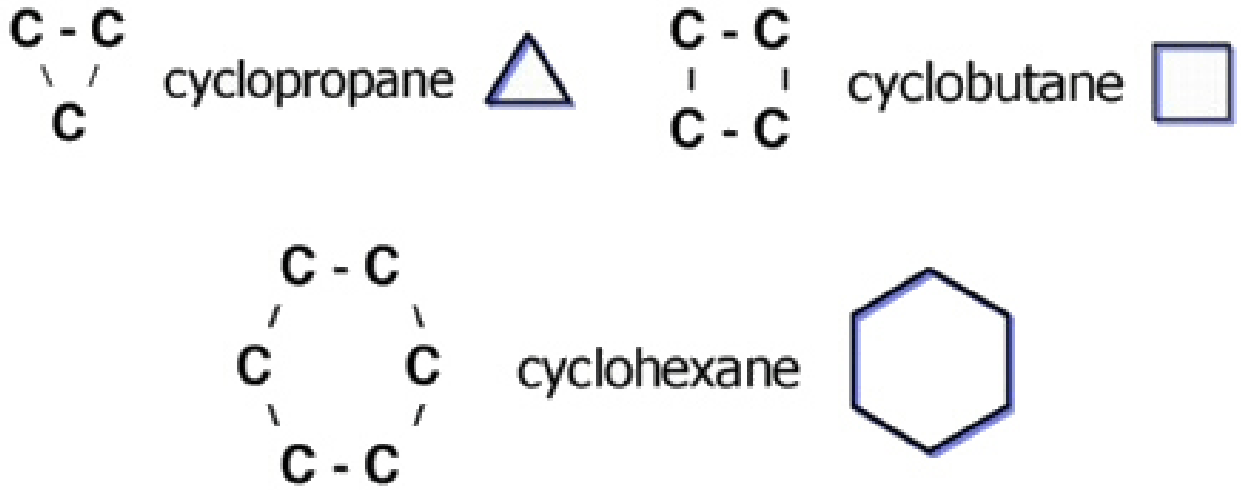


This will be more important later where the isomers can result in different functional groups.

CYCLOALKANES

Cyclic alkanes
General formula: C_nH_{2n}

Named as parent alkane with cyclo prefix



REACTIONS OF ALKANES

1. Combustion

$$CH_4 + 2\,O_2 \rightarrow CO_2 + 2\,H_2O$$

Many alkanes used as fuel

Methane: natural gas
Propane: cooking
Butane: lighters
Gasoline: mixture of hydrocarbons

REACTIONS OF ALKANES

2. Halogenation

$$CH_4 + Cl_2 \rightarrow CH_3Cl + HCl$$

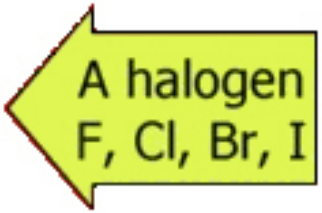
Halogen replaces hydrogen

Dichloromethane: paint stripper
Chloroform: anesthesia
1,2-dichloroethane: dry cleaning

ALKYL HALIDES

Alkanes with at least 1 halogen replacing hydrogen

General formula: R-X



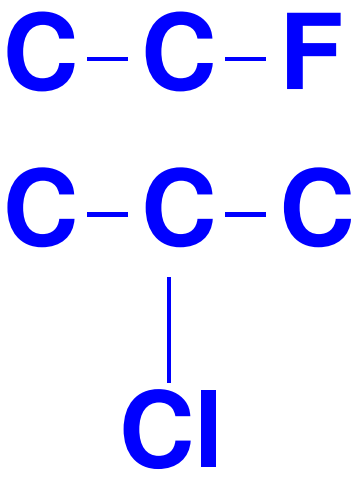
Structure and naming similar to alkanes

ALKYL HALIDES

Halogen	Name	Symbol
fluorine	fluoro	–F
chlorine	chloro	–Cl
bromine	bromo	–Br
iodine	iodo	–I

