Structure 3.2

Structural formulas



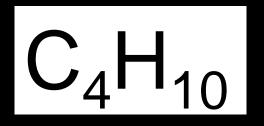
Structural formulas

- Molecular formula: actual number of atoms in the compound.
- Empirical formula: lowest whole number ratio of atoms in the compound.
- Full structural formula: shows all atoms and bonds between the atoms.
- Condensed structural formula: shows only the atoms and omits the bonds.
- Skeletal formula: C atoms and H atoms bonded to C atoms are omitted leaving only the carbon skeleton.

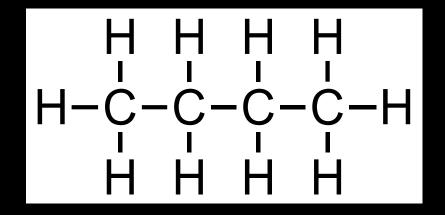


Structural formulas

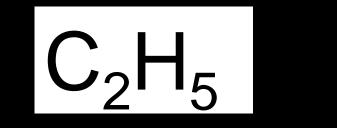
Butane molecular formula



full structural formula



empirical formula condensed structural formula





skeletal formula





Structural formula

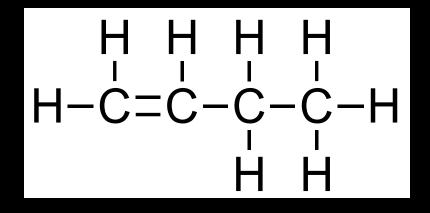
But-1-ene

molecular formula



empirical formula

full structural formula

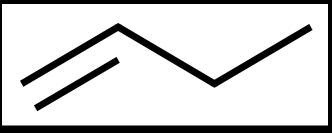


condensed structural formula





skeletal formula





Structural formula

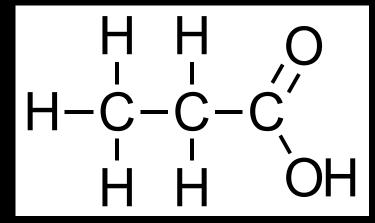
Propanoic acid molecular formula

$$C_3H_6O_2$$

 $C_3H_6O_2$

empirical formula



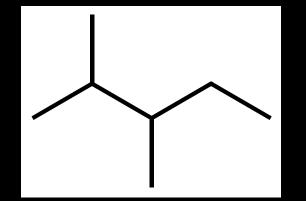


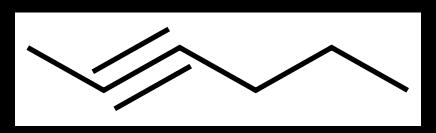
condensed structural formula

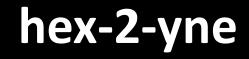
CH₃CH₂COOH CH₃CH₂CO₂H

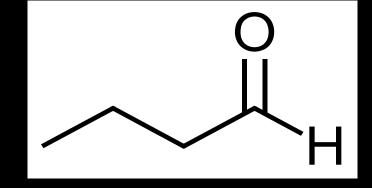
skeletal formula

Skeletal formulas



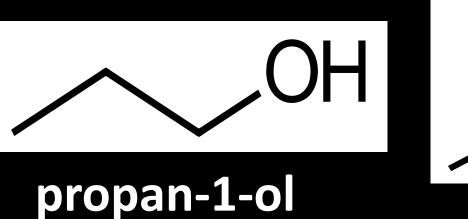


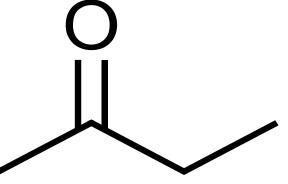


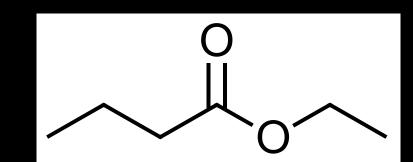


2,3-dimethylpentane

butanal







ethyl butanoate

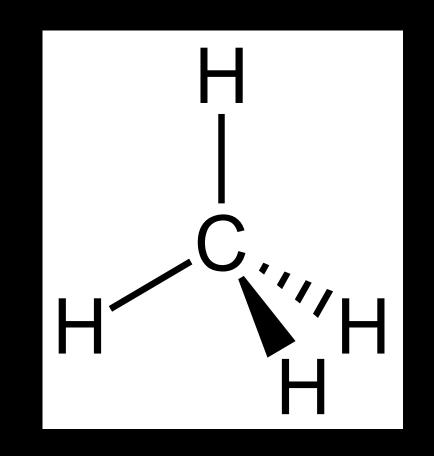
butanone



Stereochemical formula

The two solid lines are in the plane of the paper.

The solid wedge is coming out from the paper.





The dashed wedge is going into the paper.

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Functional groups

MSJChem Tutorials for IB Chemistry FUNCTIONAL GYOUDS

A functional group is a group of atoms within a molecule that are responsible for the characteristic chemical reactions of the molecule.

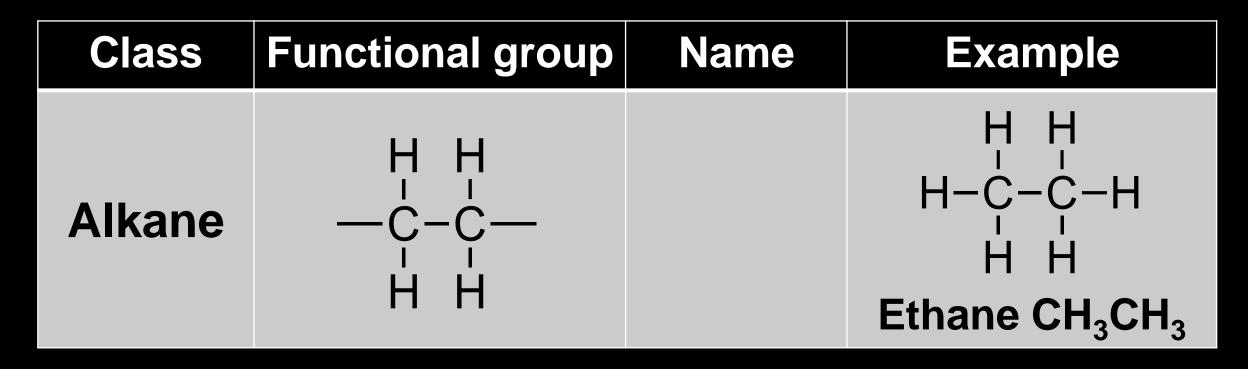
Class: alcohol Functional group: OH hydroxyl group

pentan-1-ol

Compounds with the same functional group belong to the same class.

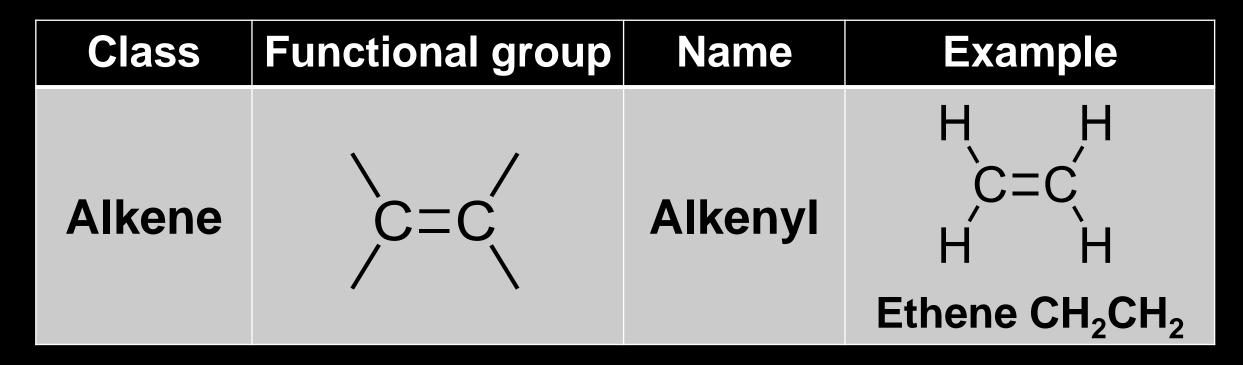


Functional groups



General formula	Type of reactions	
C _n H _{2n+2}	Combustion Free-radical substitution	



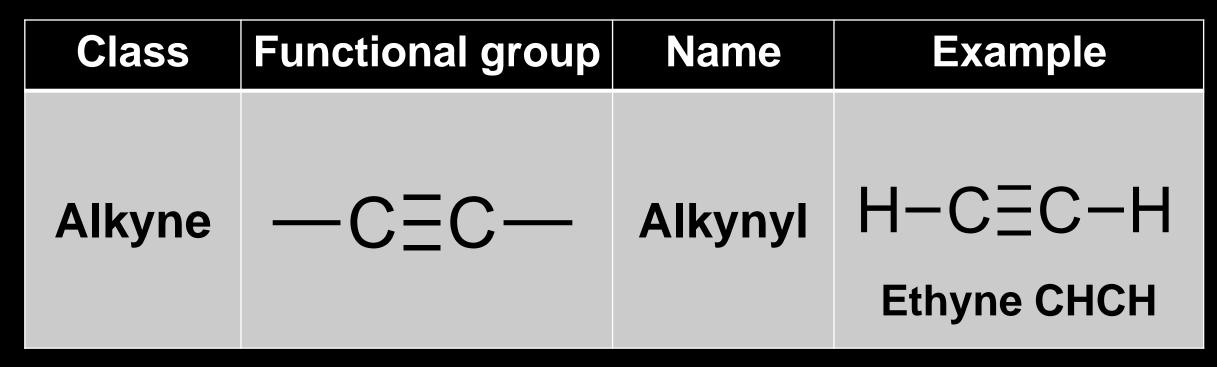


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General formula	Type of reactions	
C _n H _{2n}	Combustion Electrophilic addition	





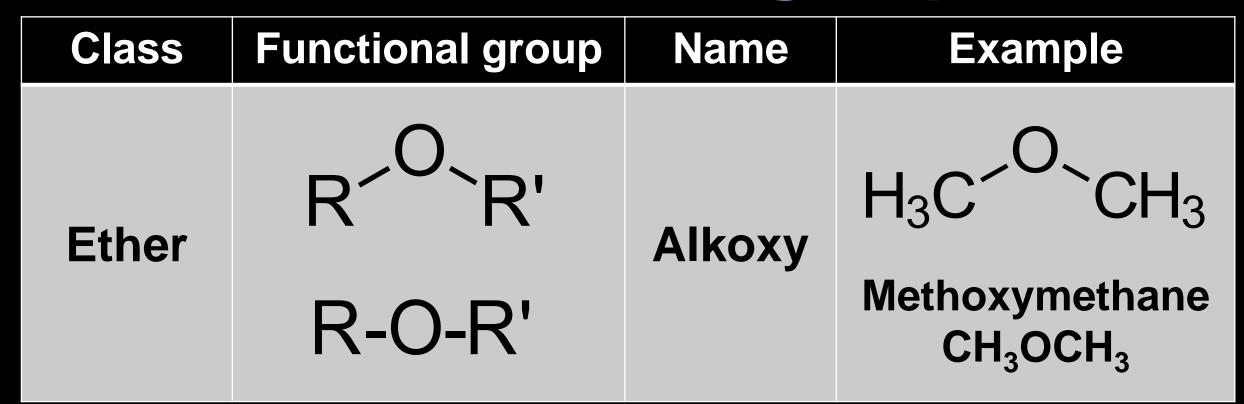
General formula	Type of reactions
C _n H _{2n-2}	Combustion Electrophilic addition

Class	Function	al group	Name	Example
Aldehyde	R-C, H R-CHO		Carbonyl	$H_3C - C'_1$ H Ethanal CH ₃ CHO
General formula		Type of reactions		
C _n H _{2n} O			Oxidat Reductio	

Class	Functional gro	up Name	Example	
Ketone	O C R'R' R-CO-R'	Carbonyl	$H_3C^{-}CH_3$ Propanone CH_3COCH_3	
General	formula	Type of reactions		
C _n ⊦	I _{2n} O	Oxidat Reductio		

Class	Functional	group	Name	Example
Ester	0 ,'' C_OR' R^OOR' R-C00-R' R-C0 ₂ -R'		Ester	$O_{II} O_{C} O_{C} O_{I}$ $H^{-}O^{-}OH_{3}$ Methyl methanoate HCOOCH ₃ or HCO ₂ CH ₃
Genera	al formula		Туре с	of reactions
C _n	$H_{2n}O_2$			

