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Topic 10 Organic chemistry SL

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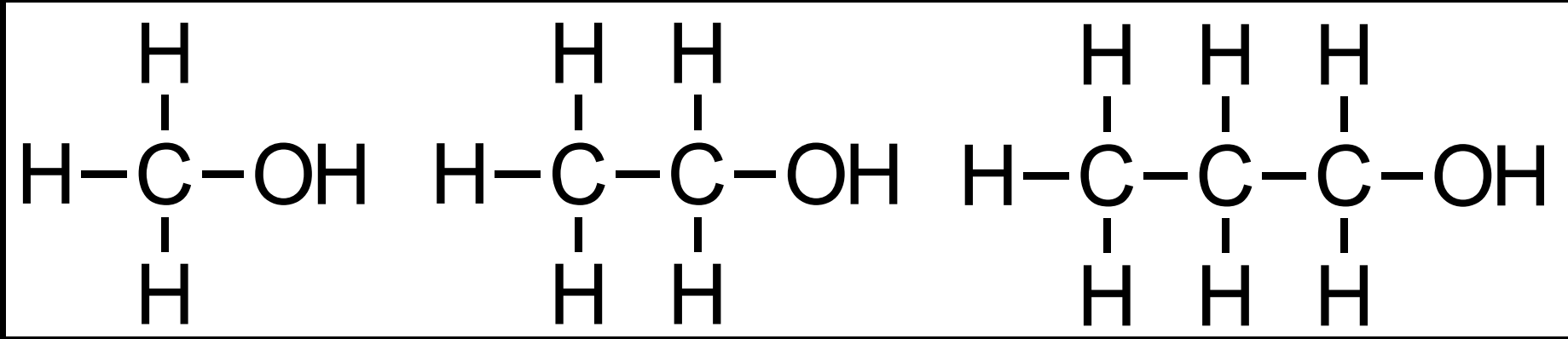
Homologous series

Homologous series

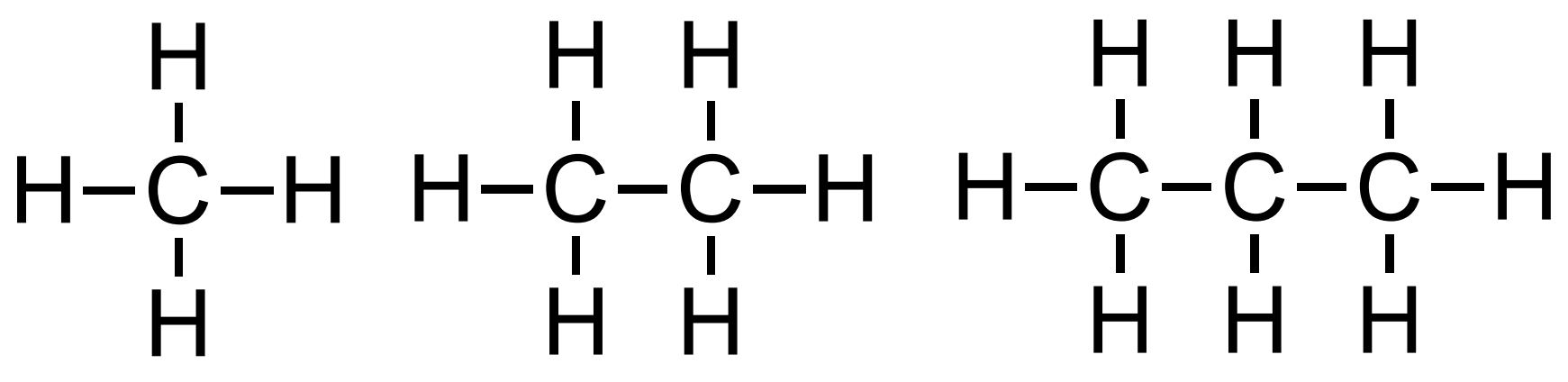
A homologous series is a series of organic compounds of the same family which differ by a common structural unit.



Functional group: hydroxyl (OH) – each member differs by CH_2

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 CH_2
- 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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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.

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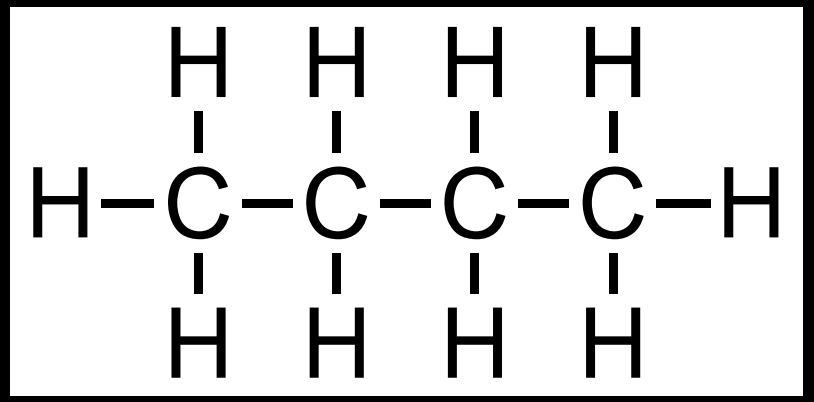
Structural formulas

Butane

molecular formula

C_4H_{10}

full structural formula



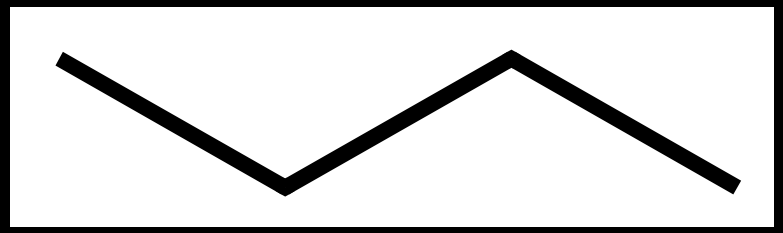
empirical formula

C_2H_5

condensed structural formula

$CH_3CH_2CH_2CH_3$

skeletal formula



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Structural formula

But-1-ene

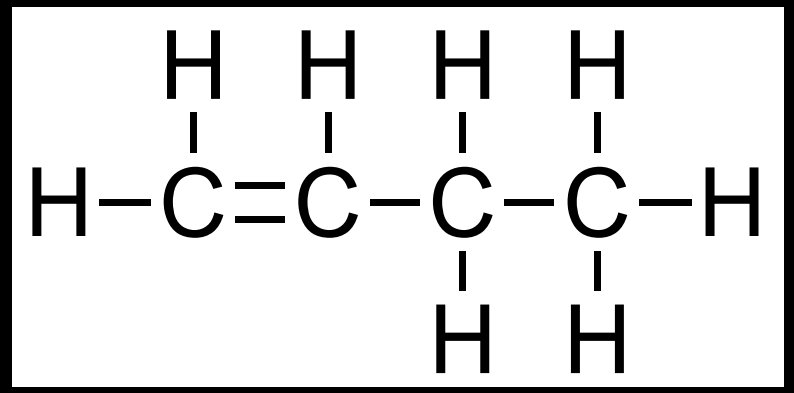
molecular formula

C_2H_8

empirical formula

CH_4

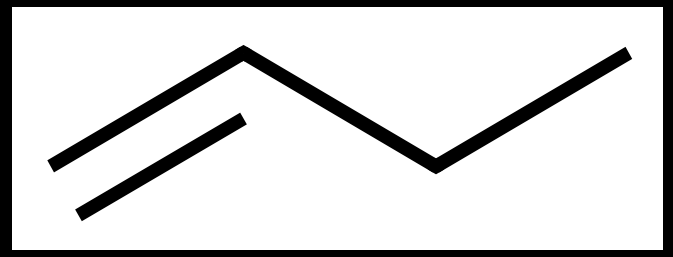
full structural formula



condensed structural formula

$CH_2CHCH_2CH_3$

skeletal formula



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Structural formula

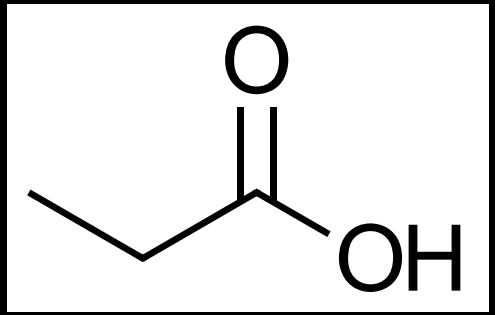
Propanoic acid

molecular formula

$C_3H_6O_2$

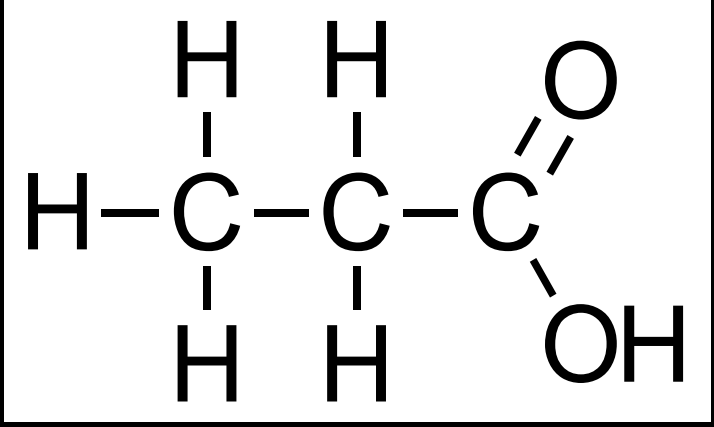
empirical formula

$C_3H_6O_2$



skeletal formula

full structural formula



condensed structural formula

CH_3CH_2COOH

$CH_3CH_2CO_2H$

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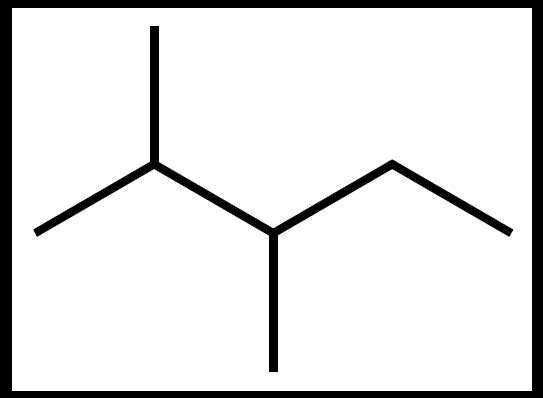
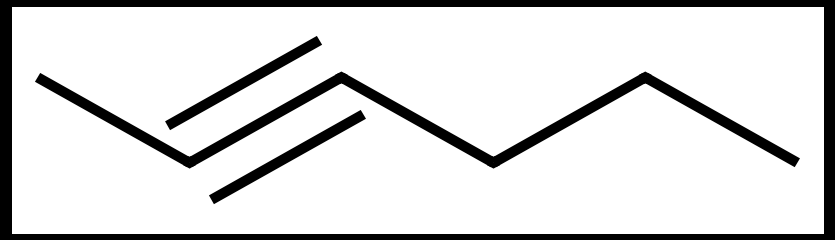
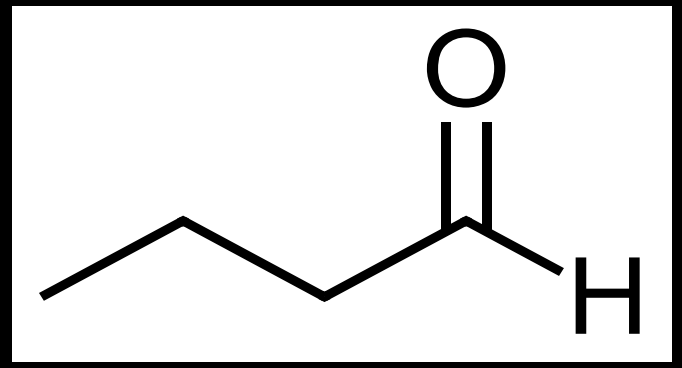
Skeletal formulas



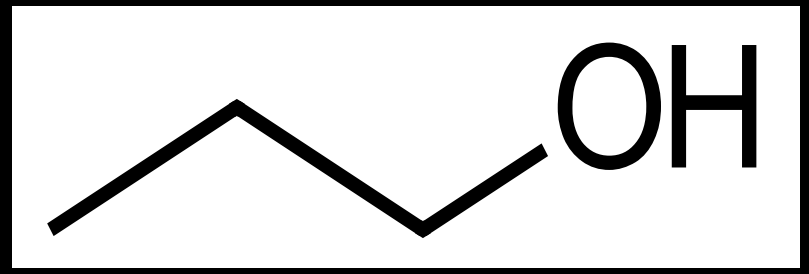
2,3-dimethylpentane



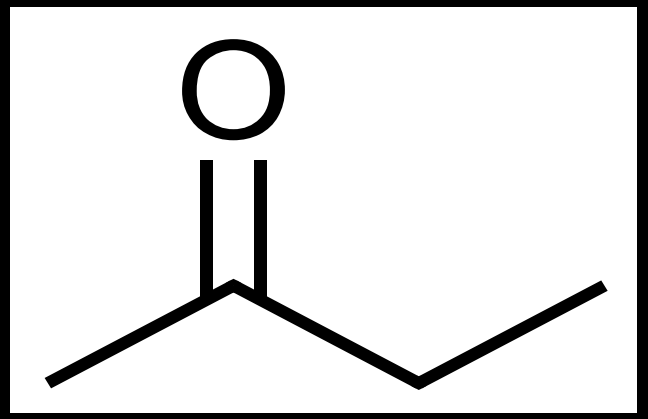
hex-2-yne



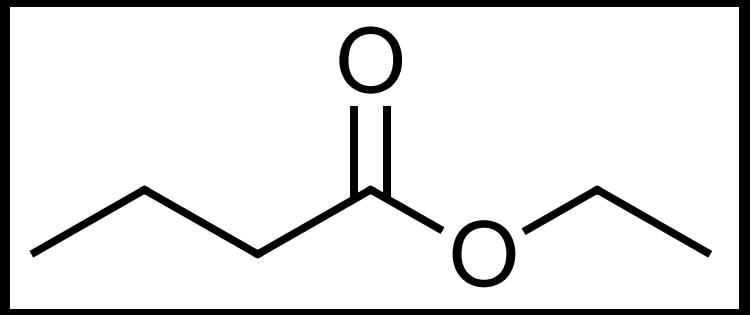
butanal



propan-1-ol



butanone



ethyl butanoate

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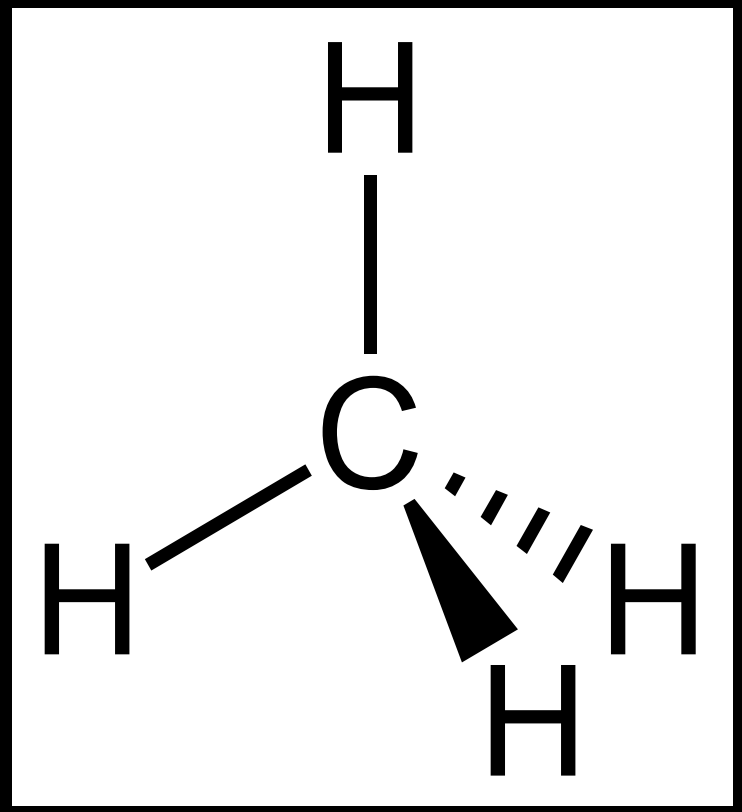
Stereochemical formula

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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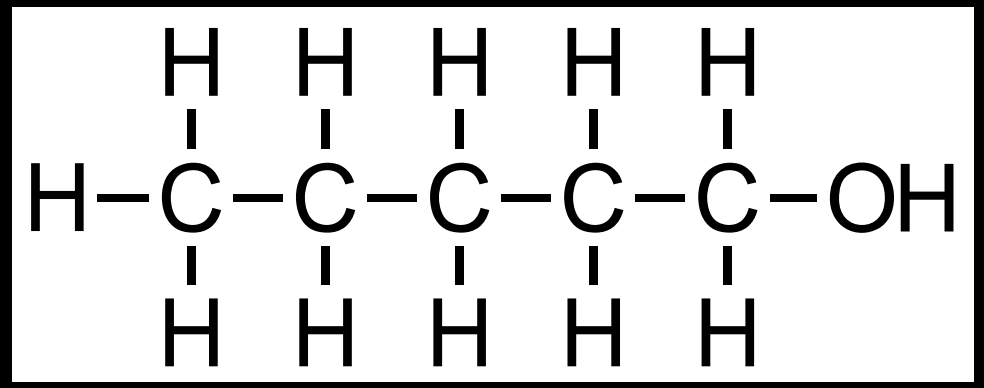
Functional groups

Functional groups

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



pentan-1-ol

Class: alcohol
Functional group: OH
hydroxyl group

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

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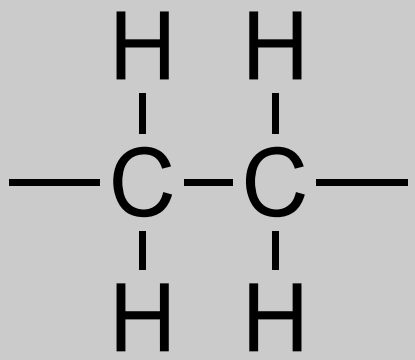
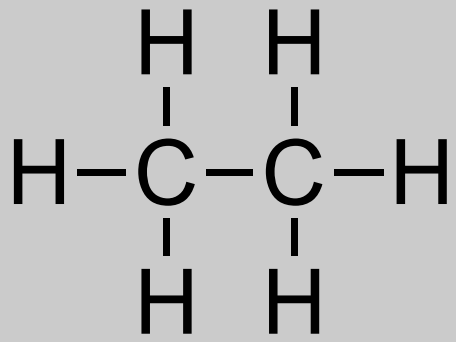
Functional groups

Class	Functional group	Name	Example
Alkane		**Alkyl**	 **Ethane CH_3CH_3**

General formula	Type of reactions
C_nH_{2n+2}	**Combustion** **Free-radical substitution**

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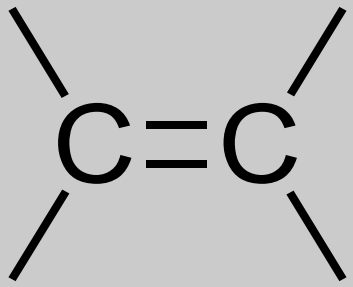
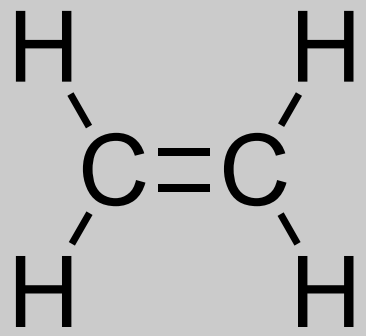
Functional groups

Class	Functional group	Name	Example
Alkene		**Alkenyl**	 **Ethene CH_2CH_2**

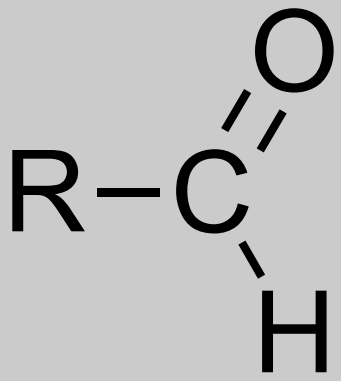
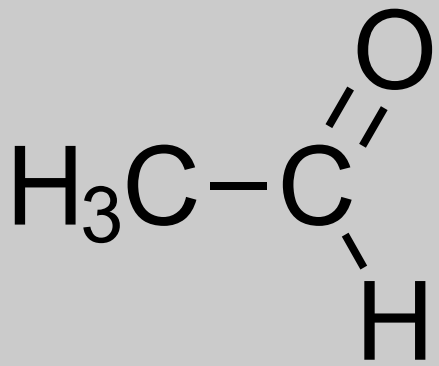
General formula	Type of reactions
C_nH_{2n}	**Combustion** **Electrophilic addition**

Functional groups

Class	Functional group	Name	Example
Alkyne	—C≡C—	Alkynyl	H–C≡C–H Ethyne CHCH

General formula	Type of reactions
C_nH_{2n-2}	Combustion Electrophilic addition

Functional groups

Class	Functional group	Name	Example
Aldehyde	 R-CHO	**Carbonyl**	 **Ethanal** CH_3CHO

General formula	Type of reactions
$C_nH_{2n}O$	**Oxidation** **Reduction (HL)**

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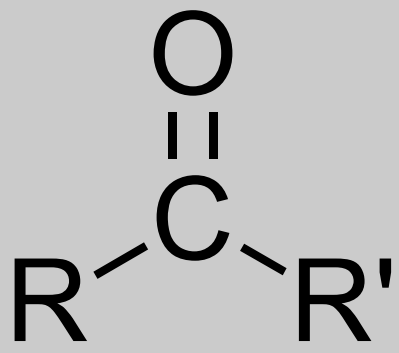
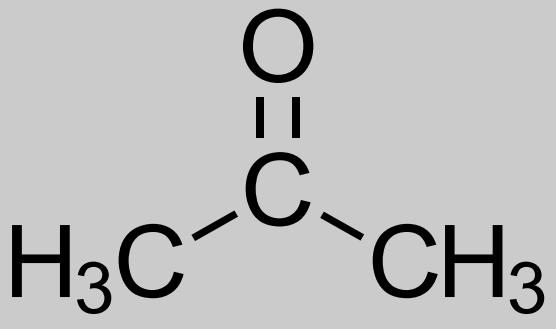
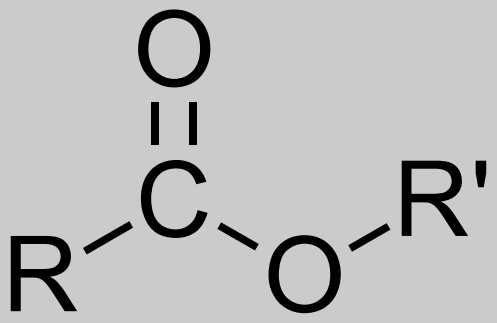
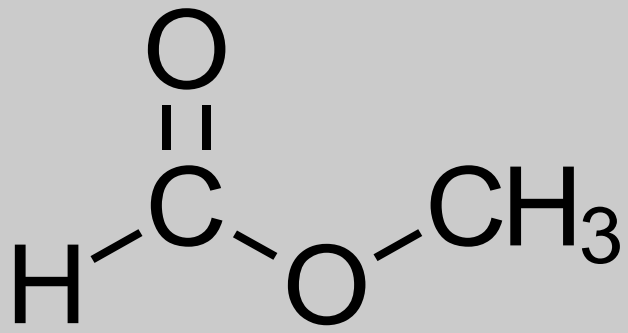
Functional groups

Class	Functional group	Name	Example
Ketone	 R-CO-R'	**Carbonyl**	 **Propanone** **CH_3COCH_3**

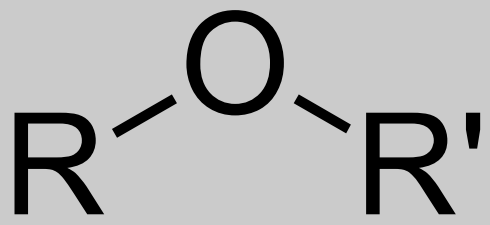
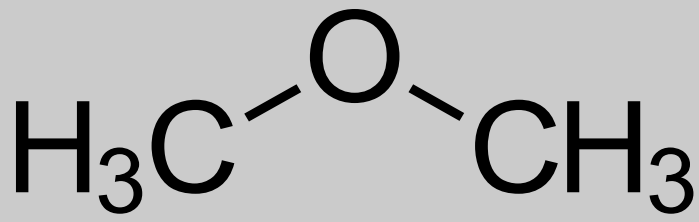
General formula	Type of reactions
$C_nH_{2n}O$	**Oxidation** **Reduction (HL)**

Functional groups

Class	Functional group	Name	Example
Ester	 R-COO-R' R-CO_2-R'	**Ester**	 **Methyl methanoate** **$HCOOCH_3$ or HCO_2CH_3**

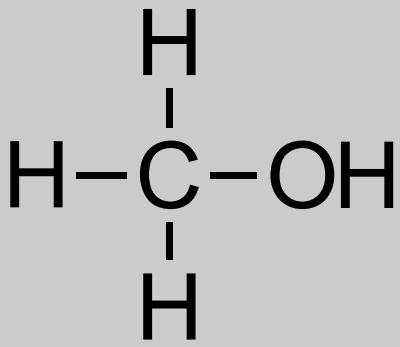
General formula	Type of reactions
$C_nH_{2n}O_2$	

Functional groups

Class	Functional group	Name	Example
Ether	 R-O-R'	Ether	 Methoxymethane CH_3OCH_3

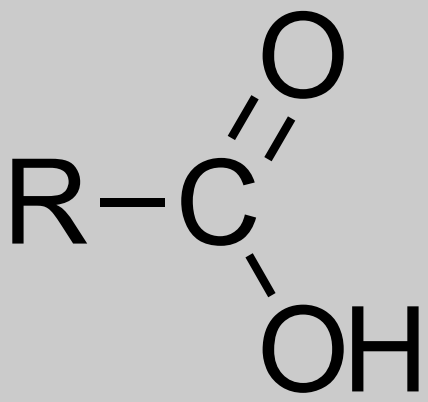
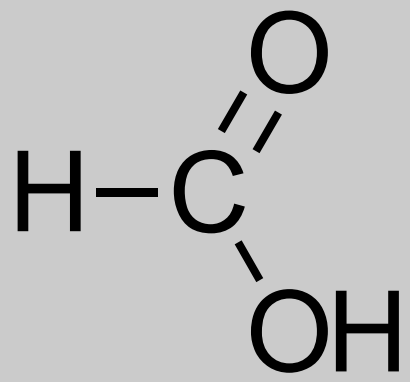
General formula	Type of reactions
$C_nH_{2n+2}O$	Not covered in IB chemistry

Functional groups

Class	Functional group	Name	Example
Alcohol	R−OH	**Hydroxyl**	 **Methanol** CH_3OH

General formula	Type of reactions
$C_nH_{2n+2}O$	**Combustion** **Oxidation**

Functional groups

Class	Functional group	Name	Example
Carboxylic acid	 R-COOH R-CO_2H	**Carboxyl**	 **Methanoic acid** **HCOOH or HCO_2H**

General formula	Type of reactions
$C_nH_{2n}O_2$	**Nucleophilic substitution (with alcohols)** **Reduction (HL)**

Functional groups

Class	Functional group	Name	Example
Nitrile	R−C≡N	**Nitrile**	H−C≡N **Methanenitrile** **HCN**

General formula	Type of reactions
$C_nH_{2n-1}N$	**Not covered in IB chemistry**

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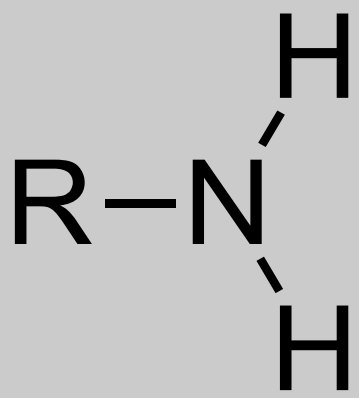
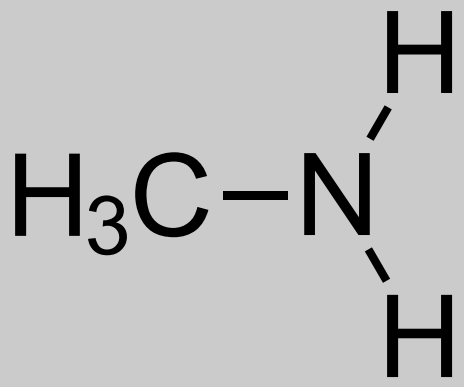
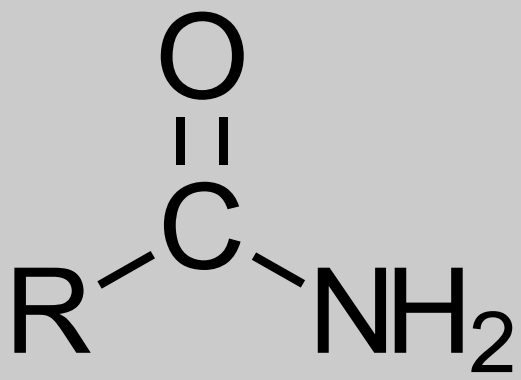
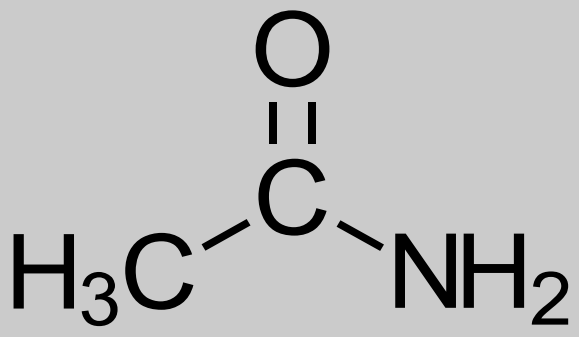
Functional groups

Class	Functional group	Name	Example
Amine	 $R\text{-}NH_2$	**Amine** **Amino**	 **Methanamine** **CH_3NH_2**

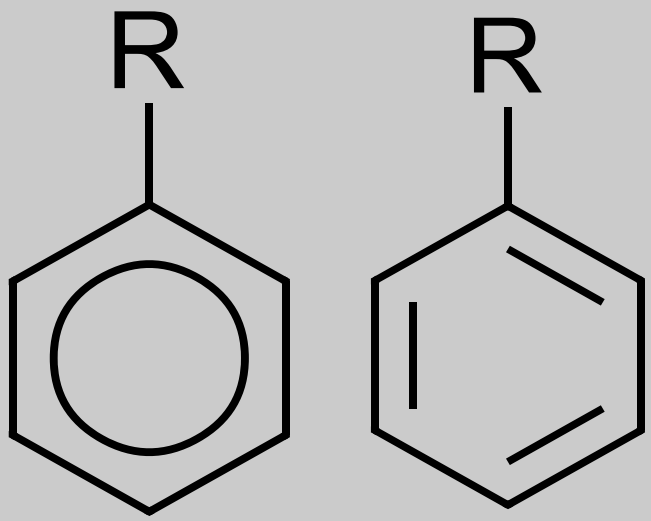
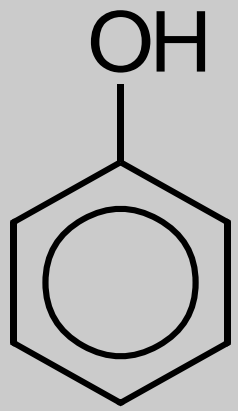
General formula	Type of reactions
$C_nH_{2n+3}N$	Can act as Bronsted-Lowry bases and Lewis bases (HL)

Functional groups

Class	Functional group	Name	Example
Amide	 $R\text{-}CONH_2$	**Carboxamide** **Amido**	 **Methanamide** **CH_3CONH_2**

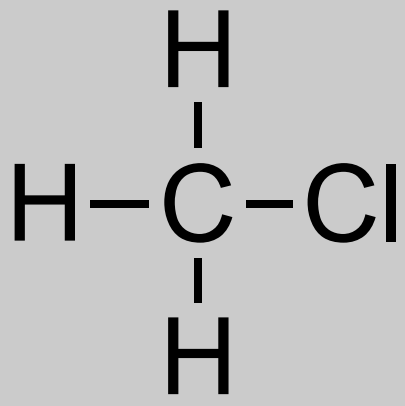
General formula	Type of reactions
$C_nH_{2n+1}NO$	**Not covered in IB chemistry**

Functional groups

Class	Functional group	Name	Example
Arene	 C_6H_5-	Phenyl	 Phenol C_6H_5OH

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

Functional groups

Class	Functional group	Name	Example
Halogeno-alkane	R-X where X is a F, Cl, Br or I atom	Fluoro- Chloro- Bromo- Iodo-	 Chloromethane CH_3Cl

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

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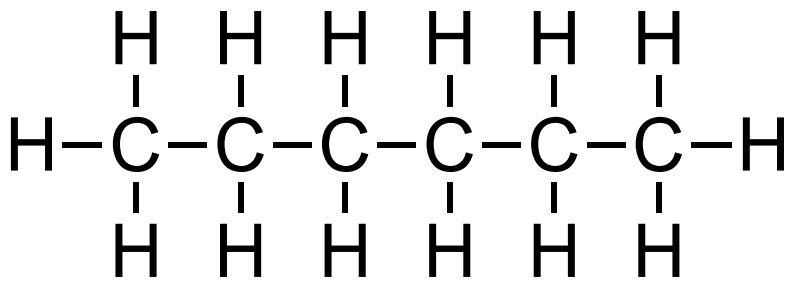
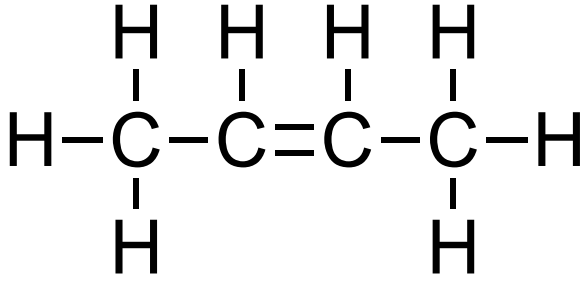
Identifying functional groups

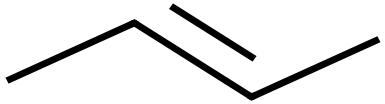
Identifying functional groups



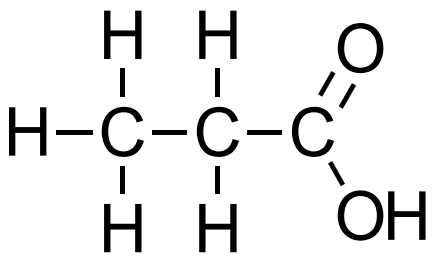
$CH_3CH_2CH_2CH_2CH_2CH_3$



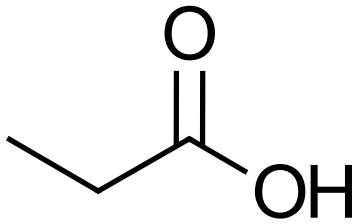
$CH_3CHCHCH_3$



Identifying functional groups



CH_3CH_2COOH



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Naming alkanes

Naming alkanes

Alkanes are saturated hydrocarbons (C-C single bonds).

They have the general formula C_nH_{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.