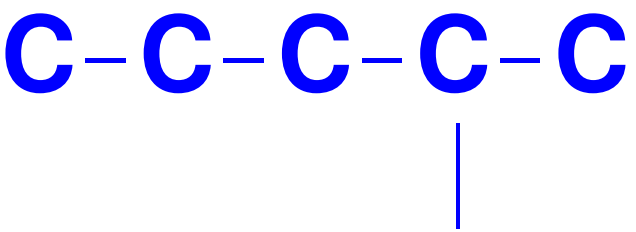
ALKYL HALIDES

Give name and carbon number for halide just like a side branch



1-fluoroethane

2-chloropropane



1-bromo-2-methylpentane

ALKENES AND ALKYNES

Unsaturated hydrocarbons

Contain C–C multiple bonds

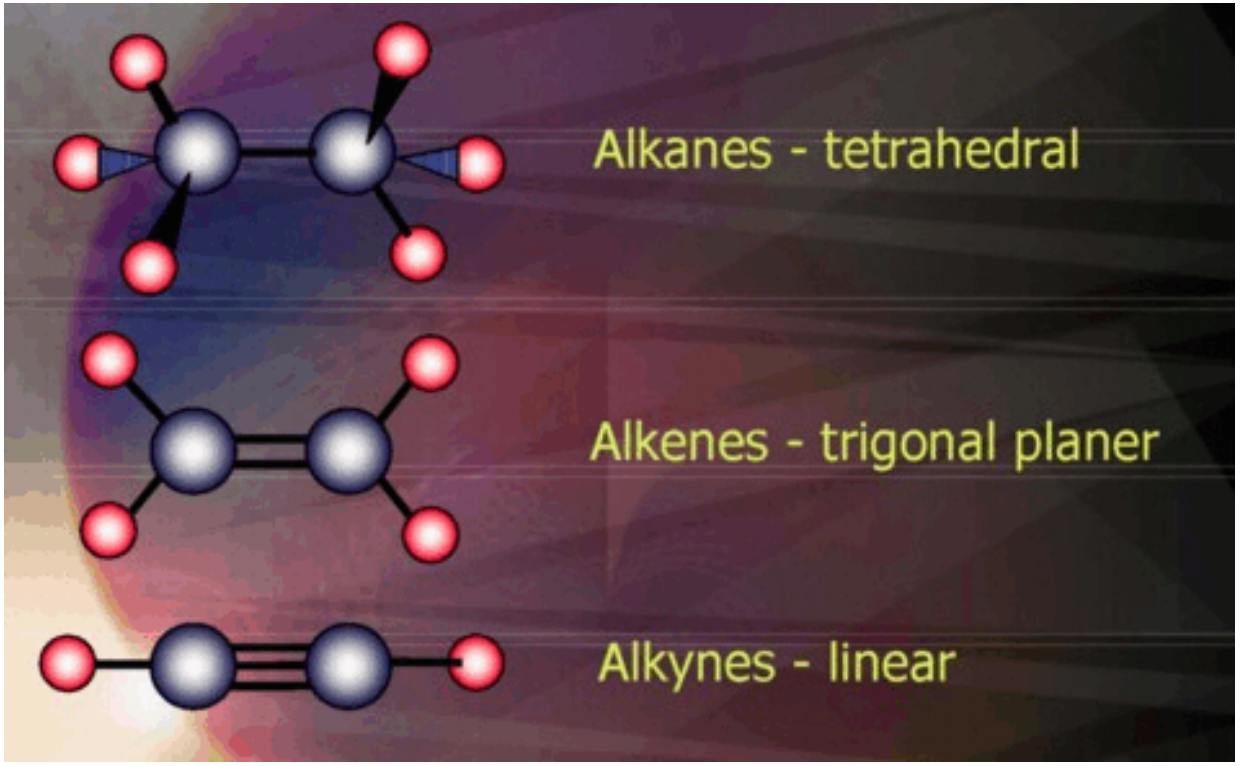
Alkenes: R–C=C–R C_nH_{2n}

Alkynes: R–C≡C–R C_nH_{2n-2}

Examples: steroids, unsaturated fats, polymers, prostaglandins

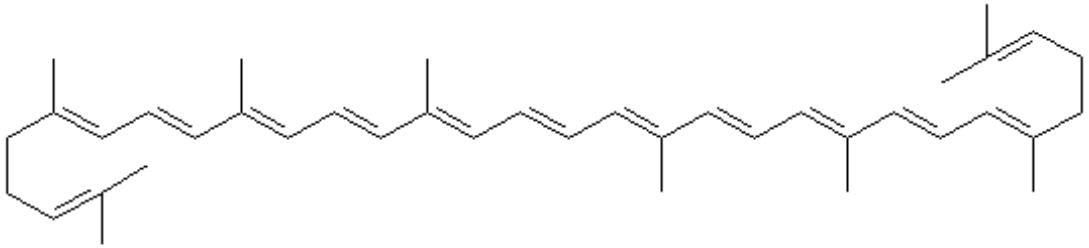
ALKENES AND ALKYNES

Geometry



COLORED ALKENES

Molecules with many double bonds can be colored



Molecular Weight: 536.89

Molecular Formula: $C_{40}H_{56}$

100mg Organic
Tomato Concentrate

10mg Lycopene
Nutritional Factor

Lycopene

NAMING ALKENES

Indicate position of double bond

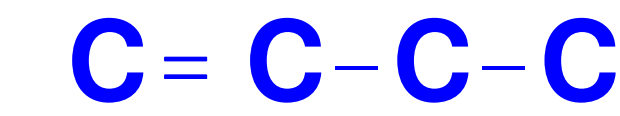
1. Longest C chain must contain double bond
2. Number carbons so double bond has lowest number
3. Indicate position of double bond