Functional groups



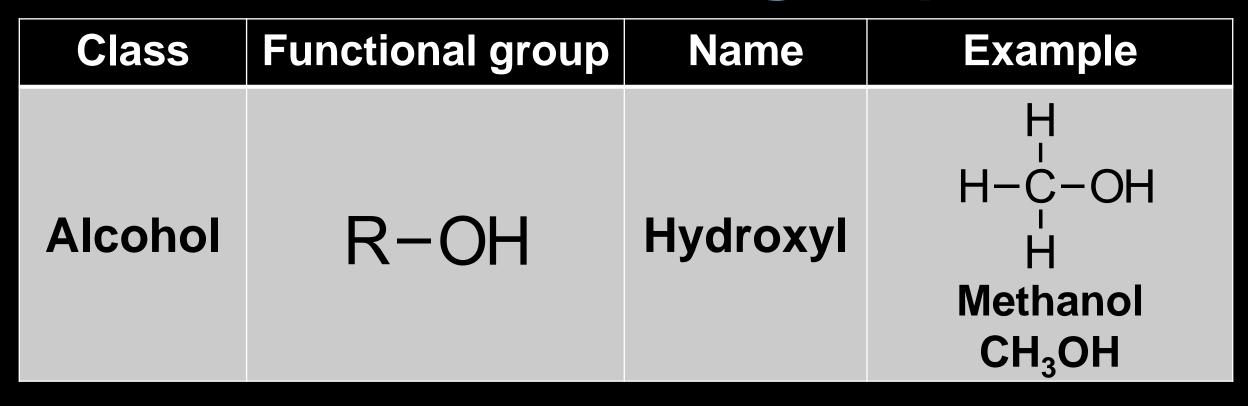
MSJChem

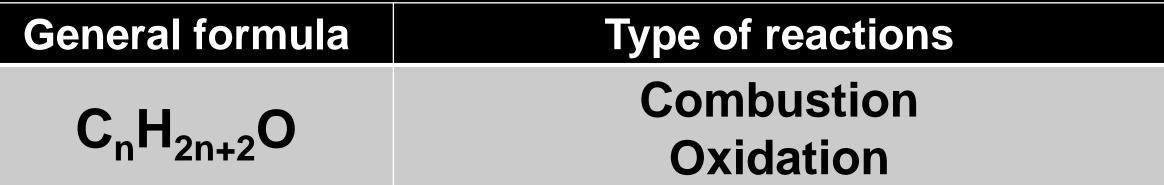
Tutorials for IB Chemistry

General formula	Type of reactions	
$C_nH_{2n+2}O$	Not covered in IB chemistry	



Functional groups



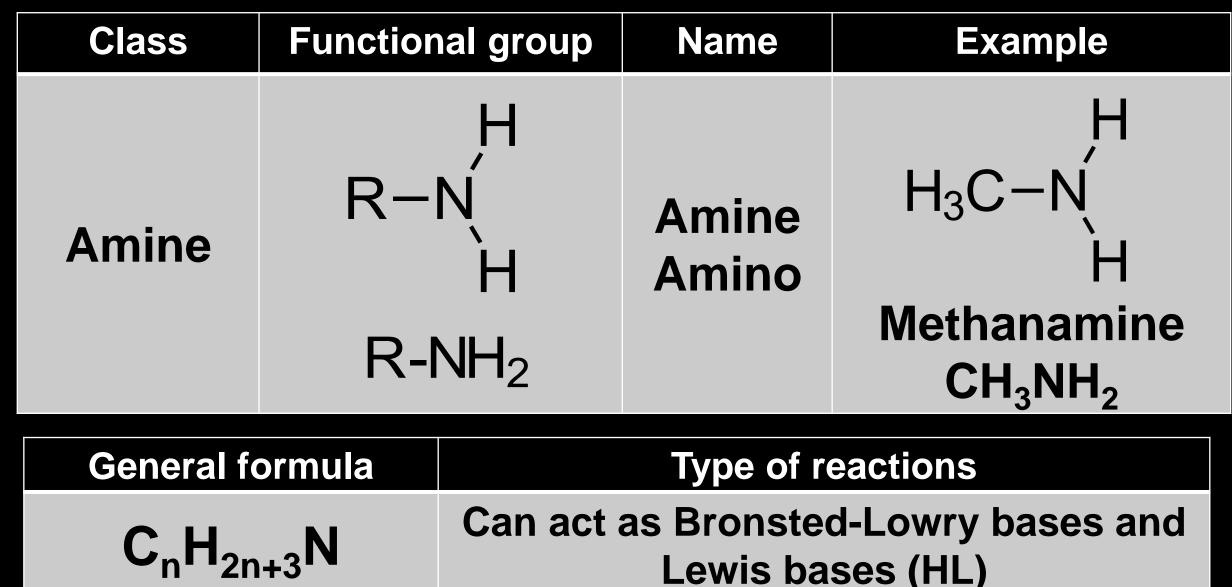


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Tutorials for IB Chemistry FUNCtional groups

Class	Functional group		Name	Example
Carboxylic acid	$R-C'_{OH}$ R-COOH R-CO2H		Carboxyl	$H - C'_{OH}$ Methanoic acid HCOOH or HCO ₂ H
General formula		Type of reactions		
$C_n H_{2n} O_2$		Nucleophilic substitution (with alcohols) Reduction (HL)		



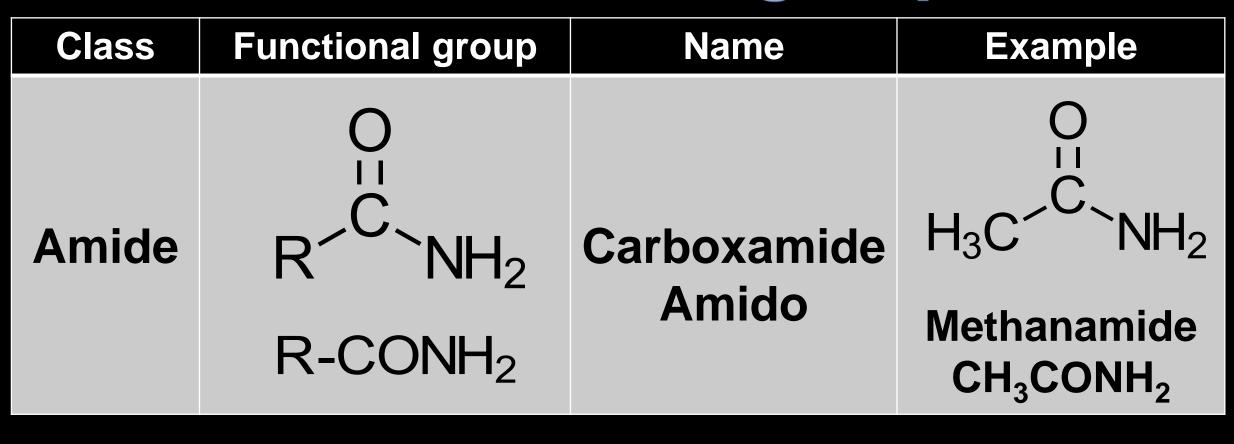


Chem

Tutorials for IB Chemistry

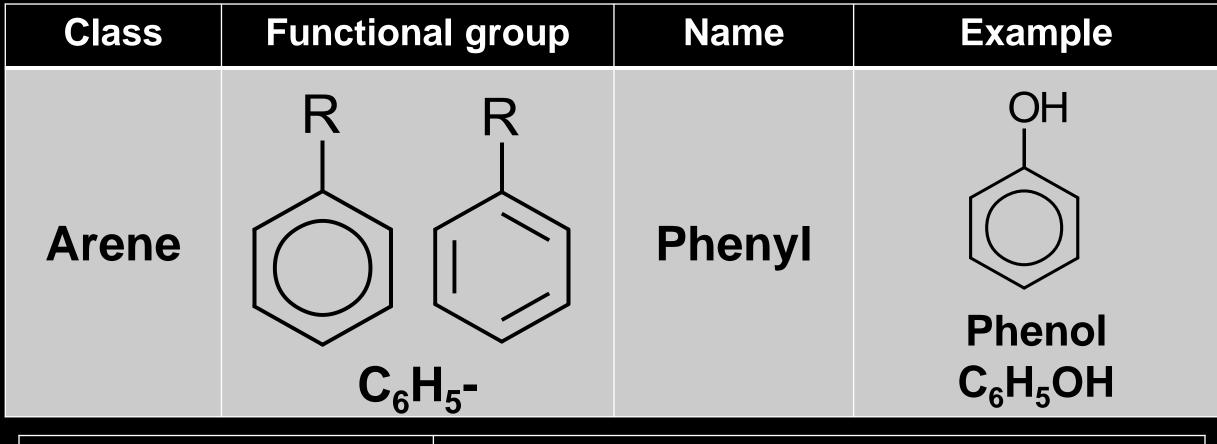


Functional groups



General formulaType of reactions $C_nH_{2n+1}NO$ Not covered in IB chemistry

Functional groups



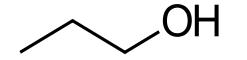
General formula	Type of reactions	
N/A	Reactions involving compounds with phenyl groups are covered in HL only	



Class	Functional group	Name	Example
Halogeno- alkane	R-X where X is a F, CI, Br or I atom	Fluoro- Chloro- Bromo- lodo-	H - C - CI $H - C - CI$ H

General formula	Type of reactions	
$C_n H_{2n+1} X$	Nucleophilic substitution	

Identifying functional groups



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CH₃CH₂CH₂OH

H-C-C-C-OH

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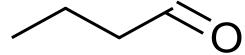
Tutorials for IB Chemistry

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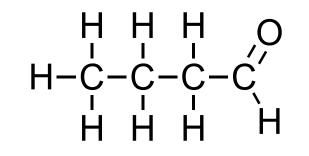
H-C-C-C-C-C-H

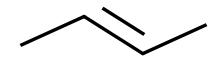
CH₃CH₂CH₂CH₂CH₂CH₂CH₃

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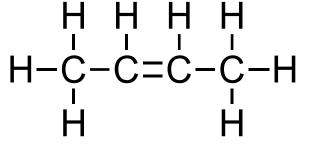


 $CH_3CH_2CH_2CHO$

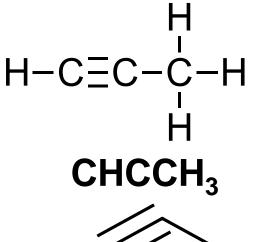




CH₃CHCHCH₃



Identifying functional groups



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 $H-\dot{C}-\dot{C}-\dot{C}-C-C-H$

CH₃COCH₂CH₂CH₃



MSJChem Identifying functional groups Tutorials for IB Chemistry НН $\begin{array}{cccc} H & H & O & H & H \\ H - C - C - C - C - O - C - C - H \end{array}$ ΗН $H-\dot{C}-\dot{C}-c$ H-Ċ-Ċ-O-Ċ-Ċ-H OH CH₃CH₂COOH CH₃CH₂OCH₂CH₃ CH₃CH₂COOCH₂CH₃ ŊН

> H-Ċ-Ċ-Ń H H H

CH₃CH₂NH₂

 \mathbf{MH}_{2}

CH₃CH₂CONH₂

 NH_2

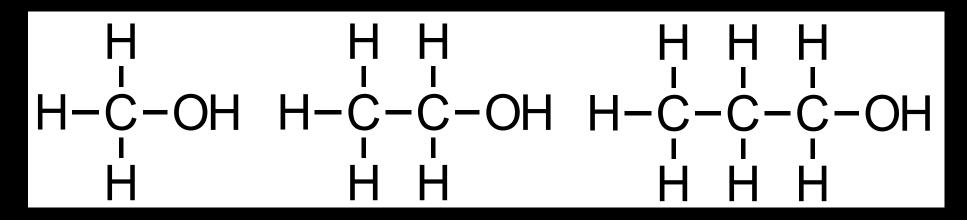
 C_6H_5CI

Homologous series



Homologous series

A homologous series is a series of organic compounds of the same family which differ by a common structural unit.

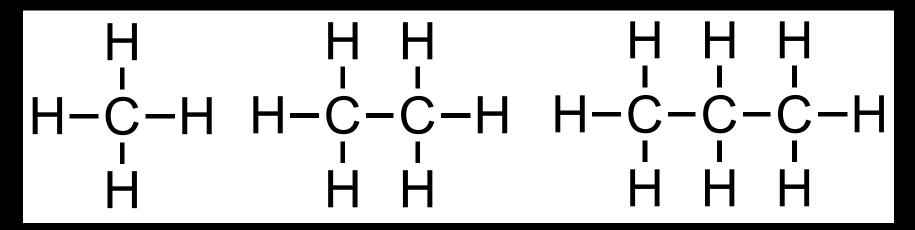


Functional group: hydroxyl (OH) – each member differs by CH₂



Homologous series

Members of a homologous series have similar chemical properties.



They also show a gradation in physical properties (such as the increasing boiling point of the alkanes).



Homologous series

Members of a homologous series:

- differ by a CH₂
- have the same general formula
- have similar chemical properties
- show a gradation (gradual increase) in physical properties such as boiling point

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Factors that affect the boiling points of organic compounds

Factors that affect the boiling points of organic compounds are:

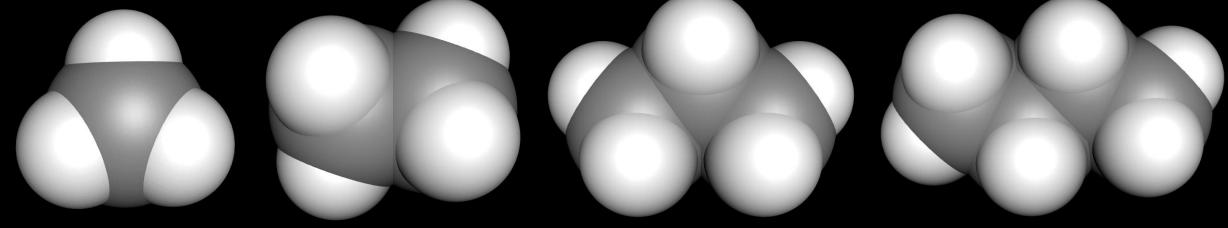
- Molar mass of the compound
- Structure of the molecule (straight-chain vs branched-chain isomers)
- Type of functional group (hydrogen bonding, dipole-dipole, London dispersion)

Boiling points of the alkanes

alkane	molar mass (gmol ⁻¹)	boiling point (°C)
methane	16	-164
ethane	30	-89
propane	44	-42
butane	58	-0.5
pentane	72	36
hexane	86	69
heptane	100	98
octane	114	125
nonane	128	151
decane	142	174

As the molar mass of the compound increases, the **boiling point** also increases.

MSJChem Tutorials for IB Chemistry Boiling points of the alkanes



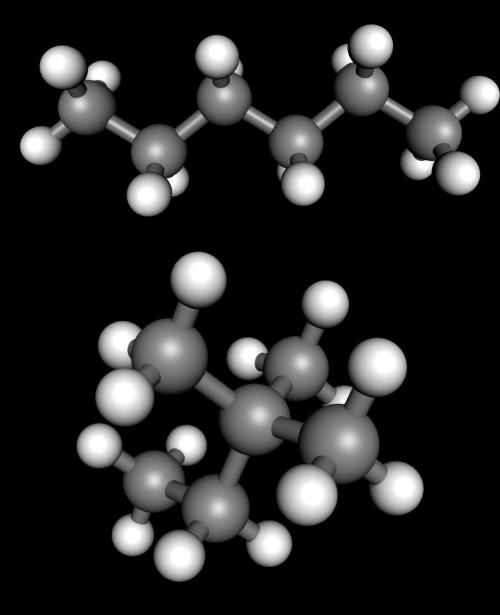
As the molar mass increases, the number of electrons within the molecule also increases.

Larger molecules are more polarisable and therefore have stronger London dispersion forces.

Larger molecules have an increased surface area over which the London dispersion forces can act.

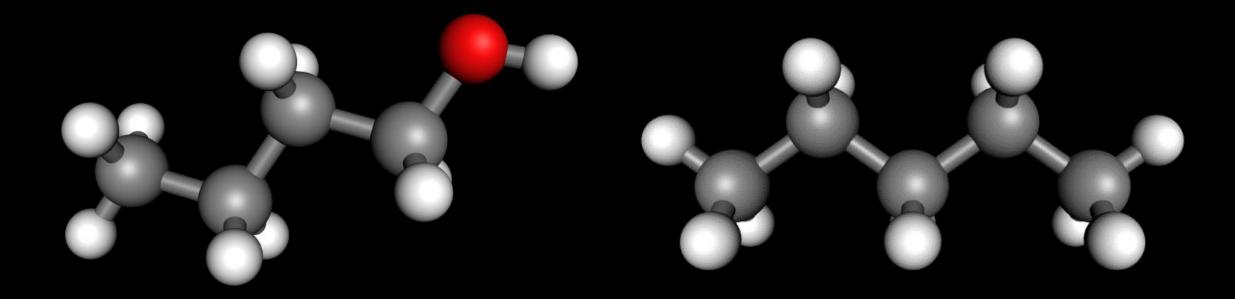


Branched vs straight-chain



Branched-chain isomers have lower boiling points than straight-chain isomers. The branches prevent the molecules getting close together (less surface area contact) which results in weaker London dispersion forces and a lower boiling point.