Naming alkanes

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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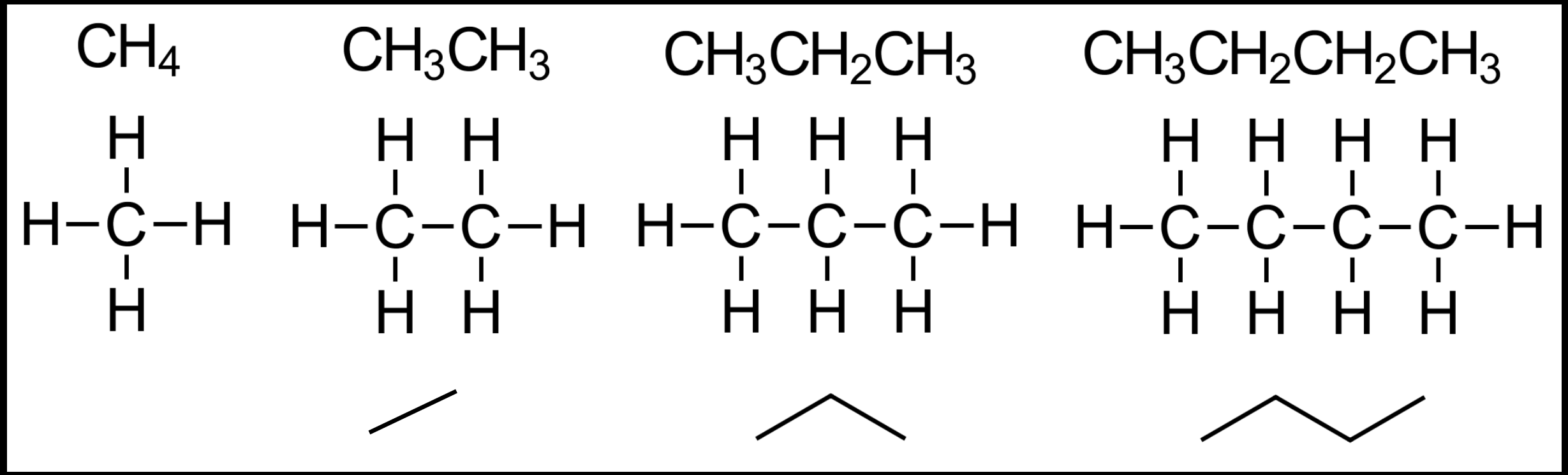
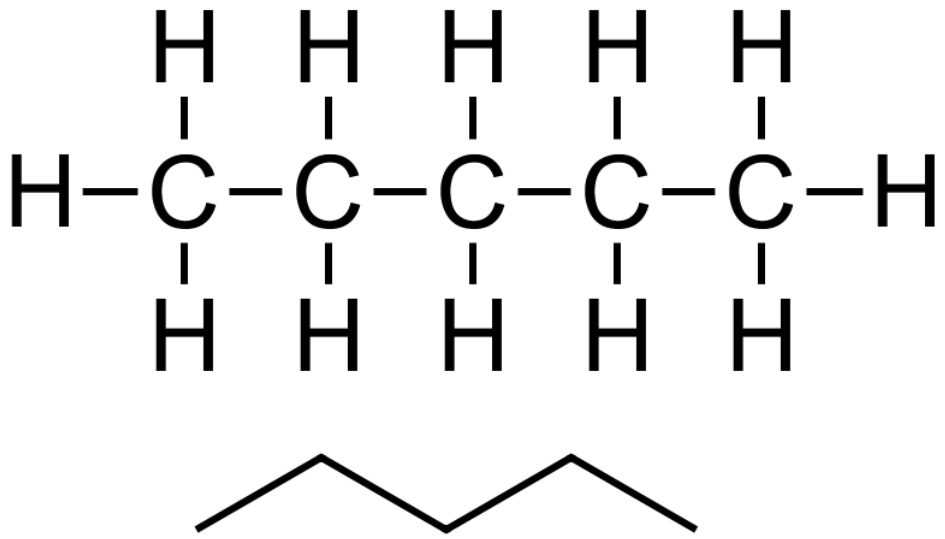
Naming alkanes



Methane	Ethane	Propane	Butane
CH_4	C_2H_6	C_3H_8	C_4H_{10}

Naming alkanes

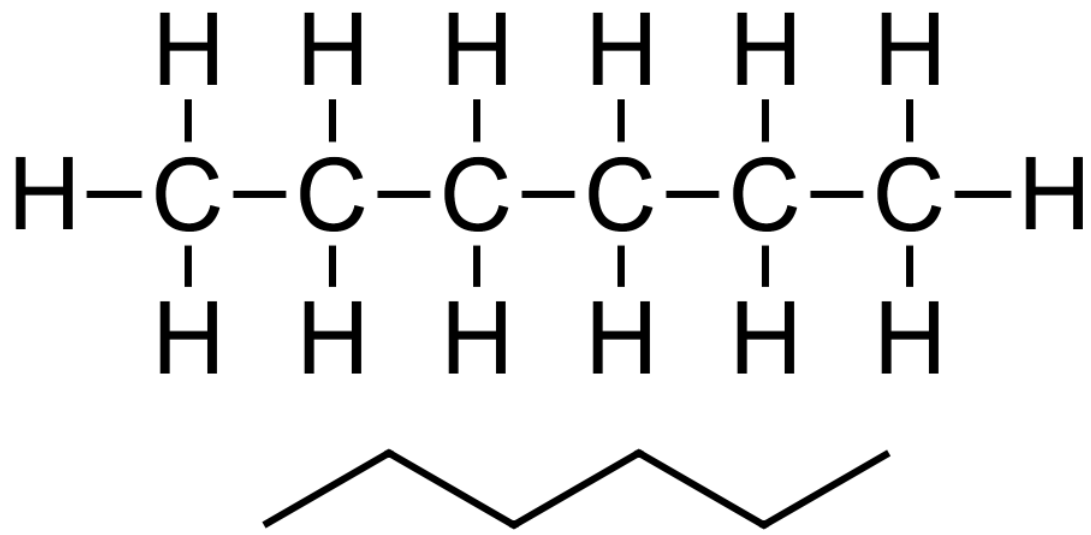
$CH_3CH_2CH_2CH_2CH_3$



Pentane

C_5H_{12}

$CH_3CH_2CH_2CH_2CH_2CH_3$



Hexane

C_6H_{14}

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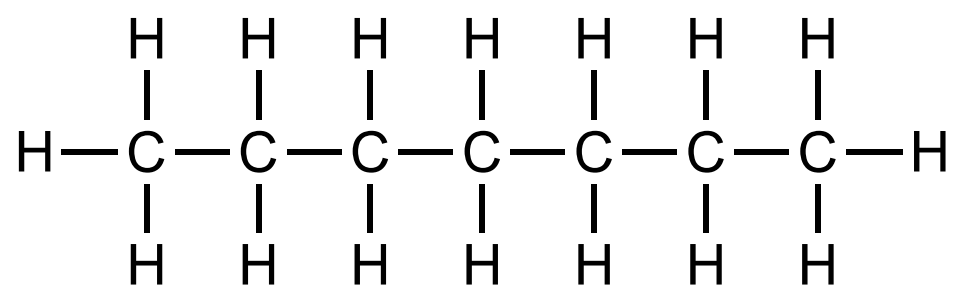
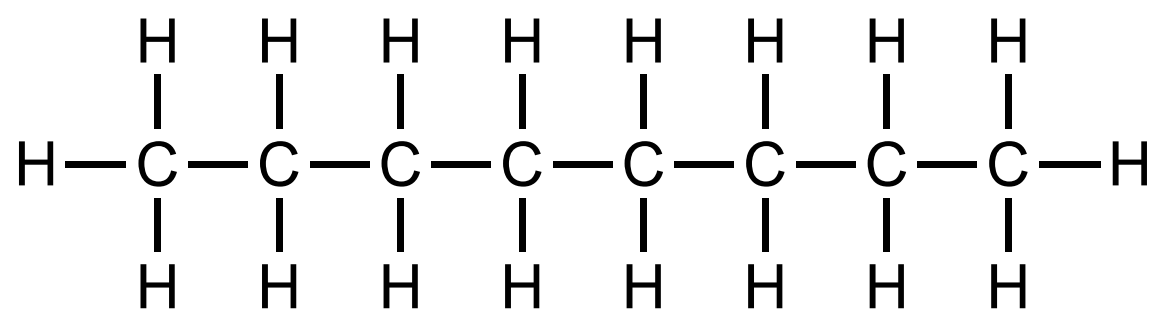
Naming alkanes

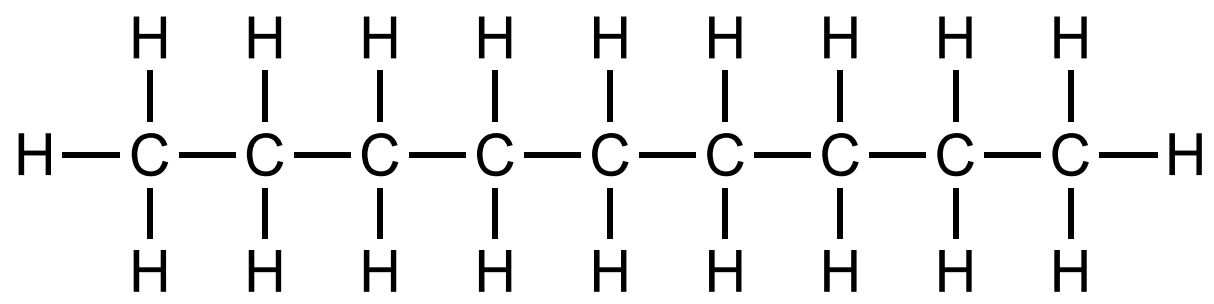
Heptane C_7H_{16}



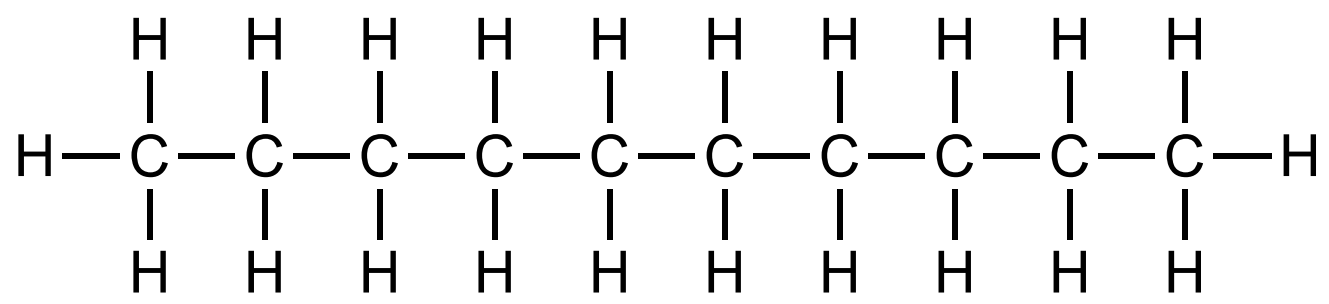
Octane C_8H_{18}



Nonane C_9H_{20}



Decane $C_{10}H_{22}$

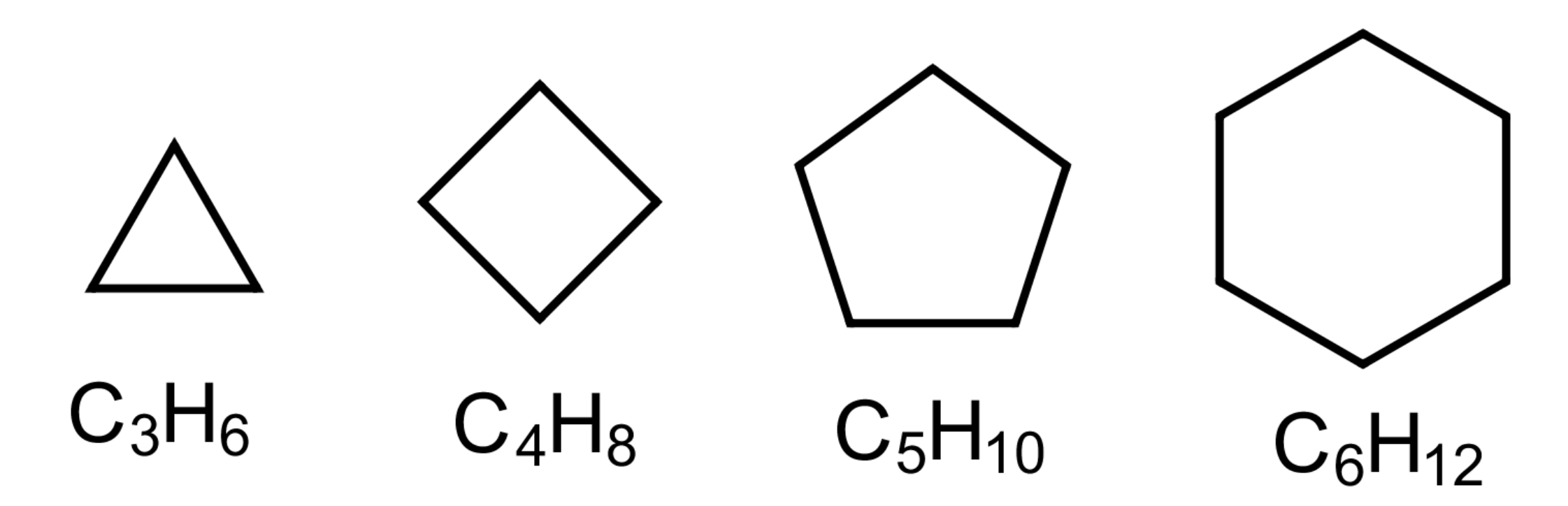


Naming alkanes

Cyclic alkanes feature a ring structure (C_nH_{2n}).

Cyclobutane

Cyclohexane



Cyclopropane

Cyclopentane

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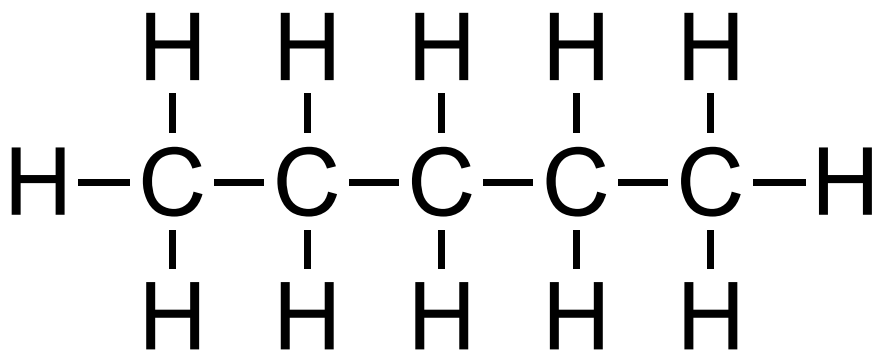
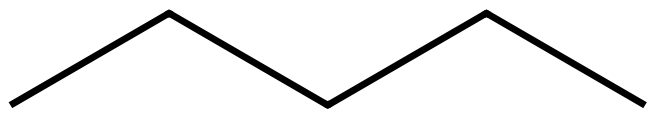
Naming branched-chain alkanes

Branched-chain alkanes

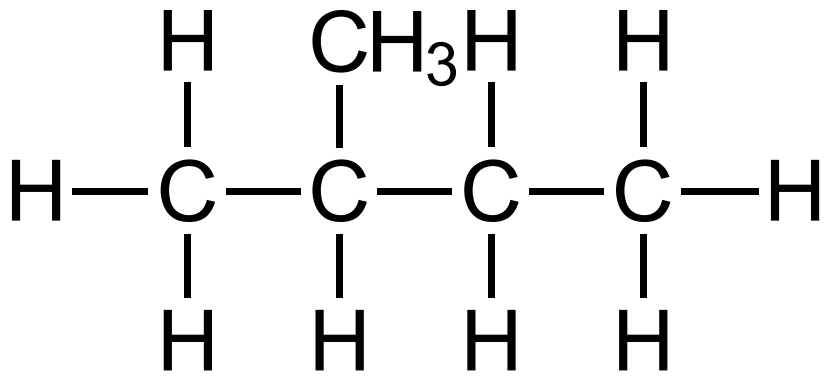
Branched-chain alkanes have branches which are alkyl substituents ($-CH_3$, $-C_2H_5$).

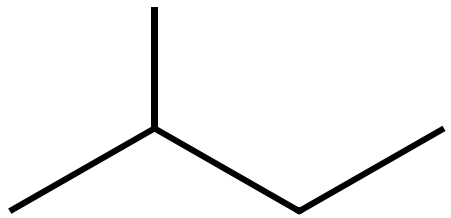
$CH_3CH_2CH_2CH_2CH_3$





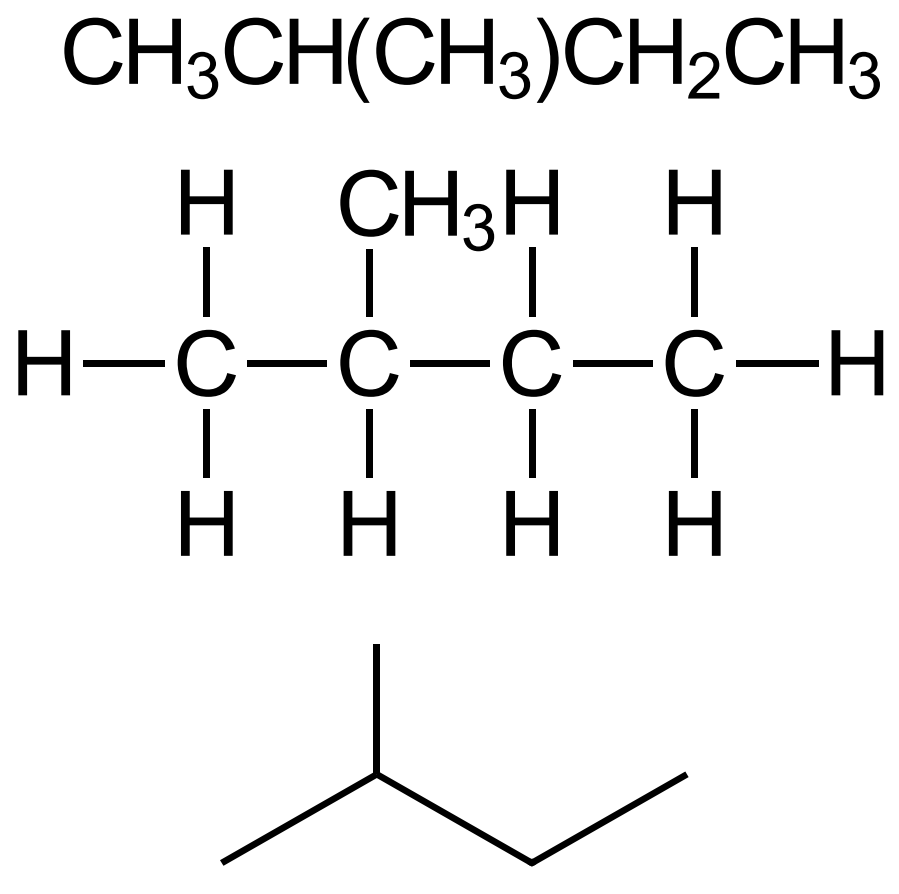
$CH_3CH(CH_3)CH_2CH_3$





Branched-chain alkanes

1. Identify the longest continuous carbon chain.

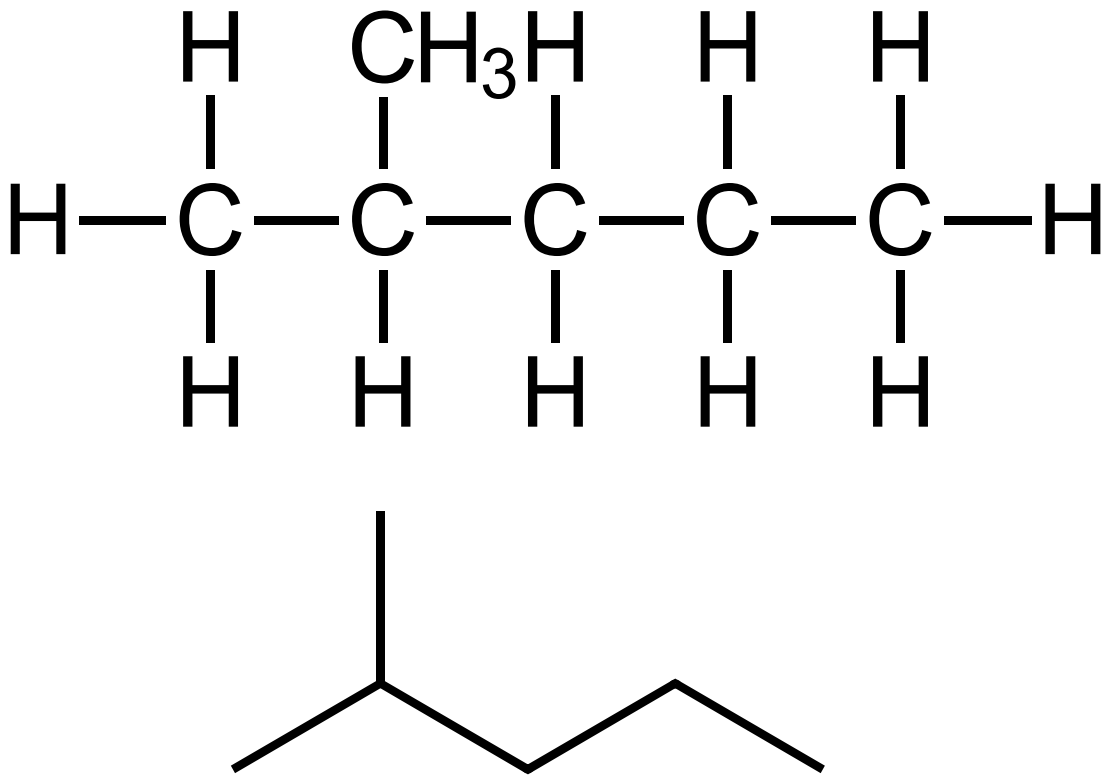


2-methylbutane

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.

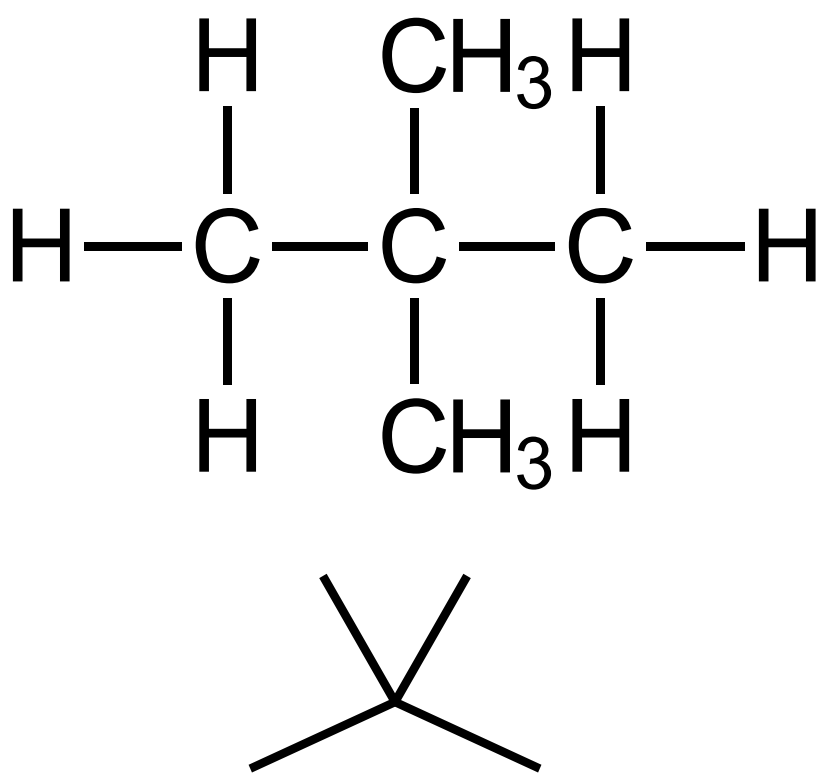
Branched-chain alkanes

$CH_3CH(CH_3)CH_2CH_2CH_3$



2-methylpentane

$CH_3C(CH_3)_2CH_3$



2,2-dimethylpropane

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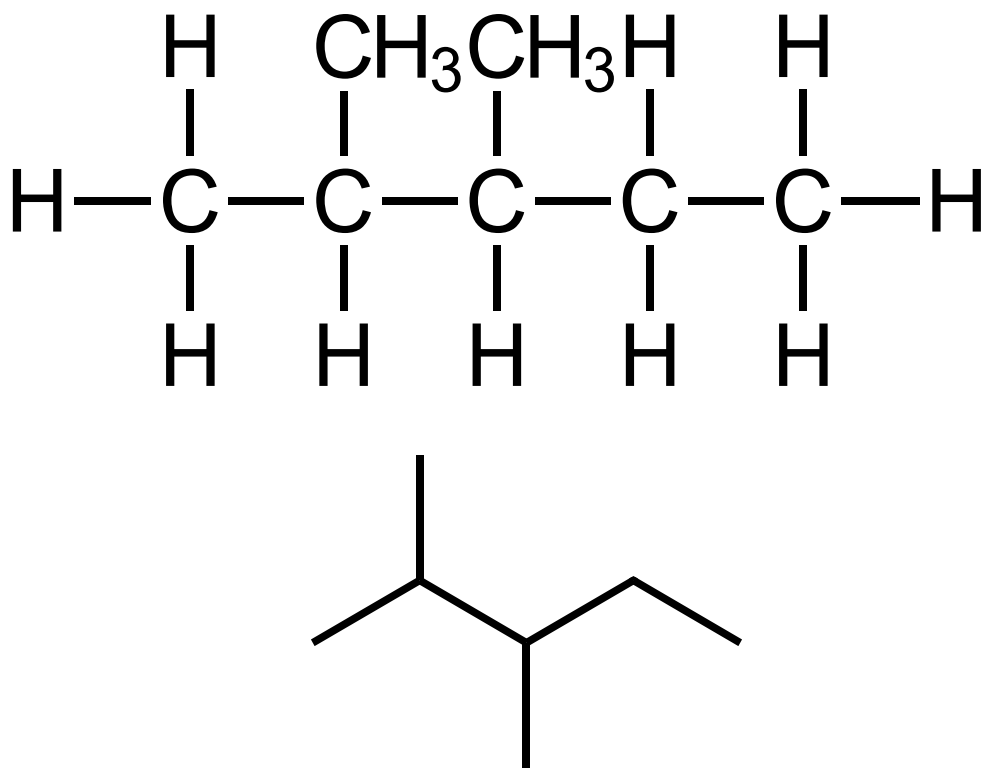
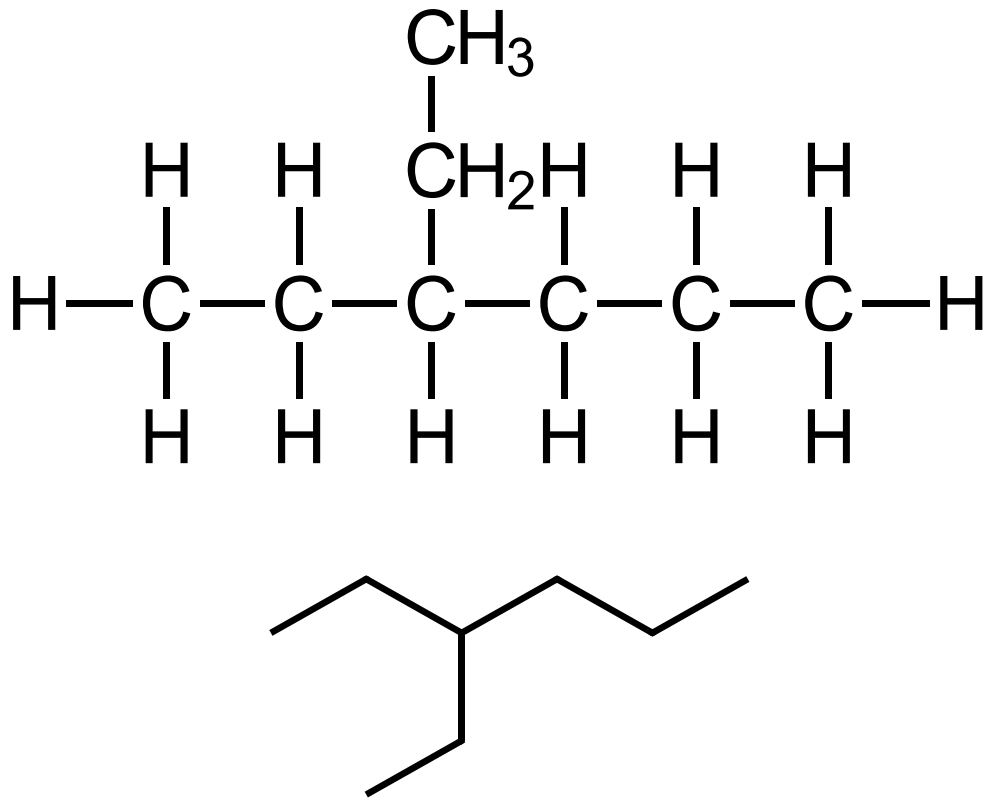
Branched-chain alkanes

$CH_3CH(CH_3)CH(CH_3)CH_2CH_3$



2,3-dimethylpentane

$CH_3CH_2CH(C_2H_5)CH_2CH_2CH_3$



3-ethylhexane

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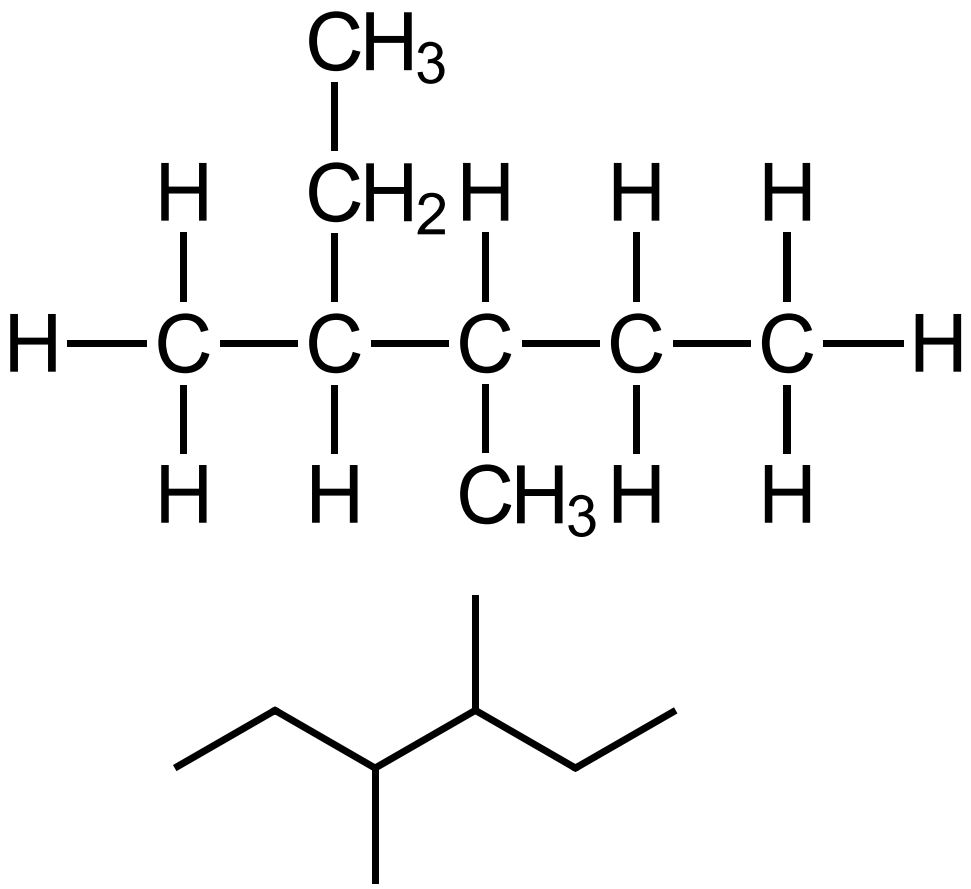
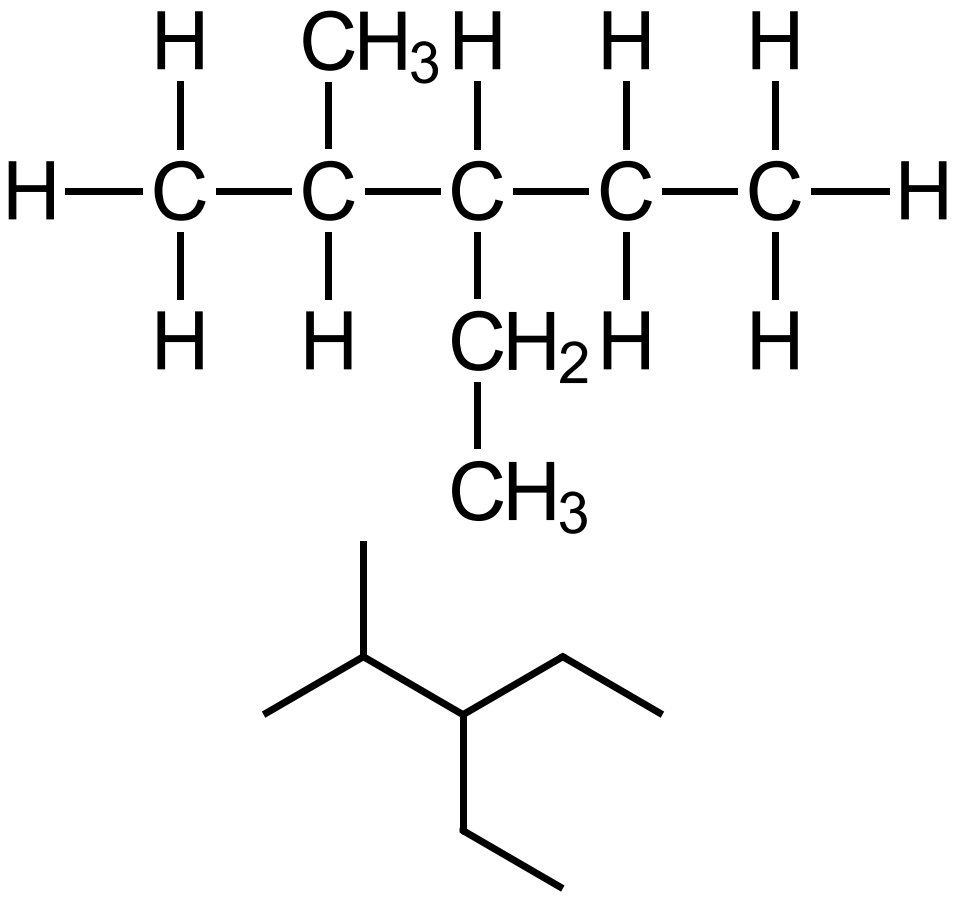
Branched-chain alkanes

$CH_3CH_2CH(CH_3)CH(CH_3)CH_2CH_3$



3,4-dimethylhexane

$CH_3CH(CH_3)CH(C_2H_5)CH_2CH_3$



3-ethyl-2-methylpentane

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Naming alkenes

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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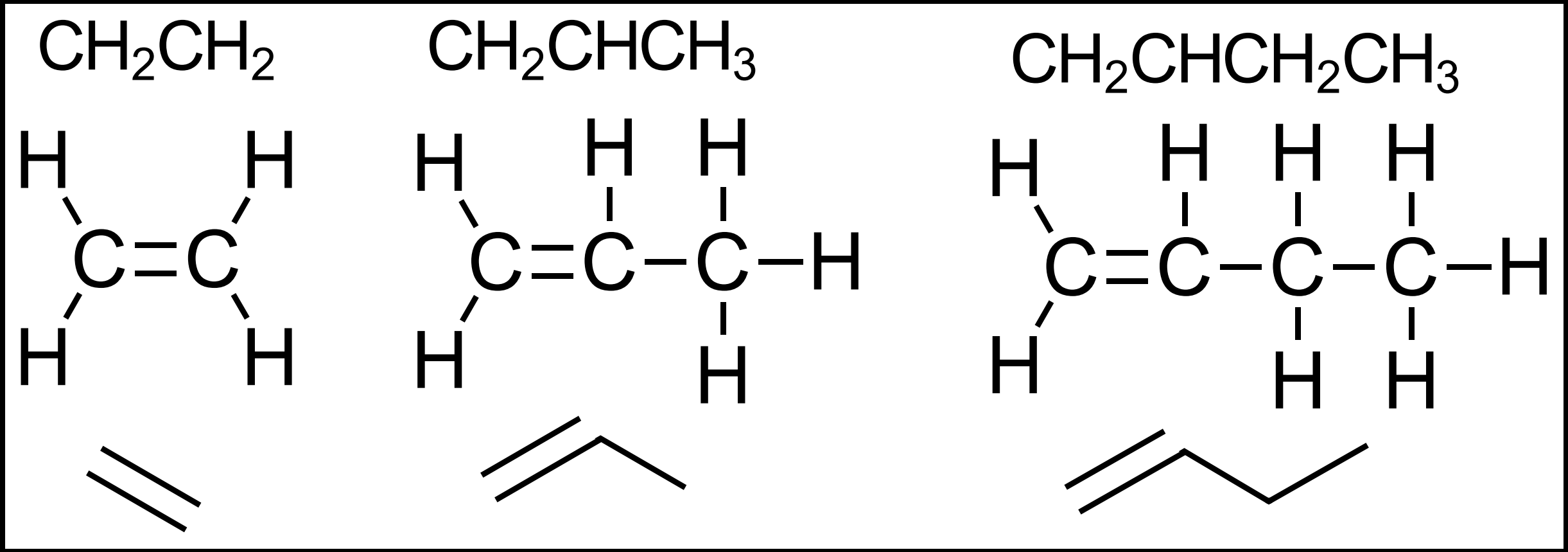
Naming alkenes