NAMING ALKENES

4. Change ending to -ene

5. Use same rules for side chains and halides

NAMING ALKENES



Four carbons: use base but-

Contains double bond: use -ene

Double bond is between first and second: number as 1

1-butene

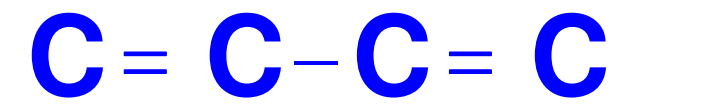
NAMING ALKENES

Multiple double bonds

Number each double bond

Use -diene for two

-triene for three, etc



1,3-butadiene

NAMING ALKYNES

Similar to alkenes

Use ending -yne

C≡C–C–C

1-butyne

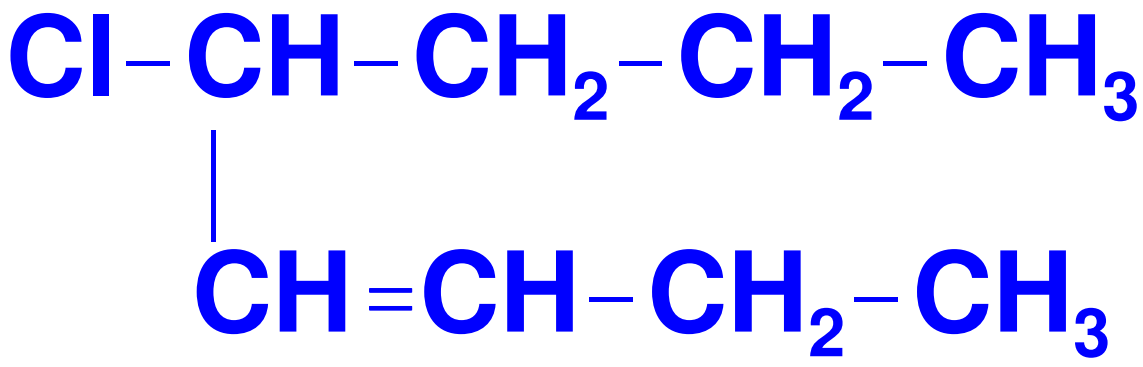
MORE EXAMPLES

2-pentene

MORE EXAMPLES

3-chloro-1-butene

MORE EXAMPLES



5-chloro-3-octene

GEOMETRIC ISOMERS

When two or more arrangements of atoms are possible

Alkanes: rotation about all bonds
no geometric isomers

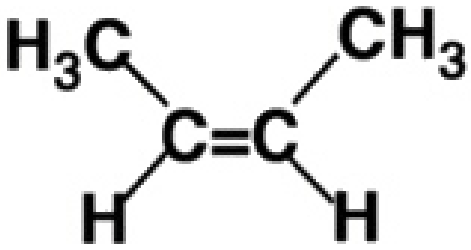
Alkenes: rigid bond
geometric isomers

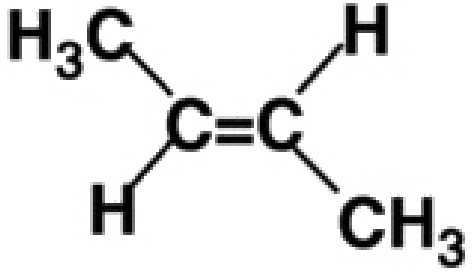
Alkynes: rigid bond & linear
geometric isomers