Butan-1-ol *M* = 74.12 g mol⁻¹ B.P. = 118 °C

Pentane *M* = 72.15 g mol⁻¹ B.P. = 36.1 °C

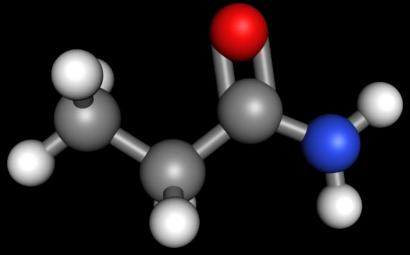
Functional group containing H bonded to O or N; hydrogen bonding between molecules

Functional group containing carbonyl group; dipole-dipole forces between molecules



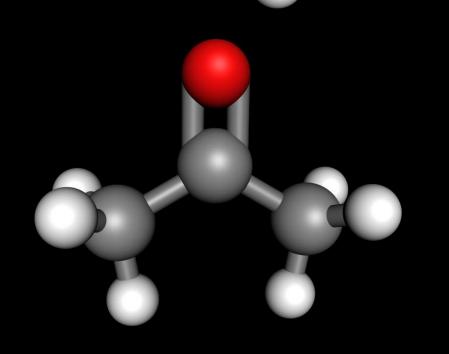
Effect of functional group

Alcohols, amides and carboxylic acids tend to have higher boiling points because they are able to form hydrogen bonds between their molecules.





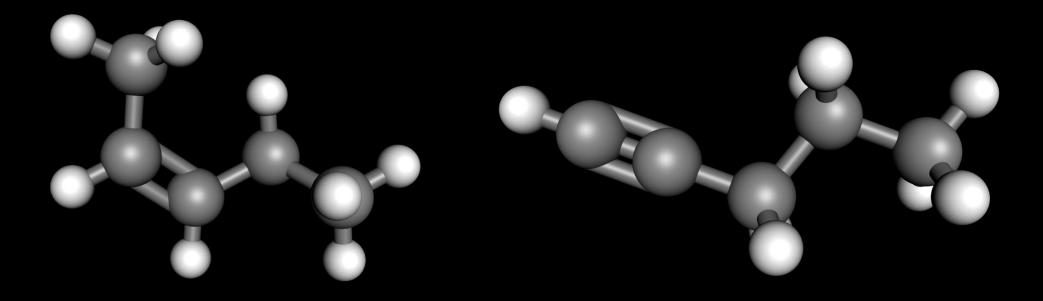
Tutorials for IB Chemistry Effect of functional group

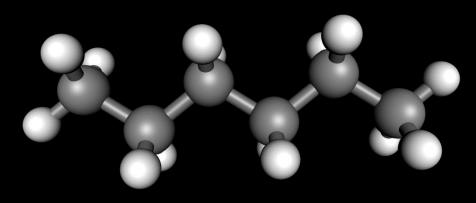


Aldehydes, ketones, and esters have dipole-dipole forces between their molecules.



Effect of functional group





Alkanes, alkenes and alkynes have London dispersion forces between their molecules.



low volatility Increasing boiling point

high volatility

Compounds that can form hydrogen bonds (alcohols, amides, amines, carboxylic acids) **Compounds that can form dipole**dipole forces (aldehydes, ketones, esters, ethers, nitriles) **Compounds that can form only** London dispersion forces (alkanes, alkenes, alkynes)

Effect of functional group

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Naming alkanes

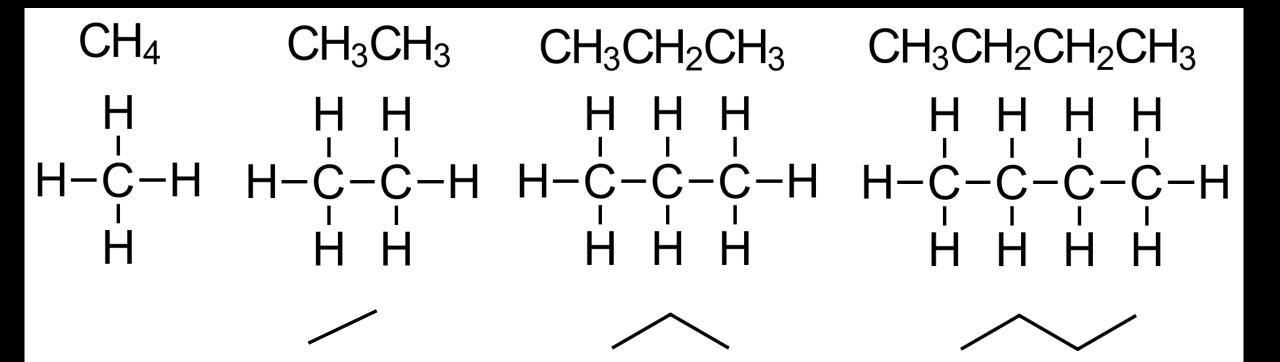




- Alkanes are saturated hydrocarbons (C-C single bonds).
- They have the general formula $C_n H_{2n+2}$ Alkanes have low reactivity for two reasons:
- the C-H bonds are non-polar (weakly polar).
- the C-C and C-H bonds are quite strong.
 Alkanes undergo combustion and free-radical substitution reactions.



Number of C atoms in the longest chain	Root/stem	Number of C atoms in the longest chain	Root/stem
1	meth-	6	hex-
2	eth-	7	hept-
3	prop-	8	oct-
4	but-	9	non-
5	pent-	10	dec-



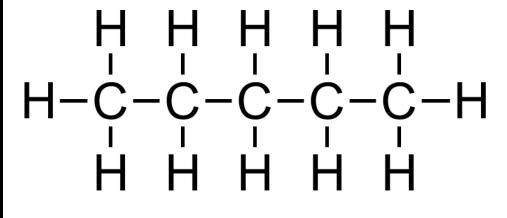
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MethaneEthanePropaneButane CH_4 C_2H_6 C_3H_8 C_4H_{10}

Pentane C_5H_{12}



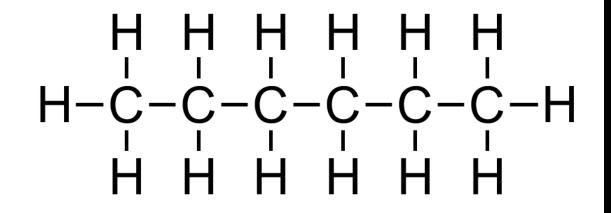


$CH_3CH_2CH_2CH_2CH_3$

Tutorials for IB Chemistry

Naming alkanes

$CH_3CH_2CH_2CH_2CH_2CH_3$

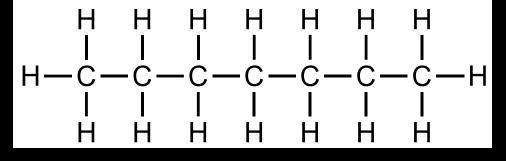


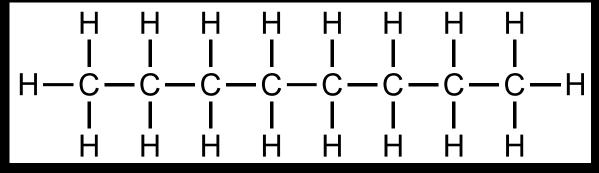
Hexane $C_{6}H_{14}$

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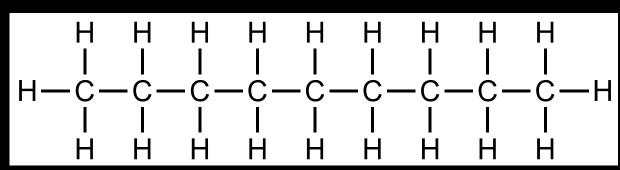
Naming alkanes

Heptane C₇H₁₆

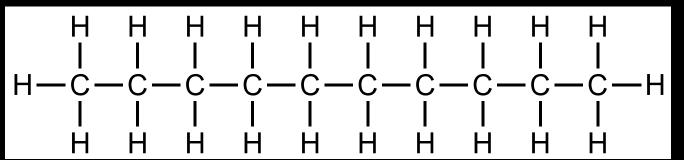




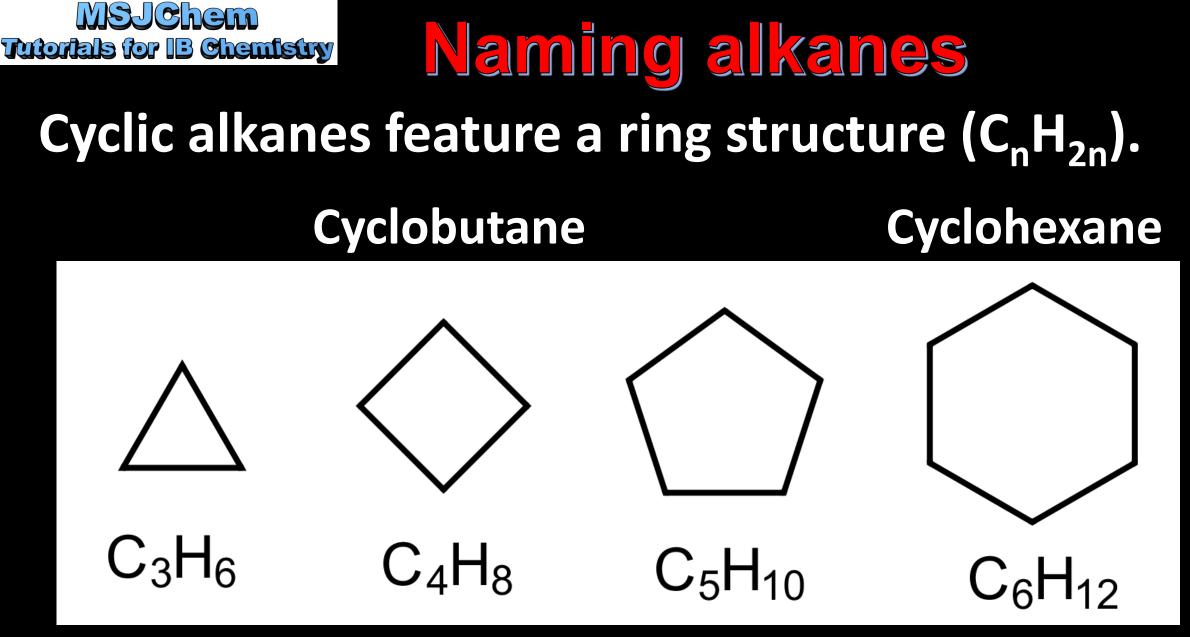
Octane C₈H₁₈



Nonane C₉H₂₀



Decane $C_{10}H_{22}$



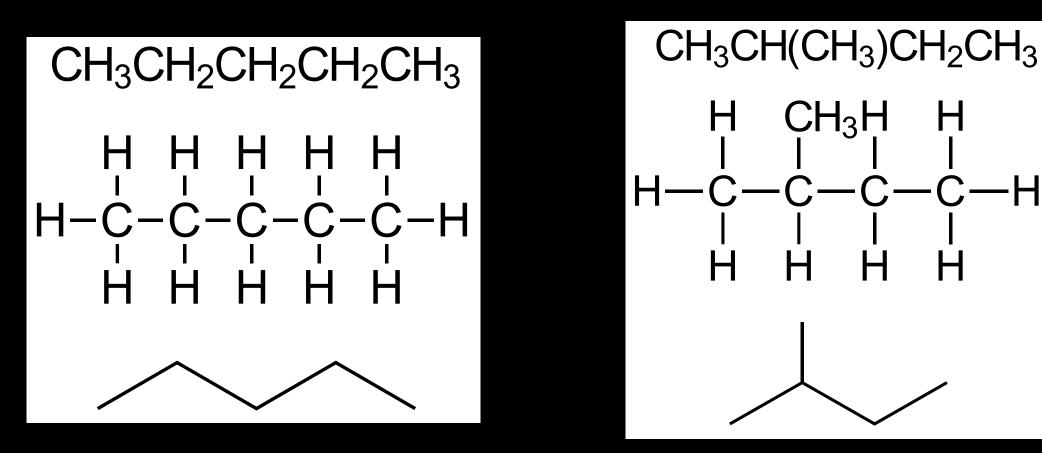
Cyclopropane

Cyclopentane

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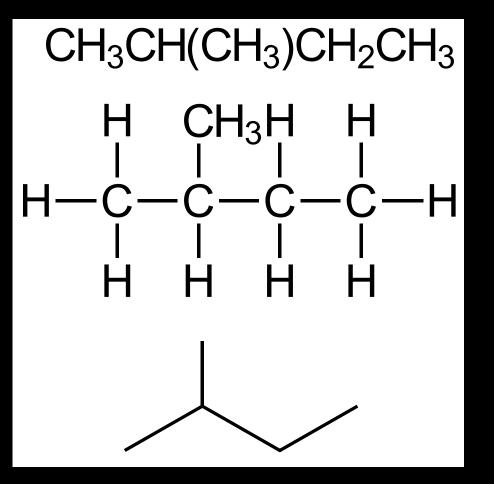
Naming branchedchain alkanes

Branched-chain alkanes Branched-chain alkanes have branches which are alkyl substituents (- CH_3 , - C_2H_5).



MSJChem prials for IB Chemistry Branched-Chain alkanes

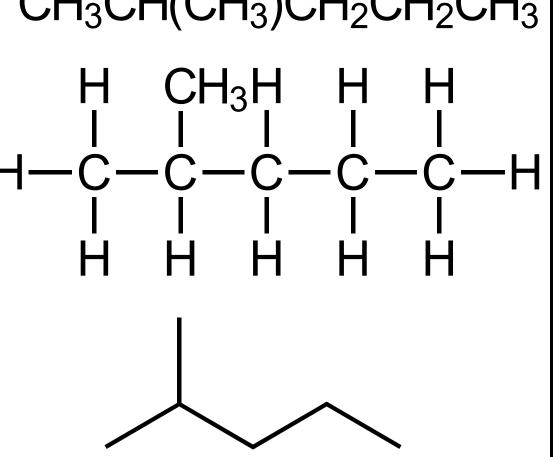
1. Identify the longest continuous carbon chain.