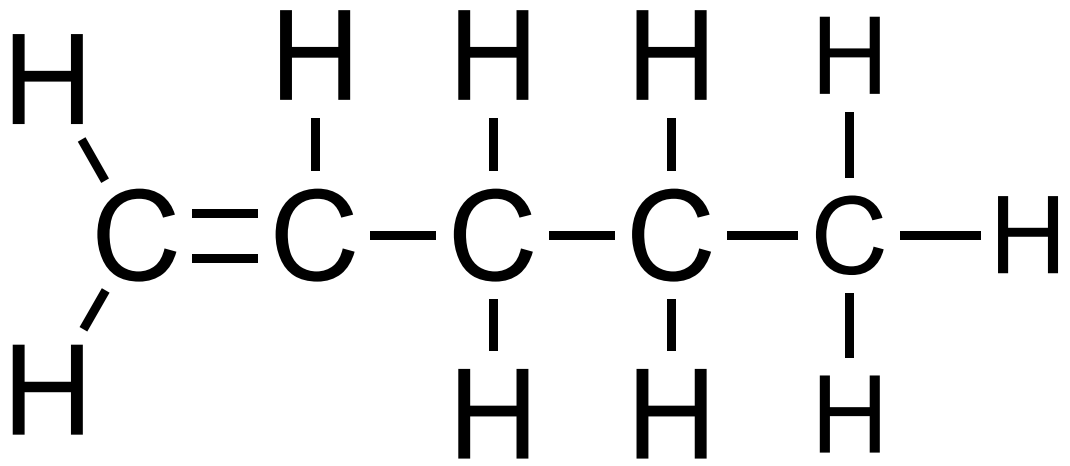
Ethene
C_2H_4

Propene
C_3H_6

But-1-ene
C_4H_8

Naming alkenes

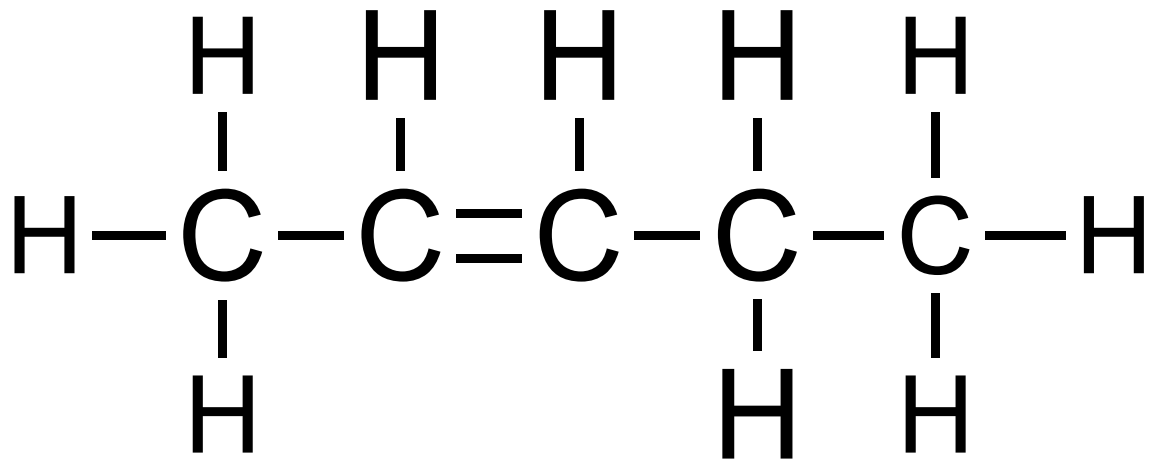
$CH_2CHCH_2CH_2CH_3$



Pent-1-ene

C_5H_{10}

$CH_3CHCHCH_2CH_3$

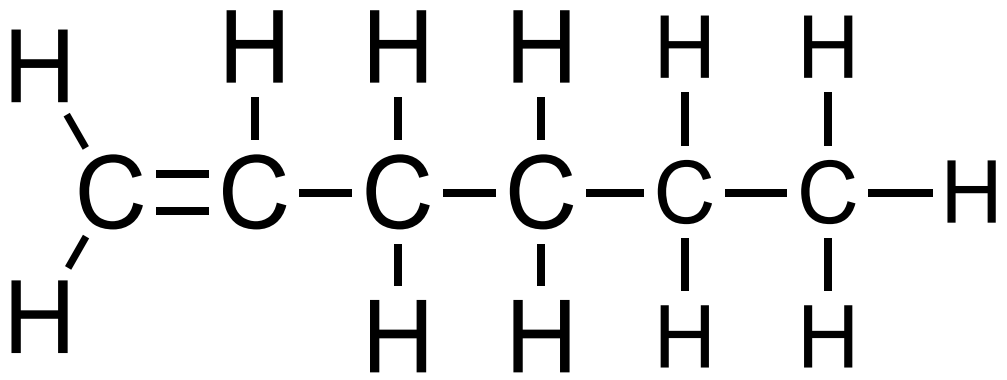


Pent-2-ene

C_5H_{10}

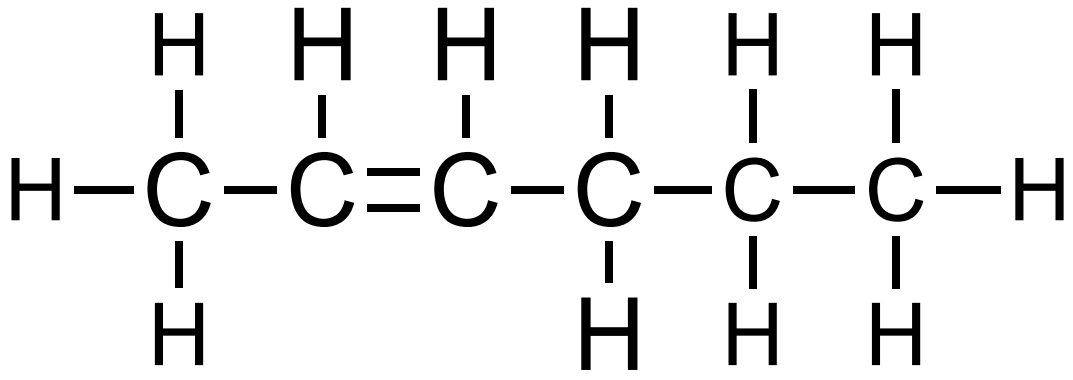
Naming alkenes

$CH_2CHCH_2CH_2CH_2CH_3$



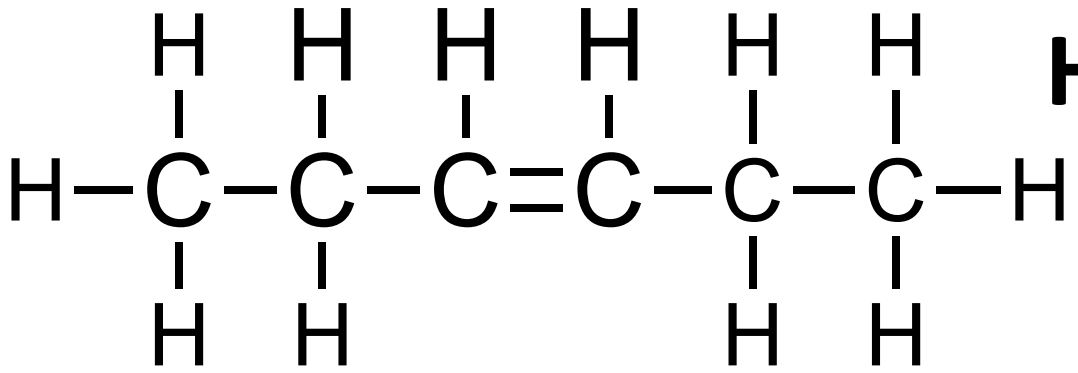
Hex-1-ene

$CH_3CHCHCH_2CH_2CH_3$



Hex-2-ene

$CH_3CH_2CHCHCH_2CH_3$



Hex-3-ene

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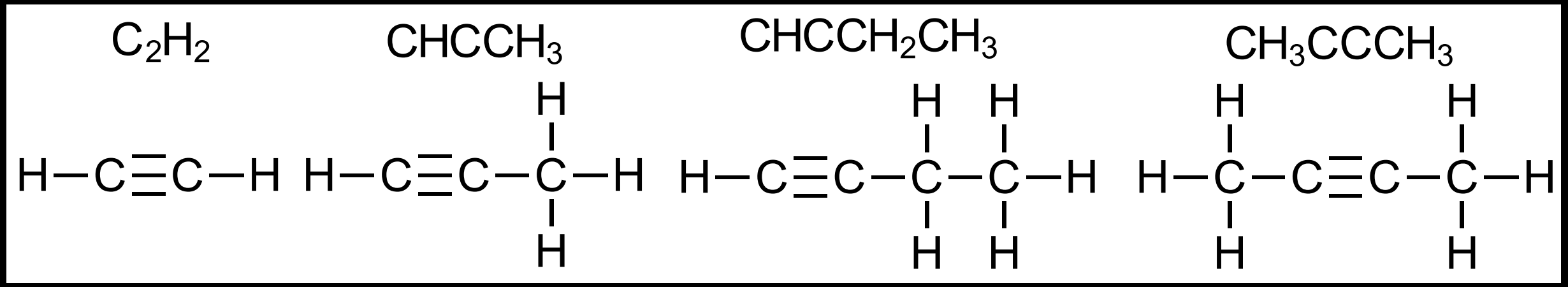
Naming alkynes

Naming alkynes

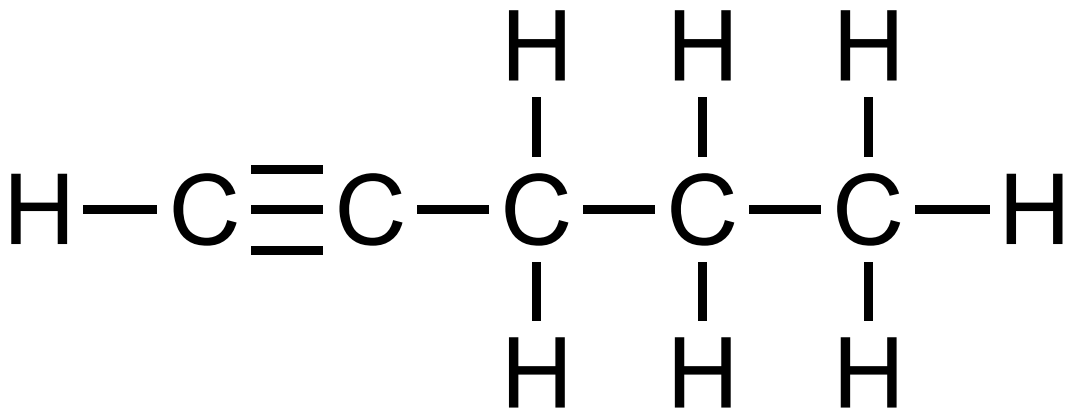
Alkynes are unsaturated hydrocarbons (C-C triple bonds).
They have the general formula C_nH_{2n-2}
Alkynes have similar reactivity to the alkenes.
Alkynes undergo electrophilic addition reactions.



Ethyne Propyne But-1-yne But-2-yne

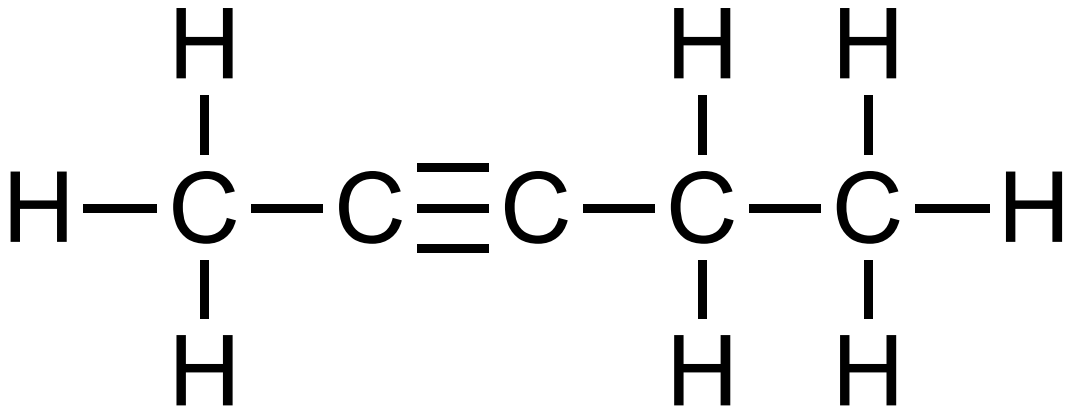
Naming alkynes

$CHCCH_2CH_2CH_3$



Pent-1-yne

$CH_3CCCH_2CH_3$



Pent-2-yne

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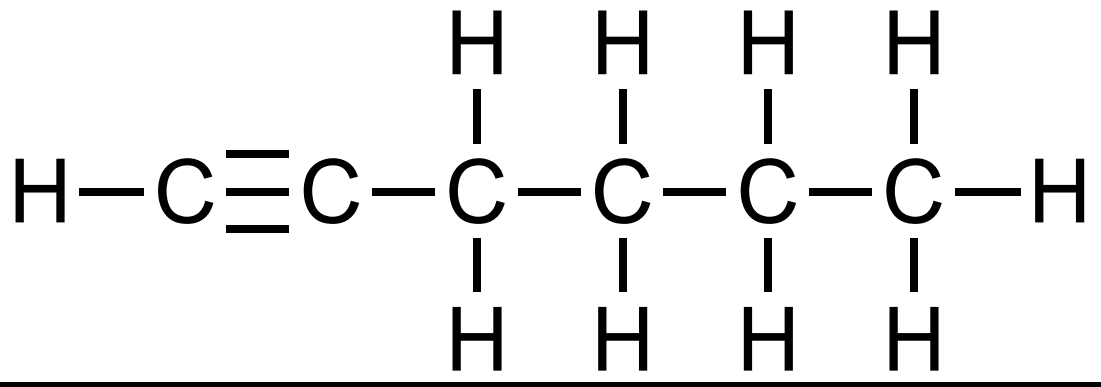
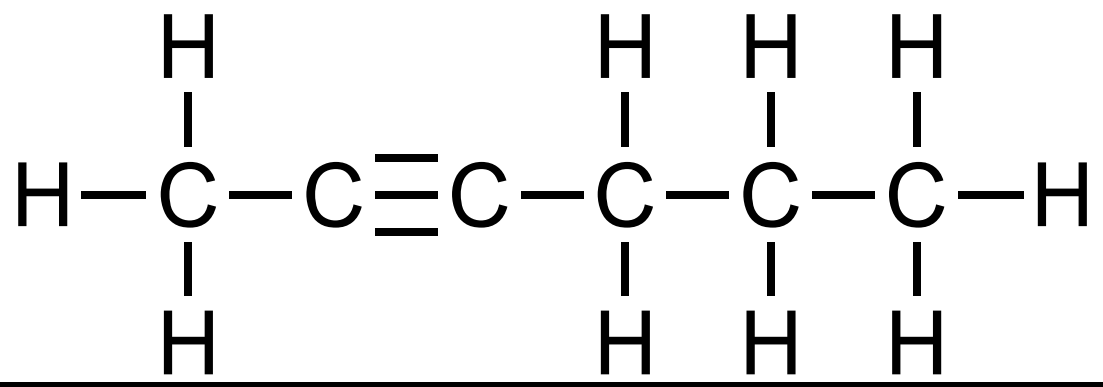
Naming alkynes

$CHCCH_2CH_2CH_2CH_3$



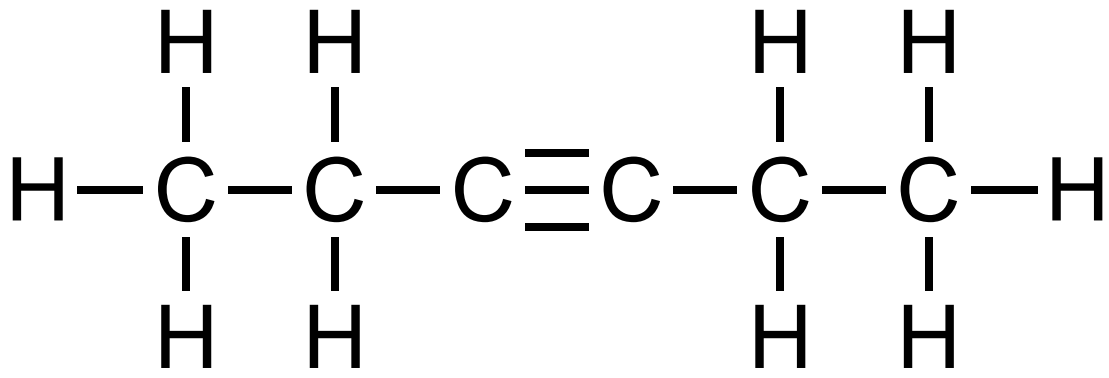
Hex-1-yne

$CH_3CCCH_2CH_2CH_3$



Hex-2-yne

$CH_3CH_2CCCH_2CH_3$



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.

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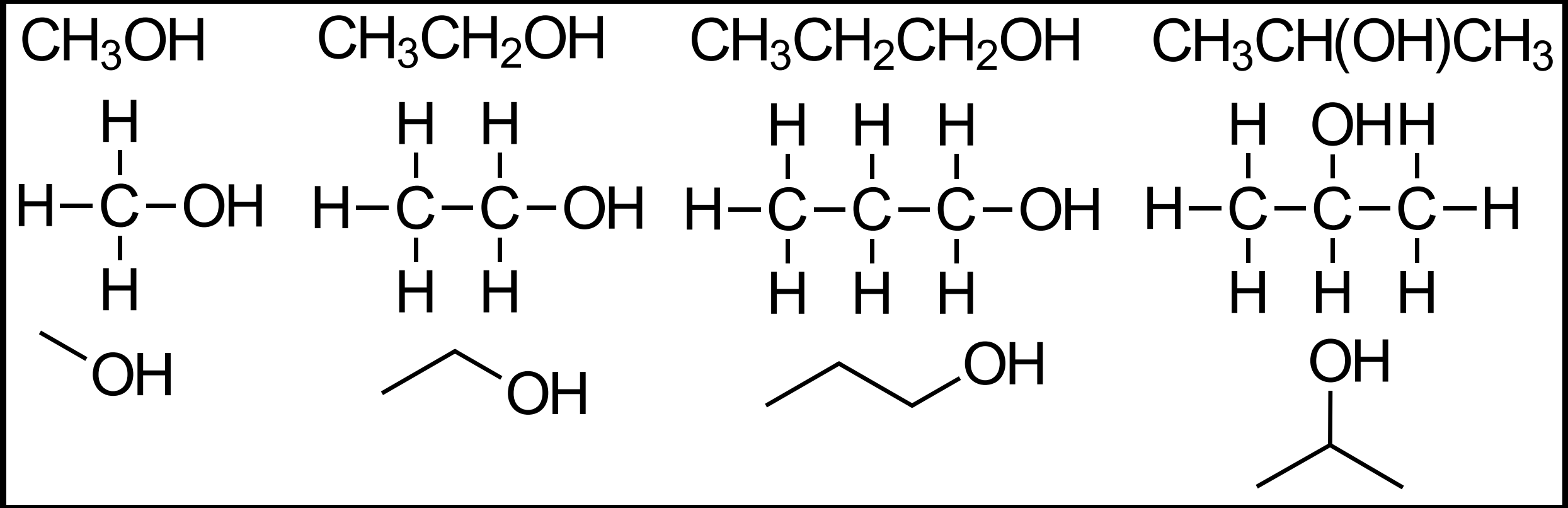
Naming alcohols



Methanol CH_3OH

Ethanol C_2H_5OH

Propan-1-ol C_3H_7OH

Propan-2-ol C_3H_7OH

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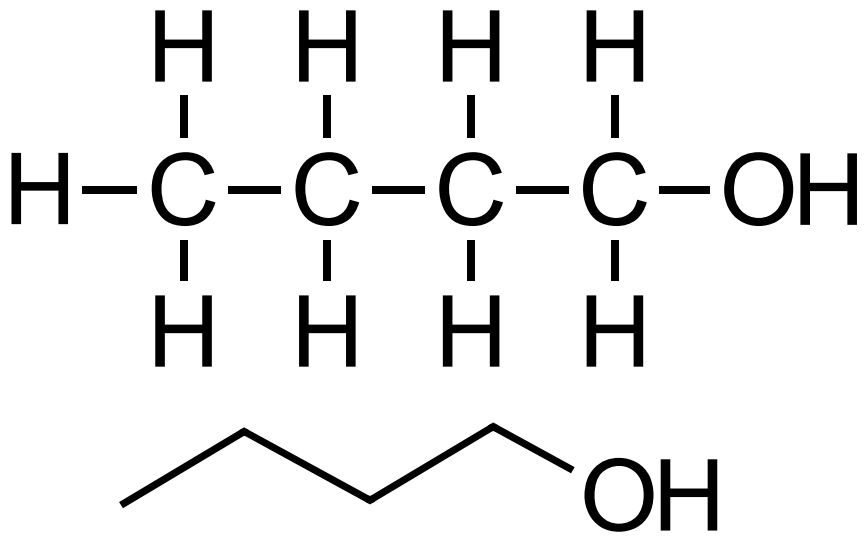
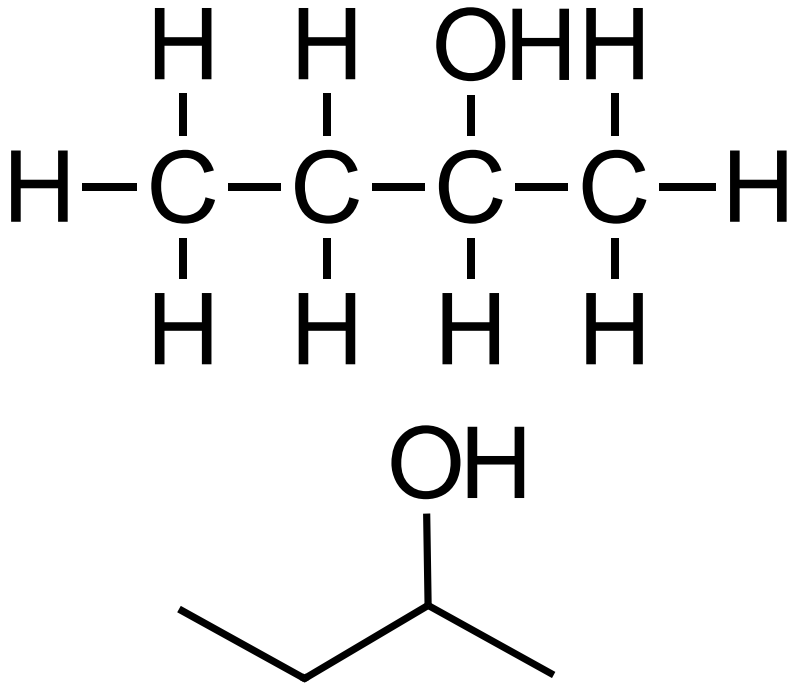
Naming alcohols

$CH_3CH_2CH_2CH_2OH$



$CH_3CH_2CH(OH)CH_3$



Butan-1-ol

C_4H_9OH

Butan-2-ol

C_4H_9OH

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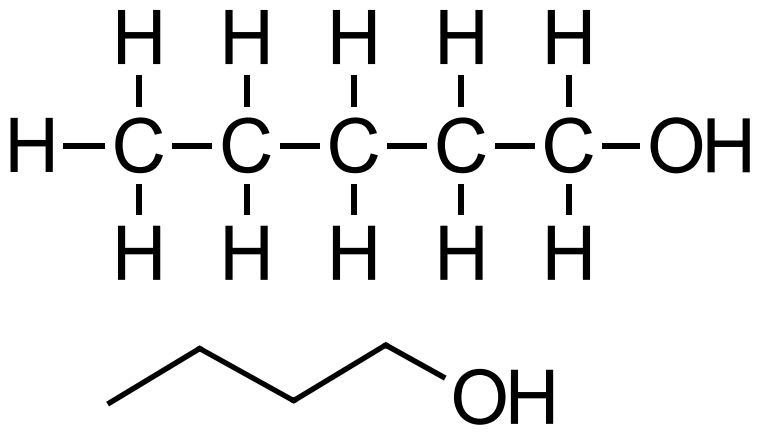
Naming alcohols

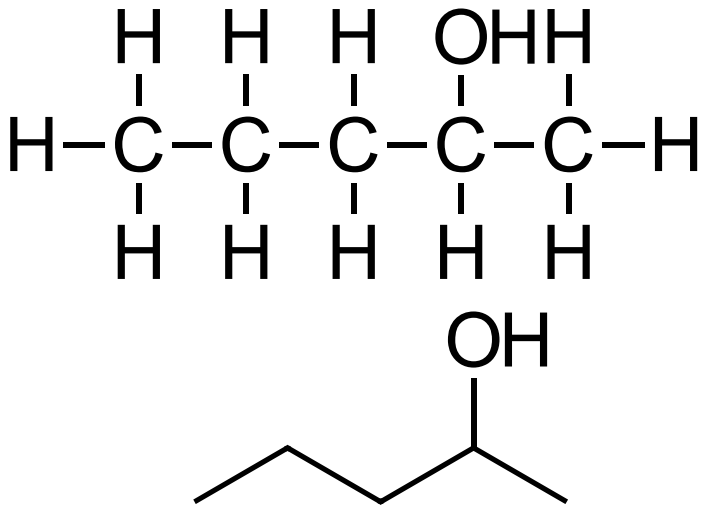
$CH_3CH_2CH_2CH_2CH_2OH$



Pentan-1-ol

$C_5H_{11}OH$

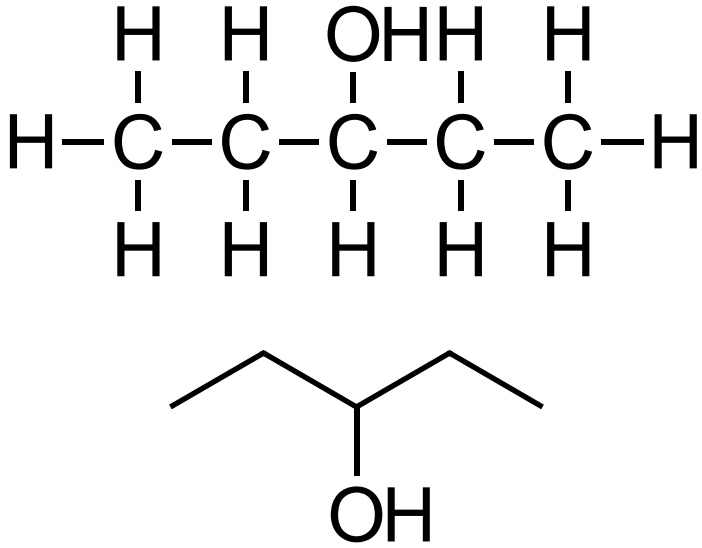
$CH_3CH_2CH_2CH(OH)CH_3$



Pentan-2-ol

$C_5H_{11}OH$

$CH_3CH_2CH(OH)CH_2CH_3$



Pentan-3-ol

$C_5H_{11}OH$

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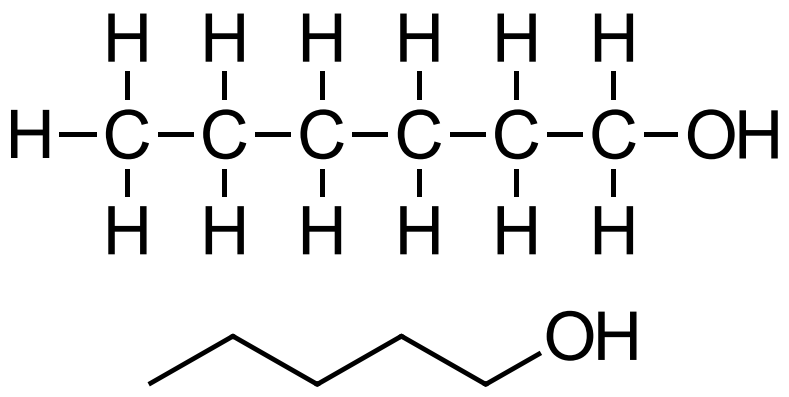
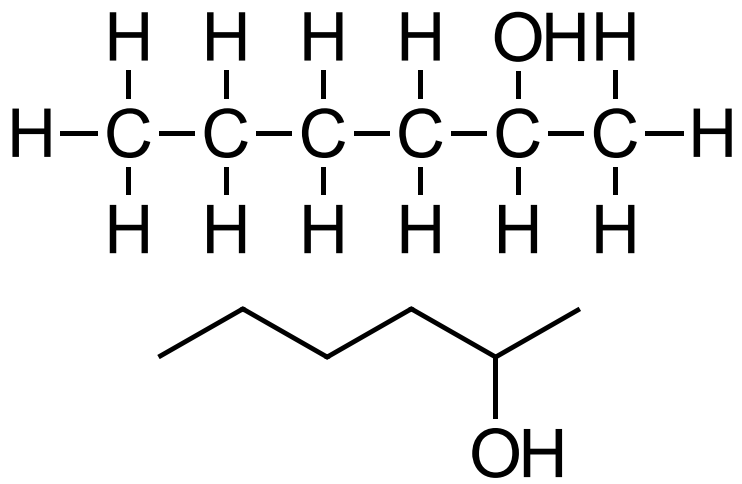
Naming alcohols

$CH_3CH_2CH_2CH_2CH_2CH_2OH$



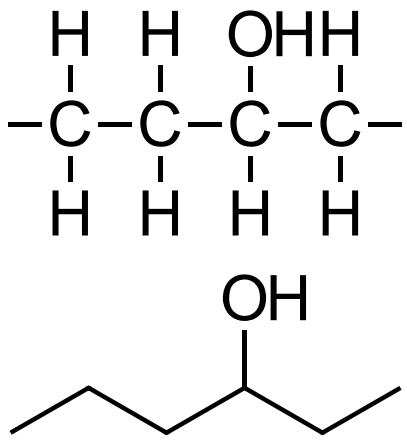
$CH_3CH_2CH_2CH_2CH(OH)CH_3$



Hexan-1-ol

$C_6H_{13}OH$

$CH_3CH_2CH_2CH(OH)CH_2CH_3$



Hexan-2-ol

$C_6H_{13}OH$

Hexan-3-ol

$C_6H_{13}OH$

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Naming carboxylic acids

Naming carboxylic acids

Carboxylic acids are organic acids that contain the carboxyl functional group (COOH or CO_2H).
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.

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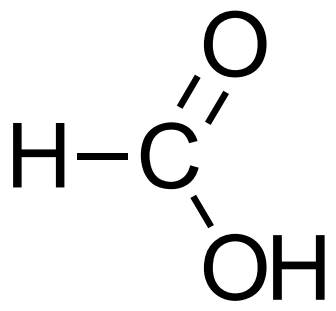
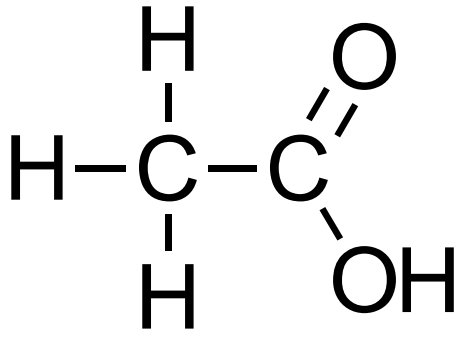
Naming carboxylic acids

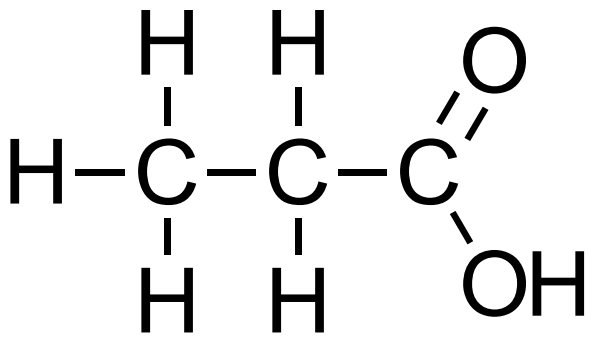
$HCOOH$



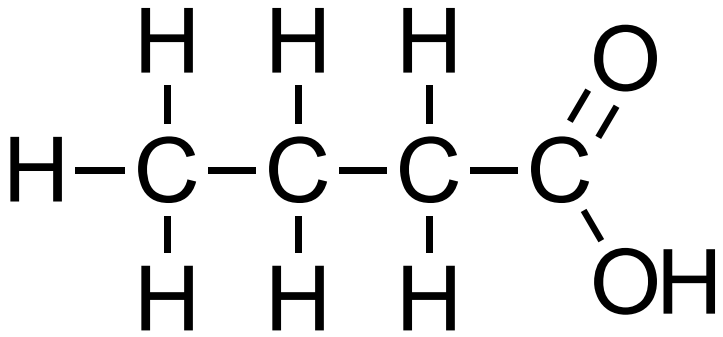
CH_3COOH



CH_3CH_2COOH



$CH_3CH_2CH_2COOH$



Methanoic acid
$HCOOH$

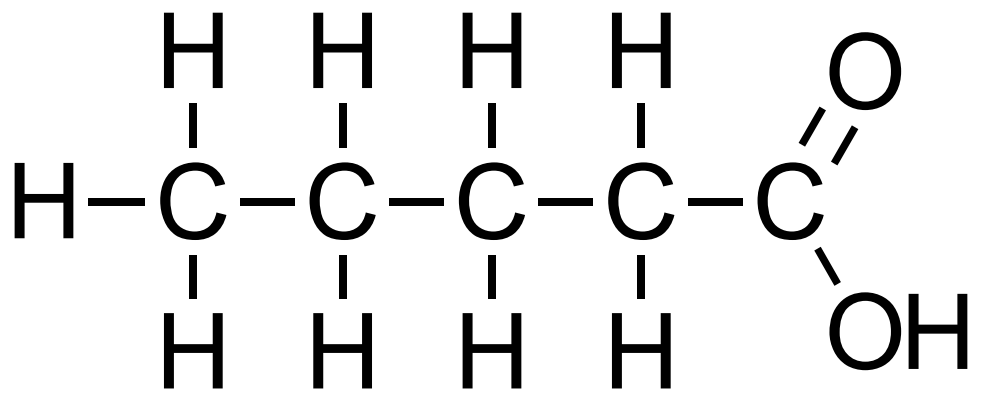
Ethanoic acid
CH_3COOH

Propanoic acid
C_2H_5COOH

Butanoic acid
C_3H_7COOH

Naming carboxylic acids

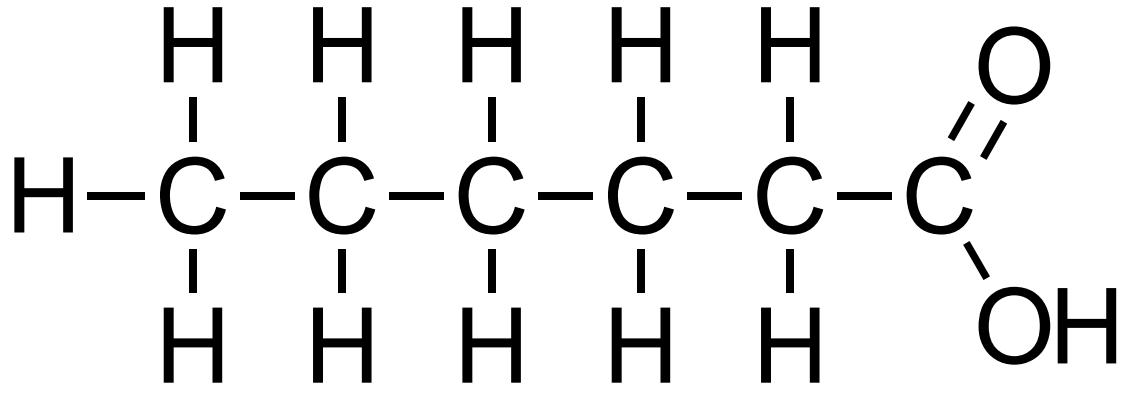
$CH_3CH_2CH_2CH_2COOH$



Pentanoic acid

C_4H_9COOH

$CH_3CH_2CH_2CH_2CH_2COOH$

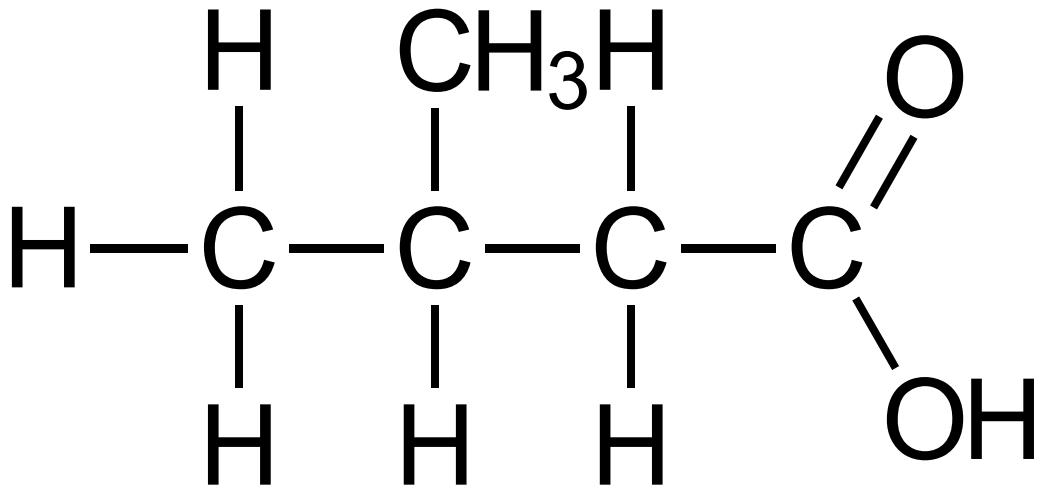


Hexanoic acid

$C_5H_{11}COOH$

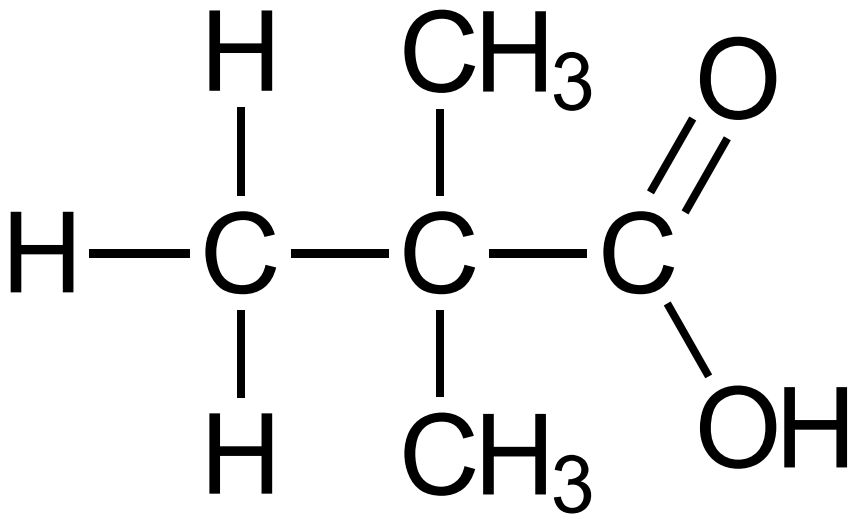
Naming carboxylic acids

$(CH_3)_2CHCH_2COOH$



3-methylbutanoic acid

$CH_3C(CH_3)_2COOH$



2,2-dimethylpropanoic acid

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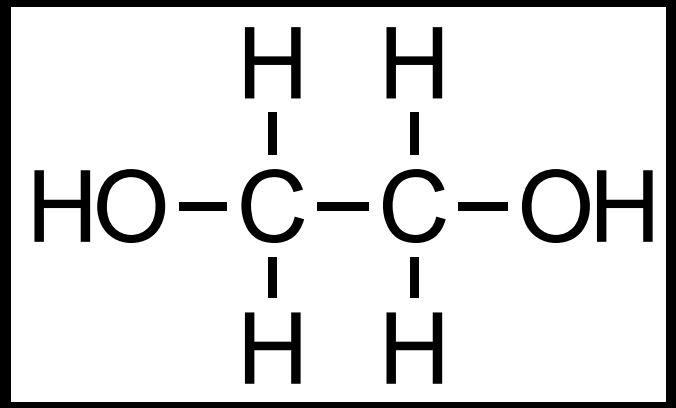
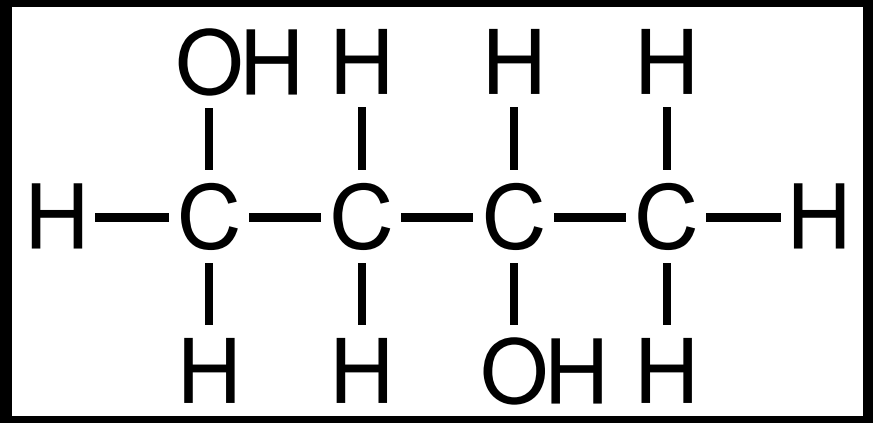
Diols and dicarboxylic acids