GEOMETRIC ISOMERS

Two possible arrangements

2-butene





cis
largest groups on same side

cis-2-butene

trans
largest groups on opposite sides

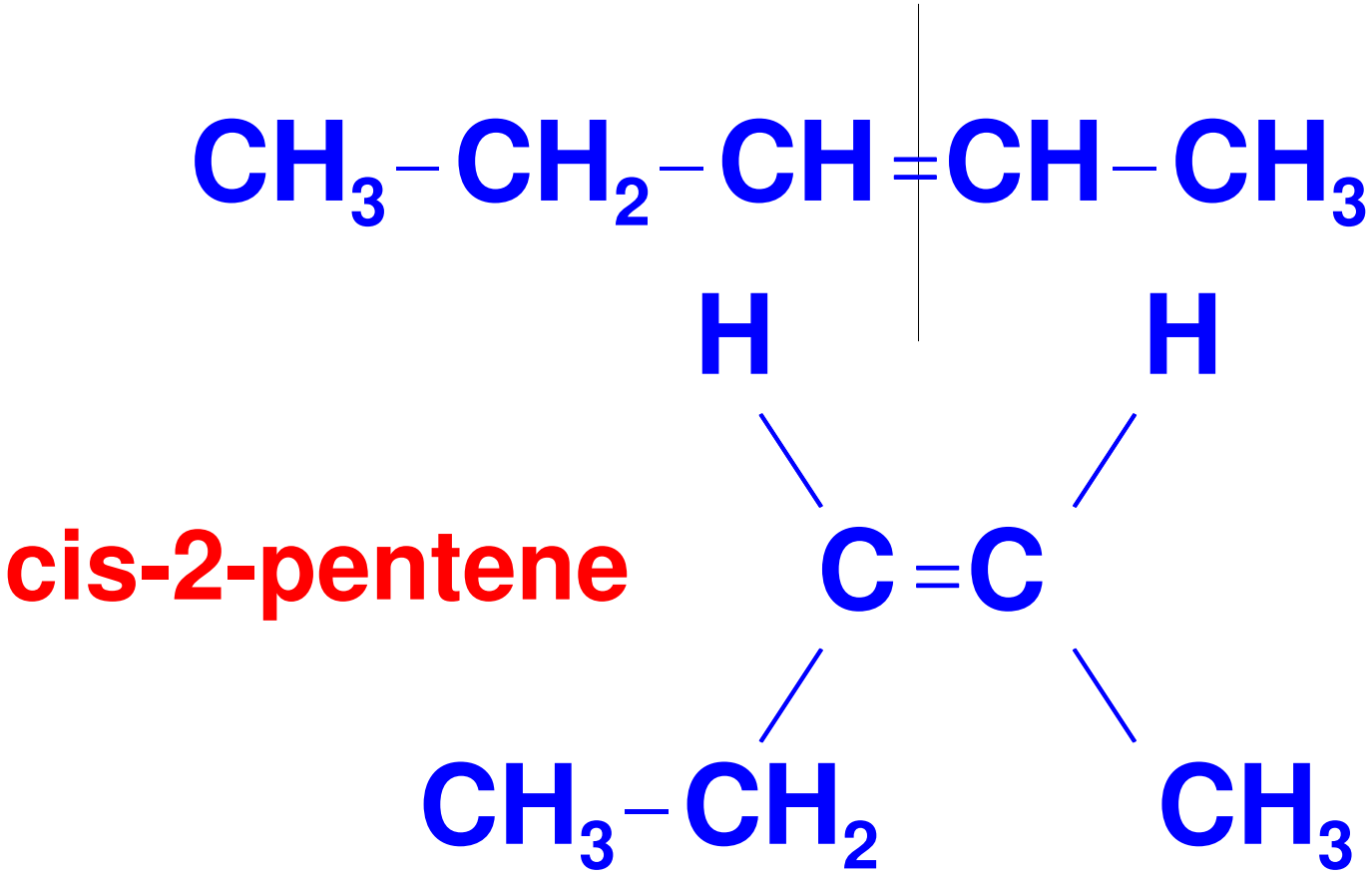
trans-2-butene

CIS/TRANS ASSIGNMENTS

1. **Locate alkene bond**

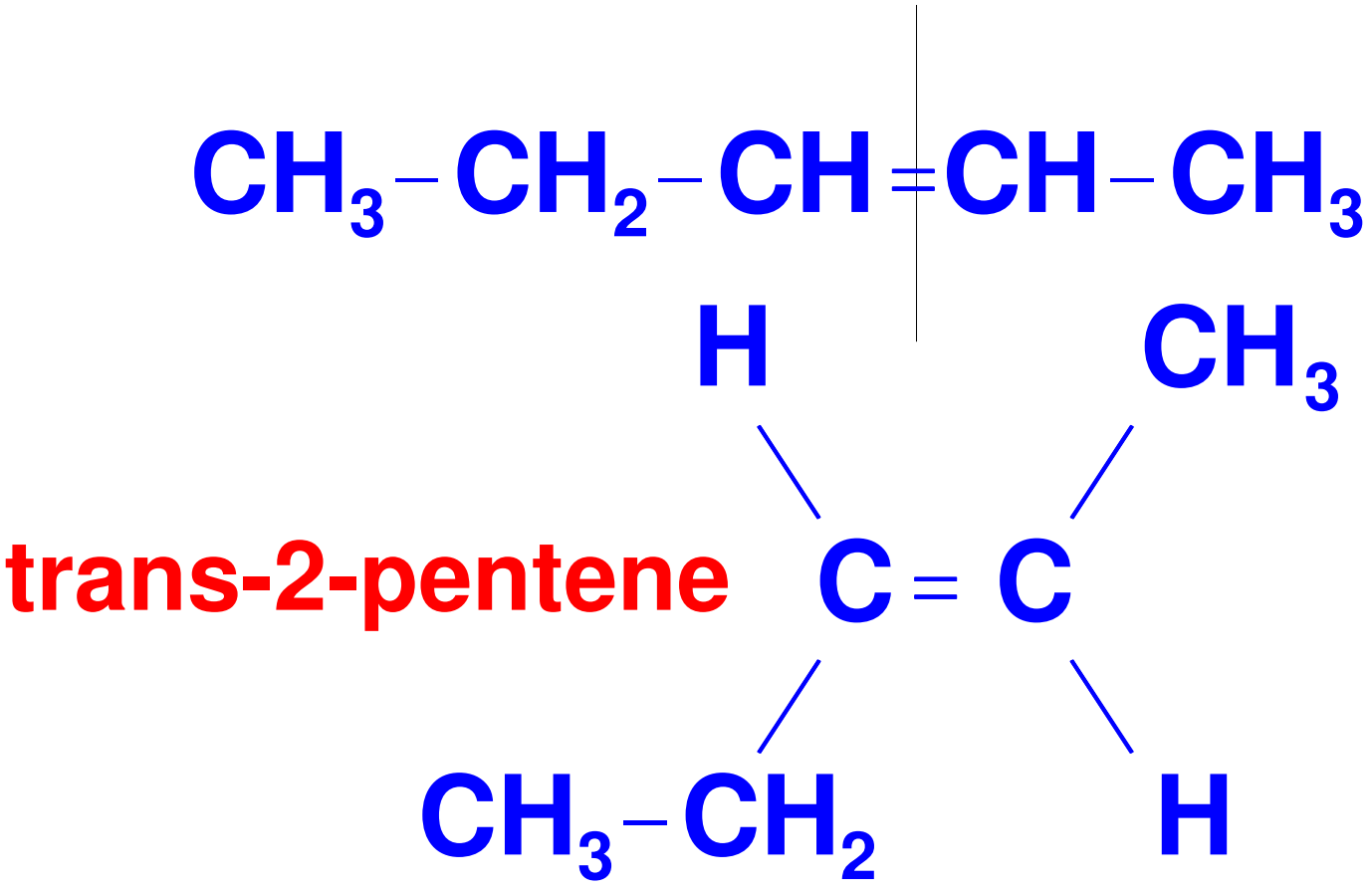
2. **Draw out structure in full**

CIS/TRANS ASSIGNMENTS

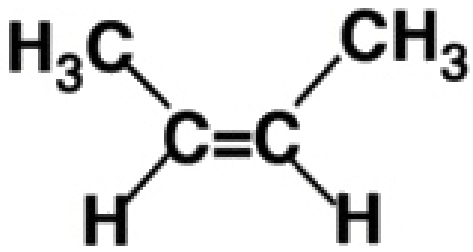


cis-2-pentene

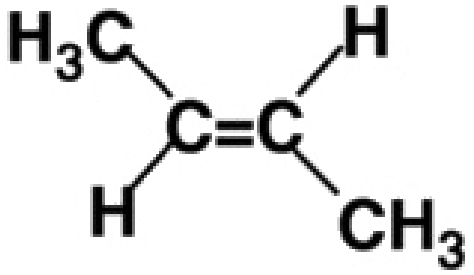