2. Identify and number the position(s) of the branch(es), giving them the lowest number possible.

3. If more than one alkyl group is attached to the main chain, use the prefixes di-, tri-, etc.

2-methylbutane



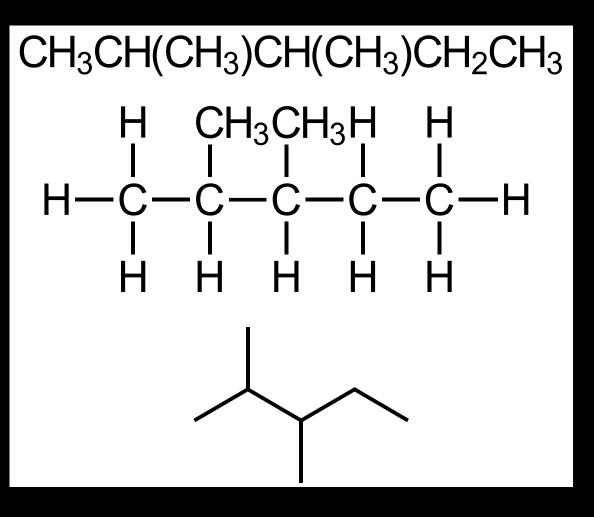


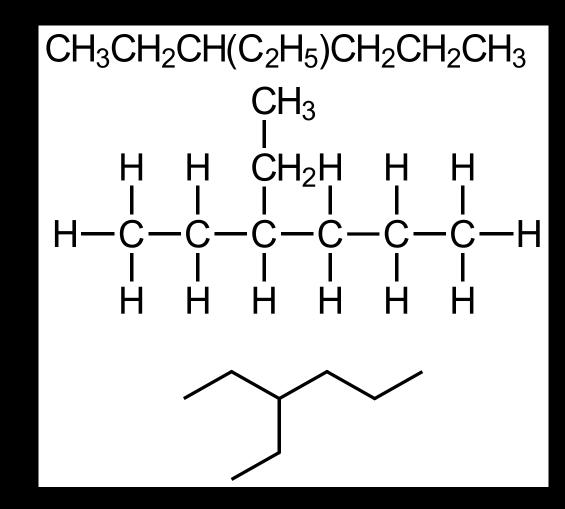
2,2-dimethylpropane

H CH_3H

 CH_3H

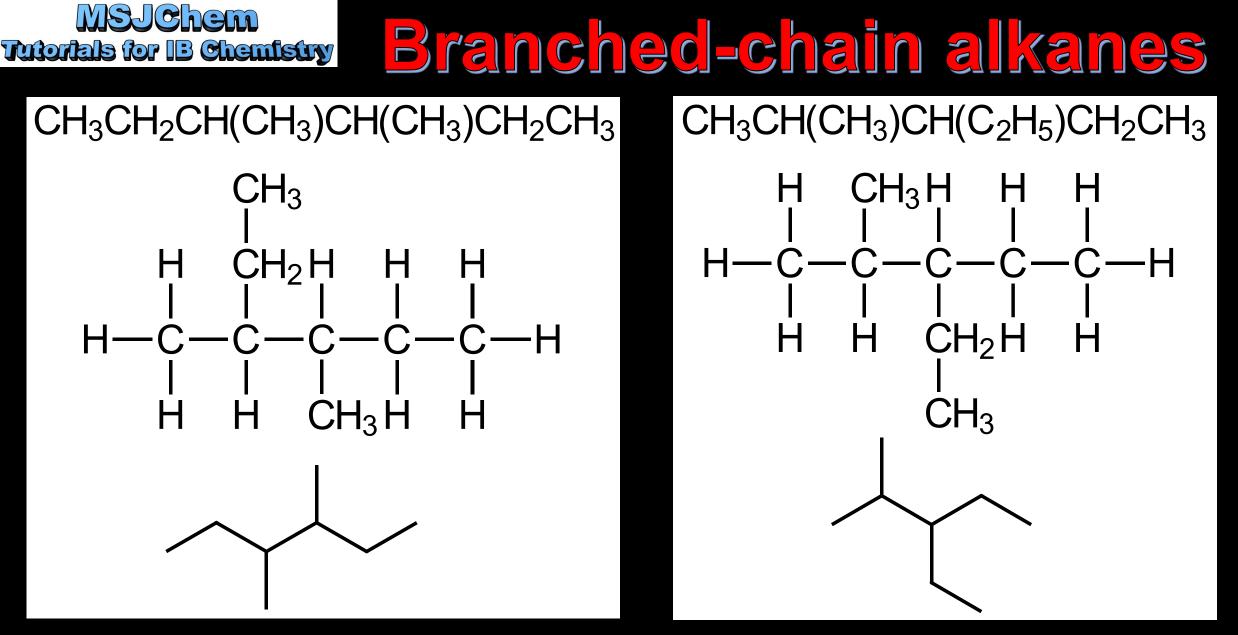
MSJChem Tutorials for IB Chemistry Branched-chain alkanes





2,3-dimethylpentane

3-ethylhexane



3,4-dimethylhexane

3-ethyl-2-methylpentane

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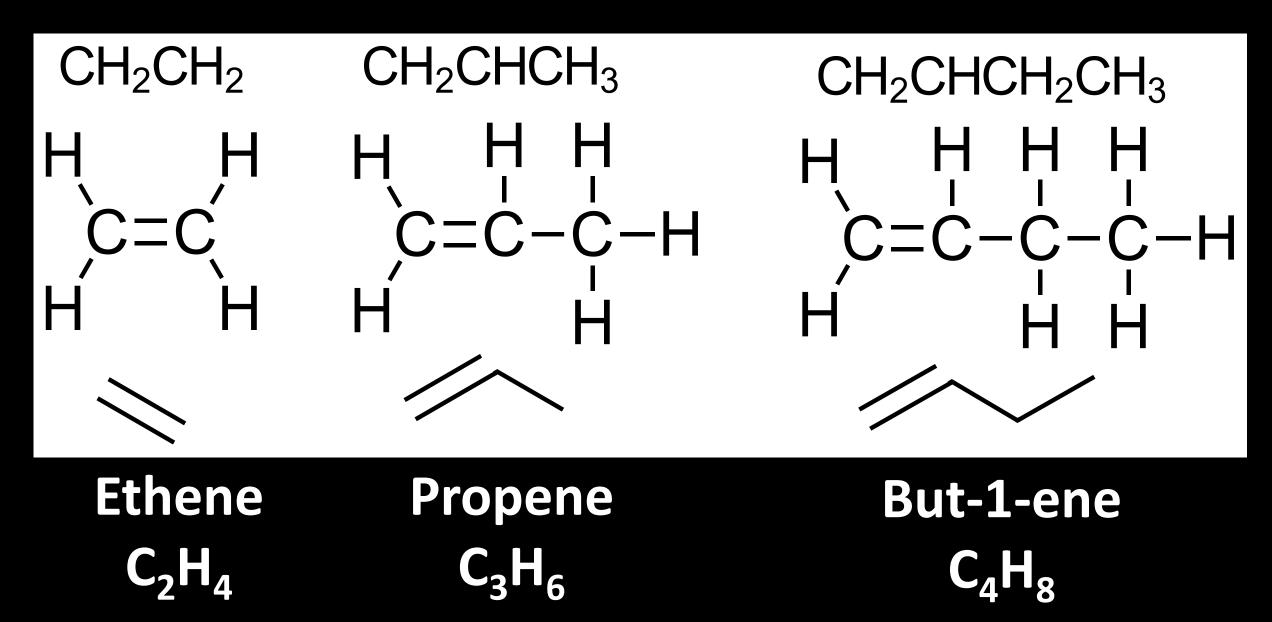
Naming alkenes



- Alkenes are unsaturated hydrocarbons (C-C double bonds).
- They have the general formula C_nH_{2n}
- Alkenes are more reactive than the alkanes for two
- reasons:
- the electron density of the C=C bond attracts electrophiles
- the pi bond is weaker than the sigma bond Alkenes undergo electrophilic addition reactions.

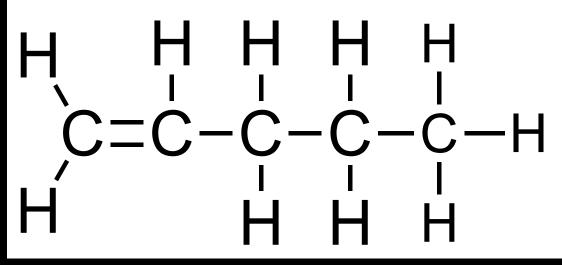
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CH₂CHCH₂CH₂CH₃



CH₃CHCHCH₂CH₃

Pent-1-ene C_5H_{10}

Pent-2-ene C_5H_{10}

Hex-1-ene

Tutorials for IB Chemistry

Hex-2-ene

 $CH_3CH_2CHCHCH_2CH_3$

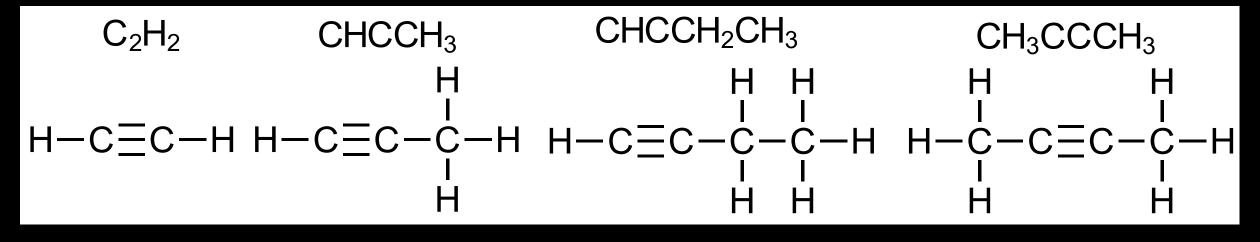
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Naming alkynes

MSJChem Tutorials for IB Chemistry

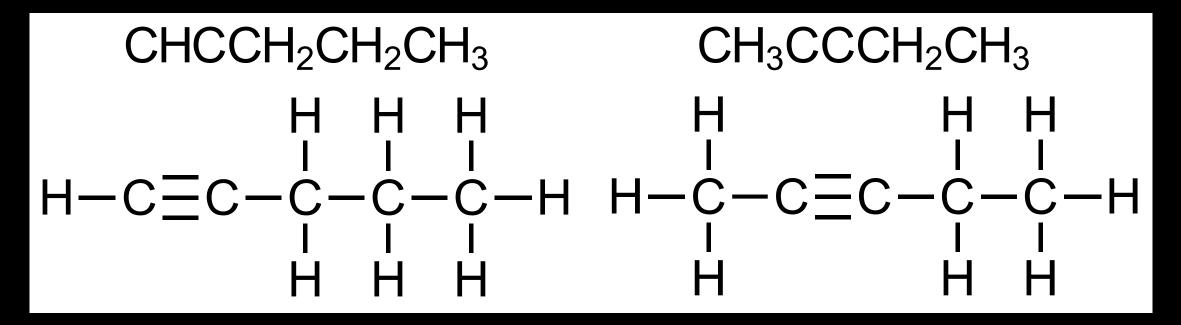
Alkynes are unsaturated hydrocarbons (C-C triple bonds). They have the general formula C_nH_{2n-2} Alkynes have similar reactivity to the alkenes. Alkynes undergo electrophilic addition reactions.

Naming alkynes



But-2-yne

Ethyne Propyne But-1-yne

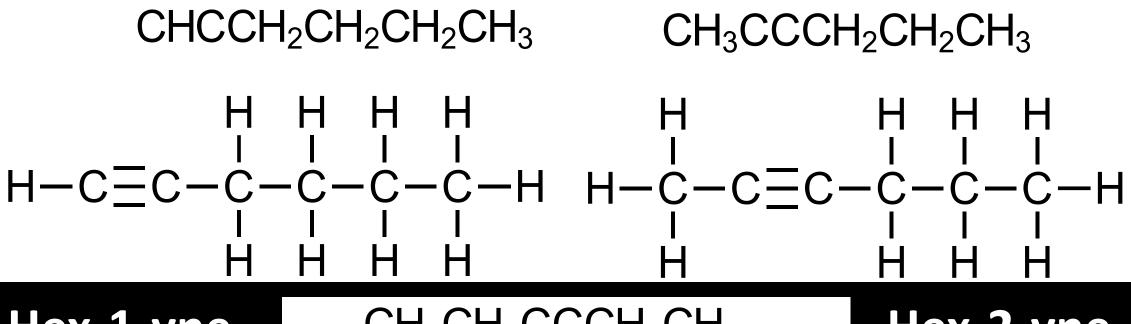


Pent-1-yne

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Pent-2-yne



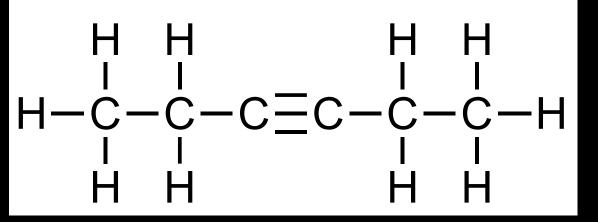
Hex-1-yne

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CH₃CH₂CCCH₂CH₃

Hex-2-yne



Hex-3-yne

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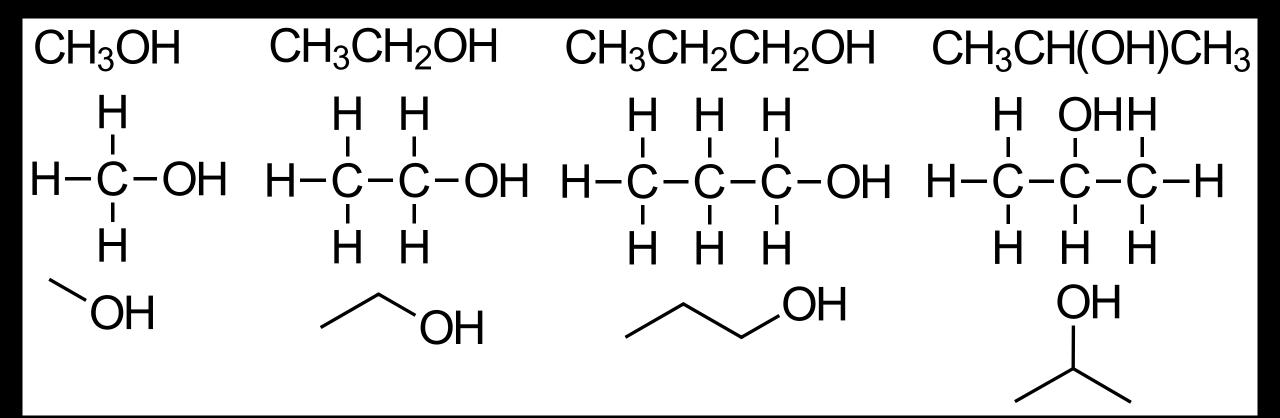
Naming alcohols



Naming alcohols

- Alcohols are organic compounds composed of carbon, hydrogen and oxygen.
- They have the hydroxyl functional group (-OH).
- Alcohols have the general formula $C_nH_{2n+1}OH$
- Alcohols undergo combustion reactions and oxidation reactions.
- They also undergo nucleophilic substitution reactions with carboxylic acids to form esters.