Diols

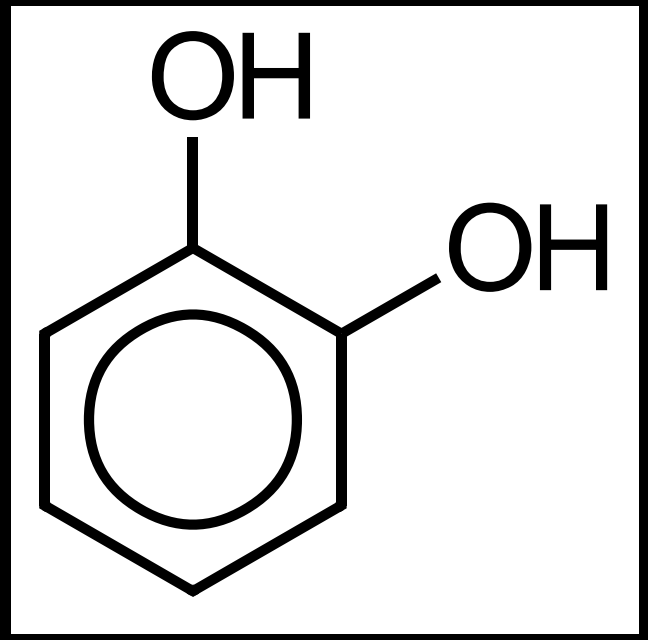
A diol is a compound that contains two hydroxyl (OH) groups.



Ethane-1,2-diol



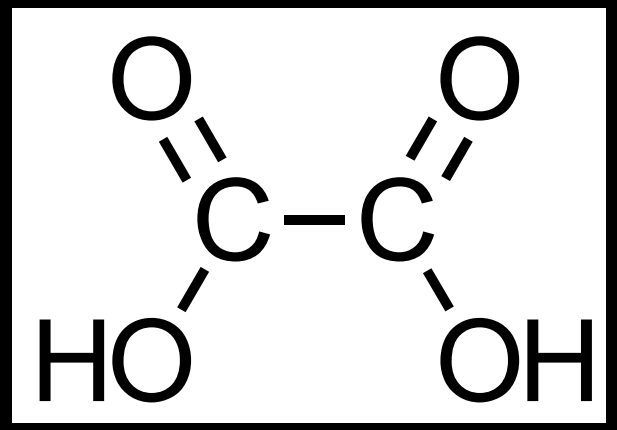
Butane-1,3-diol



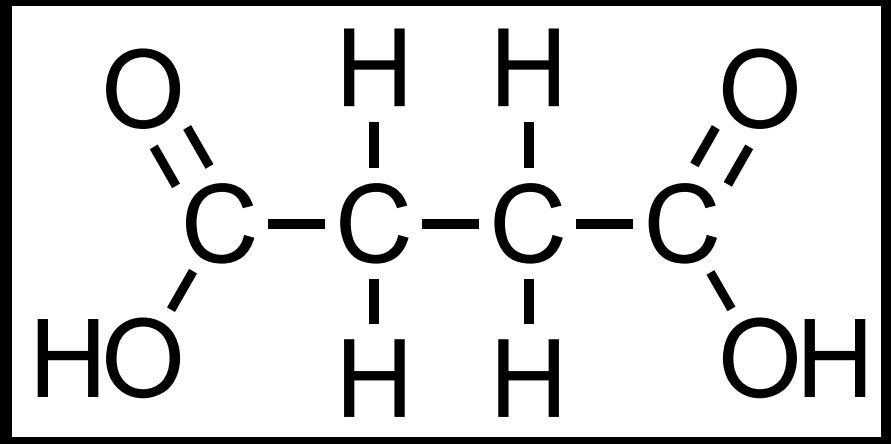
Benzene-1,2-diol

Dicarboxylic acids

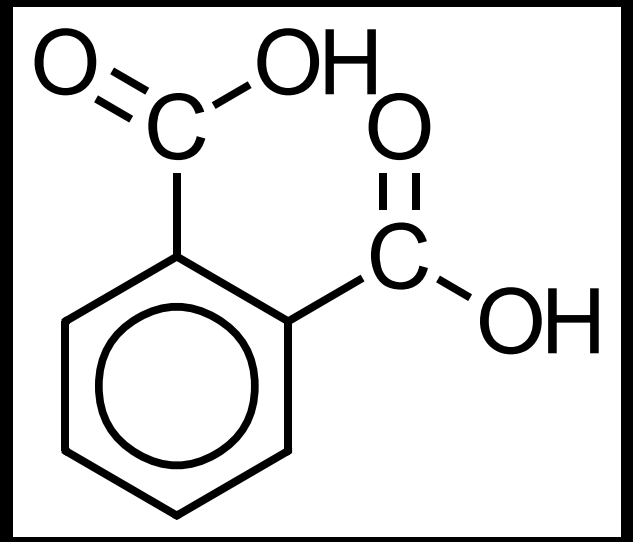
A dicarboxylic acid is a compound that contains two carboxyl (COOH) groups.



Ethanedioic acid



Butanedioic acid



Benzene-1,2-dicarboxylic acid

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Naming aldehydes and ketones

Naming aldehydes and ketones

Aldehydes and ketones both contain a carbonyl group (C=O).

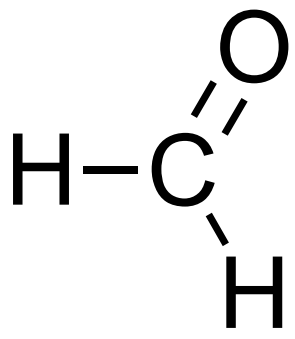
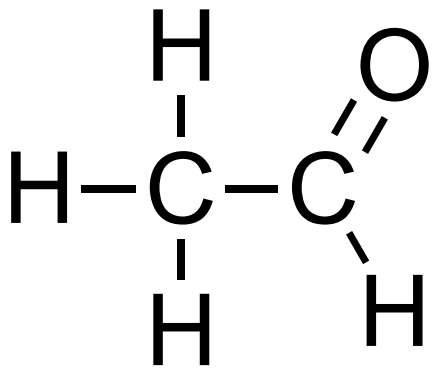
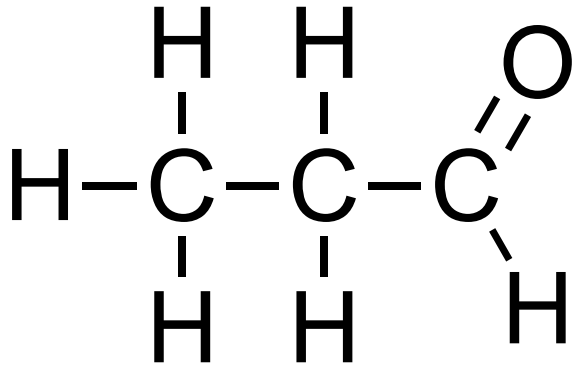
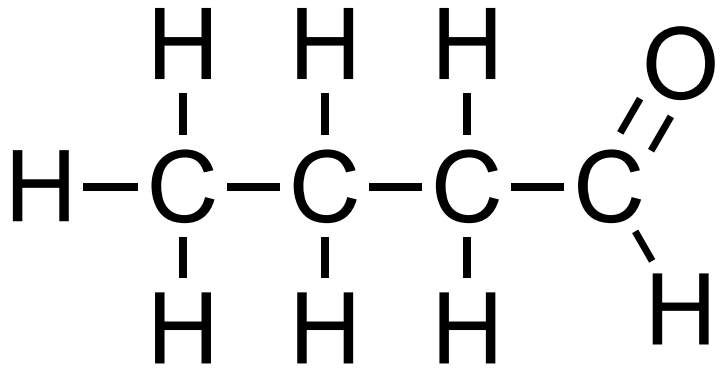
Aldehydes contain an aldehyde group (R-CHO) and ketones contain a ketone group (R-CO-R).

Aldehydes undergo oxidation to form carboxylic acids.

Ketones do not undergo oxidation.

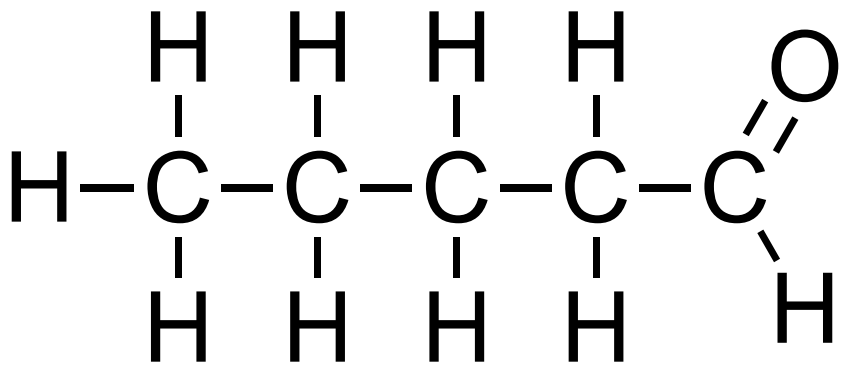
Both are polar molecules because of the difference in electronegativity between the C and O of the carbonyl group.

Naming aldehydes and ketones

HCHO	CH_3CHO	CH_3CH_2CHO	$CH_3CH_2CH_2CHO$
			
Methanal	**Ethanal**	**Propanal**	**Butanal**
CH_2O	C_2H_4O	C_3H_6O	C_4H_7O

Naming aldehydes and ketones

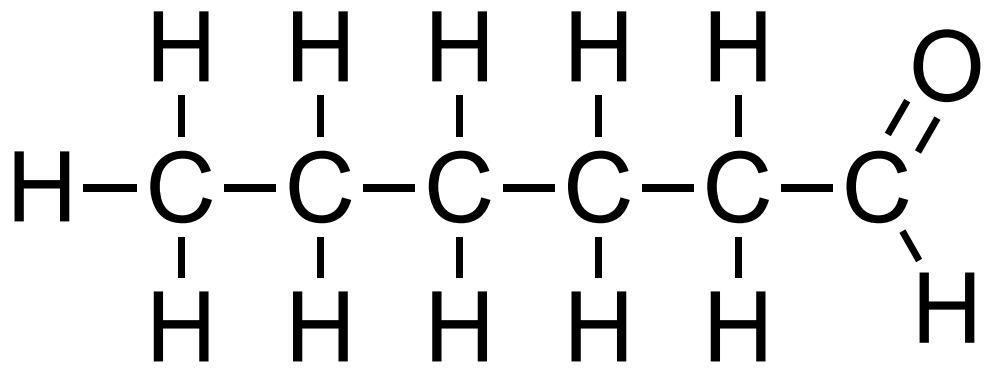
$CH_3CH_2CH_2CH_2CHO$



Pentanal

$C_5H_{10}O$

$CH_3CH_2CH_2CH_2CH_2CHO$

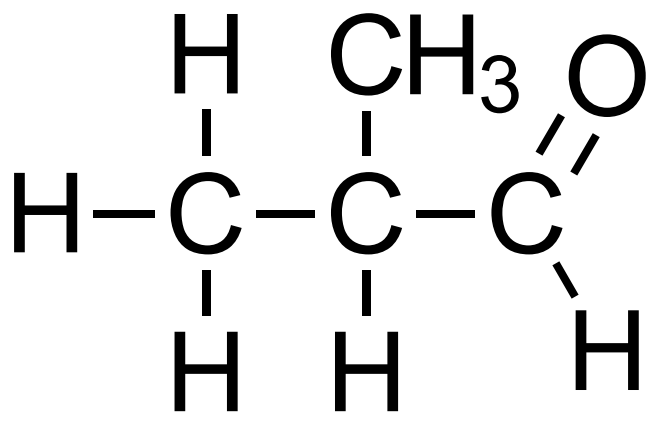


Hexanal

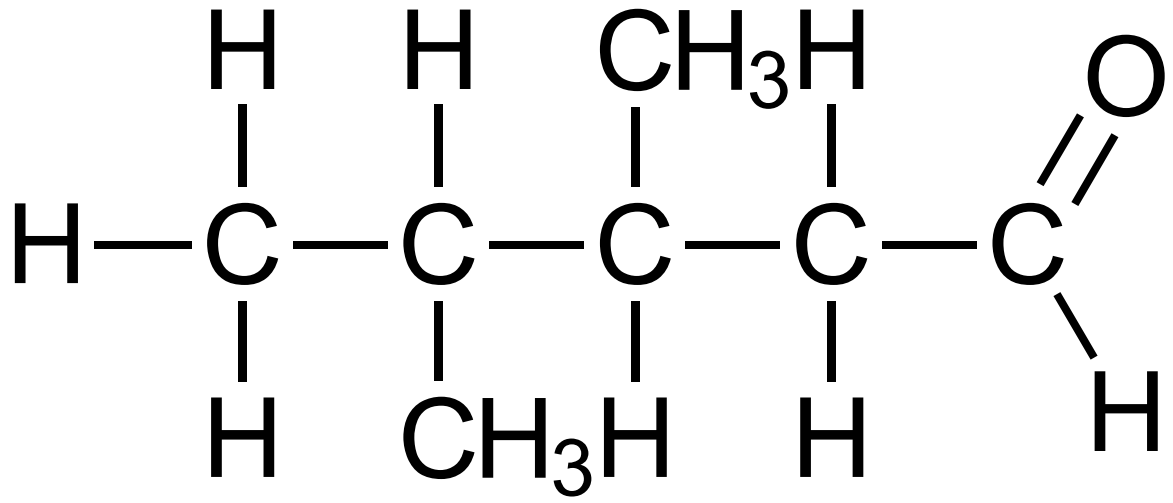
$C_6H_{12}O$

Naming aldehydes and ketones

$(CH_3)_2CHCHO$



$(CH_3)_2CHCH(CH_3)CH_2CHO$

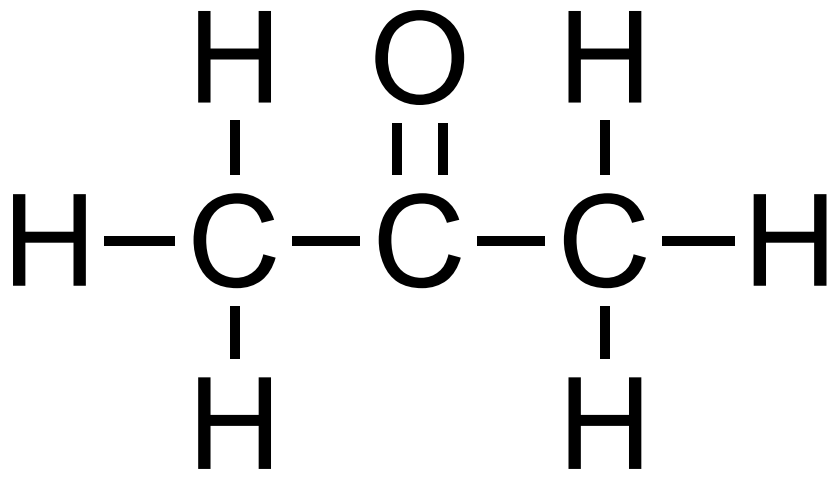


2-methylpropanal

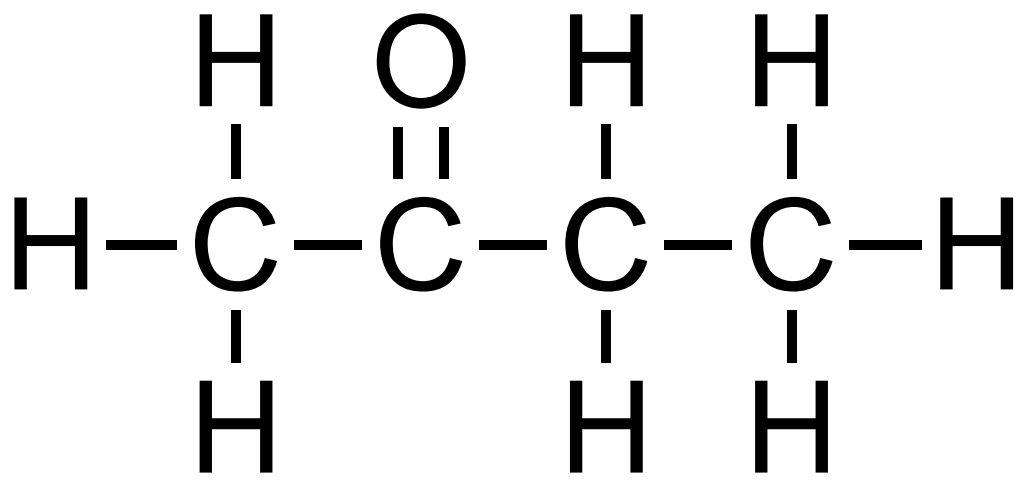
3,4-dimethylpentanal

Naming aldehydes and ketones

CH_3COCH_3



$CH_3COCH_2CH_3$



Propanone

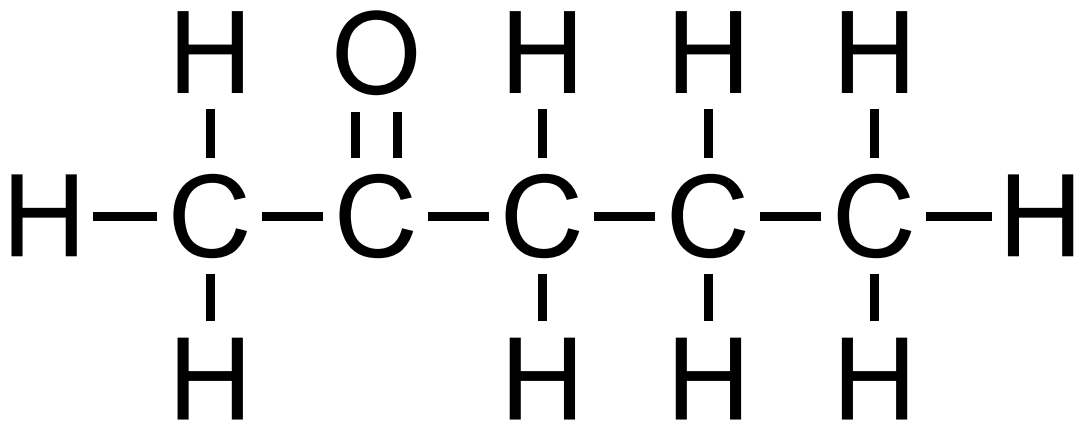
C_3H_6O

Butan-2-one

C_4H_8O

Naming aldehydes and ketones

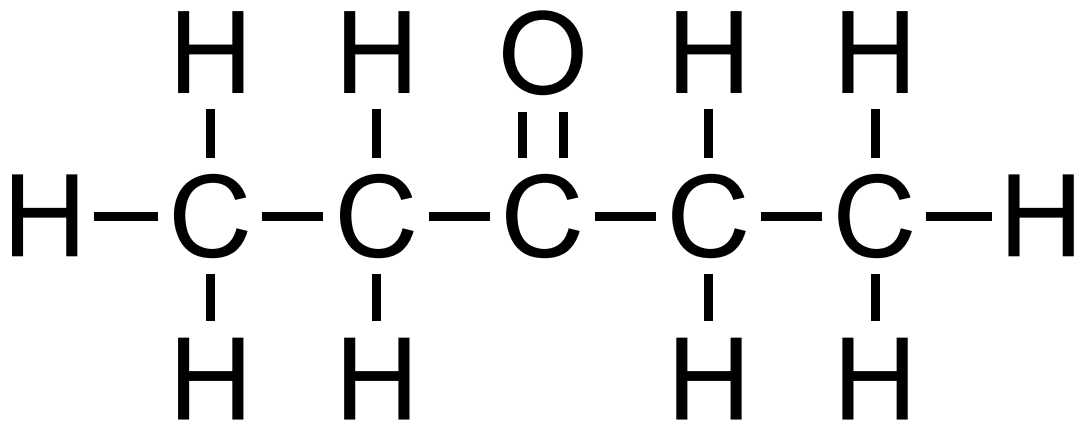
$CH_3COCH_2CH_2CH_3$



Pentan-2-one

$C_5H_{10}O$

$CH_3CH_2COCH_2CH_3$

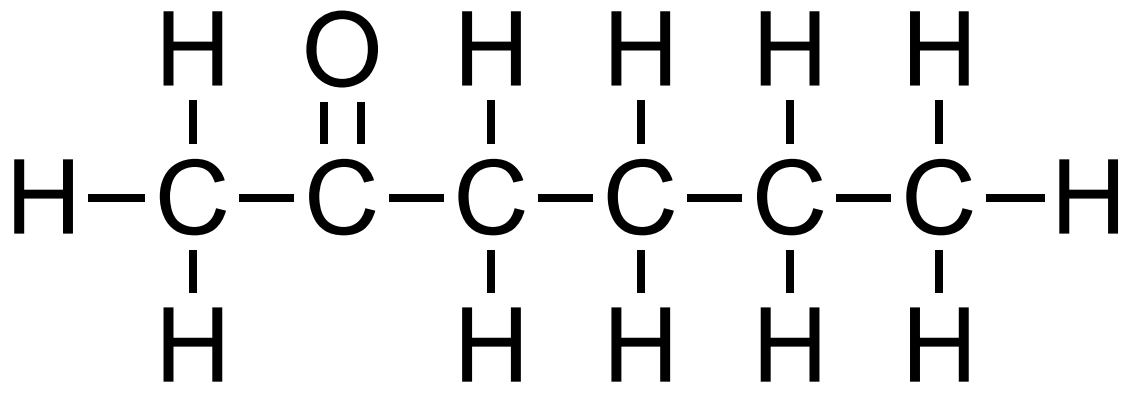


Pentan-3-one

$C_5H_{10}O$

Naming aldehydes and ketones

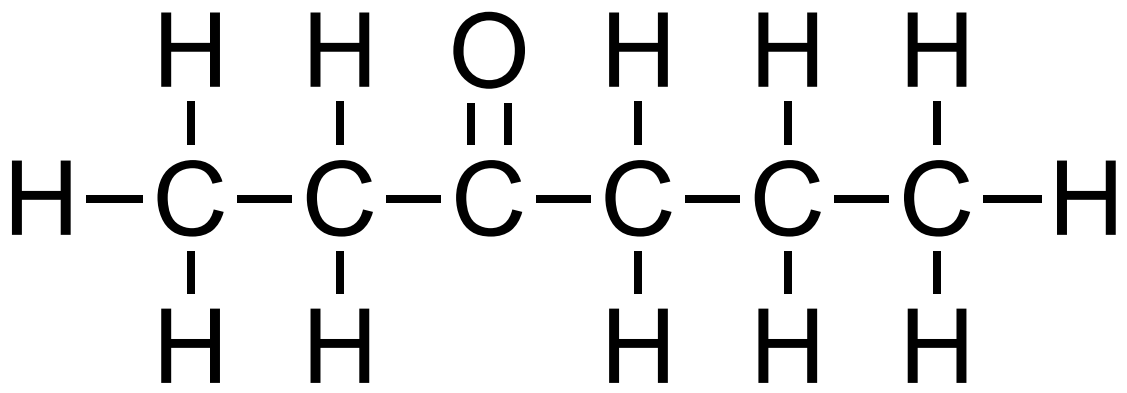
$CH_3COCH_2CH_2CH_2CH_3$



Hexan-2-one

$C_6H_{12}O$

$CH_3CH_2COCH_2CH_2CH_3$



Hexan-3-one

$C_6H_{12}O$

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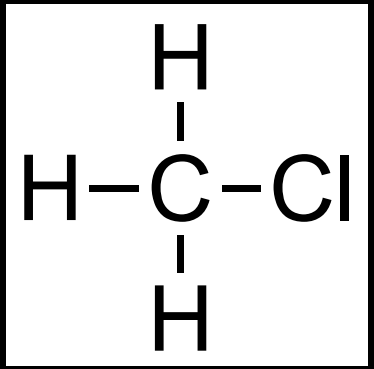
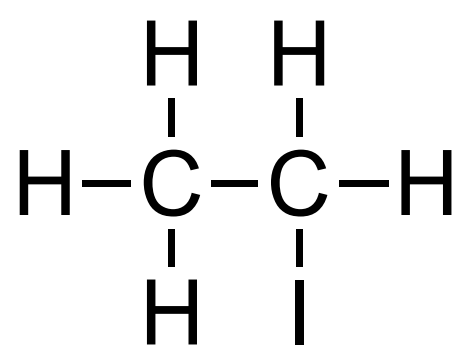
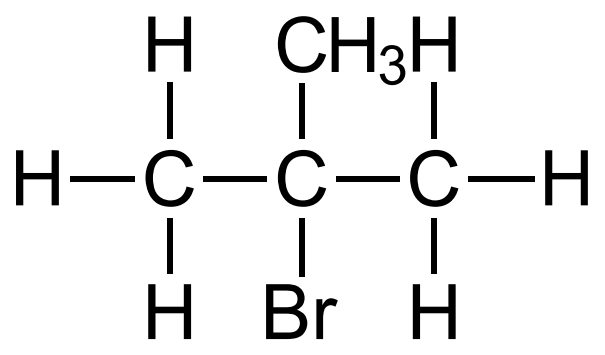
Naming halogenoalkanes

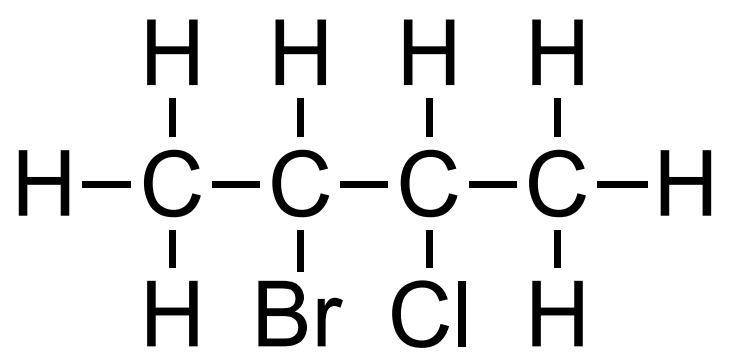
Naming halogenoalkanes

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.

Naming halogenoalkanes

The root is based on the longest chain containing the halogen atom.
The halogen atom defines the halo prefix.
The chain is numbered to give the halogen the lowest possible number.

Halogen	Prefix
Fluorine	Fluoro-
Chlorine	Chloro-
Bromine	Bromo-
Iodine	Iodo-

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

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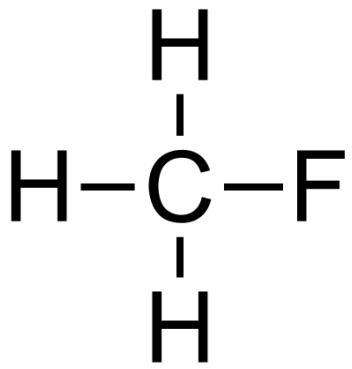
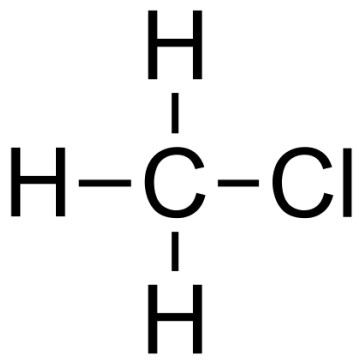
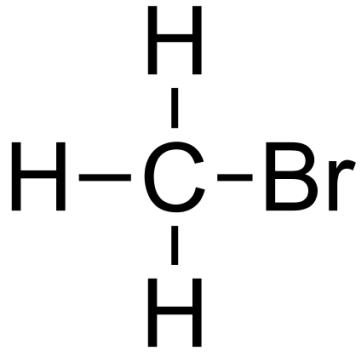
Naming halogenoalkanes