CIS/TRANS ASSIGNMENTS



GEOMETRIC ISOMERS



cis-2-butene



trans-2-butene

REACTIONS OF ALKENES

Can react like alkanes

Also react at double bond

Addition reactions common

double bond breaks

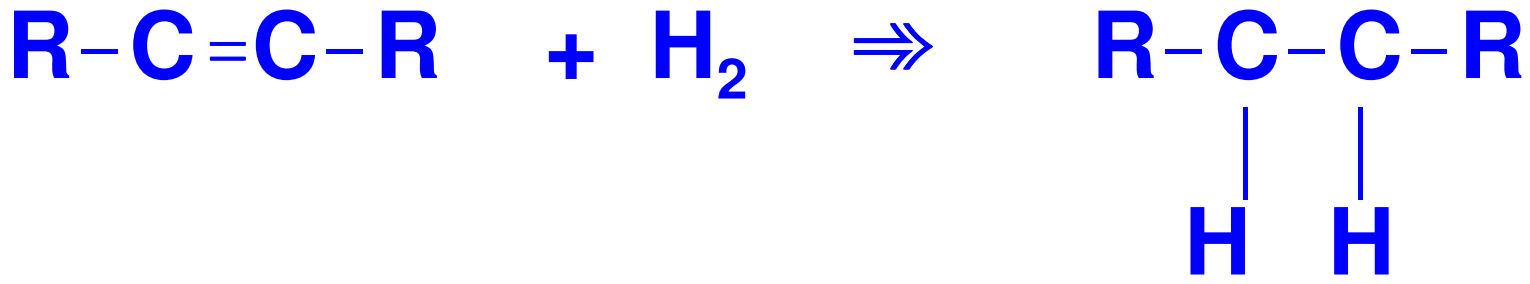
atoms added to carbons

REACTIONS OF ALKENES

Hydrogentation

Addition of H_2

Forms alkanes



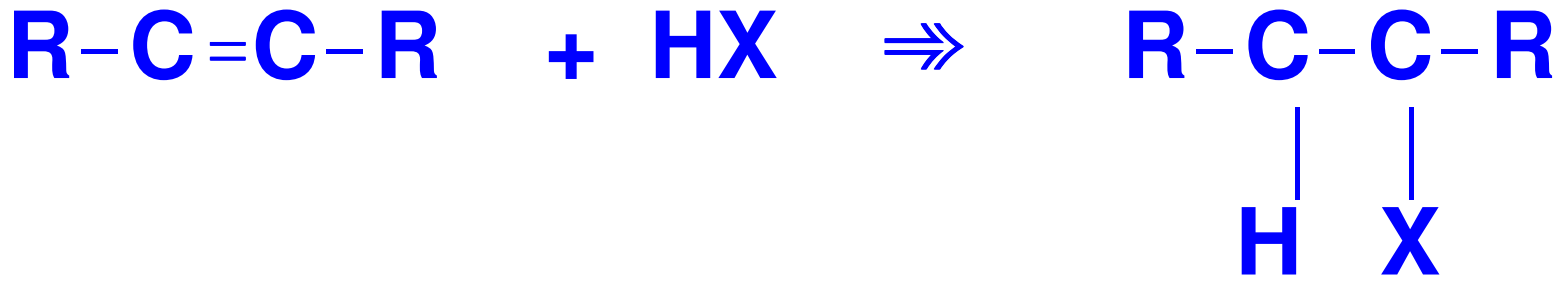
Requires heat, pressure, catalysts - Pt, Pd, Ni