Naming alcohols



MethanolEthanolPropan-1-olPropan-1-ol CH_3OH C_2H_5OH C_3H_7OH O

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Propan-2-ol C_3H_7OH

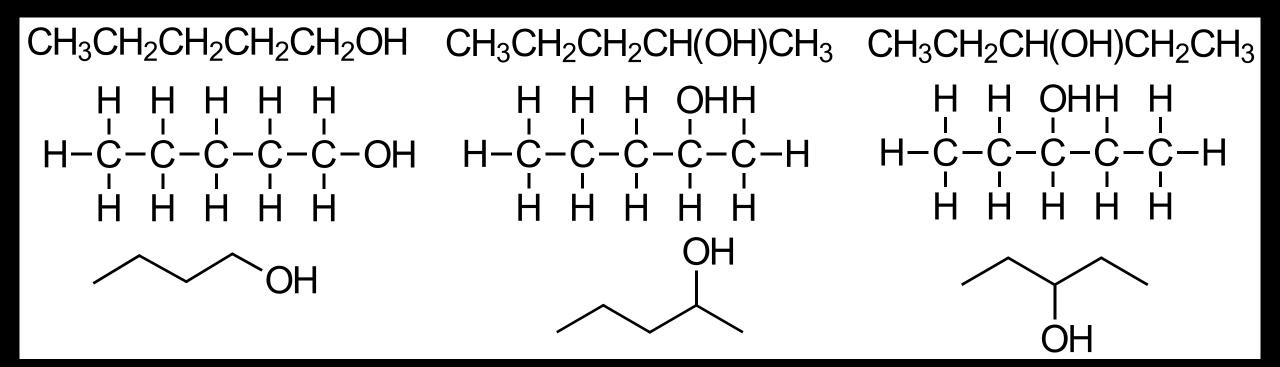
MSJChem Naming alcohols Tutorials for IB Chemistry $CH_3CH_2CH(OH)CH_3$ CH₃CH₂CH₂CH₂OH нннн H H OHH H-C-C-C-OH H-C-C-C-C-HНН OH **Butan-1-ol** Butan-2-ol

C₄H₉OH

Butan-2-ol C_4H_9OH

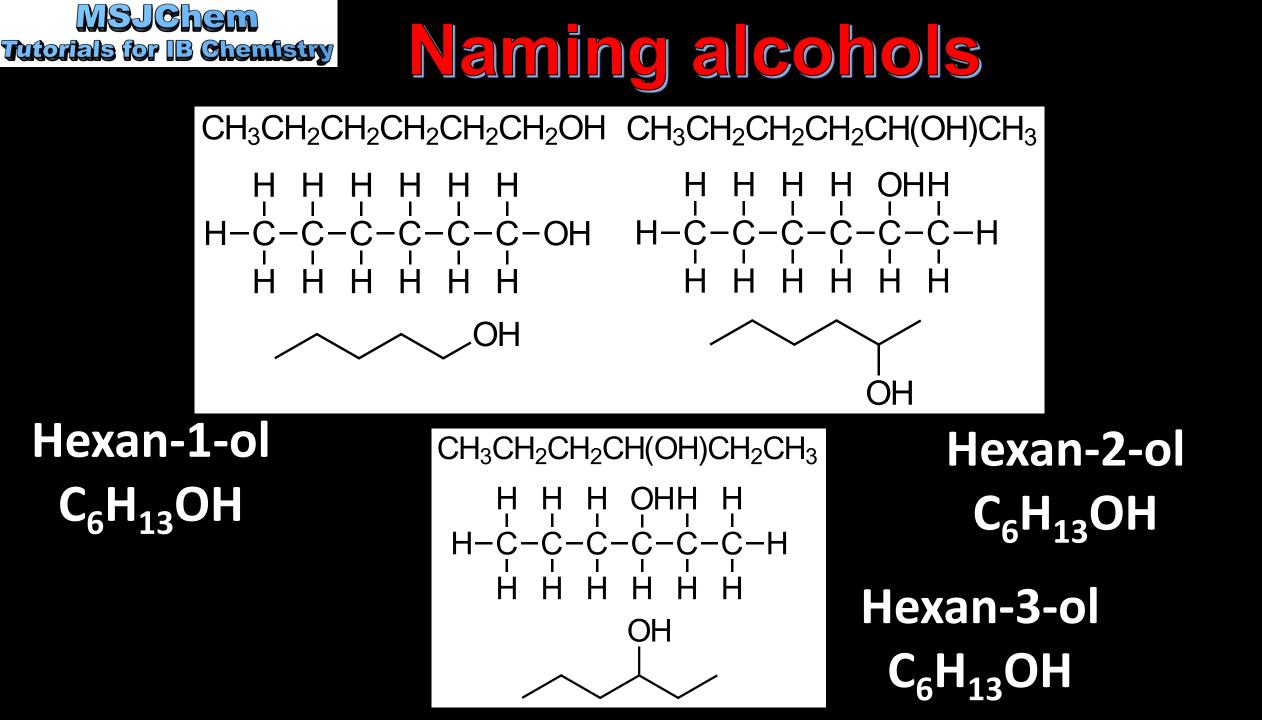
MSJChem Tutorials for IB Chemistry

Naming alcohols



Pentan-1-ol $C_5H_{11}OH$

Pentan-2-ol $C_5H_{11}OH$ Pentan-3-ol $C_5H_{11}OH$



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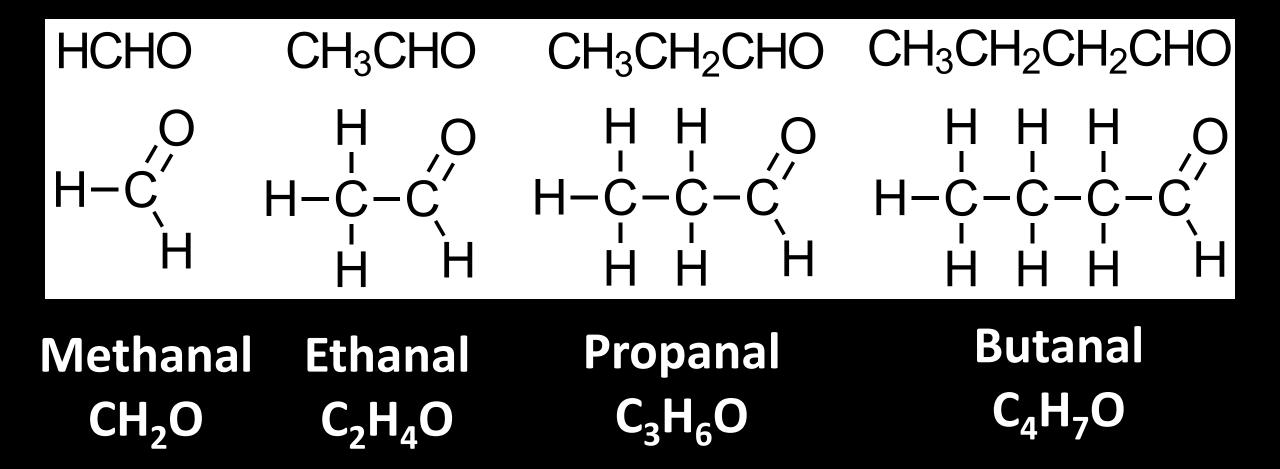
Naming aldehydes and ketones

chem

Tutorials for IB Chemistry Naming aldenydes and ketones

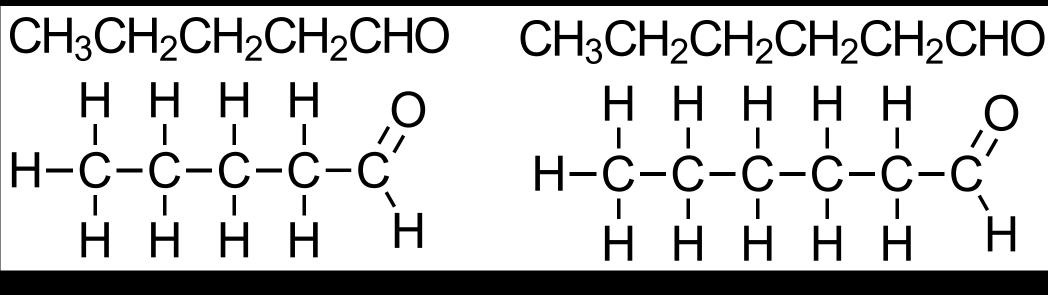
- Aldehydes and ketones both contain a carbonyl group (C=O).
- Aldehydes contain an aldehyde group (R-CHO) and ketones contain a ketone group (R-CO-R).
- Aldehydes undergo oxidation to form carboxylic acids. Ketones do not undergo oxidation.
- Both are polar molecules because of the difference in
- electronegativity between the C and O of the carbonyl
- group.

Naming aldehydes and ketones Tutorials for IB Chemistry



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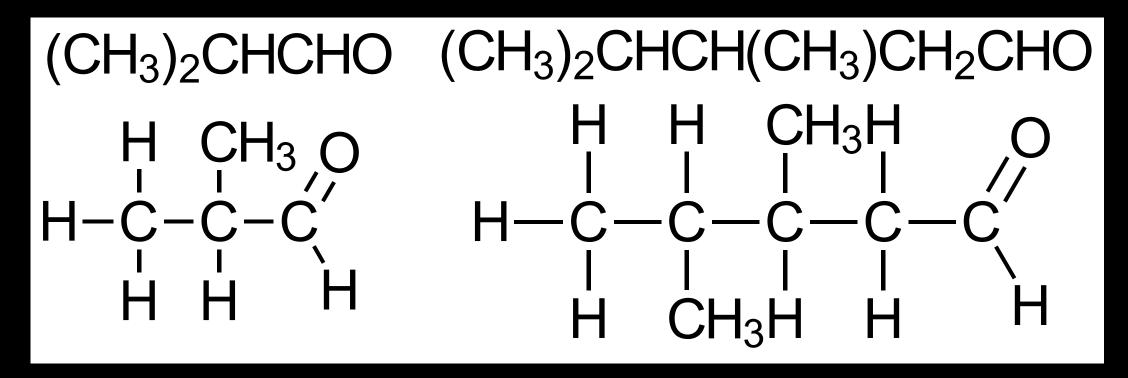
MSJChem Tutorials for IB Chemistry Naming aldehydes and ketones



Pentanal $C_5H_{10}O$

Hexanal $C_6H_{12}O$

MSJChem Tutorials for IB Chemistry Naming aldehydes and ketones



2-methylpropanal

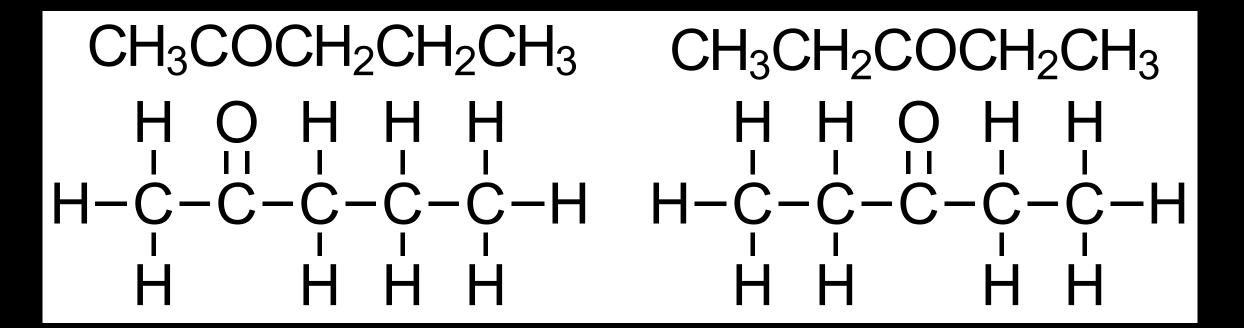
3,4-dimethylpentanal

MSJChem Tutorials for IB Chemistry Naming aldehydes and ketones CH₃COCH₃ CH₃COCH₂CH₃

Propanone C_3H_6O

Butan-2-one C_4H_8O

Naming aldehydes and ketones Tutorials for IB Chemistry

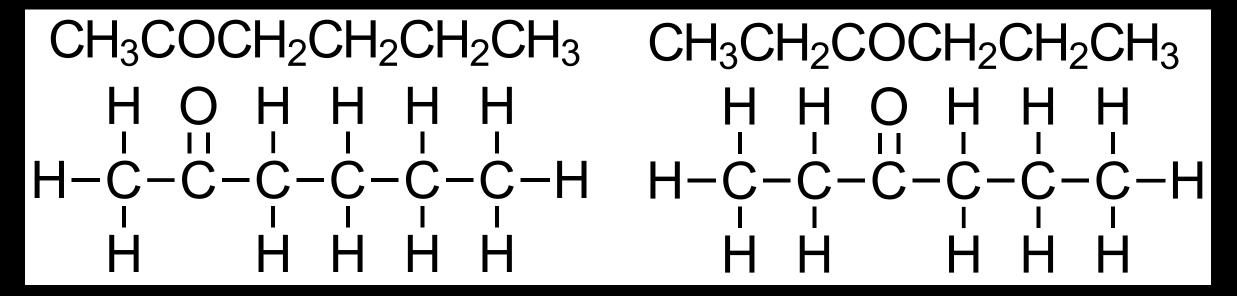


Pentan-2-one $C_5H_{10}O$

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Pentan-3-one $C_5H_{10}O$

Naming aldehydes and ketones Tutorials for IB Chemistry



Hexan-2-one $C_{6}H_{12}O$

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Hexan-3-one $C_{6}H_{12}O$

Naming carboxylic acids

MSJChem Tutorials for IB Chemistry Naming CarlooXylic acids Carboxylic acids are organic acids that contain the carboxyl functional group (COOH or CO₂H). They have the general formula $C_nH_{2n+1}COOH$. Carboxylic acids can be produced by the complete oxidation of a primary alcohol. They undergo nucleophilic substitution reactions with alcohols to produce esters.