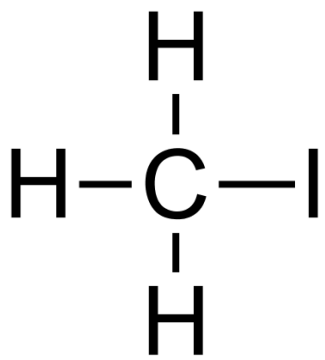
CH_3F
Fluoromethane



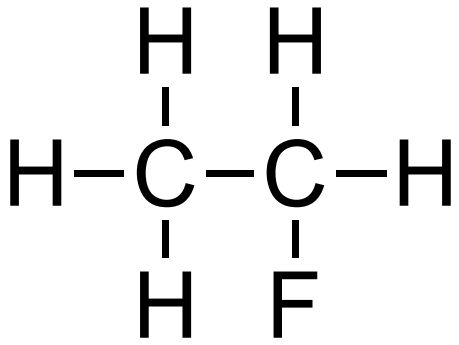
CH_3Cl
Chloromethane



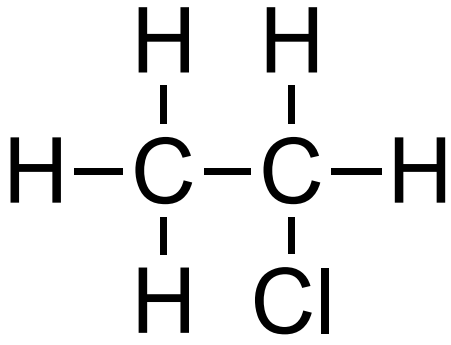
CH_3Br
Bromomethane



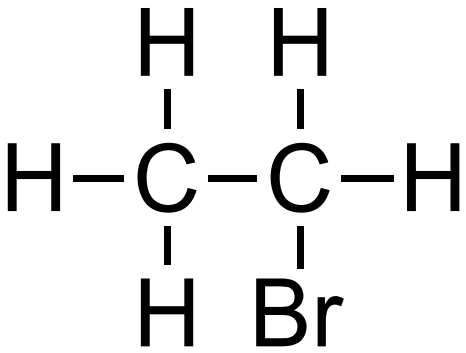
CH_3I
Iodomethane



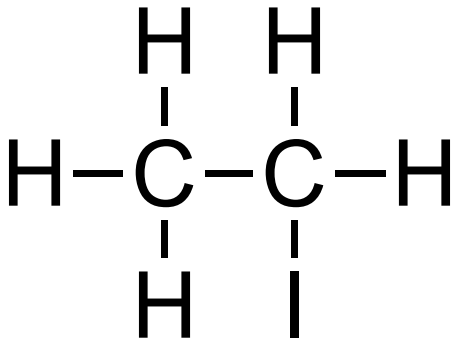
CH_3CH_2F
Fluoroethane



CH_3CH_2Cl
Chloroethane

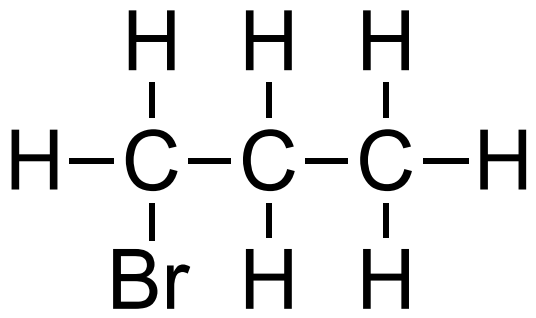


CH_3CH_2Br
Bromoethane

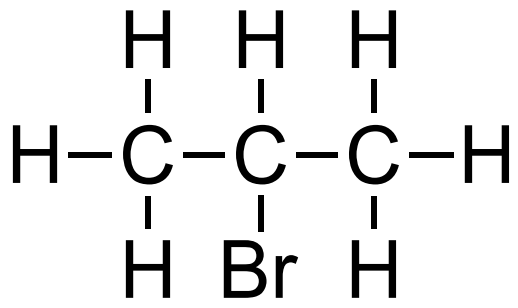


CH_3CH_2I
Iodoethane

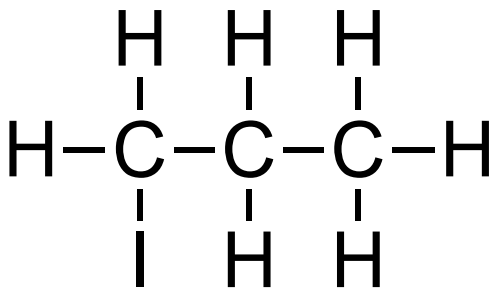
Naming halogenoalkanes



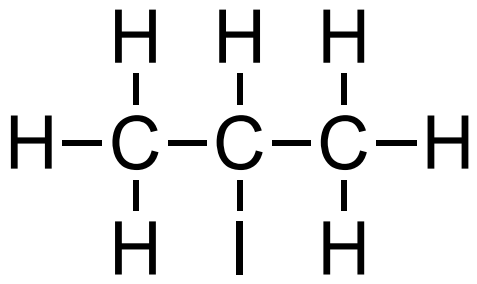
$CH_2BrCH_2CH_3$
1-bromopropane



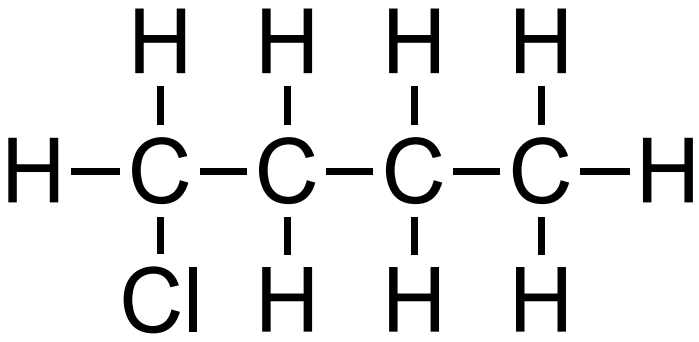
$CH_3CHBrCH_3$
2-bromopropane



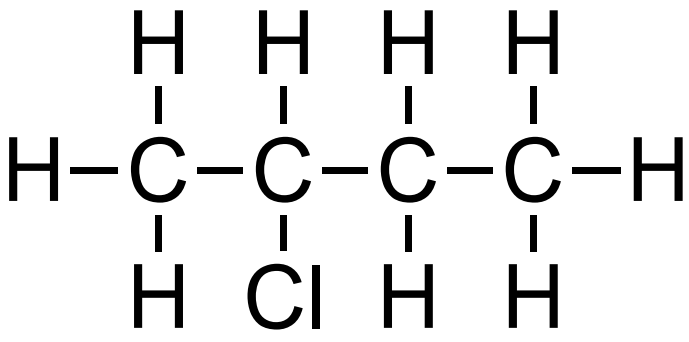
$CH_2ICH_2CH_3$
1-iodopropane



CH_3CHICH_3
2-iodopropane

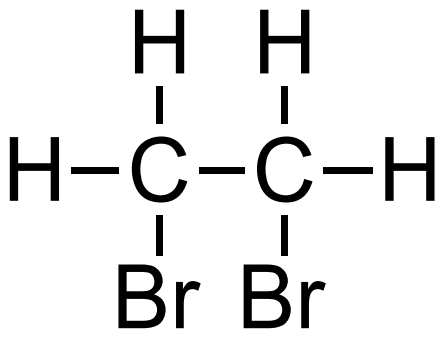


$CH_2ClCH_2CH_2CH_3$
1-chlorobutane

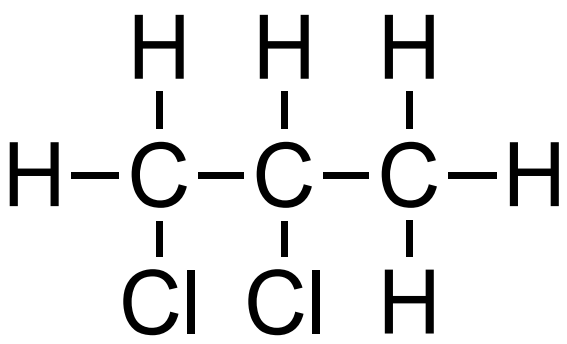


$CH_3CHClCH_2CH_3$
2-chlorobutane

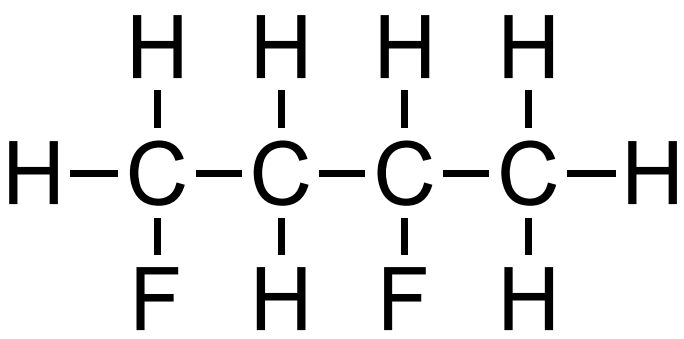
Naming halogenoalkanes



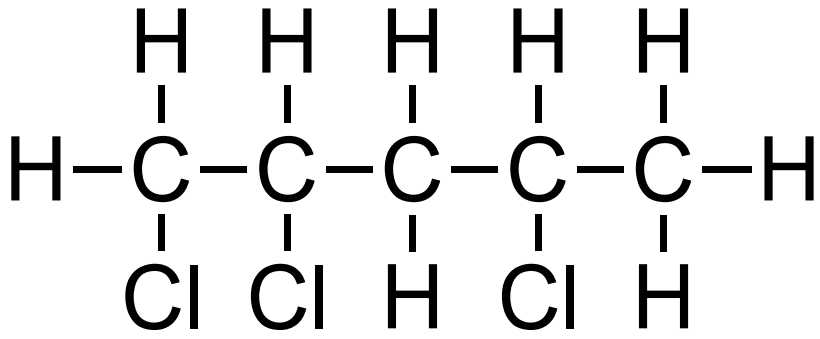
CH_2BrCH_2Br
1,2-dibromoethane



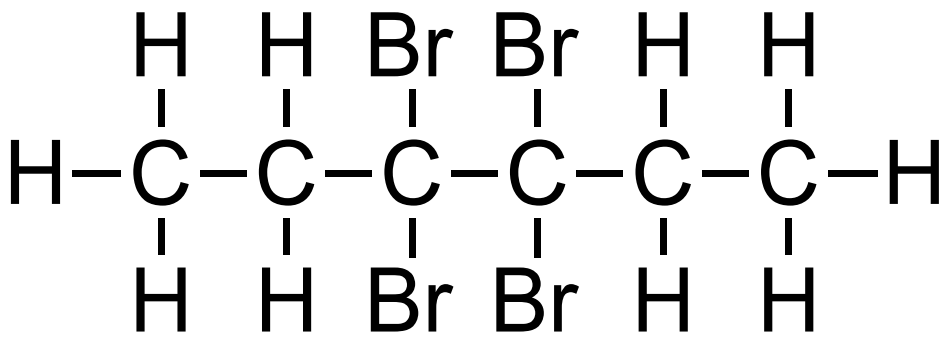
$CH_2ClCHClCH_3$
1,2-dichloropropane



$CH_2FCH_2CHFCH_3$
1,3-difluorobutane

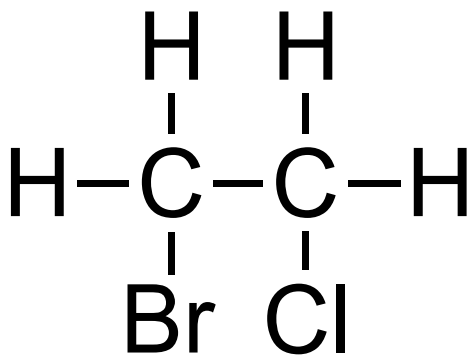


$C_5H_9Cl_3$
1,2,4-trichloropentane



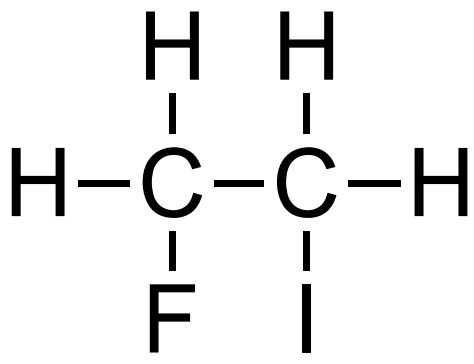
$C_6H_{10}Br_4$
3,3,4,4-tetrabromohexane

Naming halogenoalkanes



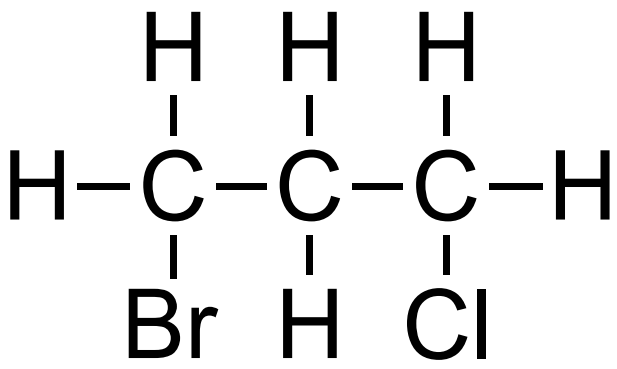
CH_2BrCH_2Cl

1-bromo-2-chloroethane



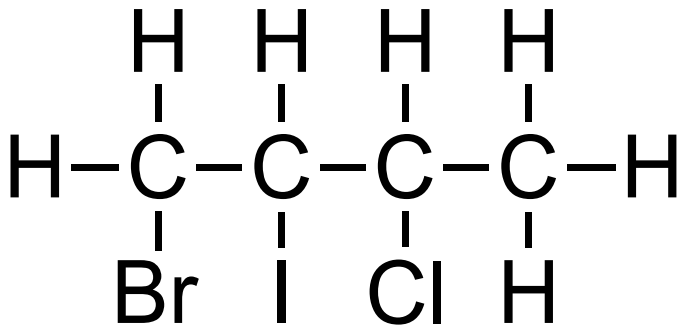
CH_2FCH_2I

1-fluoro-2-iodoethane



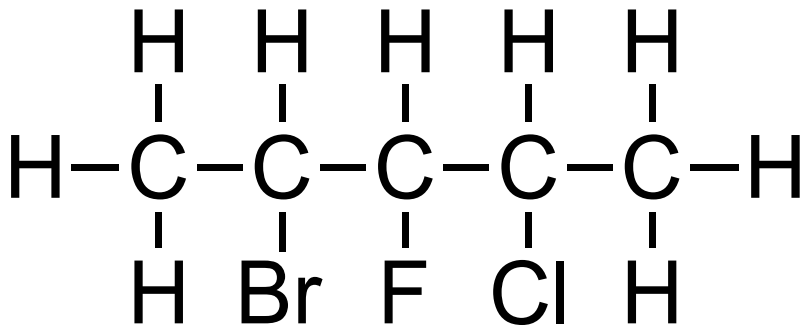
$CH_2BrCH_2CH_2Cl$

1-bromo-3-chloropropane



C_4H_7BrClI

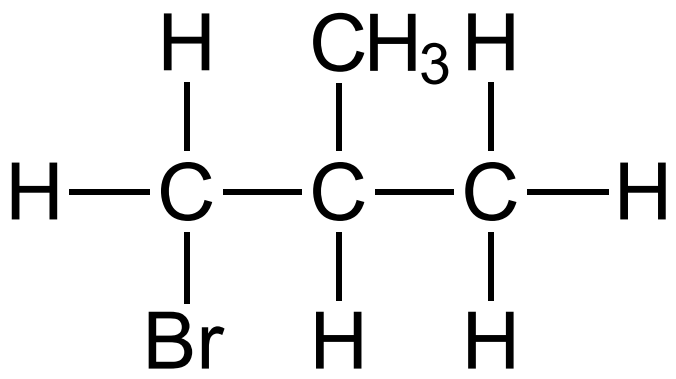
1-bromo-3-chloro-2-iodobutane



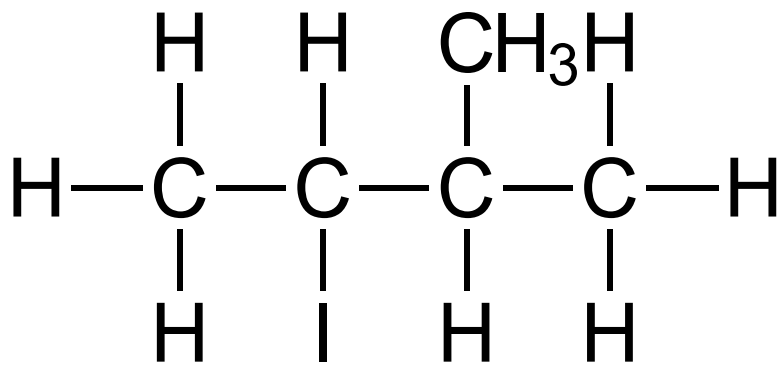
C_5H_9BrClF

2-bromo-4-chloro-3-fluoropentane

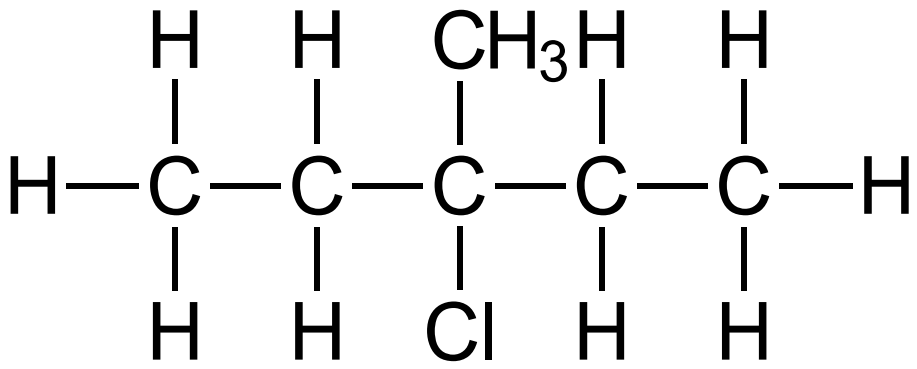
Naming halogenoalkanes



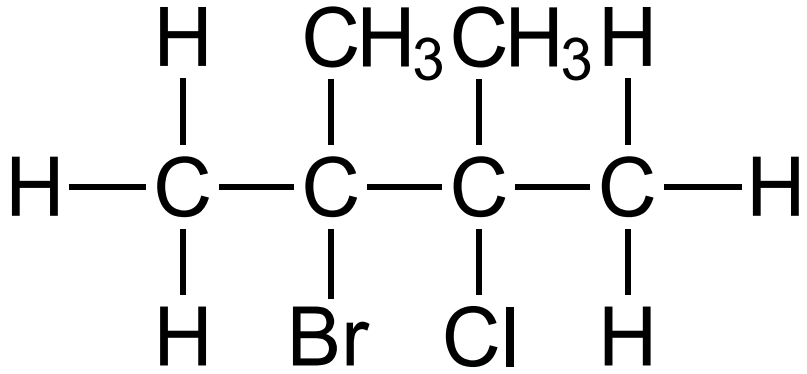
$CH_2BrCH(CH_3)CH_3$
1-bromo-2-methylpropane



$CH_3CHICH(CH_3)CH_3$
2-iodo-3-methylbutane



$CH_3CH_2CCl(CH_3)CH_2CH_3$
3-chloro-3-methylpentane



$CH_3CBr(CH_3)CCl(CH_3)CH_3$
2-bromo-3-chloro-2,3-dimethylbutane

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Esters

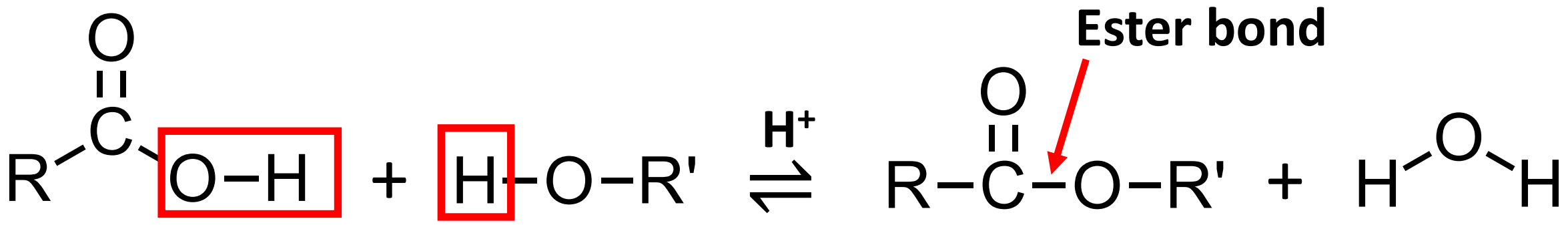
Esters

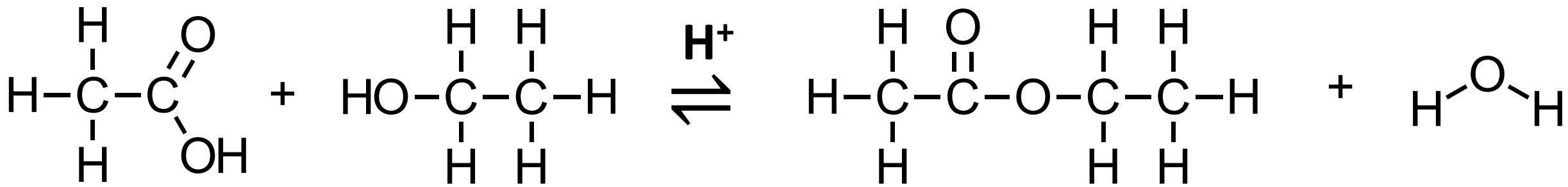
Esters (RCOOR') are derivatives of carboxylic acids. They are formed in the reaction between a carboxylic acid and an alcohol.

carboxylic acid + alcohol ⇌ ester + water

This is a nucleophilic substitution reaction; also called a condensation or esterification reaction.
The catalyst used is concentrated sulfuric acid (H_2SO_4).

Esters

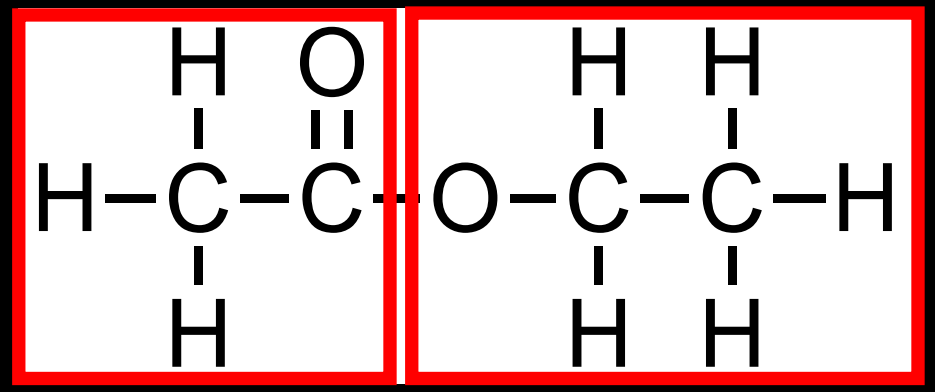




$$CH_3COOH_{(l)} + CH_3CH_2OH_{(l)} \rightleftharpoons CH_3COOCH_2CH_{3(l)} + H_2O_{(l)}$$

Naming esters

Carboxylic acid

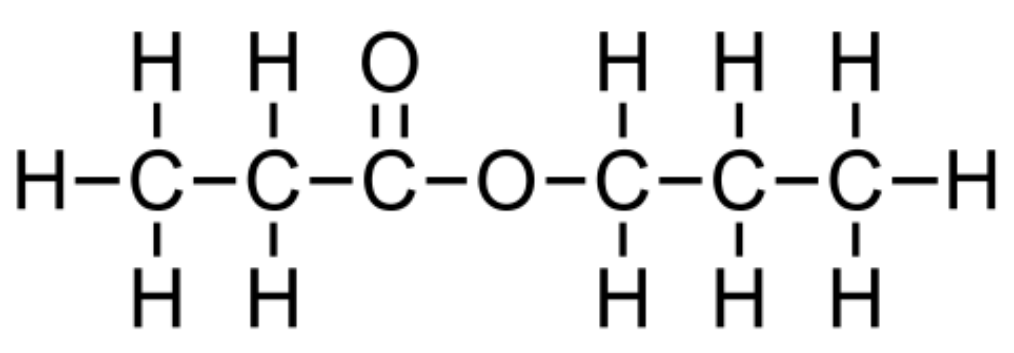


Alcohol

Number of carbons	Alcohol	Carboxylic acid
1	methyl	methanoate
2	ethyl	ethanoate
3	propyl	propanoate
4	butyl	butanoate
5	pentyl	pentanoate

Naming esters

Carboxylic acid



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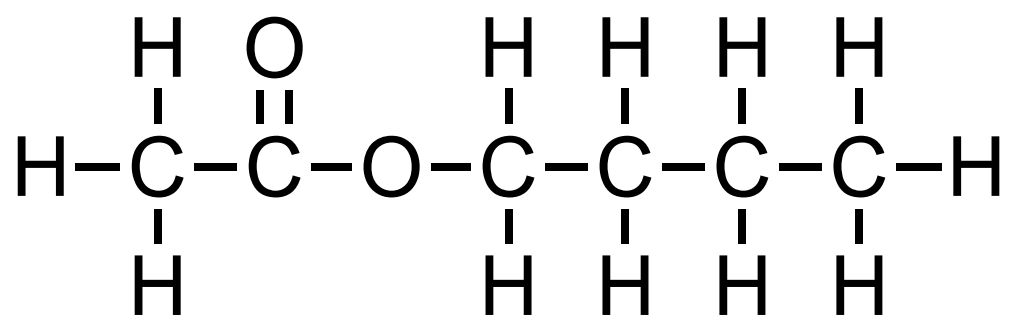
Naming esters

Carboxylic acid



Alcohol

Number of carbons	Alcohol	Carboxylic acid
1	methyl	methanoate
2	ethyl	ethanoate
3	propyl	propanoate
4	butyl	butanoate
5	pentyl	pentanoate

Naming esters

The first part of the name is derived from the alkyl chain of the alcohol.

The second part of the name is derived from the carboxylic acid (longest carbon chain including the carbonyl group.)

Alcohol	
Methanol	Methyl
Ethanol	ethyl
Propanol	propyl
Butanol	Butyl

Carboxylic acid	
Methanoic acid	methanoate
Ethanoic acid	ethanoate
Propanoic acid	propanaote
Butanoic acid	Butanoate

Naming esters

$$HCOOH_{(l)} + CH_3CH_2OH_{(l)} \rightleftharpoons HCOOCH_2CH_{3(l)} + H_2O_{(l)}$$

Ethyl methanoate

$$CH_3COOH_{(l)} + CH_3OH_{(l)} \rightleftharpoons CH_3COOCH_{3(l)} + H_2O_{(l)}$$

Methyl ethanoate

$$CH_3COOH_{(l)} + CH_3CH_2CH_2CH_2OH_{(l)} \rightleftharpoons CH_3COOCH_2CH_2CH_2CH_{3(l)} + H_2O_{(l)}$$

Butyl ethanoate

$$CH_3CH_2COOH_{(l)} + CH_3CH_2CH_2OH_{(l)} \rightleftharpoons CH_3CH_2COOCH_2CH_2CH_{3(l)} + H_2O_{(l)}$$

Propyl propanoate

Esters

Ester	Molar mass (g mol^{-1})	Boiling point (°C)
CH_3COOCH_3	74.08	57.1
$CH_3COOCH_2CH_3$	88.11	77.1
$CH_3COOCH_2CH_2CH_3$	102.13	102
$CH_3COOCH_2CH_2CH_2CH_3$	116.16	126
$CH_3COOCH_2CH_2CH_2CH_2CH_3$	130.19	149

Properties of esters

Esters are used as artificial food flavourings, solvents and plasticisers.

Ester	Flavour/fragrance
Methyl butanoate	apples
Ethyl butanoate	pineapple
Pentyl ethanoate	bananas
Pentyl butanoate	pears
Ethyl heptanoate	grapes

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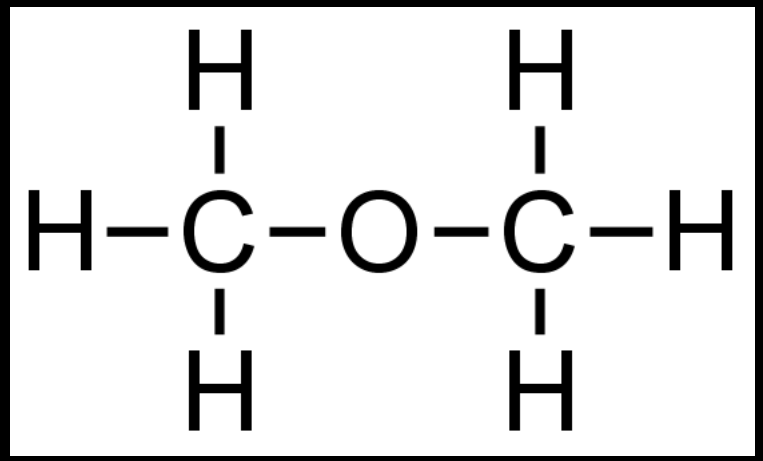
Naming ethers

Naming ethers

Ethers have the ether functional group R-O-R', where R and R' can be alkyl or aryl groups.



Ethers are weakly polar molecules because of the C-O-C bond. CH_3OCH_3 boils at -24°C.

Ethers with up to 3 carbon atoms are soluble in water but the solubility decreases with an increasing number of carbon atoms.

Naming ethers

Ethers have two alkyl groups bonded to an oxygen atom. The shorter alkyl group (with the oxygen) becomes the alkoxy substituent.

The longer alkyl group becomes the alkane stem.

Alkoxy group	Name	Alkane stem	Name
CH_3O-	Methoxy	-CH_3	methane
CH_3CH_2O-	Ethoxy	-CH_2CH_3	ethane
$CH_3CH_2CH_2O$-	Propoxy	-$CH_2CH_2CH_3$	propane
$CH_3(CH_2)_3O$-	Butoxy	-$(CH_2)_3CH_3$	butane

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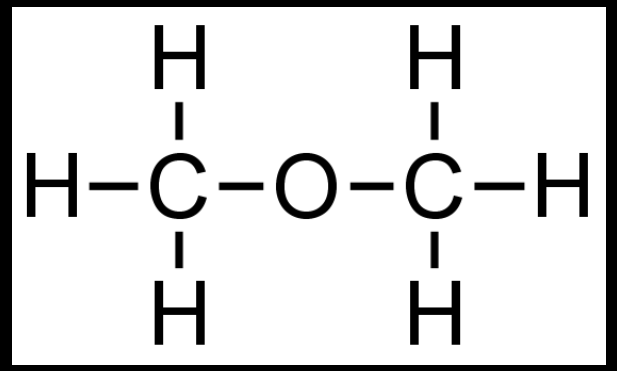
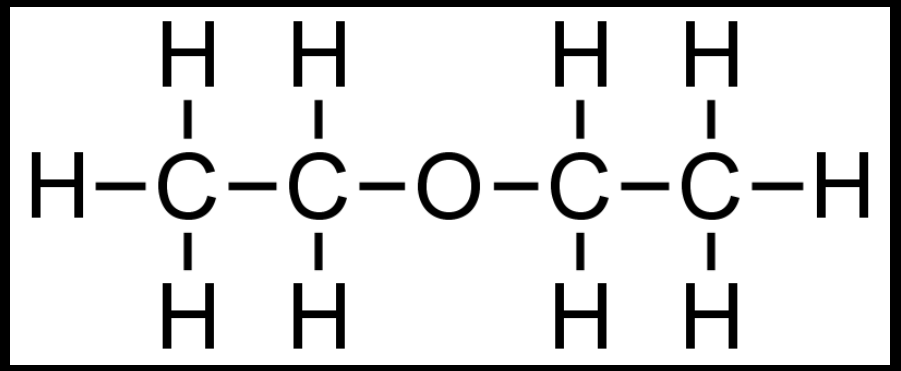
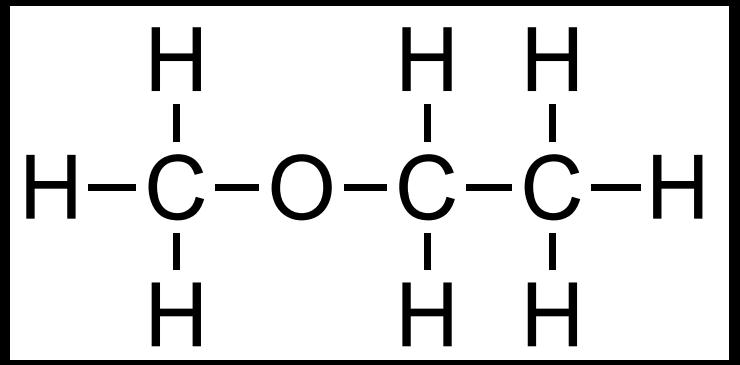
Naming ethers



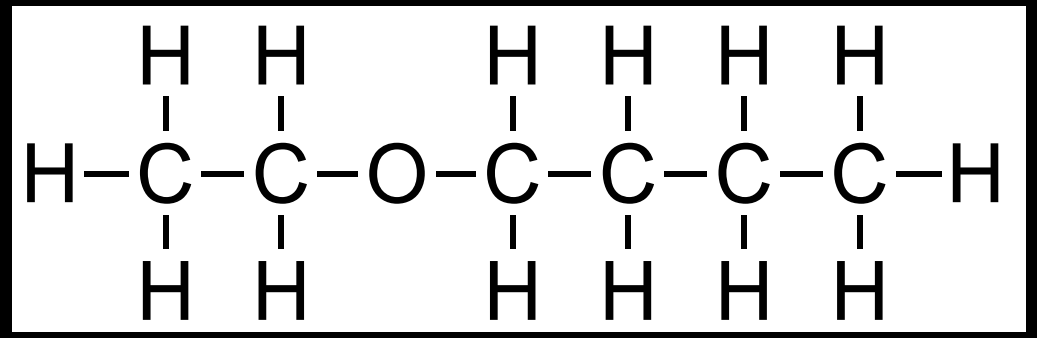
Methoxymethane
CH_3OCH_3



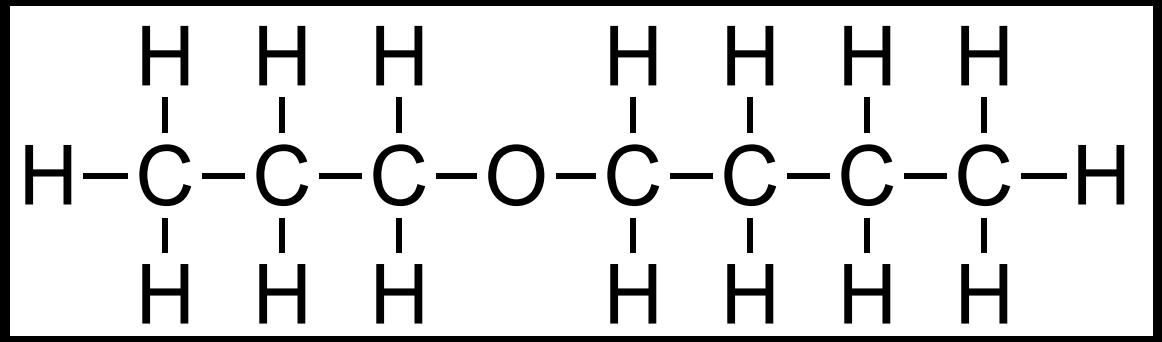
Ethoxyethane
$CH_3CH_2OCH_2CH_3$



Methoxyethane
$CH_3OCH_2CH_3$



1-ethoxybutane
$CH_3CH_2O(CH_2)_3CH_3$



1-propoxybutane
$CH_3(CH_2)_2O(CH_2)_3CH_3$

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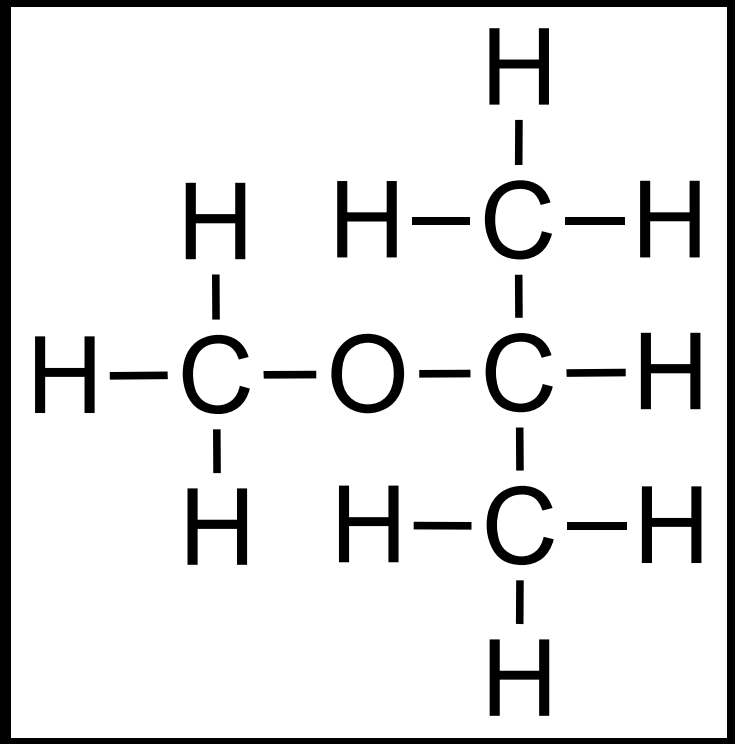
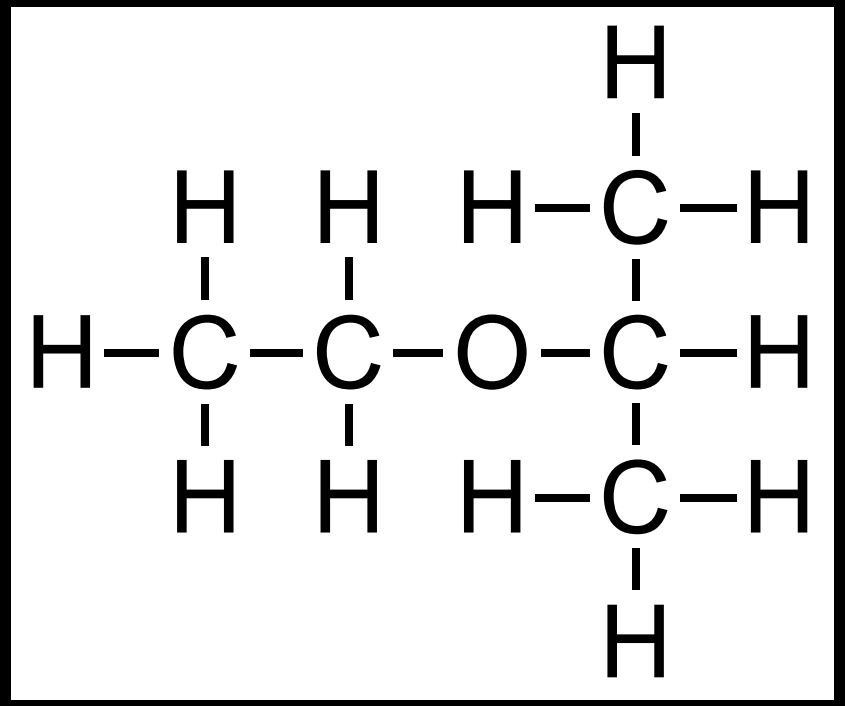
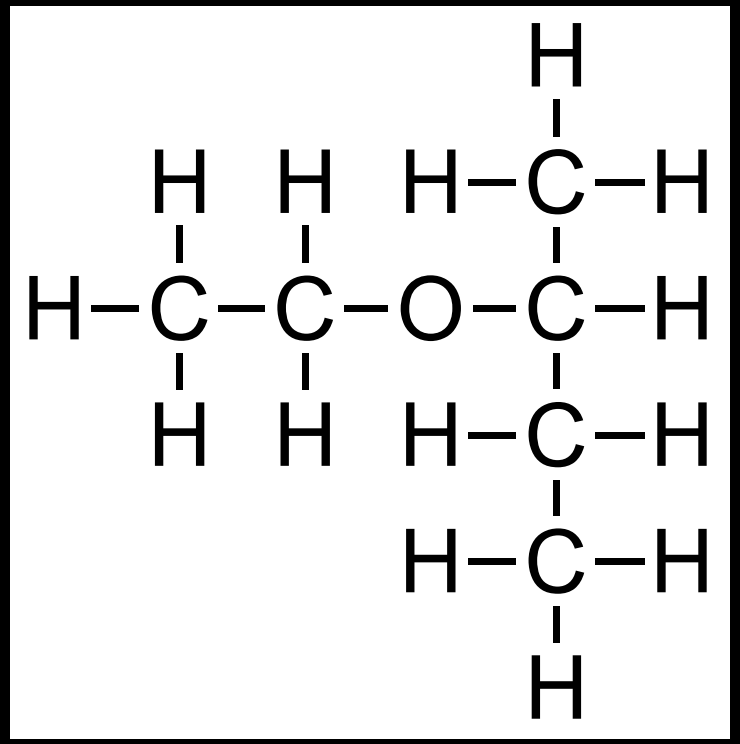
Naming ethers



2-methoxypropane
$CH_3OCH(CH_3)_2$



2-ethoxypropane
$CH_3CH_2OCH(CH_3)_2$



2-ethoxybutane
$CH_3CH_2OCH(CH_3)CH_2CH_3$

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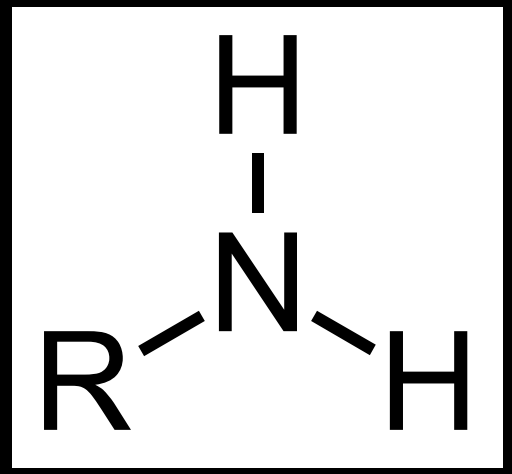
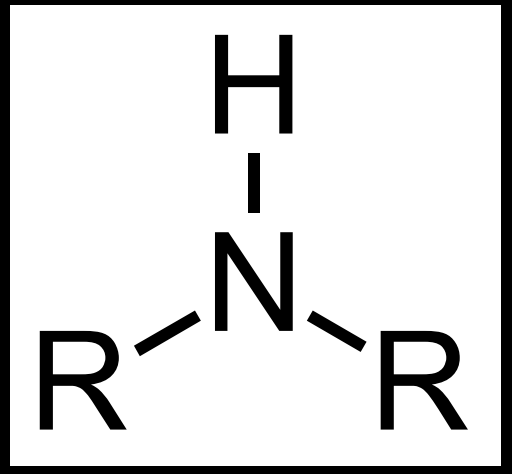
Naming amines

Amines

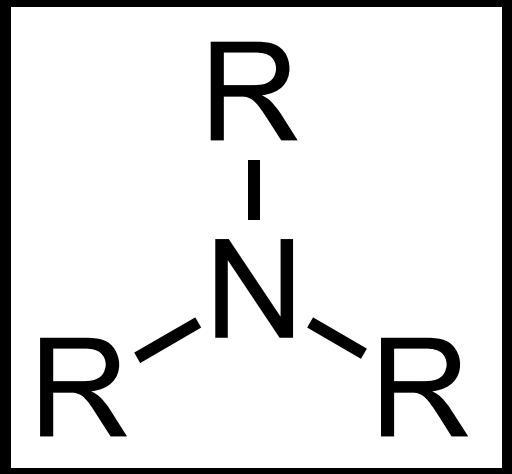
Amines are derivatives of ammonia (NH_3) in which the hydrogen atoms have been replaced by hydrocarbon (alkyl) groups.