REACTIONS OF ALKENES

Hydrohalogentation

Addition of HX - HF, HCl, HBr, HI

Forms haloalkanes



AROMATIC HYDROCARBONS

Best represented by benzene

A six carbon ring

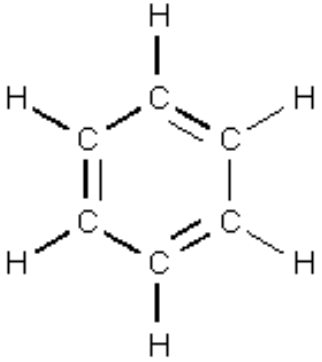
Three alternating double bonds

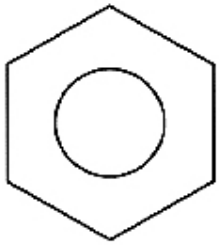
Electrons in bonds spread out

Exists as resonance structure (average)

AROMATIC HYDROCARBONS

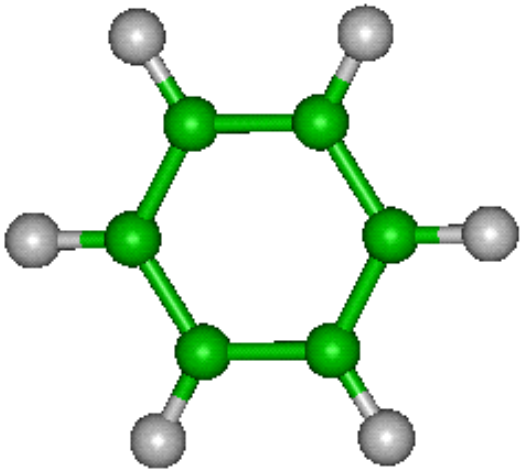
Best represented by benzene

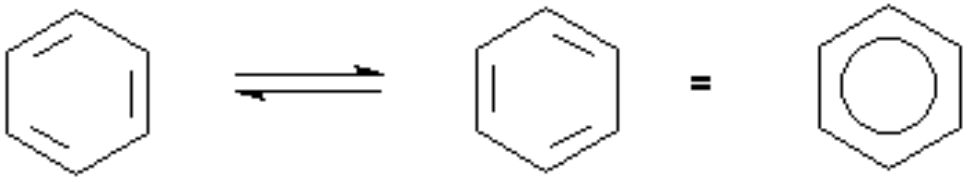




Benzene

C_6H_6

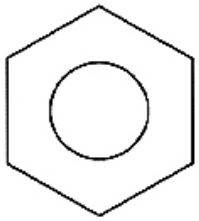




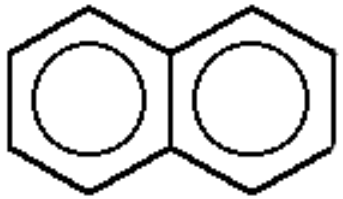
Resonance Forms of Benzene

AROMATIC HYDROCARBONS

Fused rings common



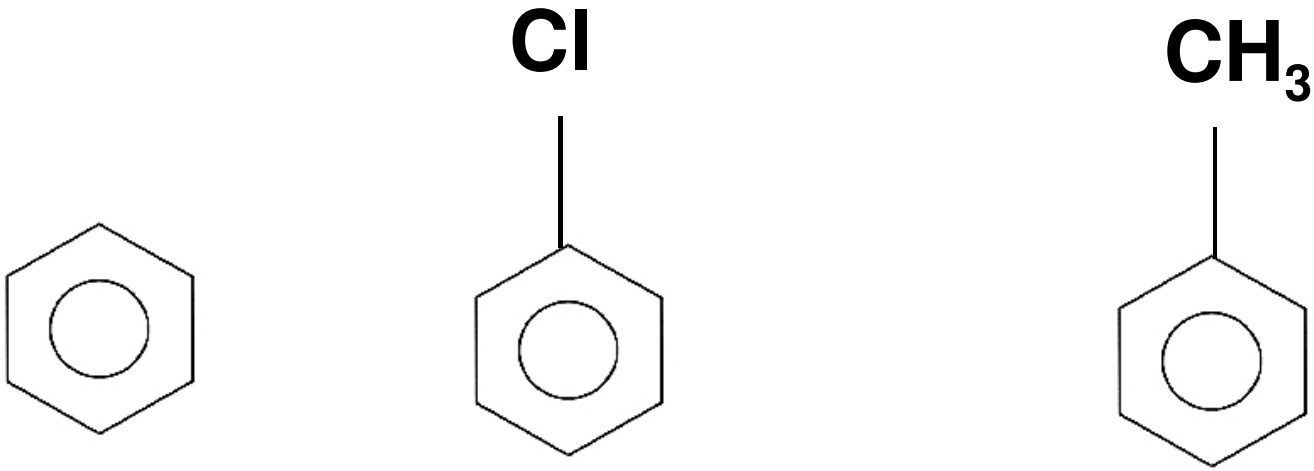
benzene



napthalene

AROMATIC HYDROCARBONS

Name benzene derivatives