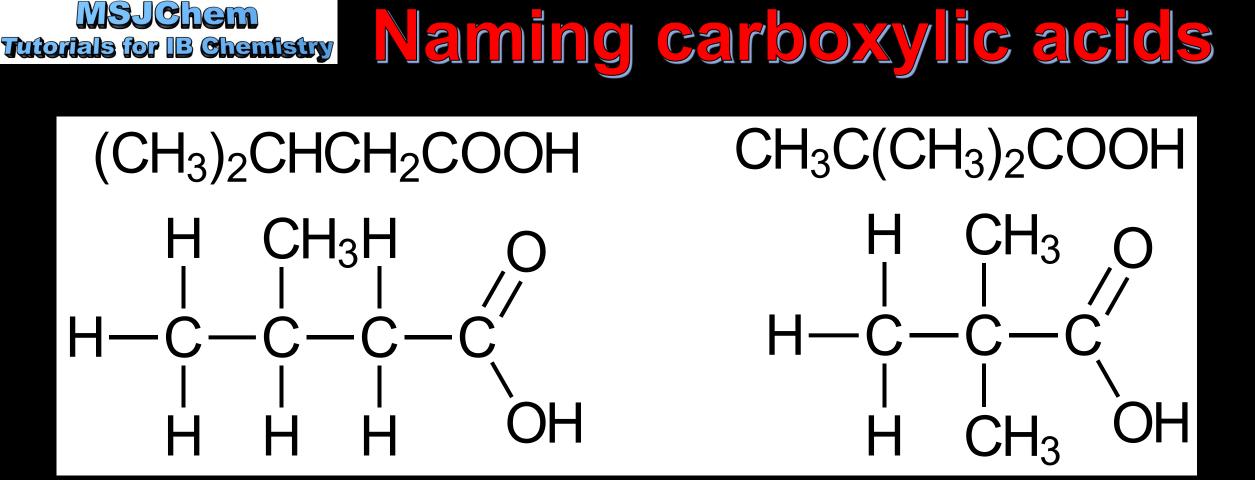
CH₃CH₂CH₂CH₂CH₂COOH CH₃CH₂CH₂CH₂COOH $\begin{array}{ccccccc} H & H & H & H & H & O \\ I & I & I & I & I & I \\ H - C - C - C - C - C - C & O \\ I & I & I & I & O \end{array}$ OH OH нннн нннн

Tutorials for IB Chemistry Naming CarlooXylic acids

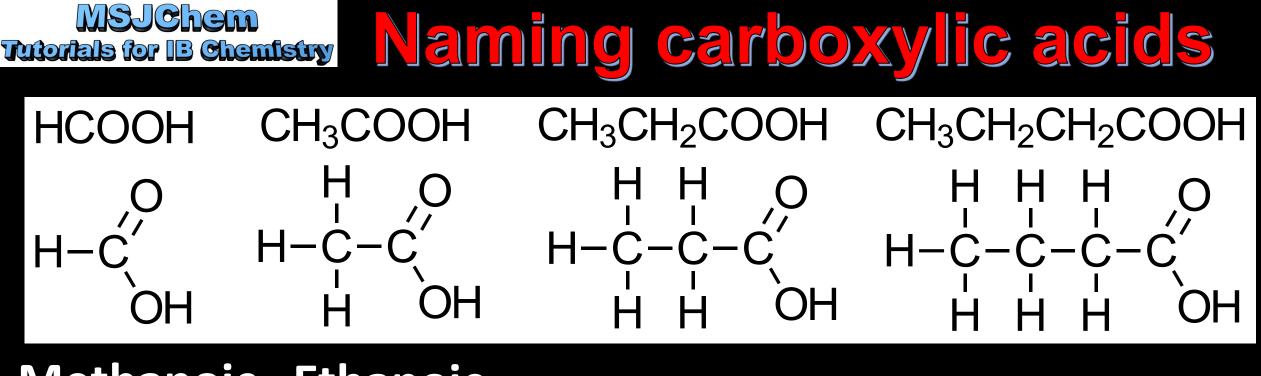
Pentanoic acid C₄H₉COOH

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Hexanoic acid $C_5H_{11}COOH$



3-methylbutanoic acid 2,2-dimethylpropanoic acid



MethanoicEthanoicPropanoic acidButanoic acidacidacid C_2H_5COOH C_3H_7COOH HCOOH CH_3COOH C_2H_5COOH C_2H_5COOH C_3H_7COOH

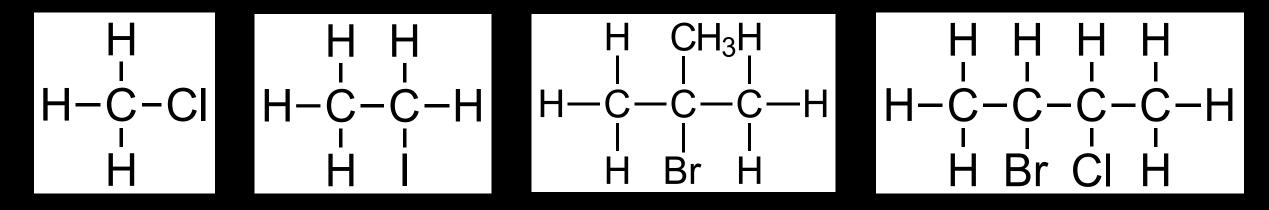
Naming

halogenoalkanes



Naming halogenoalkanes

Halogenoalkanes are alkanes in which one (or more) hydrogen atoms have been replaced with halogen atoms (fluorine, chlorine, bromine, iodine).



Halogenoalkanes are produced in nucleophilic substitution reactions with alkanes and electrophilic addition reactions with alkenes.

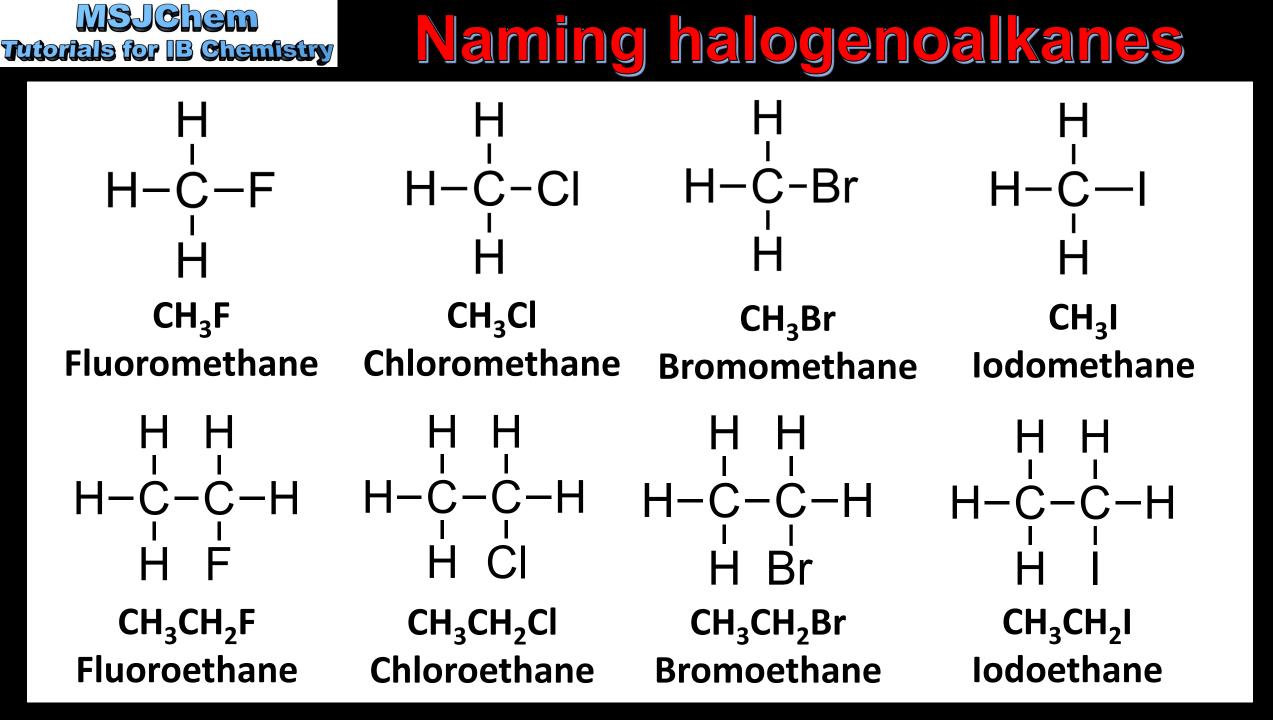
The root is based on the longest chain containing the halogen atom. The halogen atom defines the halo prefix.

Naming halogenoalkanes

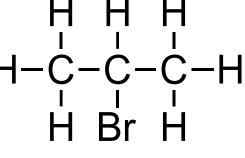
The chain is numbered to give the halogen the lowest possible number.

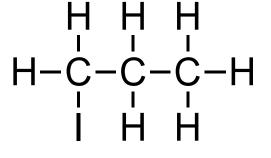
Halogen	Prefix
Fluorine	Fluoro-
Chlorine	Chloro-
Bromine	Bromo-
lodine	lodo-

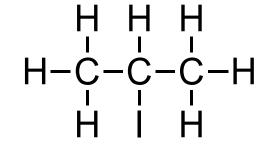
Number of C atoms in the longest chain containing the halogen atom	Root/stem
1	methane
2	ethane
3	propane
4	butane
5	pentane
6	hexane



Naming halogenoalkanes







CH₂BrCH₂CH₃ 1-bromopropane

CH₃CHBrCH₃ 2-bromopropane

CH₂ICH₂CH₃ **1-iodopropane**

НННН

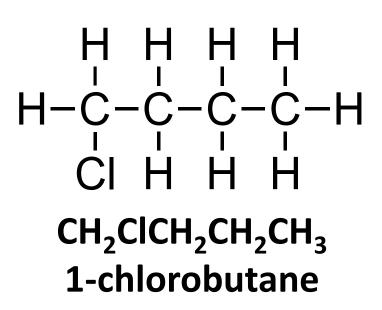
H-C-C-C-C-H

CH₃CHClCH₂CH₃

2-chlorobutane

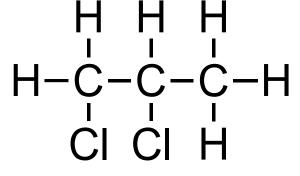
H CI

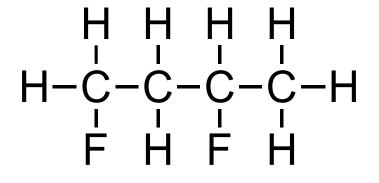
CH₃CHICH₃ 2-iodopropane



Naming halogenoalkanes

H H H-C-C-H Br Br

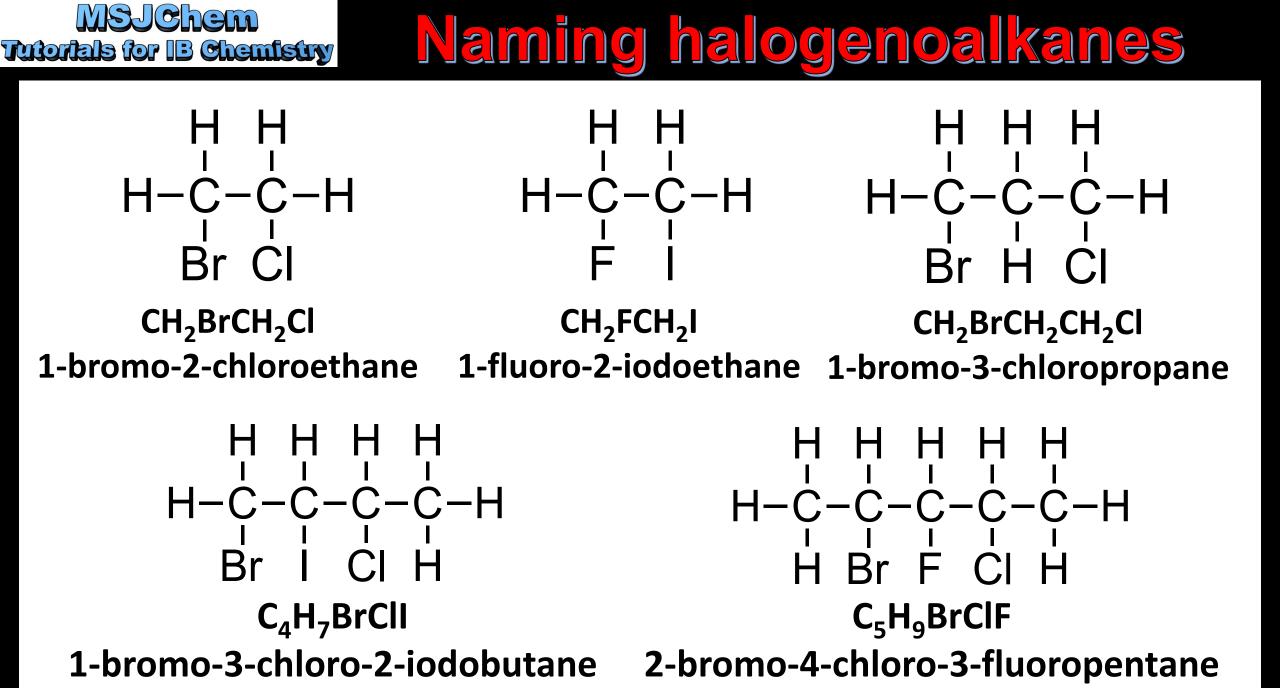




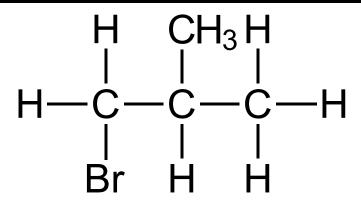
CH₂BrCH₂Br 1,2-dibromoethane CH₂CICHCICH₃ 1,2-dichloropropane

CH₂FCH₂CHFCH₃ 1,3-difluorobutane

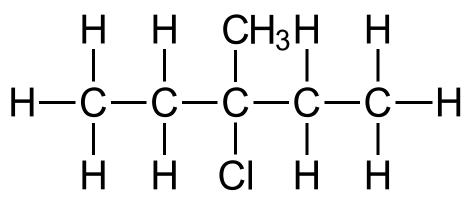
H H Br Br H H H-C-C-C-C-C-C-C-H H H Br Br H H $C_6H_{10}Br_4$ 3,3,4,4-tetrabromohexane