Primary amine



Secondary amine



Tertiary amine

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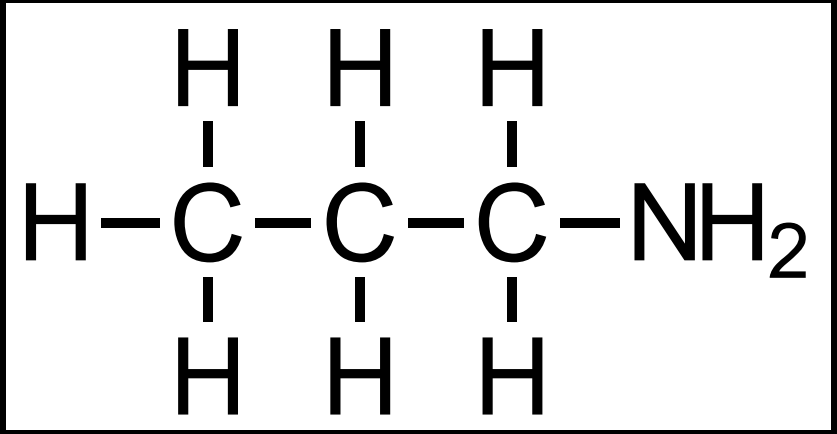
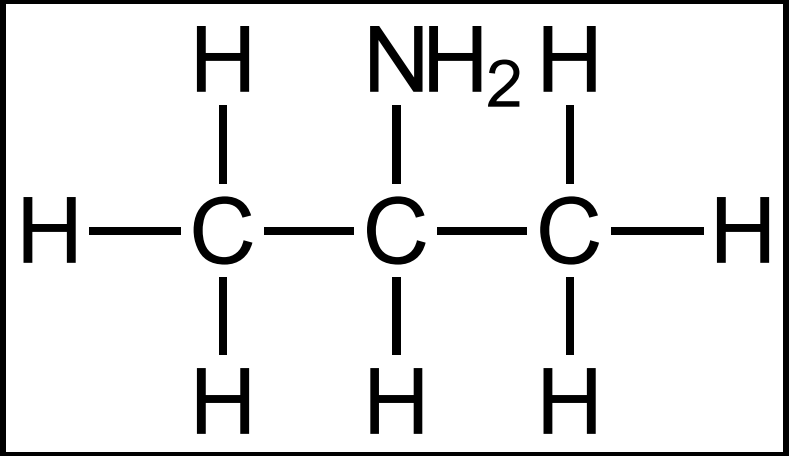
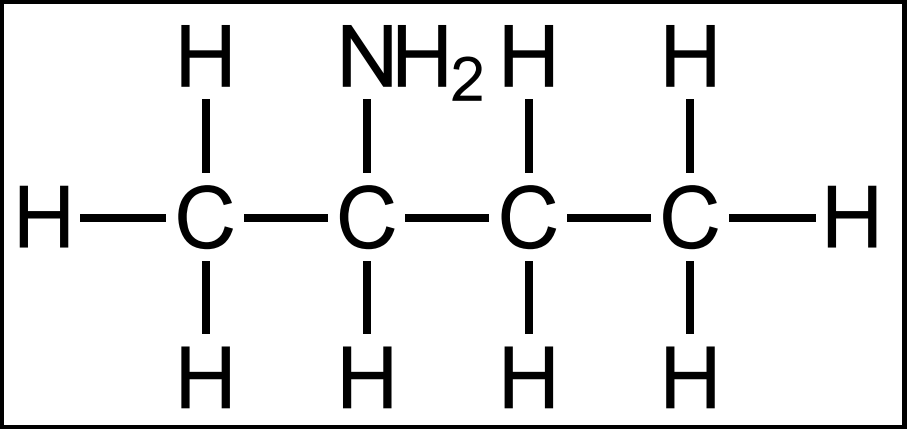
Primary amines



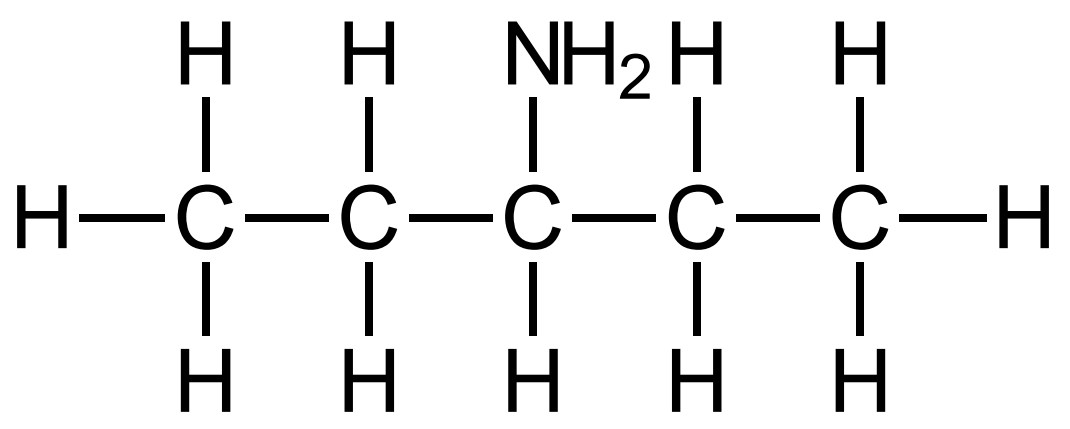
Propan-1-amine



Propan-2-amine

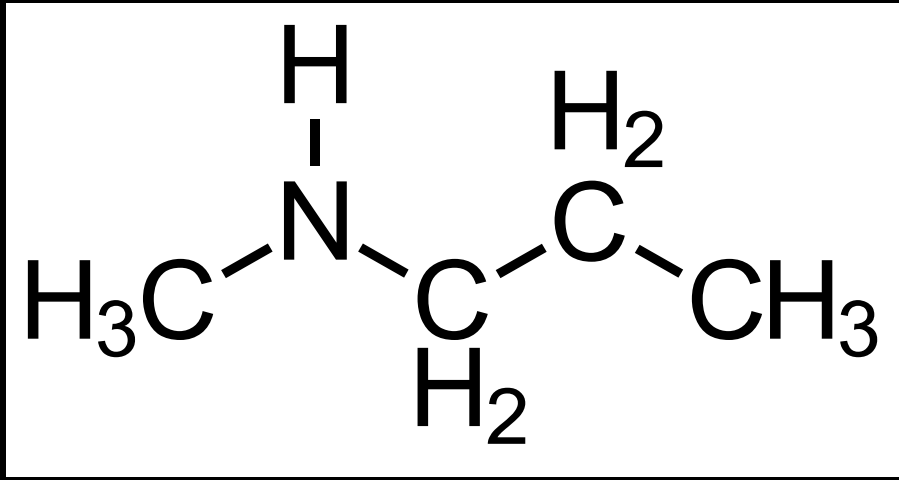


Butan-2-amine

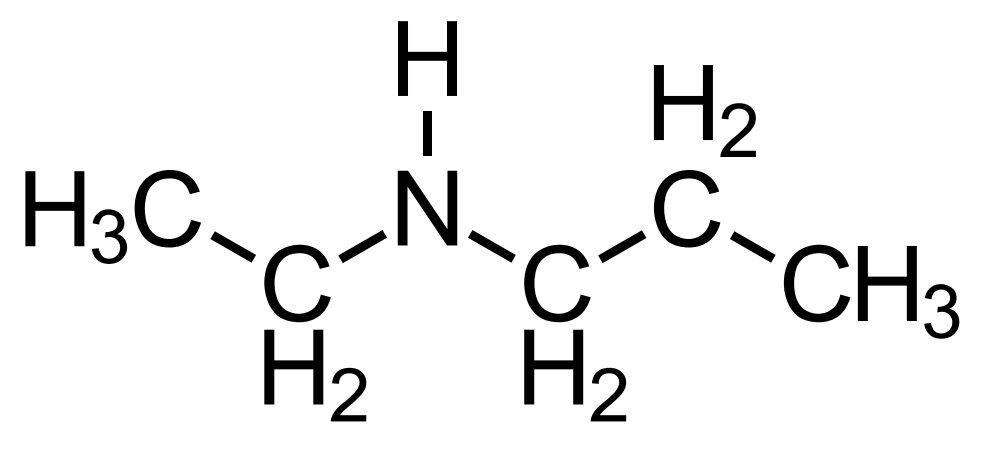


Pentan-3-amine

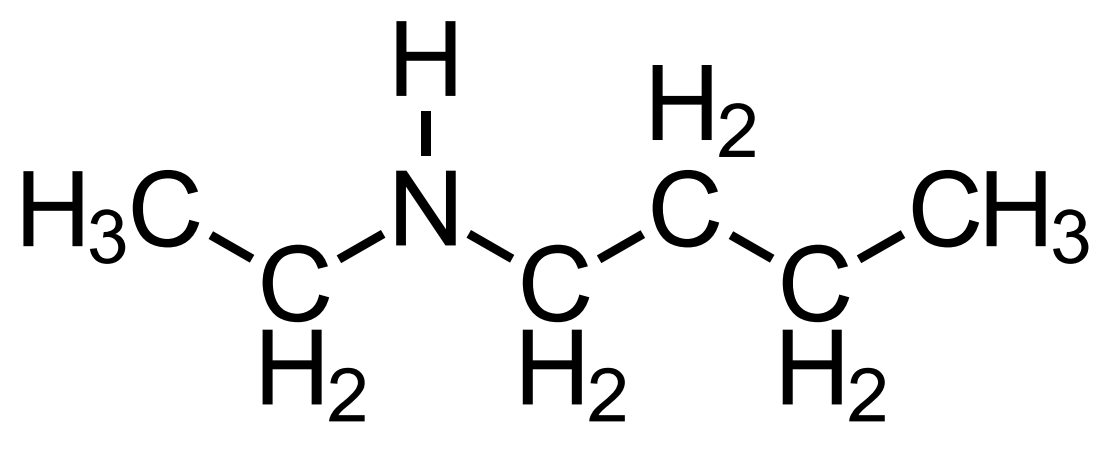
Secondary amines



N-methylpropanamine

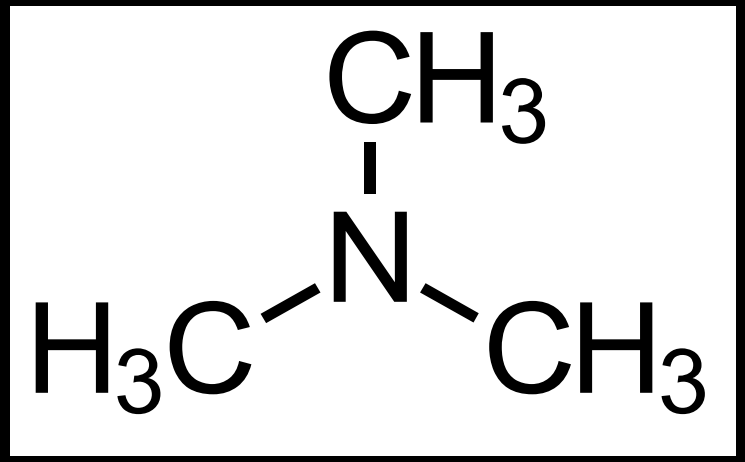


N-ethylpropanamine

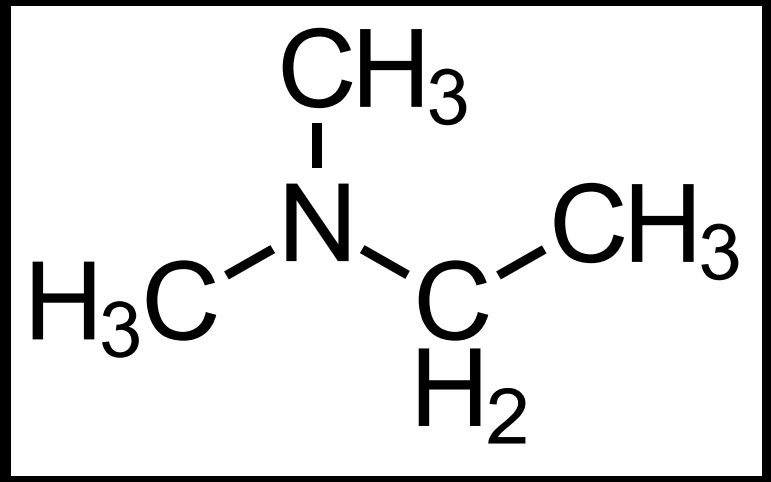


N-ethylbutanamine

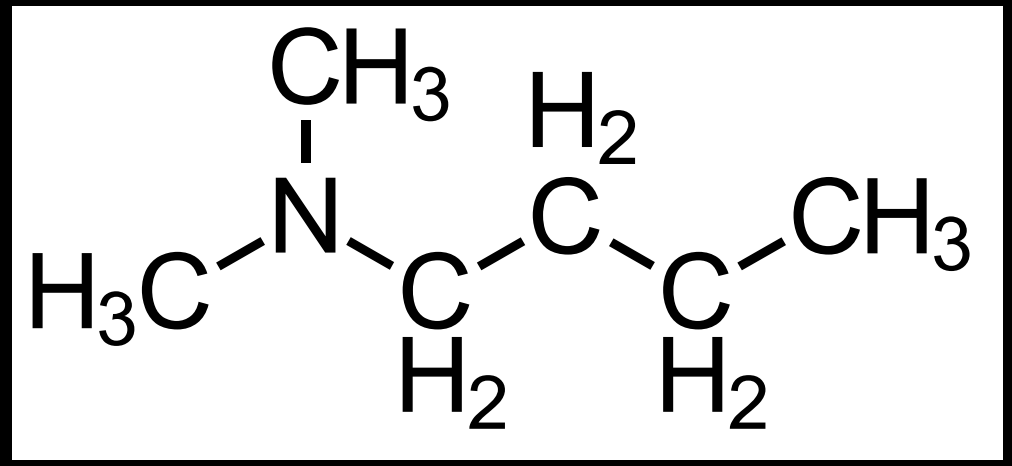
Tertiary amines



N,N-dimethylmethanamine



N,N-dimethylethanamine



N,N-dimethylbutanamine

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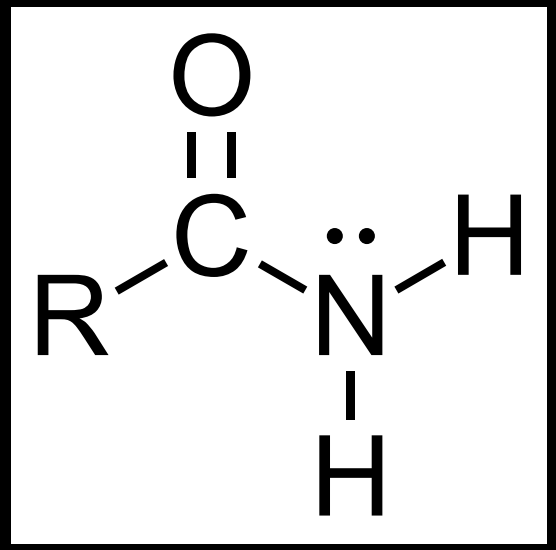
Naming amides

Naming amides

Amides are derivatives of carboxylic acids in which the –OH of the COOH group is replaced by an $–NH_2$ group.

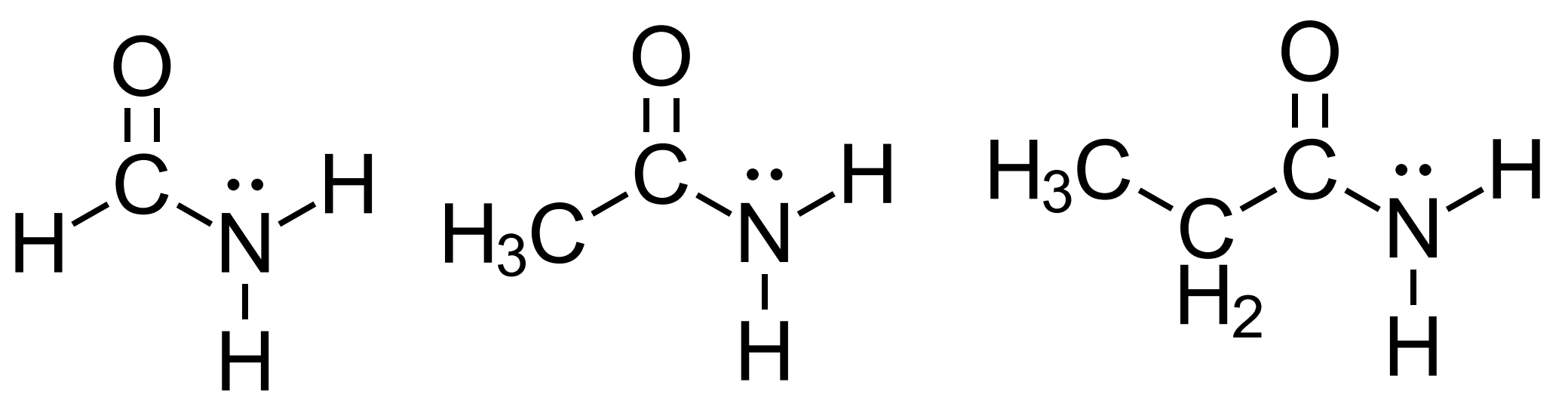
Amides contain the carboxamide (amido) functional group $R\text{-}CONH_2$



Amides have high boiling points as they are able to form hydrogen bonds between molecules. They are also soluble in water as they are able to form hydrogen bonds with water molecules.

Naming amides

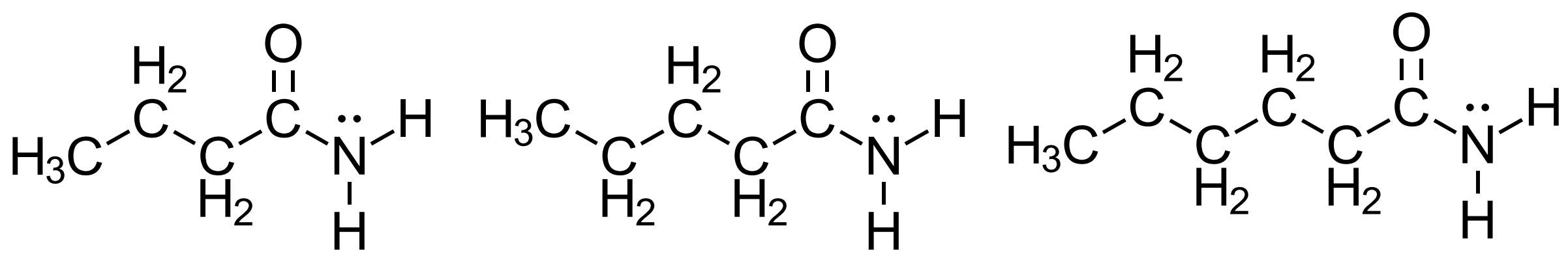
Primary amides are named by replacing the –oic of the carboxylic acid name with –amide.



Methanamide	Ethanamide	Propanamide
$HCONH_2$	CH_3CONH_2	$CH_3CH_2CONH_2$

Naming amides

Primary amides are named by replacing the –oic of the carboxylic acid name with –amide.



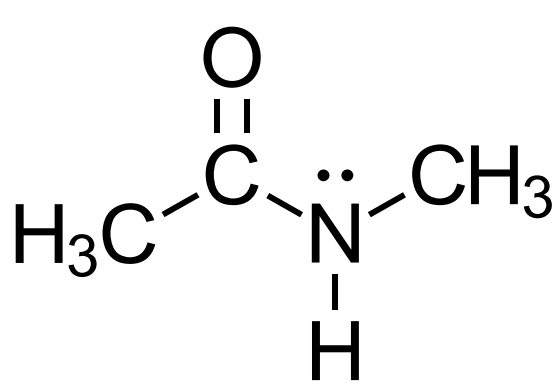
Butanamide	Pentanamide	Hexanamide
$CH_3(CH_2)_2CONH_2$	$CH_3(CH_2)_3CONH_2$	$CH_3(CH_2)_4CONH_2$

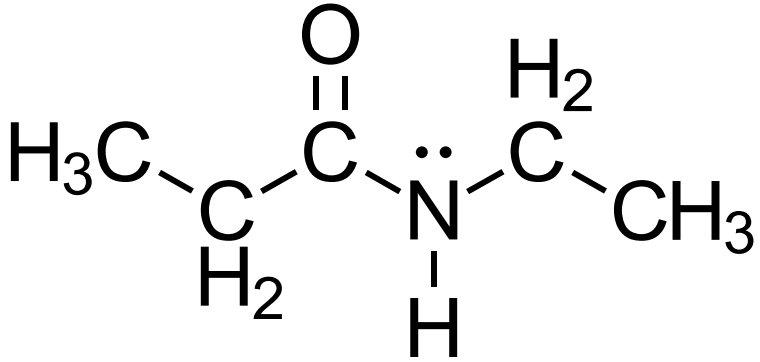
Naming amides

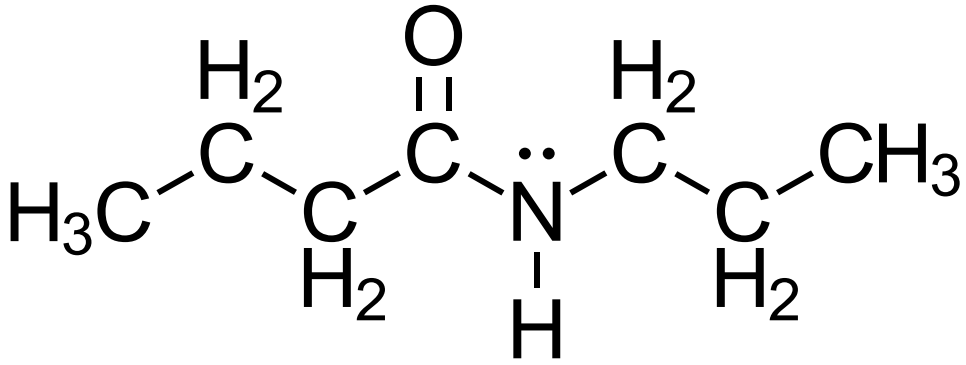
Secondary amides are named using an uppercase *N* to designate the alkyl group attached to nitrogen atom.

***N*-methylethanamide**
$CH_3CONHCH_3$

***N*-propylbutanamide**
$CH_3CH_2CH_2CONHCH_2CH_2CH_3$





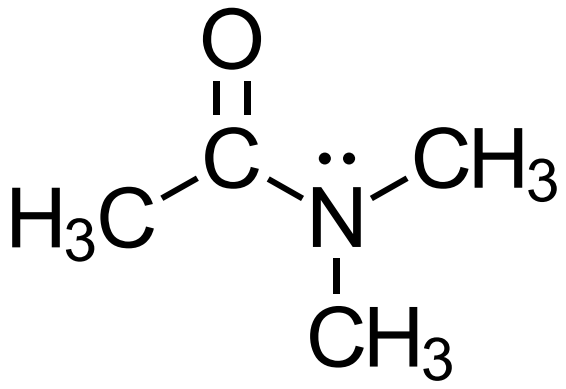


***N*-ethylpropanamide**
$CH_3CH_2CONHCH_2CH_3$

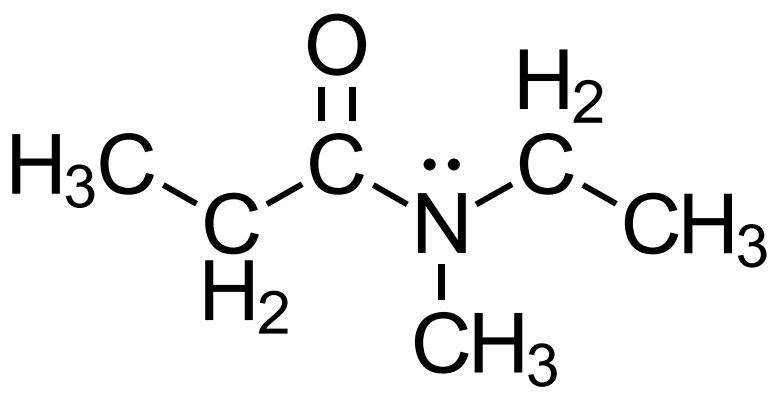
Naming amides

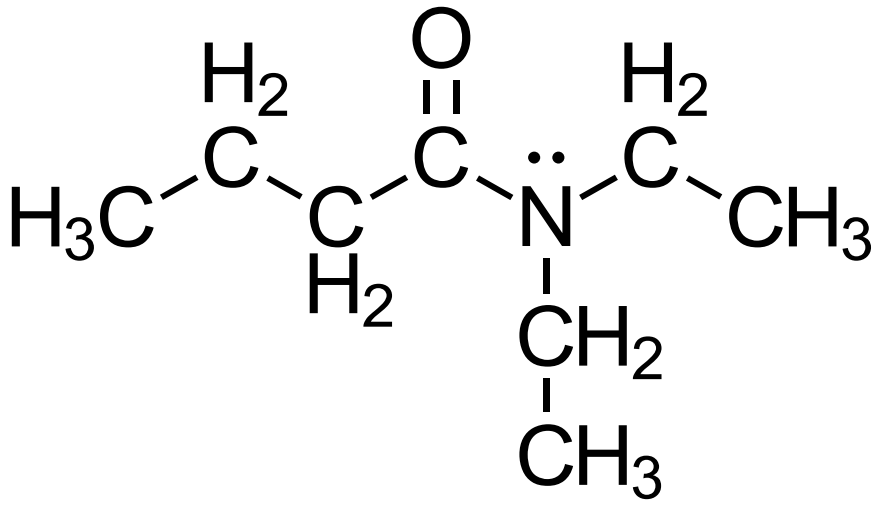
Tertiary amides are named using uppercase *N,N*- to designate the alkyl groups attached to the nitrogen atom.

***N,N*-dimethylethanamide**



***N,N*-diethylbutanamide**





***N*-ethyl-*N*-methylpropanamide**

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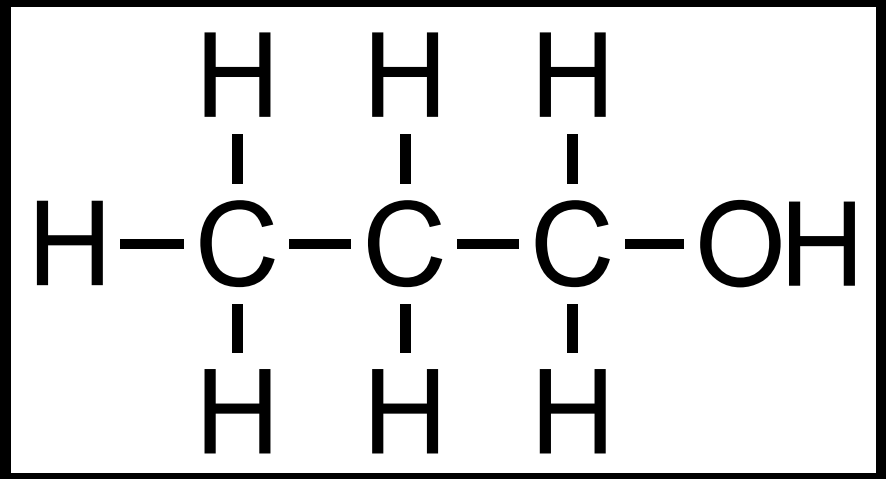
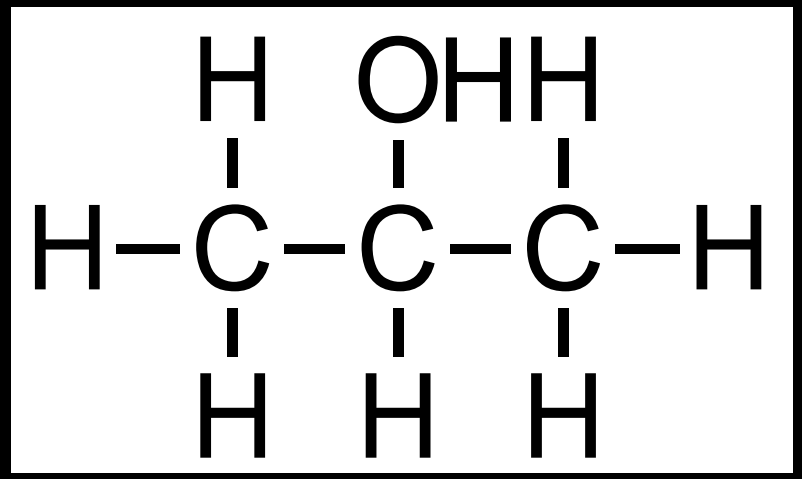
Classification of organic compounds

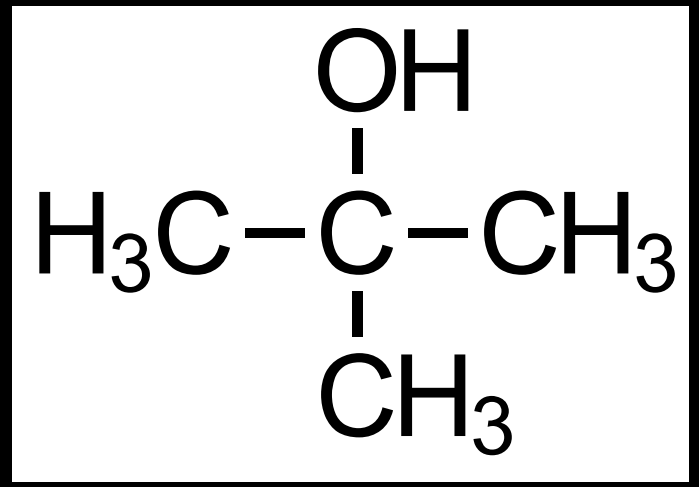
Classification of alcohols



propan-1-ol
primary (1°) alcohol

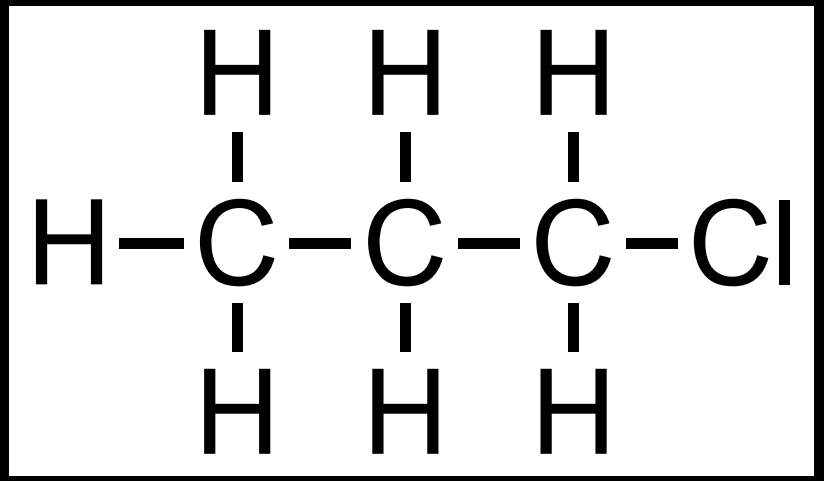


propan-2-ol
secondary (2°) alcohol

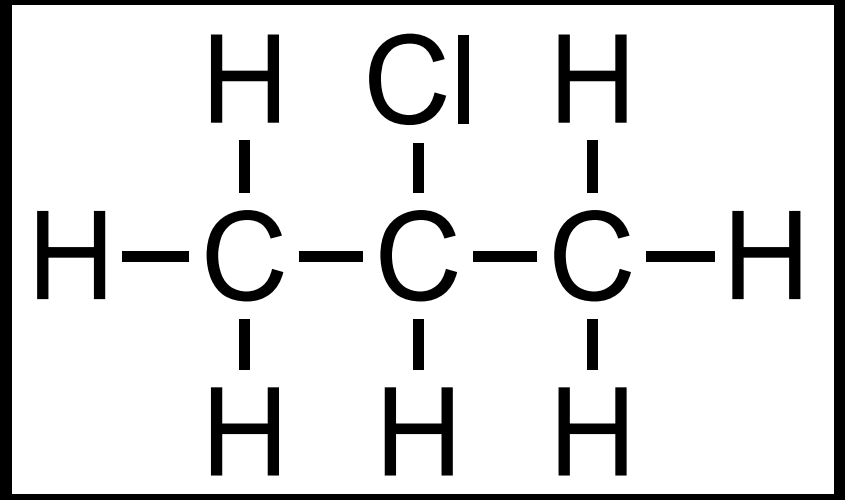


2-methylpropan-2-ol
tertiary (3°) alcohol

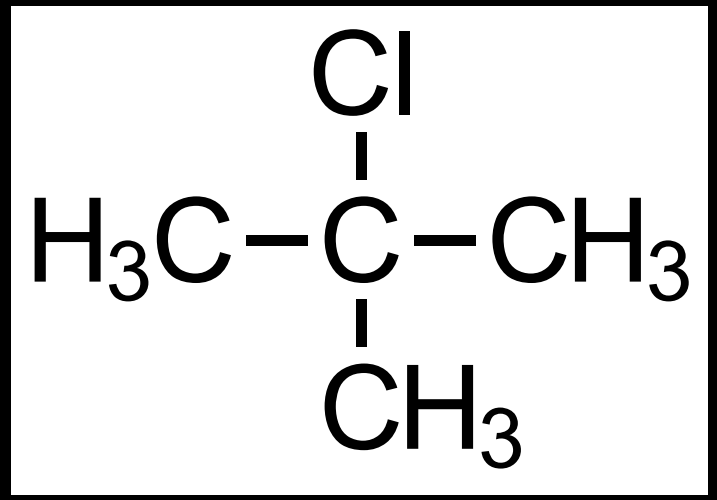
Classification of halogenoalkanes



1-chloropropane
primary halogenoalkane



2-chloropropane
secondary halogenoalkane



2-chloro-2-methylpropane
tertiary halogenoalkane

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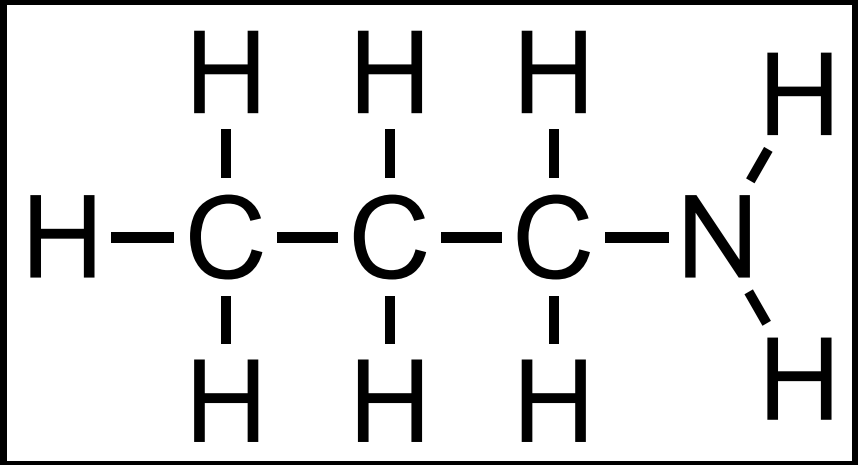
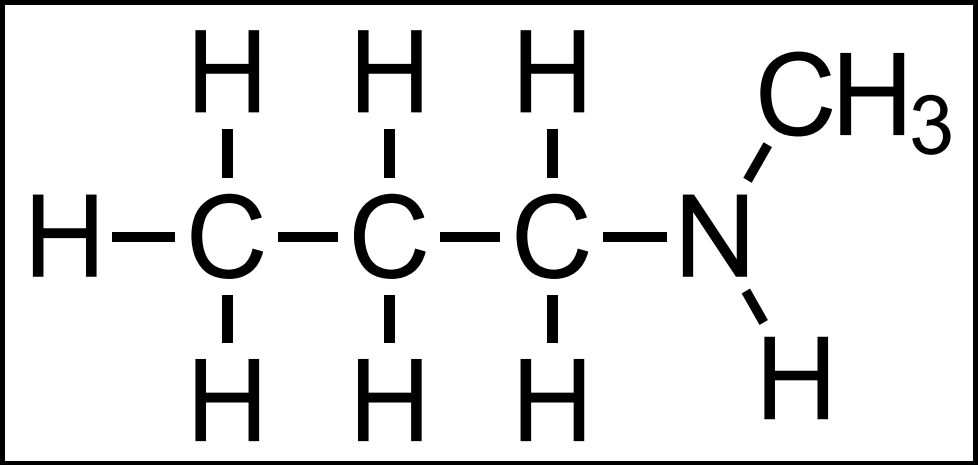
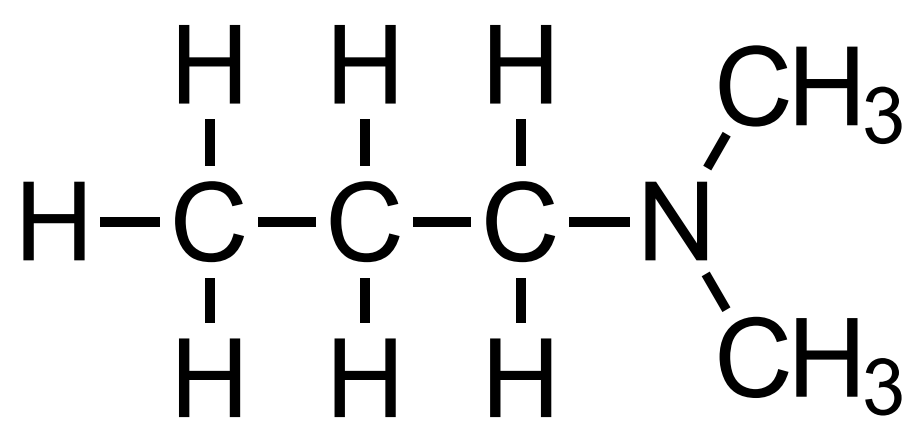
Classification of amines



Propanamine
primary amine



***N*-methylpropanamine**
secondary amine



***N*,*N*-dimethylpropanamine**
tertiary amine

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Structural isomerism

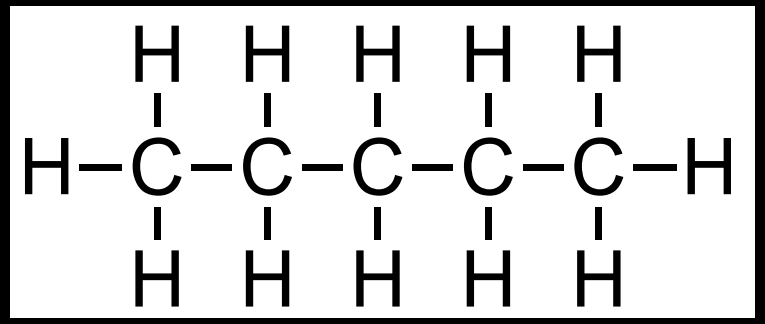
Structural isomerism

Structural isomers are compounds with the same molecular formula but different arrangements of atoms (different structural formulas).