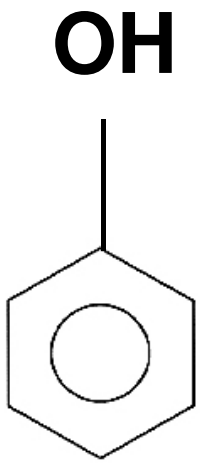


benzene chlorobenzene methylbenzene

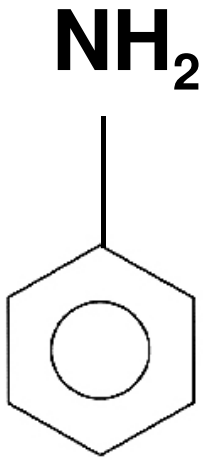
nitro: NO_2 amino: NH_2

AROMATIC HYDROCARBONS

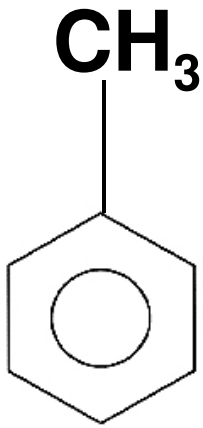
Common names



phenol



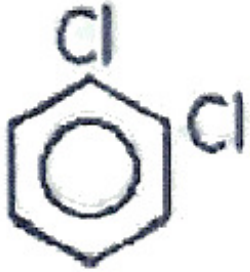
aniline

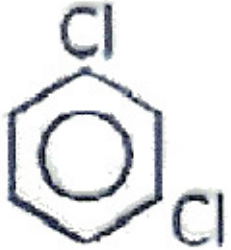


toluene

AROMATIC HYDROCARBONS

Disubstituted rings





1,2-dichlorobenzene

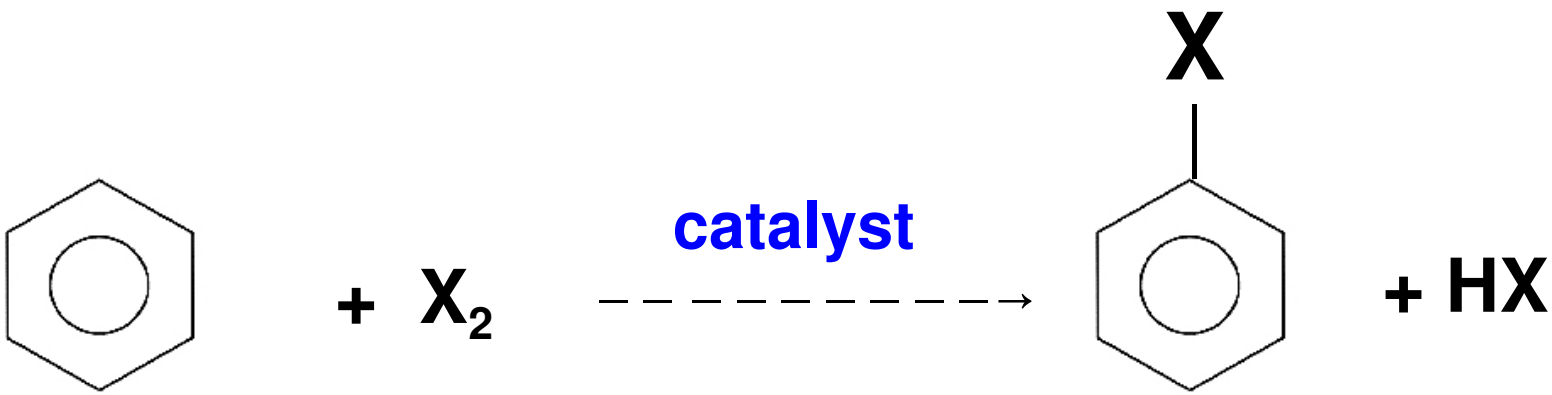
1,3- dichlorobenzene

1,4-dichlorobenzene

dichlorobenzene

AROMATIC HYDROCARBONS

Reactions of benzene



A substitution reaction

Functional groups

specific combinations of atoms

alcohols R–OH **acids R–COOH**

amines R–NH_2 **ethers R–O–R'**

aldehydes R–CHO

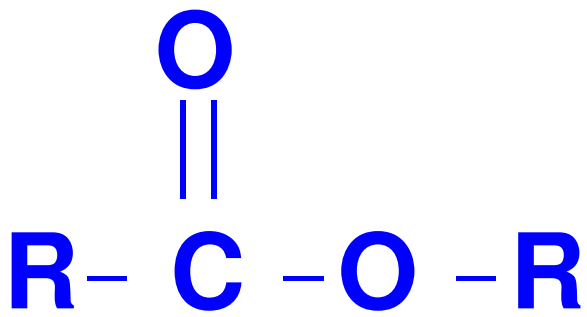
ketones R(C=O)R'

esters R–COOR'