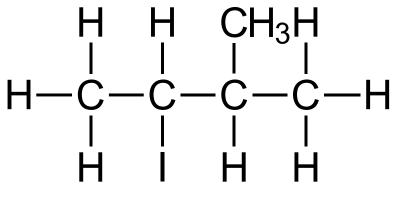
Naming halogenoalkanes



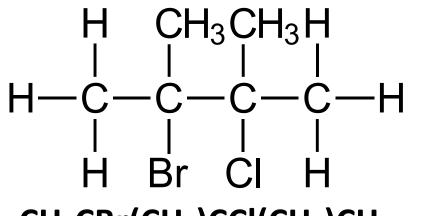
CH₂BrCH(CH₃)CH₃ 1-bromo-2-methylpropane



CH₃CH₂CCl(CH₃)CH₂CH₃ 3-chloro-3-methylpentane



CH₃CHICH(CH₃)CH₃ 2-iodo-3-methylbutane



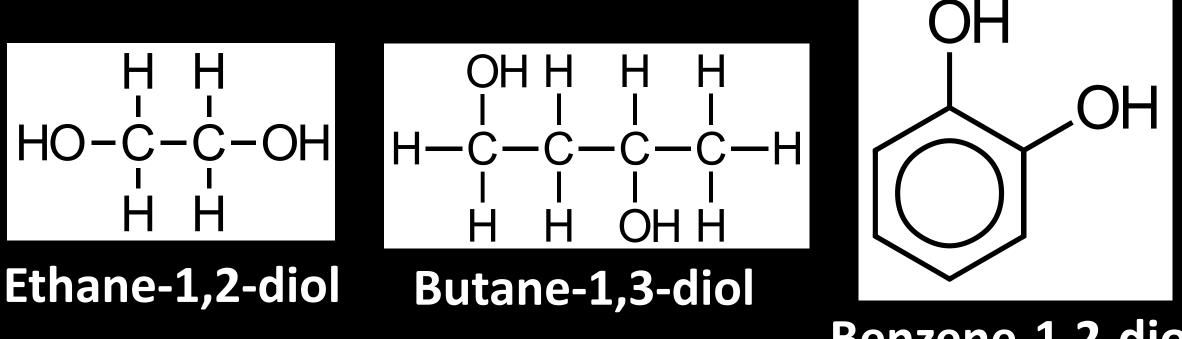
CH₃CBr(CH₃)CCl(CH₃)CH₃ 2-bromo-3-chloro-2,3-dimethylbutane

Diols and dicarboxylic acids





A diol is a compound that contains two hydroxyl (OH) groups.

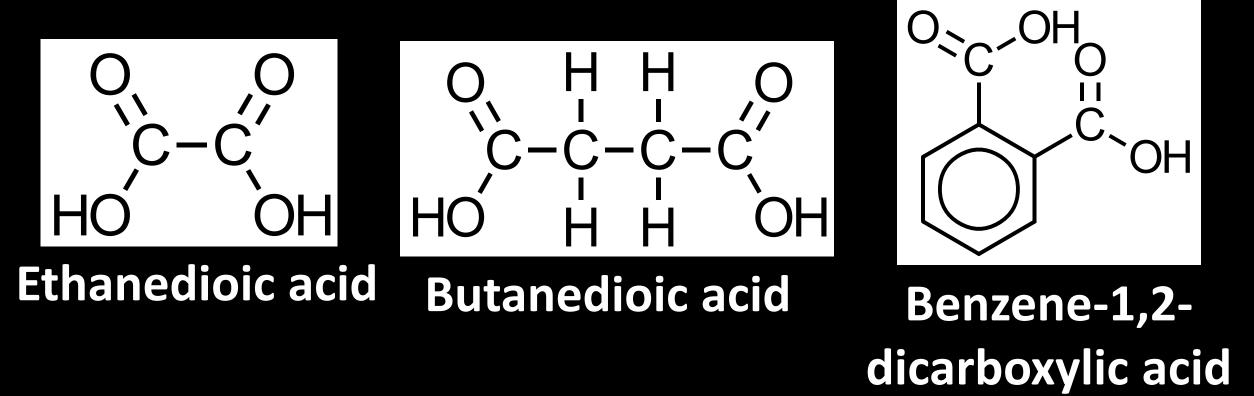


Benzene-1,2-diol



Dicarboxylic acids

A dicarboxylic acid is a compound that contains two carboxyl (COOH) groups.

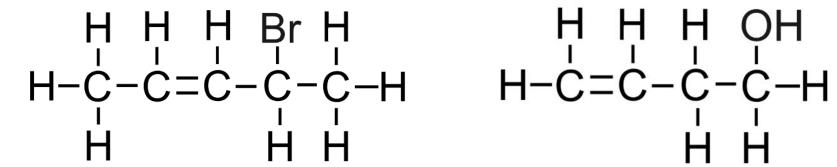


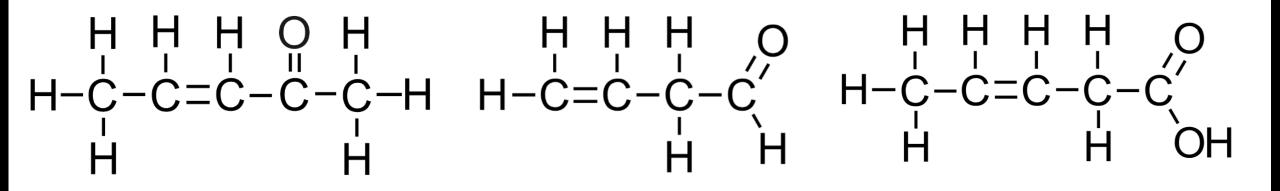
Naming unsaturated compounds

Apply IUPAC nomenclature to mono-unsaturated compounds that have up to six carbon atoms in the parent chain and contain one type of the following functional groups: halogeno, hydroxyl, carbonyl, carboxyl.

Tutorials for IB Chemistry Naming Unsaturated compounds

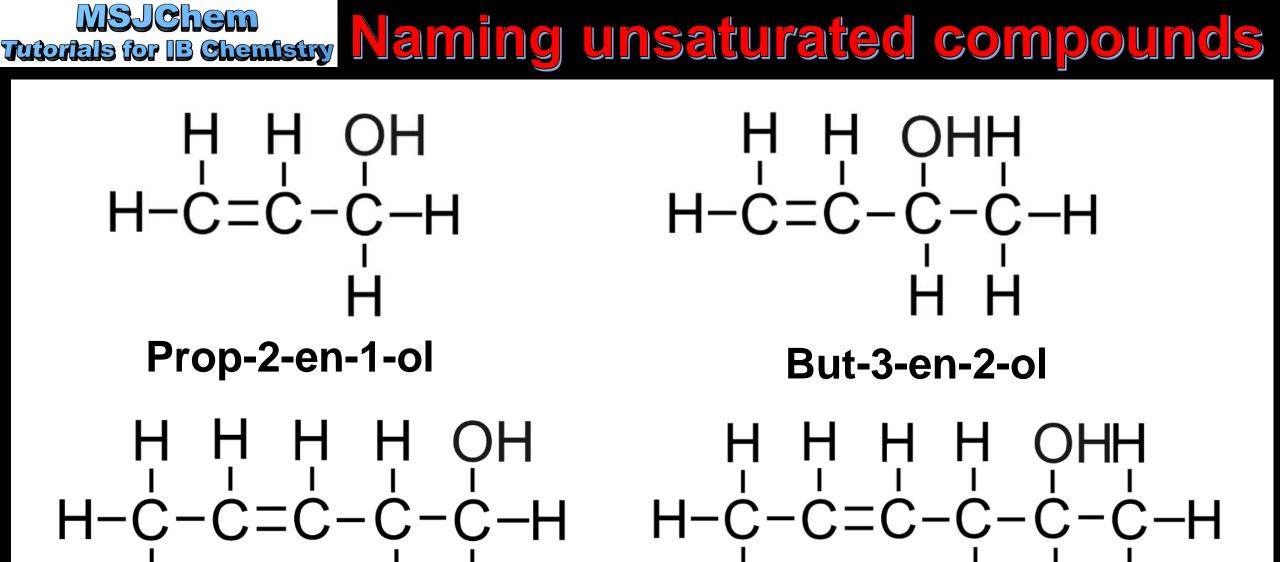
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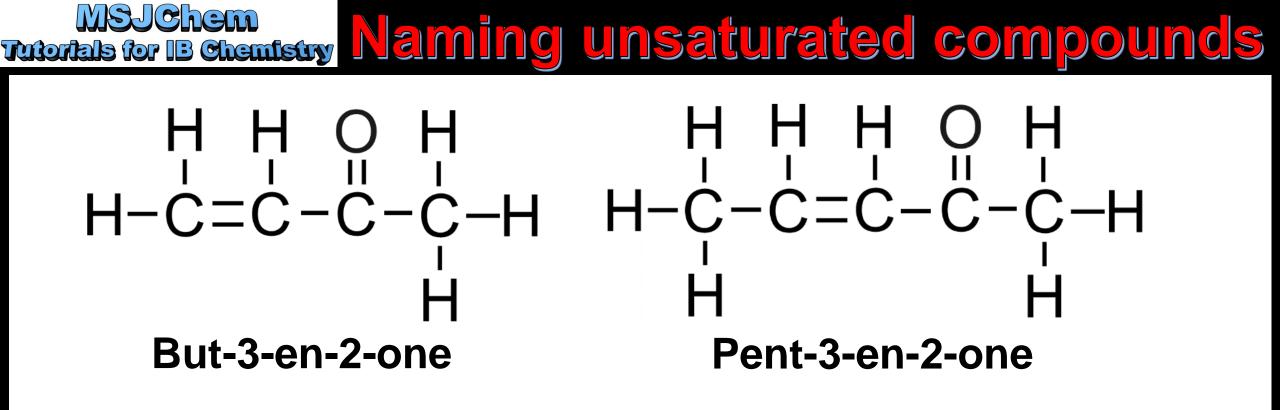
MSJChem Tutorials for IB Chemistry Naming Unsaturated compounds

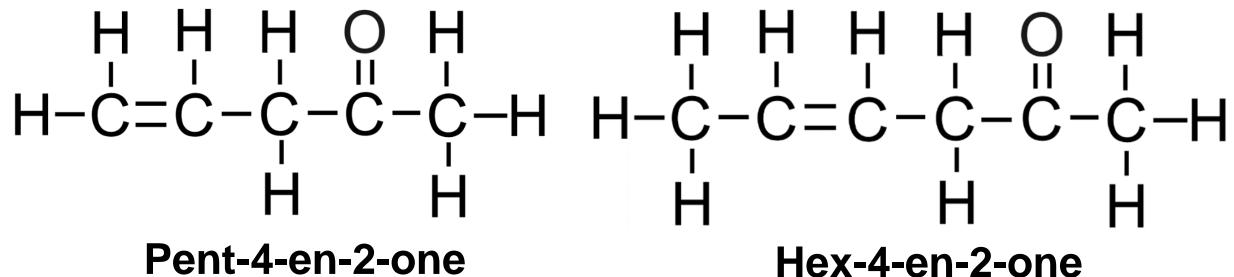
Priority	Class / functional group	Suffix / prefix
1	Carboxylic acid / carboxyl	-oic acid
2	Aldehyde / carbonyl	-al
3	Ketone / carbonyl	-one
4	Alcohol / hydroxyl	-ol
5	Alkene	-ene
6	Halogenoalkane / halogeno	chloro / bromo / iodo