- Chain isomerism: straight-chain and branched-chain molecules
- Position isomerism: functional group attached in a different position
- Functional group isomerism: molecules with different functional groups

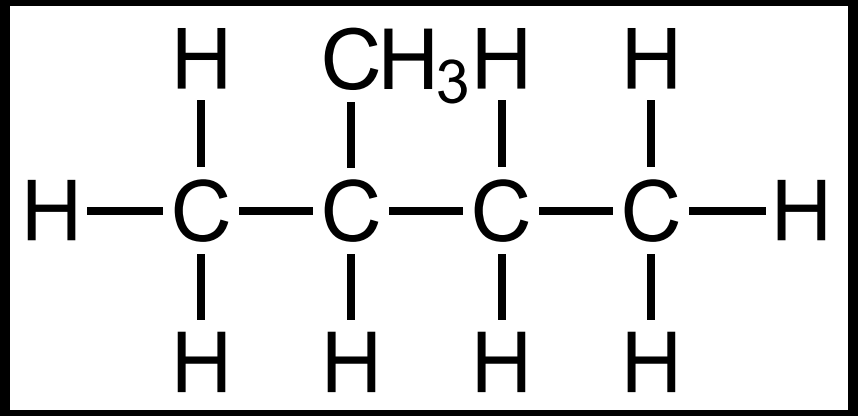
Structural isomerism

Structural isomers of C_5H_{12}



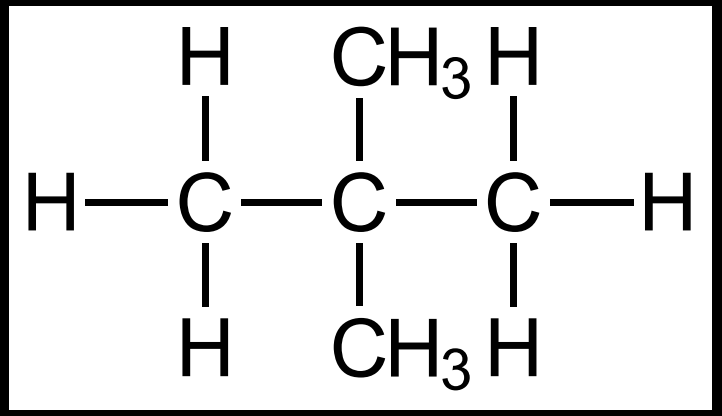
pentane

$CH_3(CH_2)_3CH_3$



2-methylbutane

$CH_3CH(CH_3)CH_2CH_3$

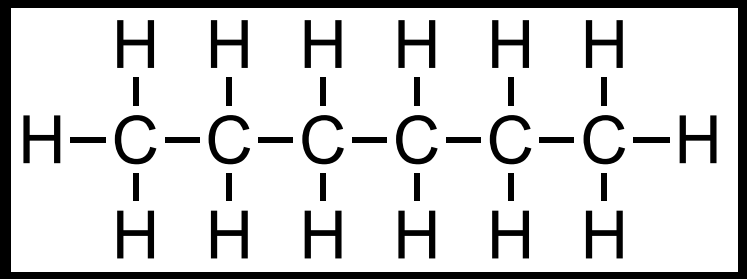


2,2-dimethylpropane

$CH_3C(CH_3)_2CH_3$

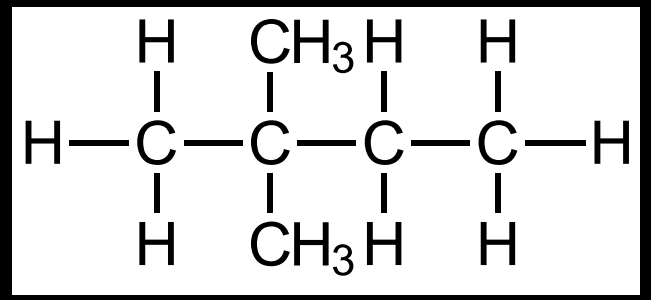
Structural isomerism

Structural isomers of C_6H_{14}



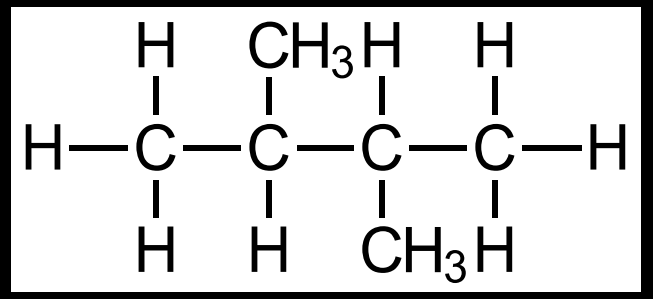
hexane

$CH_3(CH_2)_4CH_3$



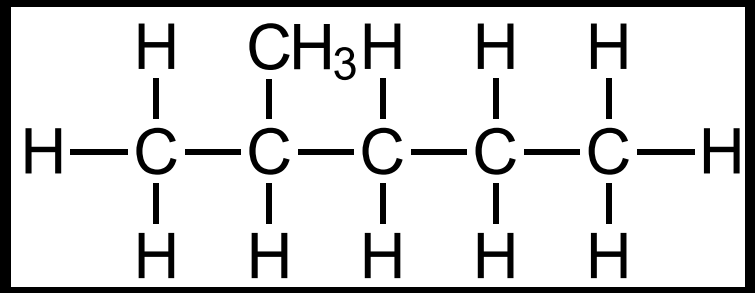
2,2-dimethylbutane

$(CH_3)_3CCH_2CH_3$



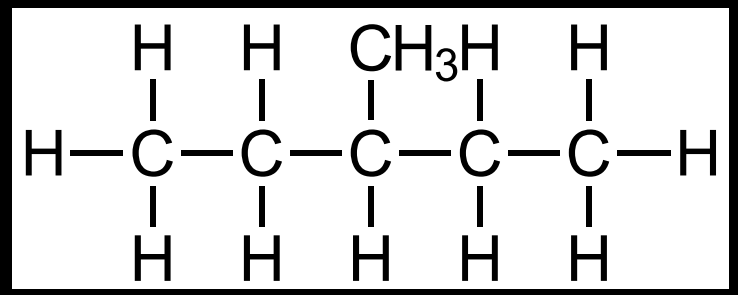
2,3-dimethylbutane

$(CH_3)_2CHCH(CH_3)_2$



2-methylpentane

$(CH_3)_2CHCH_2CH_2CH_3$

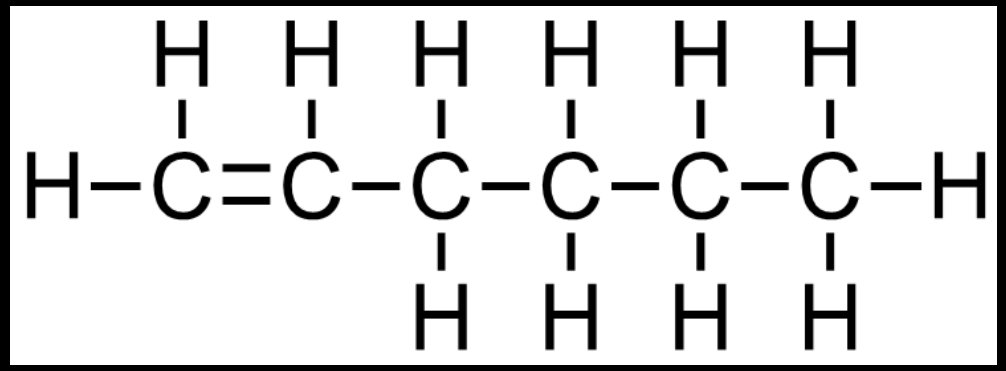


3-methylpentane

$CH_3CH_2CH(CH_3)CH_2CH_3$

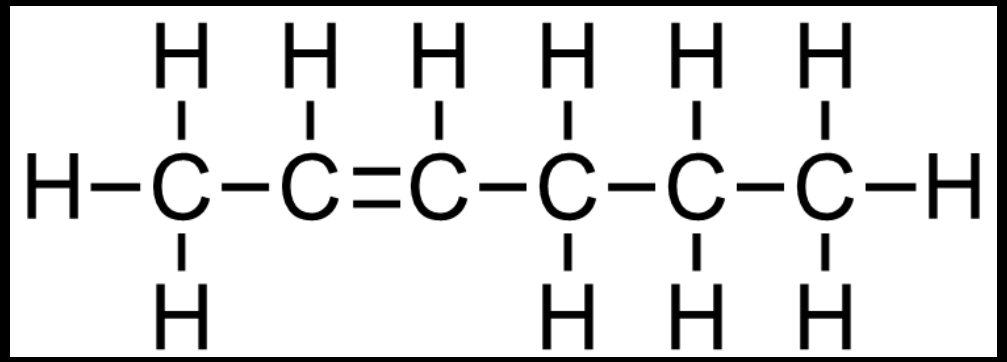
Structural isomerism

Structural isomers of C_6H_{12}



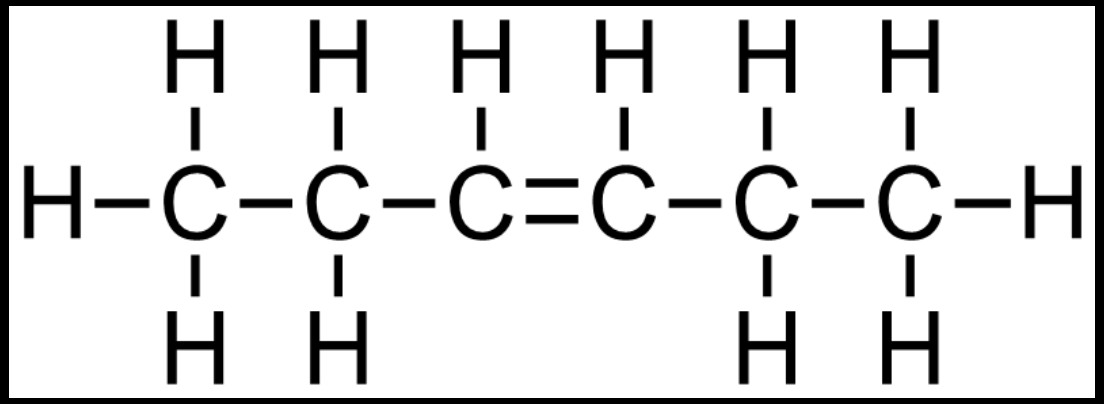
hex-1-ene

$CHCH(CH_2)_3CH_3$



hex-2-ene

$CH_3CHCH(CH_2)_2CH_3$

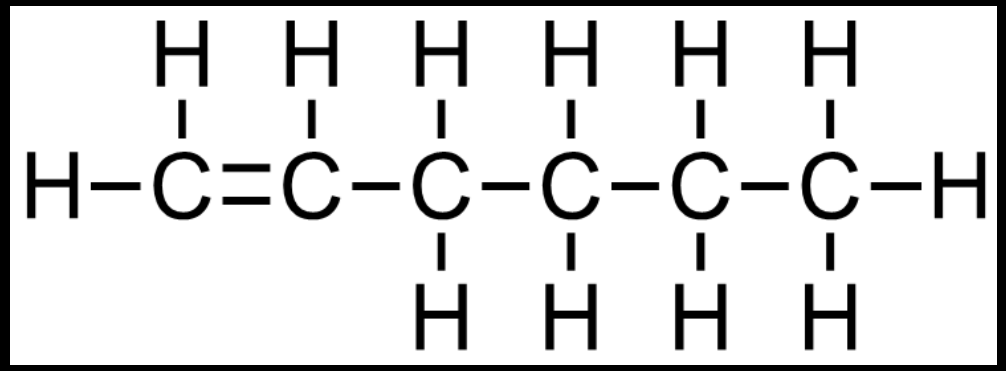


hex-3-ene

$CH_3CH_2CHCHCH_2CH_3$

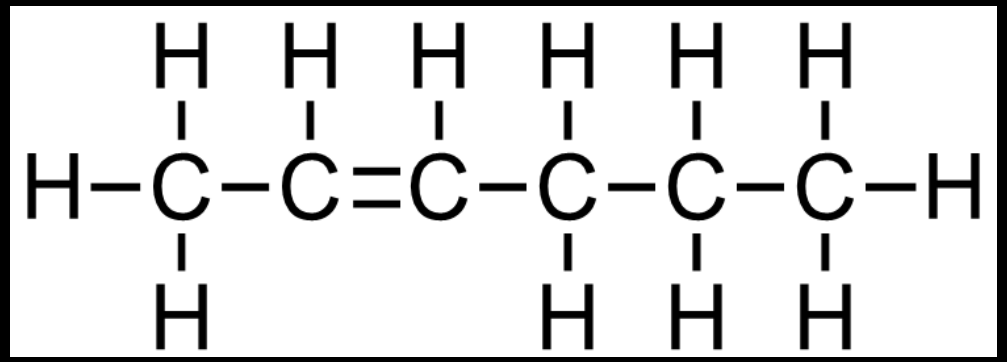
Structural isomerism

Structural isomers of C_6H_{12}



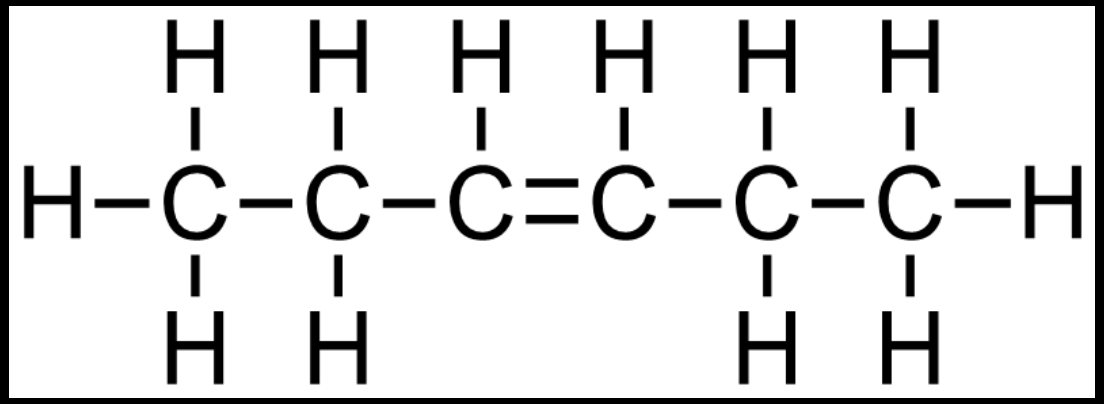
hex-1-ene

$CHCH(CH_2)_3CH_3$



hex-2-ene

$CH_3CHCH(CH_2)_2CH_3$



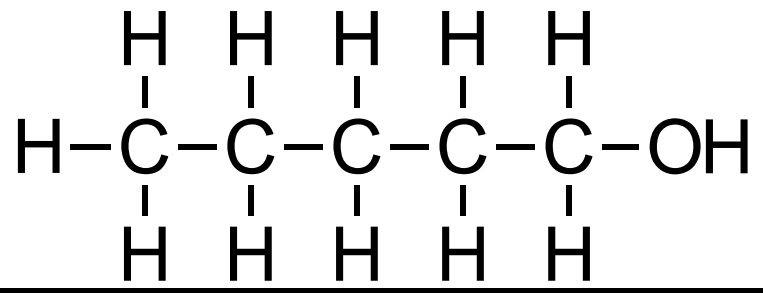
hex-3-ene

$CH_3CH_2CHCHCH_2CH_3$

Structural isomerism

Structural isomers of $C_5H_{12}O$

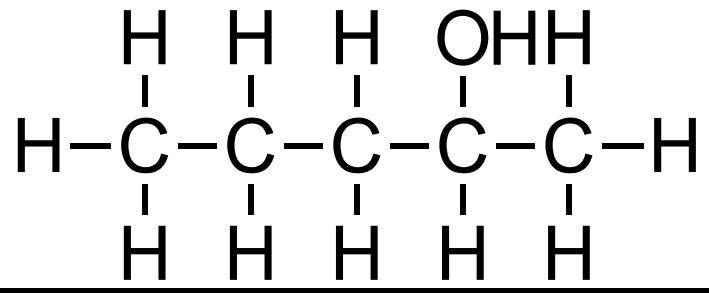
$CH_3CH_2CH_2CH_2CH_2OH$



Pentan-1-ol

$C_5H_{11}OH$

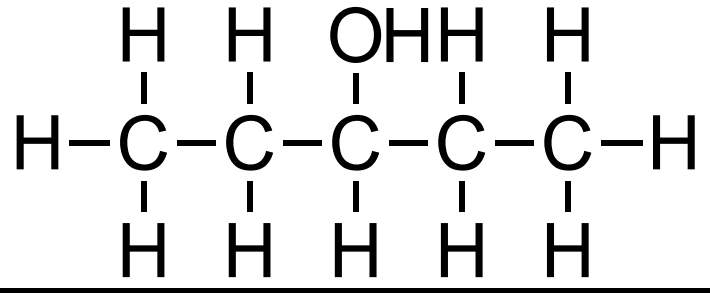
$CH_3CH_2CH_2CH(OH)CH_3$



Pentan-2-ol

$C_5H_{11}OH$

$CH_3CH_2CH(OH)CH_2CH_3$



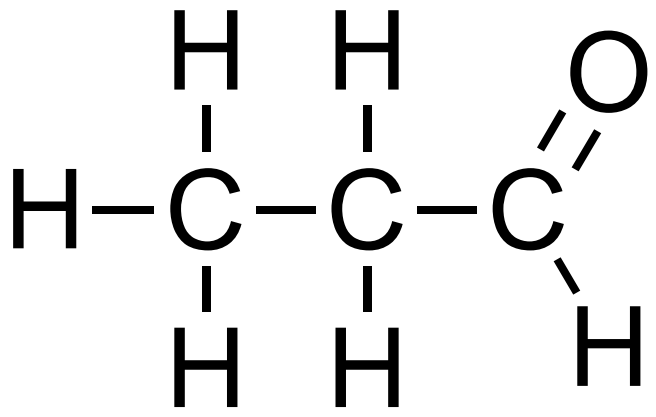
Pentan-3-ol

$C_5H_{11}OH$

Structural isomerism

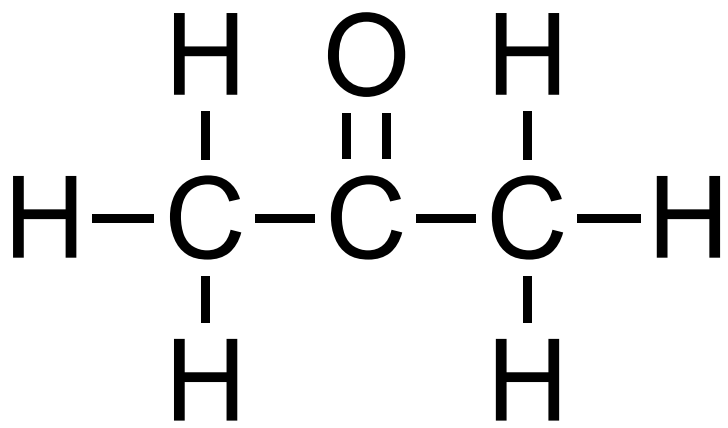
Structural isomers of C_3H_6O

CH_3CH_2CHO



Propanal

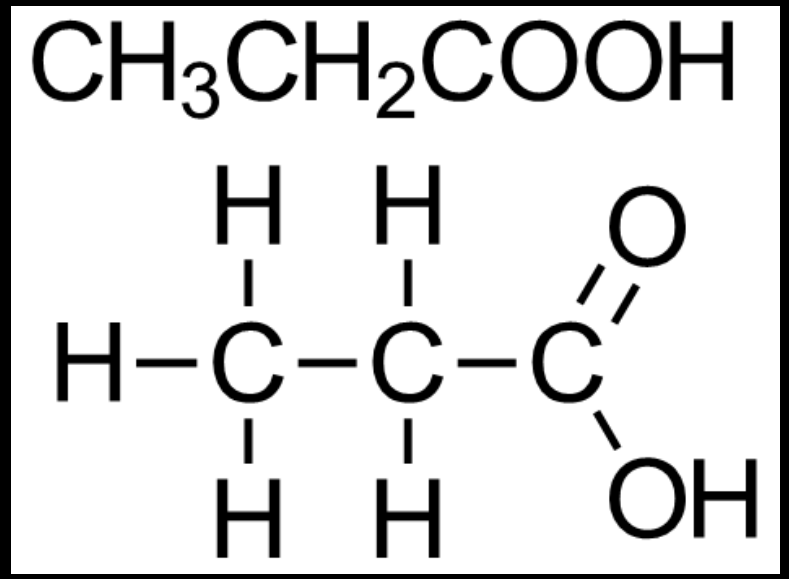
CH_3COCH_3



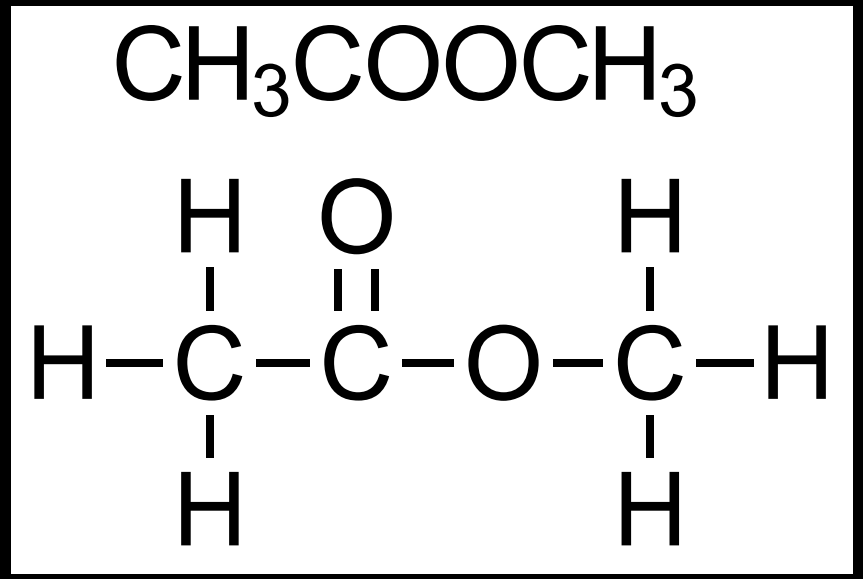
Propanone

Structural isomerism

Structural isomers of $C_3H_6O_2$



Propanoic acid



Methyl ethanoate

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Tutorials for IB Chemistry

Factors that affect the boiling points of organic compounds

Boiling points of organic compounds

Factors that affect the boiling points of organic compounds are:

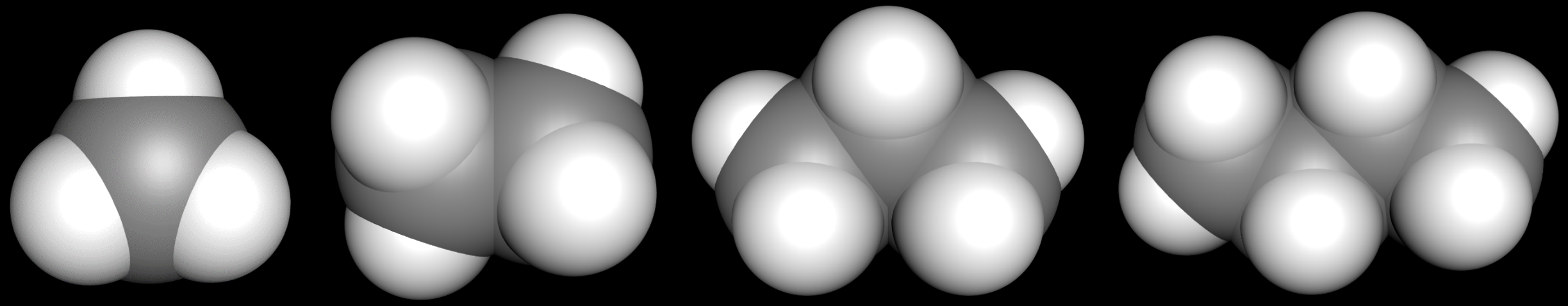
- Molar mass of the compound
- Structure of the molecule (straight-chain vs branched-chain isomers)
- Type of functional group (hydrogen bonding, dipole-dipole, London dispersion)

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.

Boiling points of the alkanes

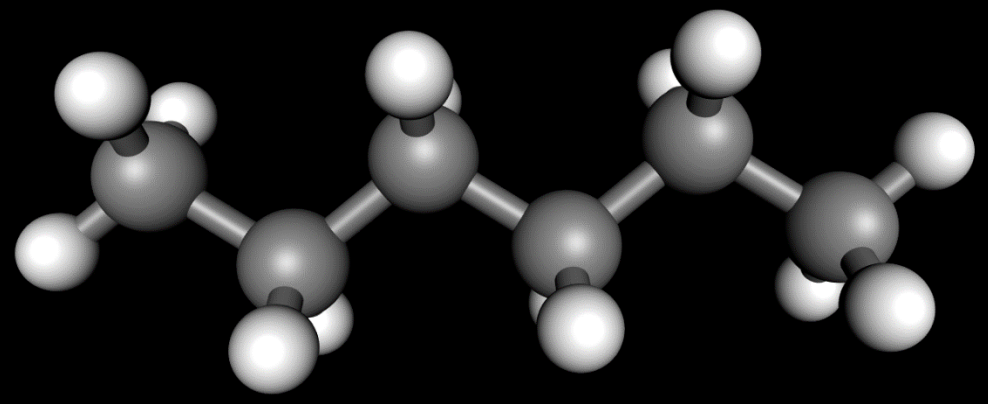


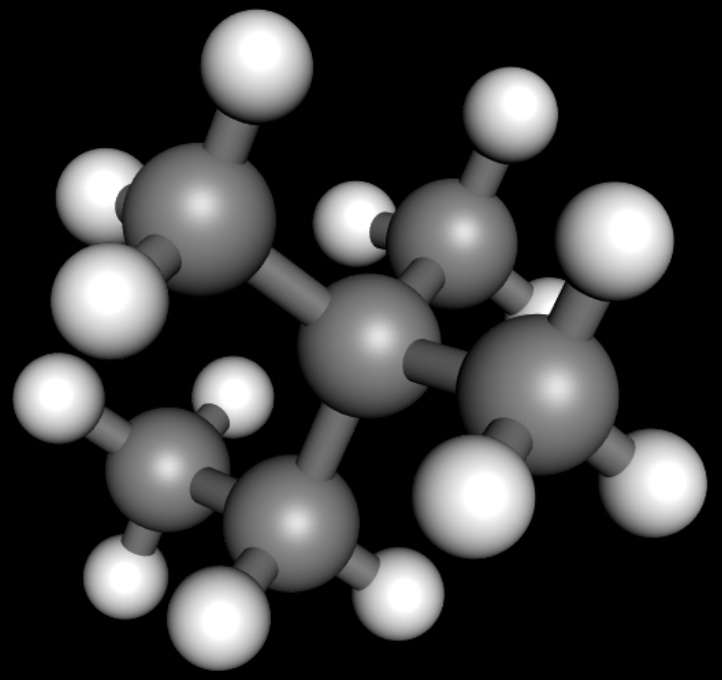
As the molar mass increases, the number of electrons within the molecule also increases.

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.

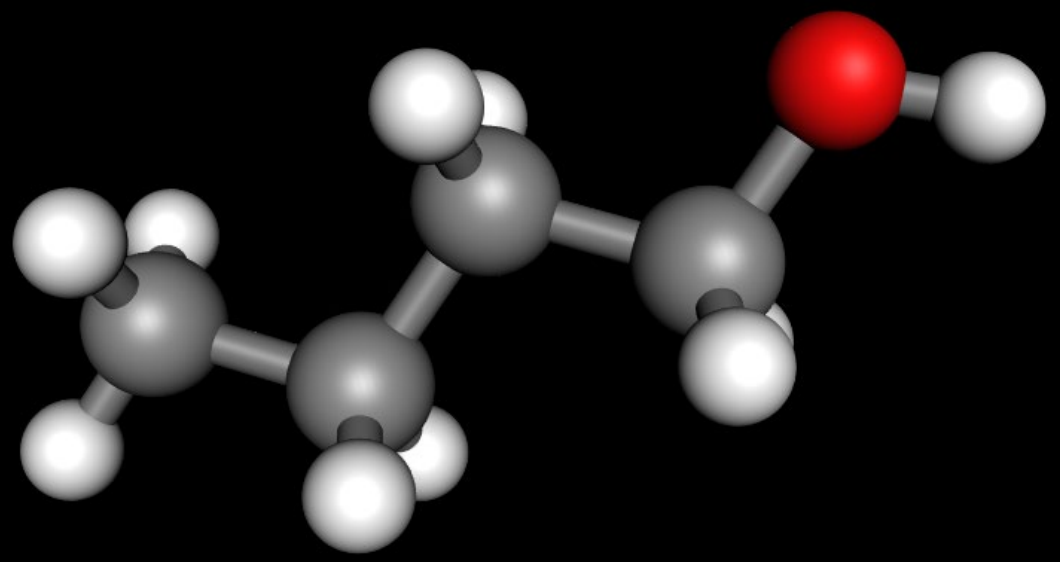
Branched vs straight-chain

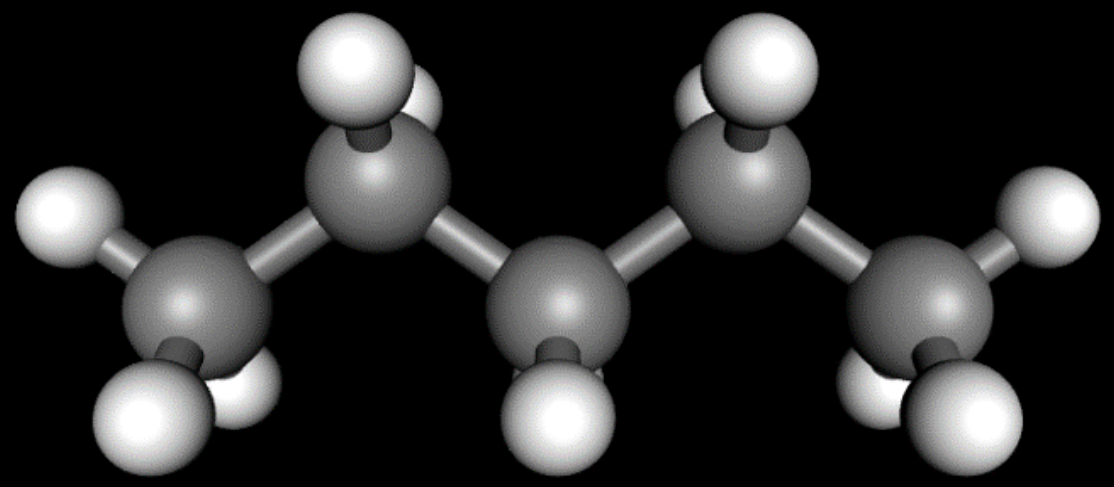




Branched-chain isomers have lower boiling points than straight-chain isomers.
The branches prevent the molecules getting close together (less surface area contact) which results in weaker London dispersion forces and a lower boiling point.