Esters

–OH of acid replaced by –OR

R- COOR



Isomerism

Stereoisomers

Two types: geometric isomers
optical isomers

cis-trans isomers

Mirror image molecules

enantiomers

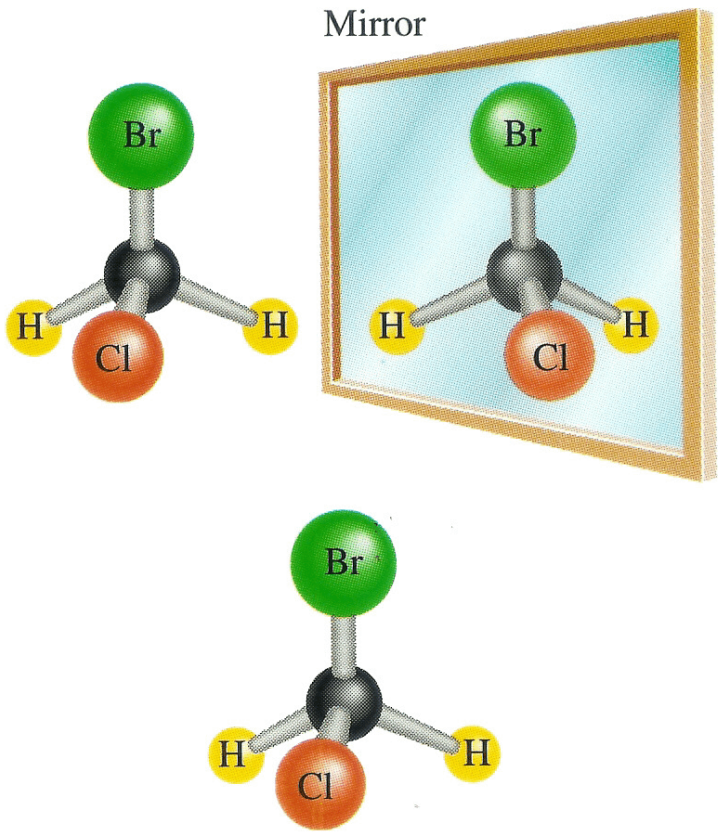
Isomerism

Stereoisomers

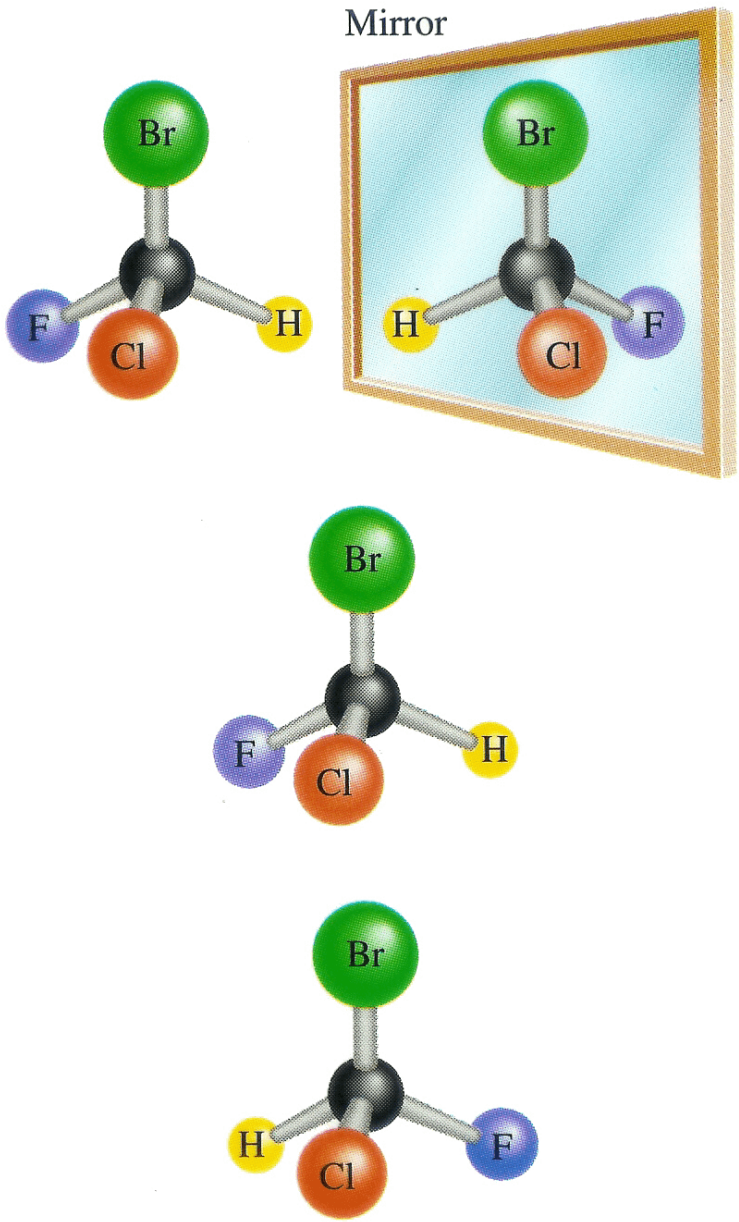
Compare left and right hands

Non-superimposable mirror images

Distinguish by D- or L- prefix in name



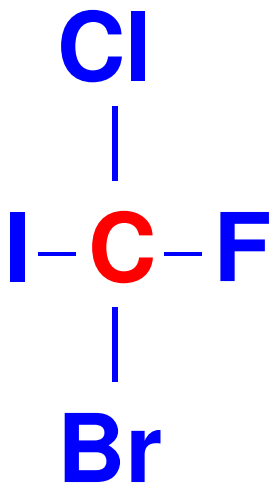
Not optical isomers



Optical isomers

Isomerism

Optical isomers have chiral center or asymmetric carbon atom



4 different atoms or groups attached

Stereoisomers

Is the red carbon chiral?

Isomerism