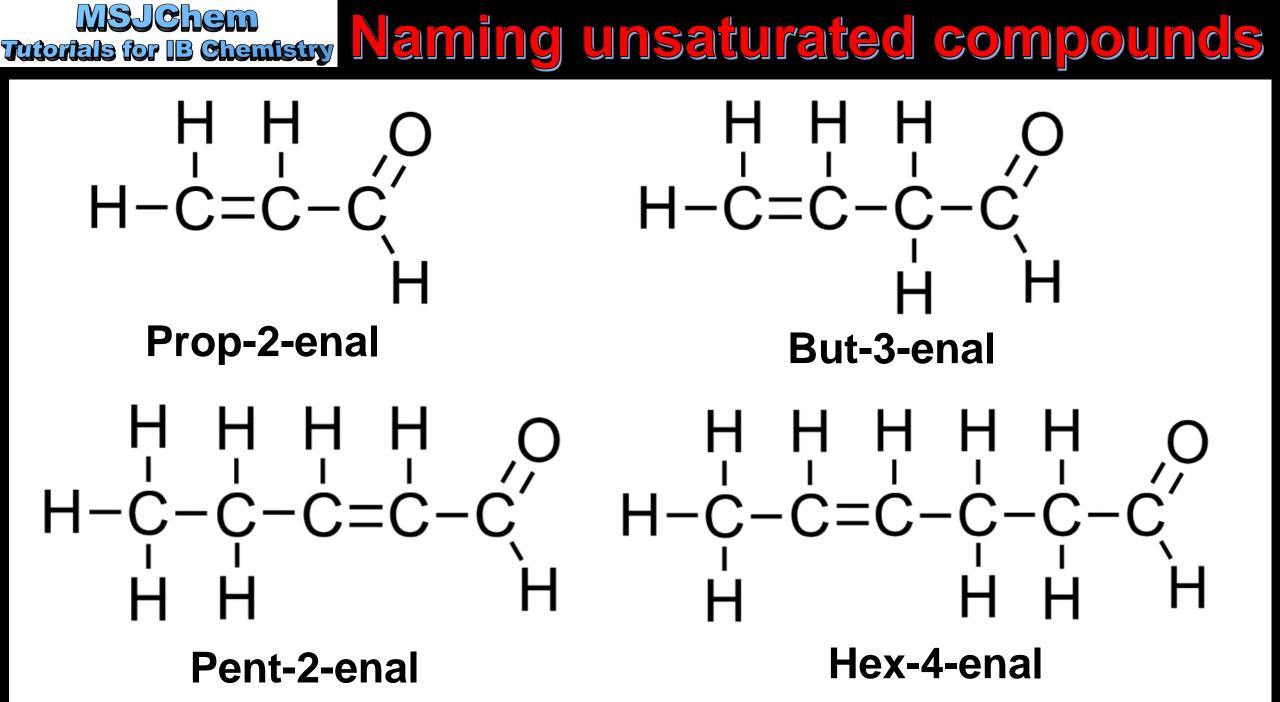


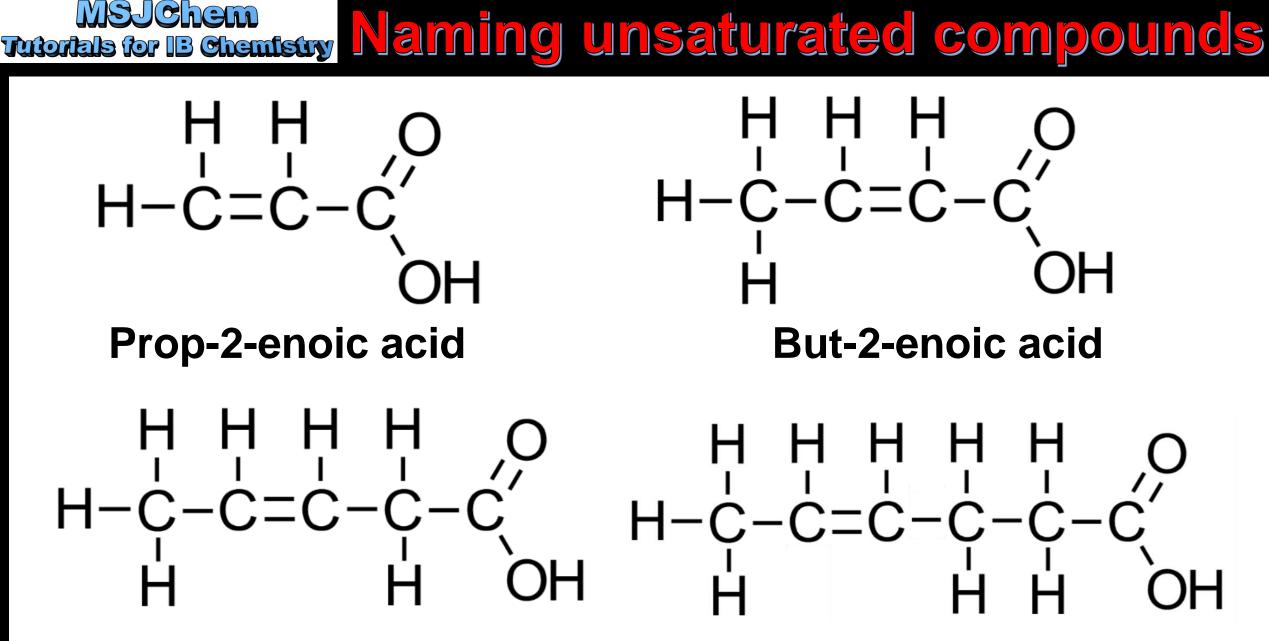
Pent-3-en-1-ol

Hex-4-en-2-ol





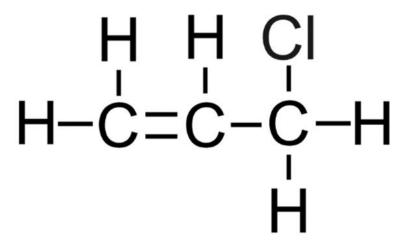




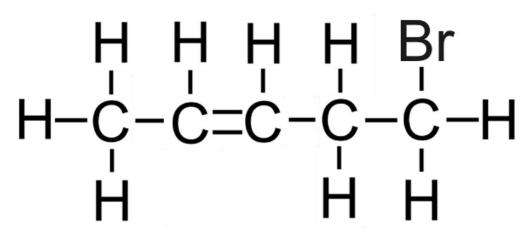
Pent-3-enoic acid

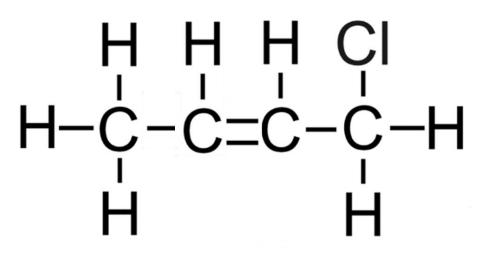
Hex-4-enoic acid

MSJChem Tutorials for IB Chemistry Naming Unsaturated compounds









1-chlorobut-2-ene

H H H Br H H H-C=C-C-C-C-C-H H H H H

5-bromopent-2-ene

4-bromohex-1-ene

Structural isomerism

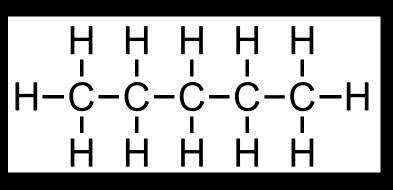


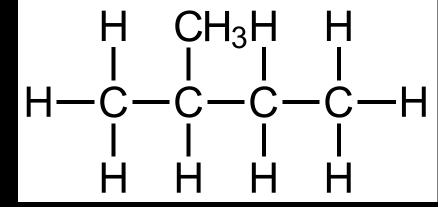
Tutorials for IB Chemistry Structural isometry

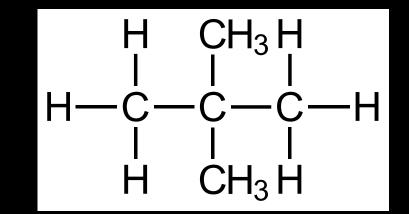
- Structural isomers are compounds with the same molecular formula but different arrangements of atoms (different structural formulas).
- Chain isomerism: straight-chain and branchedchain molecules
- Position isomerism: functional group attached in a different position
- Functional group isomerism: molecules with different functional groups



Structural isomers of C₅H₁₂





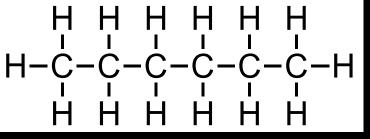


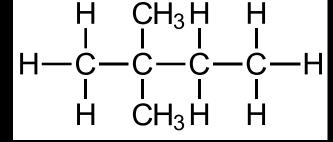
pentane $CH_3(CH_2)_3CH_3$

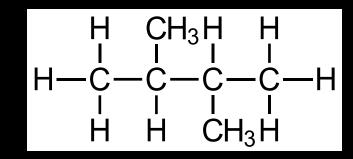
2-methylbutane 2,2-dimethylpropane $CH_3CH(CH_3)CH_2CH_3$ $CH_3C(CH_3)_2CH_3$



Structural isomers of C₆H₁₄

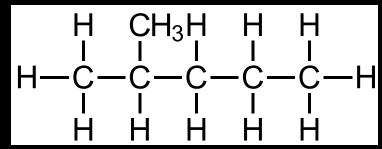




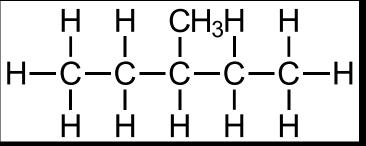


hexane CH₃(CH₂)₄CH₃

2,2-dimethylbutane 2,3-dimethylbutane $(CH_3)_3CCH_2CH_3$ $(CH_3)_2CHCH(CH_3)_2$



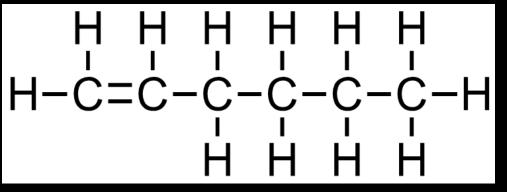
2-methylpentane (CH₃)₂CHCH₂CH₂CH₂CH₃

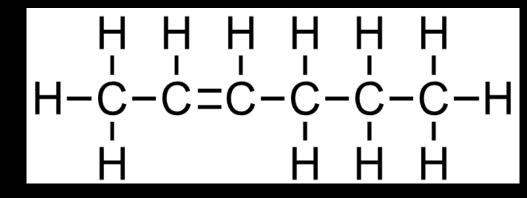


3-methylpentane CH₃CH₂CH(CH₃)CH₂CH₃



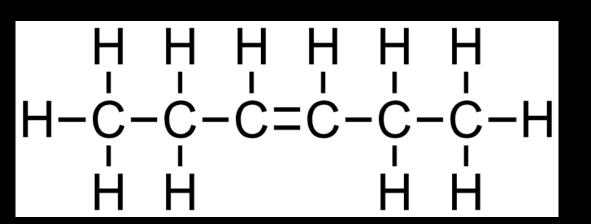
Structural isomers of C₆H₁₂





hex-1-ene CH₂CH(CH₂)₃CH₃

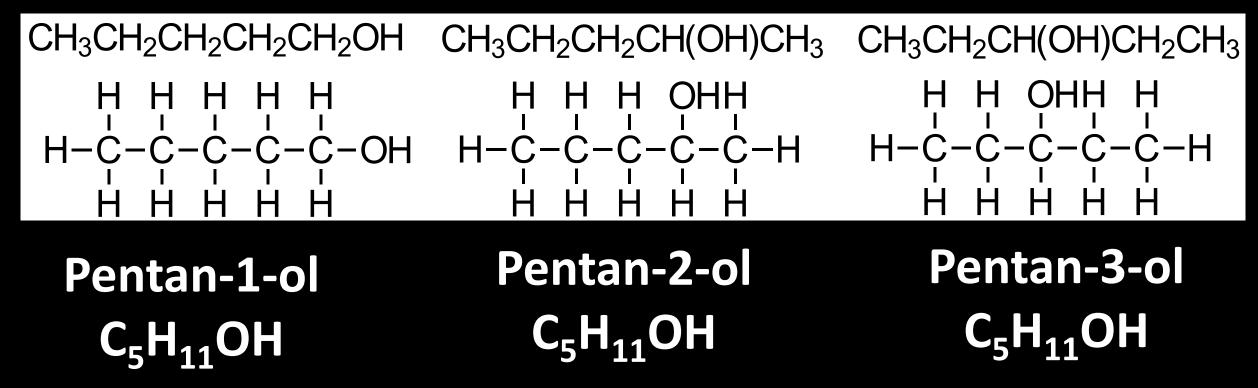
hex-2-ene $CH_3CHCH(CH_2)_2CH_3$



$hex-3-ene \\ CH_3CH_2CHCHCH_2CH_3$

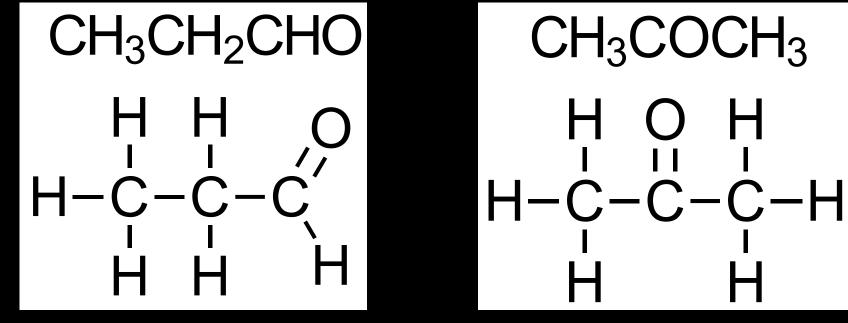


Structural isomers of C₅H₁₂O





Structural isomerism Structural isomers of C₃H₆O

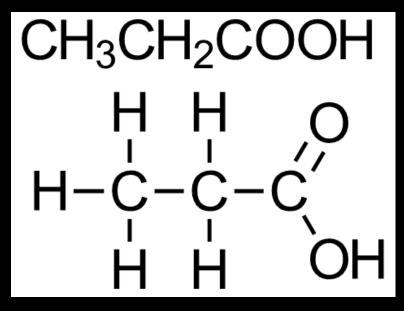


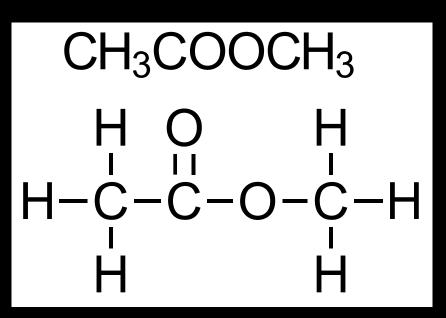
Propanal

Propanone



Structural isomerism Structural isomers of $C_3H_6O_2$





Propanoic acid

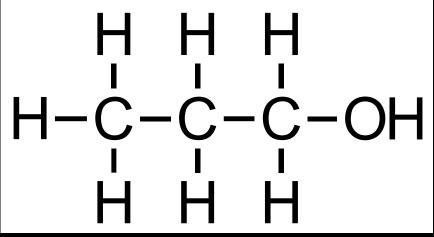
Methyl ethanoate

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Classification of organic compounds



Classification of alcohols



H-C-C-C-H H H H propan-2-ol secondary (2°) alcohol

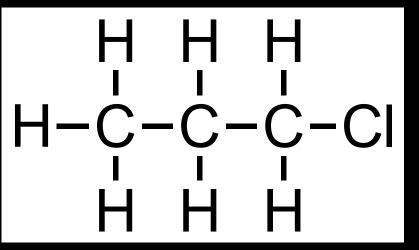
OHH

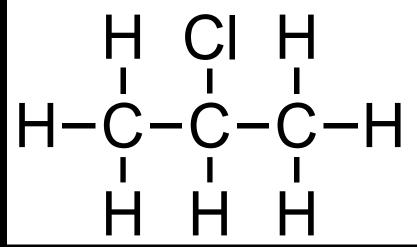
propan-1-ol primary (1°) alcohol

$$\begin{array}{c} \mathsf{OH} \\ \mathsf{I} \\ \mathsf{H}_3\mathsf{C} - \overset{\mathsf{I}}{\mathsf{C}} - \mathsf{CH}_3 \\ \mathsf{CH}_3 \end{array}$$

2-methylpropan-2-ol tertiary (3°) alcohol

Classification of halogenoalkanes



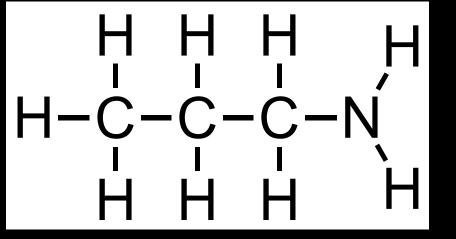


1-chloropropane primary halogenoalkane

2-chloro-2-methylpropane tertiary halogenoalkane

Classification of amines

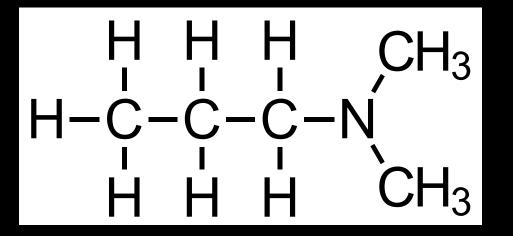
H-C-C-C-N







 H_3



N,N-dimethylpropanamine tertiary amine