Effect of functional group





Butan-1-ol

M = 74.12 g mol^{-1}

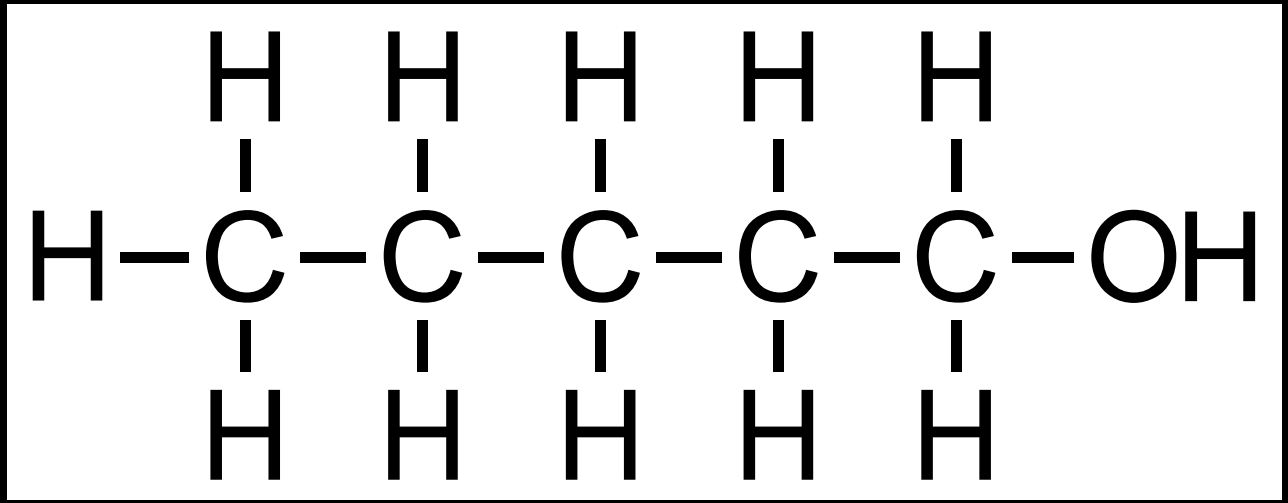
B.P. = 118 °C

Pentane

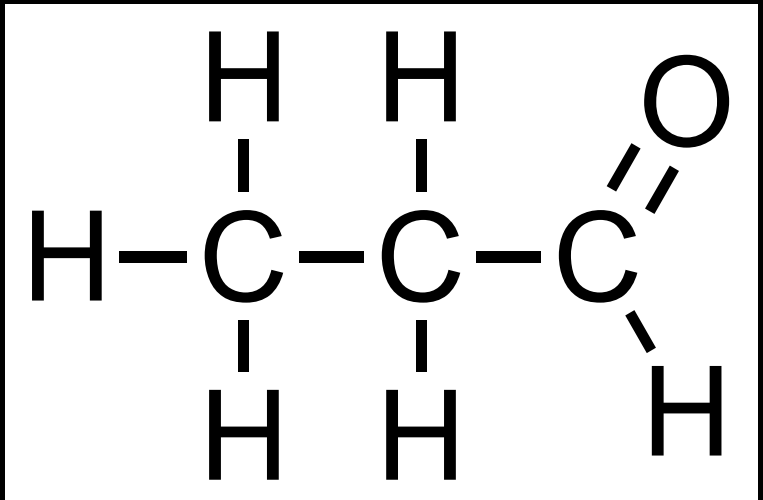
M = 72.15 g mol^{-1}

B.P. = 36.1 °C

Effect of functional group

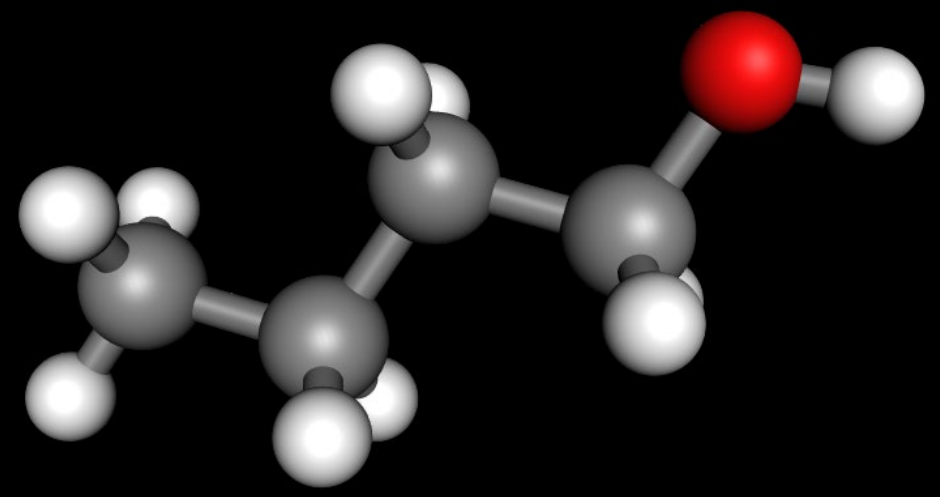


Functional group containing H bonded to O or N; hydrogen bonding between molecules

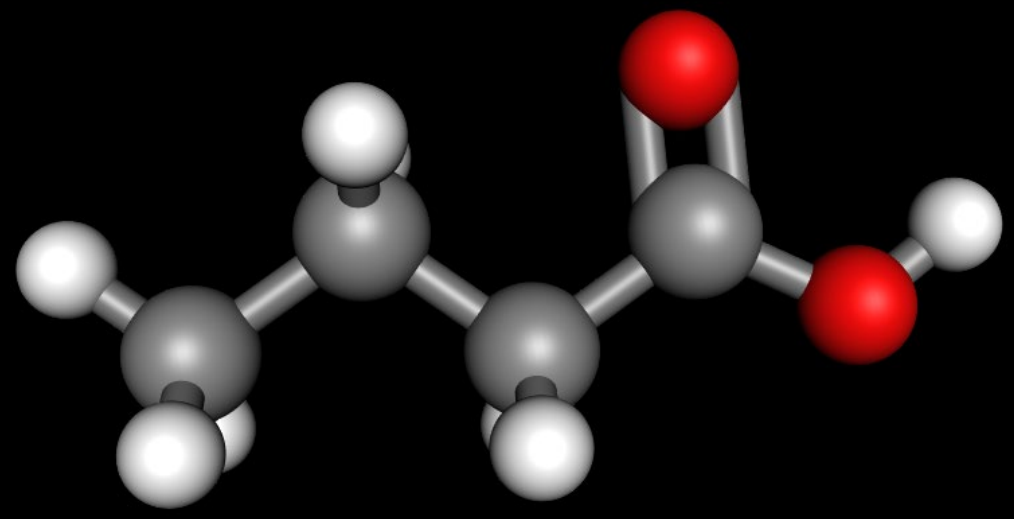


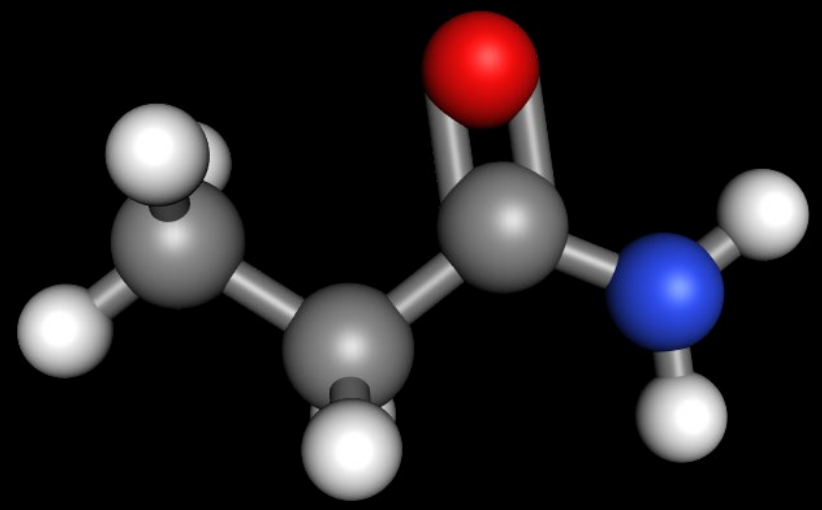
Functional group containing carbonyl group; dipole-dipole forces between molecules

Effect of functional group

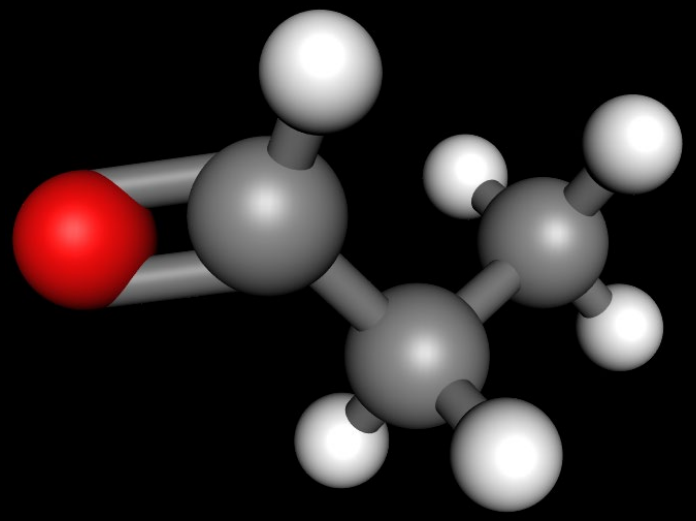


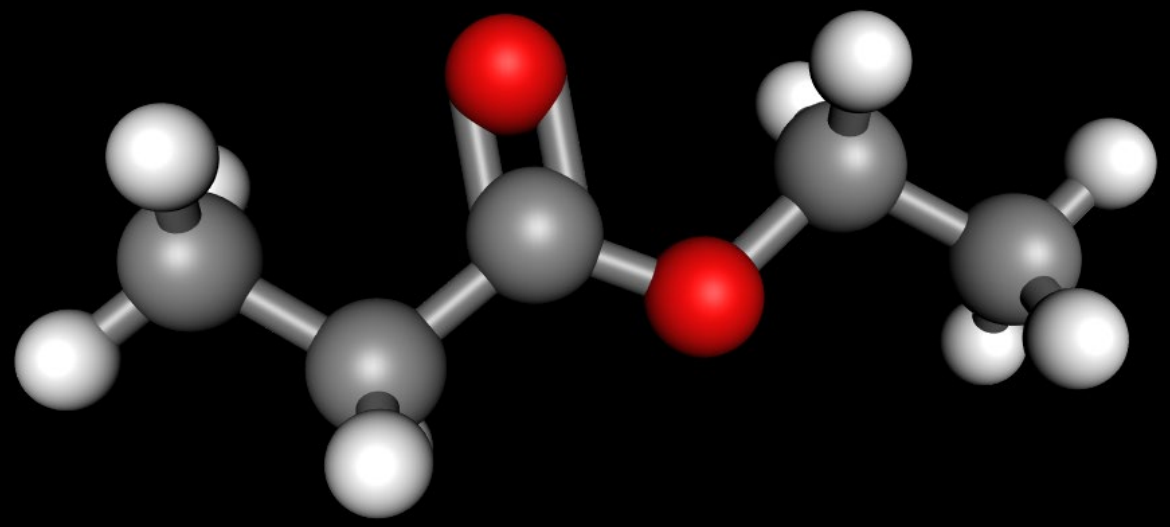
Alcohols, amides and carboxylic acids tend to have higher boiling points because they are able to form hydrogen bonds between their molecules.

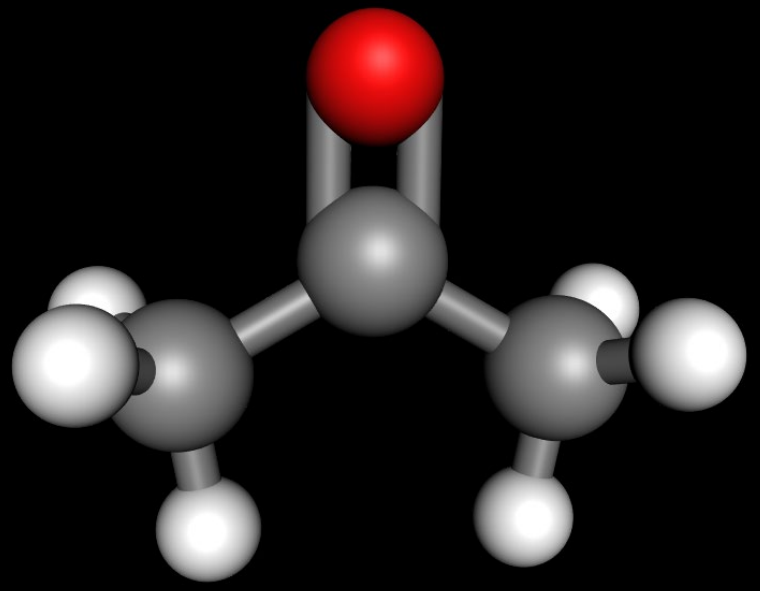




Effect of functional group

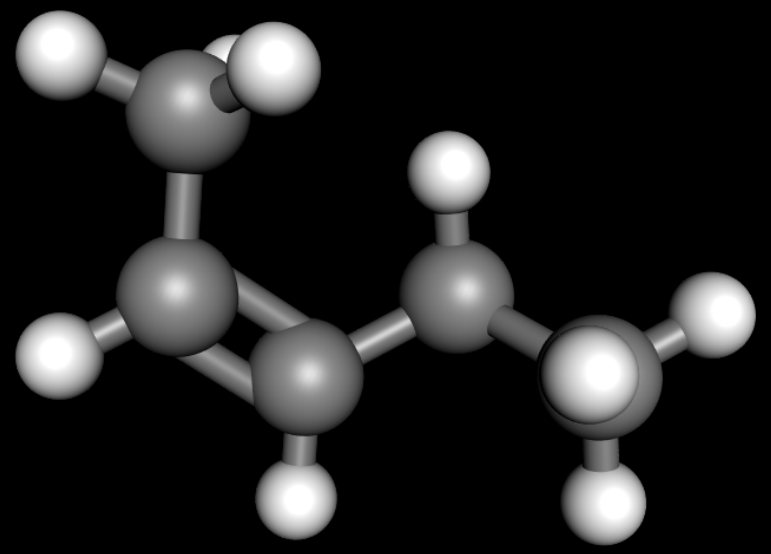


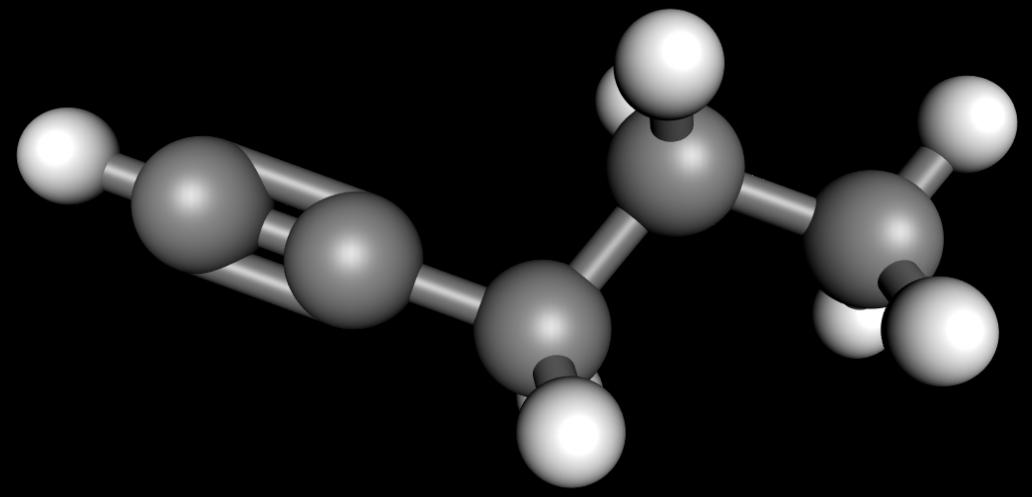


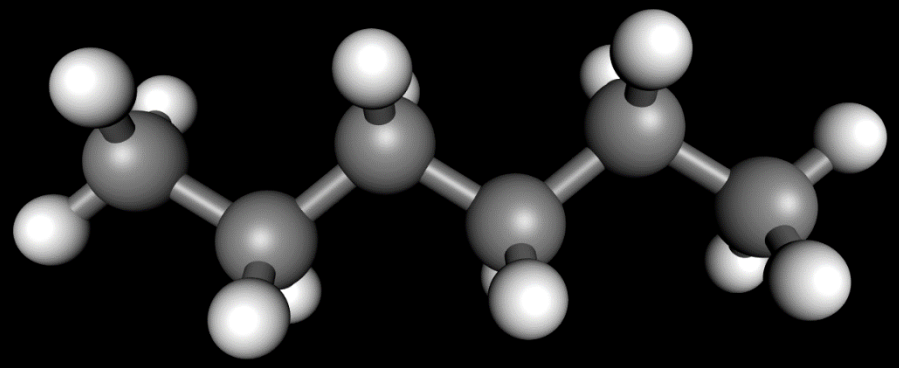


Aldehydes, ketones, and esters have dipole-dipole forces between their molecules.

Effect of functional group







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

Effect of functional group

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)

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Solubility of organic compounds

Solubility 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)

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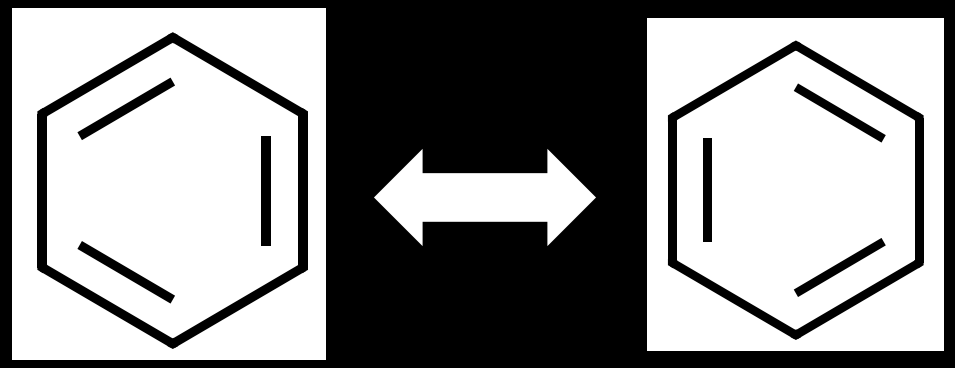
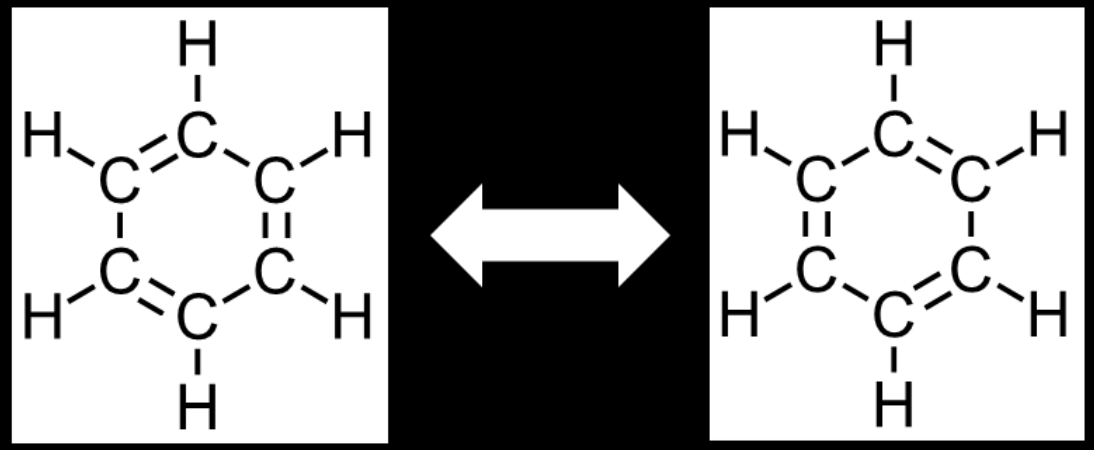
Tutorials for IB Chemistry

Evidence for the structure of benzene

Structure of benzene

The Kekulé structure of benzene consists of alternating single and double carbon to carbon bonds.





All C to C bonds would be different lengths and strengths.

The enthalpy of hydrogenation of benzene would be -360 kJ mol^{-1}

Benzene would undergo addition reactions.

Two possible isomers produced in 1,2-dibsubtituted benzene compounds.

Structure of benzene

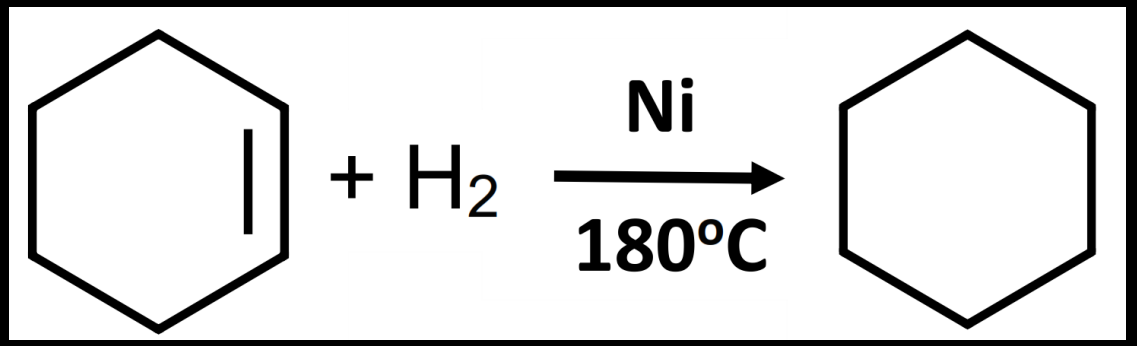
The C to C bonds in benzene are of equal length and equal strength.

Bond	Bond length ($\times 10^{-12}$ m)	Bond strength (kJ mol^{-1})
C-C	154	346
C≡C	140	507
C=C	134	614

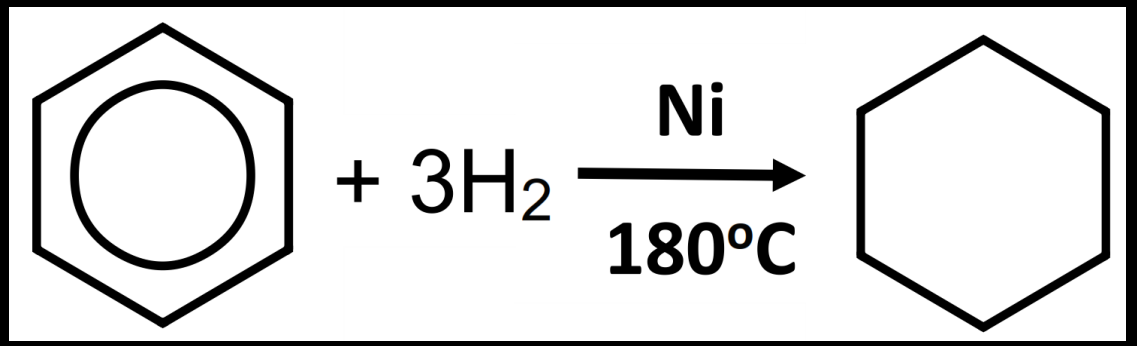
The length and strength of the C to C bonds in benzene are equal - intermediate between a single and a double bond.

Structure of benzene

The enthalpy of hydrogenation of benzene is less than predicted.



ΔH = -120 kJ mol^{-1}



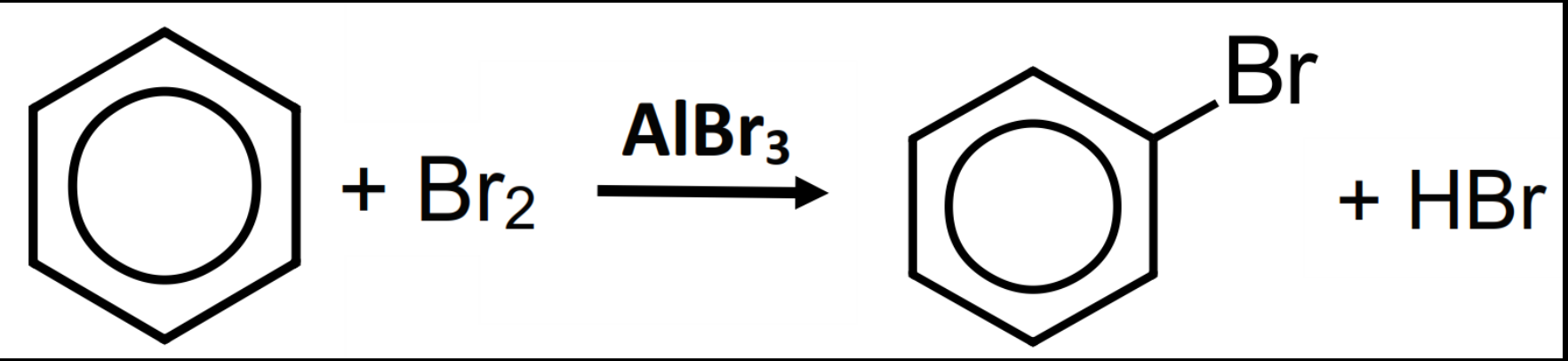
ΔH = -360 kJ mol^{-1}

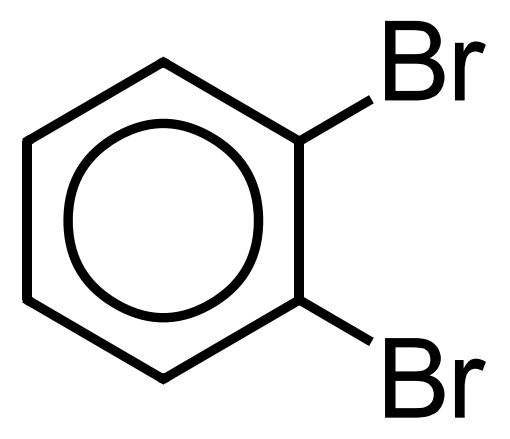
ΔH = -210 kJ mol^{-1}

The difference in energy (-150 kJ mol^{-1}) is known as the resonance energy.

Structure of benzene

Benzene undergoes substitution reactions, rather than addition reactions.





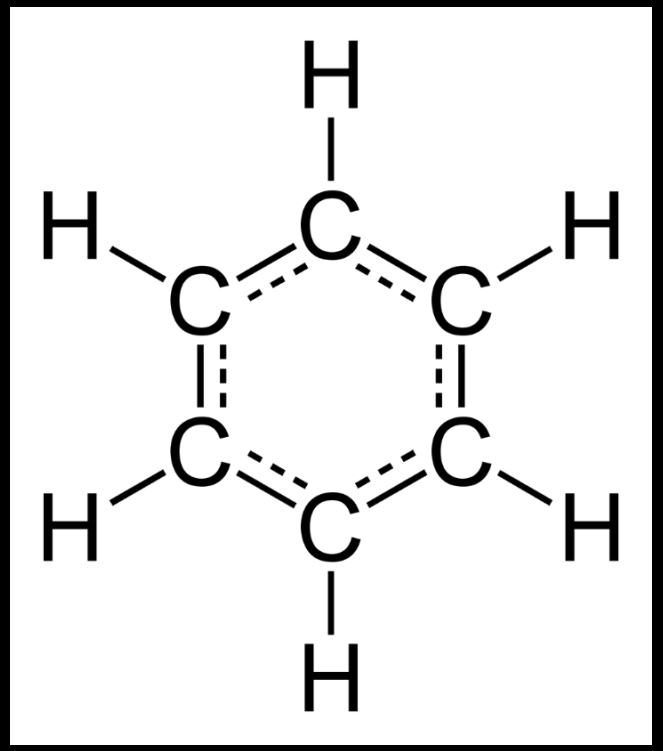
Only one isomer exists for 1,2-disubstituted compounds such as 1,2-dibromobenzene.

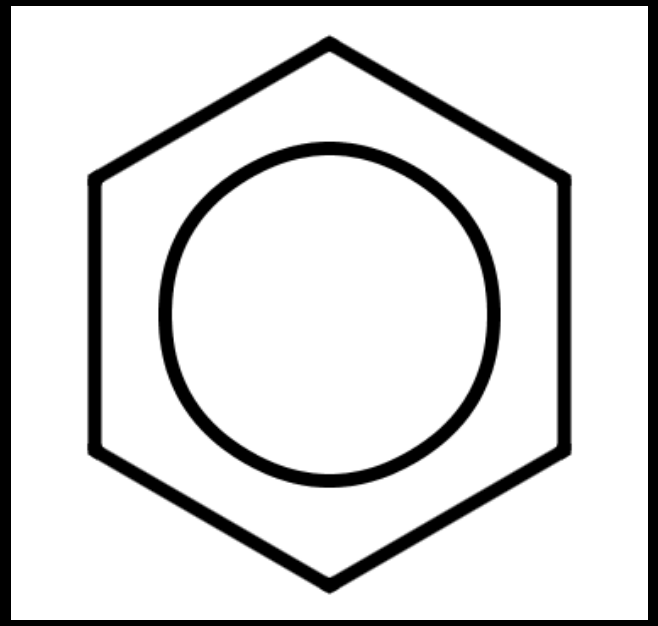
Structure of benzene

Kekule structure	Actual structure
Alternating single and double C-C bonds	All C-C bonds are of equal length and equal strength
Enthalpy of hydrogenation is –360 kJ mol^{-1}	Enthalpy of hydrogenation is –210 kJ mol^{-1}
Benzene undergoes addition reactions	Benzene undergoes substitution reactions
Two isomers produced in the reactions with the halogens	Only one isomers exists

Structure of benzene

The actual structure of benzene is a planar regular hexagon (bond angles of 120º).





The ring represents the delocalised electrons within the benzene molecule.

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Homolytic and heterolytic bond fission

Homolytic bond fission

In homolytic bond fission, a covalent bond between two atoms in a molecule breaks with each atom taking one electron from the bond.

$$X : Y \longrightarrow X\cdot + Y\cdot$$

Homolytic bond fission results in the formation of free radicals (radicals) - highly reactive species with unpaired electrons.

Heterolytic bond fission

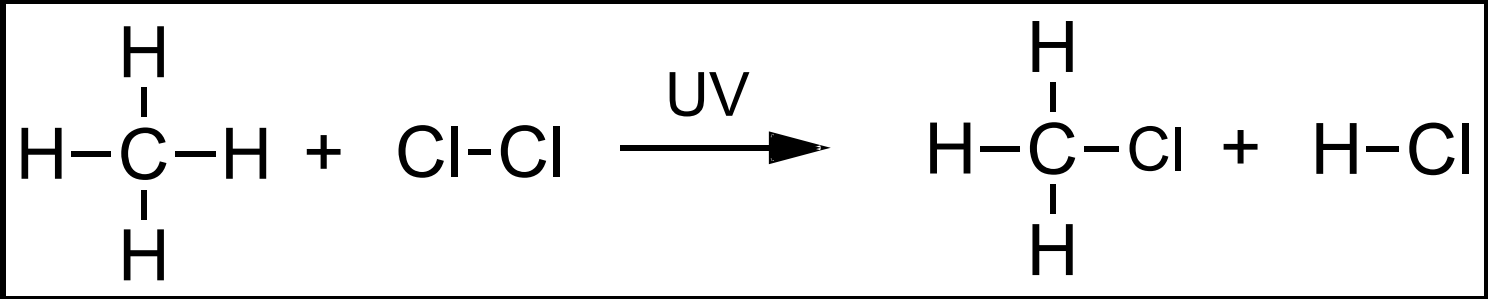
In heterolytic bond fission, a covalent bond between two atoms in a molecule breaks with one atom taking both bonding electrons.

$$X : Y \longrightarrow X^{-} : + Y^{+}$$

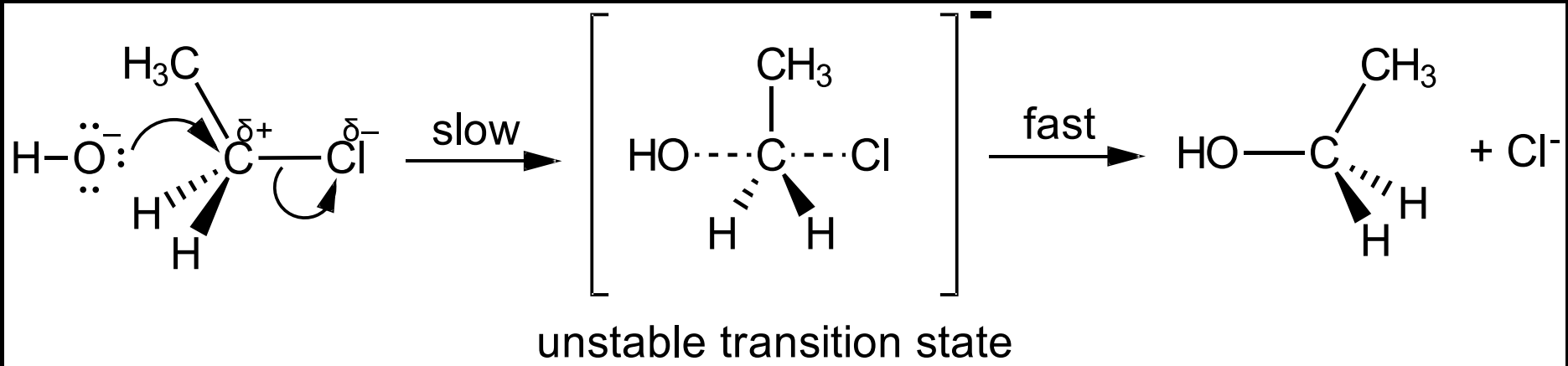
Heterolytic bond fission results in the formation of ions (cation and anion). The more electronegative atom usually takes both bonding electrons.

Bond fission

Homolytic bond fission occurs in the free radical substitution reactions of the alkanes.



Heterolytic bond fission occurs in the nucleophilic substitution reactions of halogenoalkanes.



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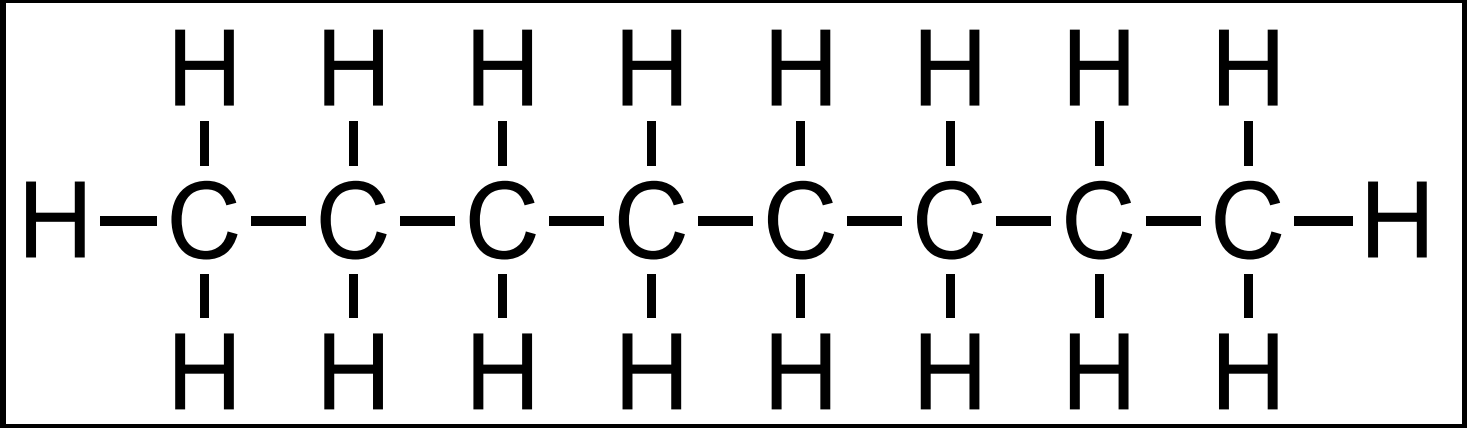
Free radical substitution reactions of the alkanes

Reactions of the alkanes

Alkanes such as octane (C_8H_{18}) are relatively unreactive.



The C-H bond is a non-polar bond.

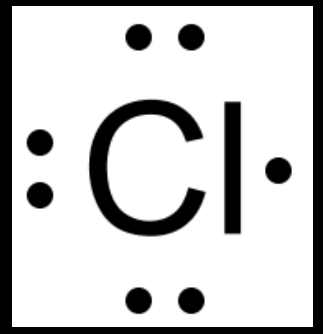
The C-C and C-H bonds are relatively strong (C-C 348 kJ mol^{-1} C-H 412 kJ mol^{-1}).

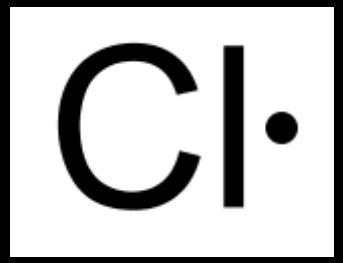
Reactions of the alkanes

Alkanes undergo **free radical substitution** reactions.

In a substitution reaction, an atom or group of atoms is replaced by another atom or group.

Free radicals (radicals) are species with unpaired electrons which are represented by a dot (•).





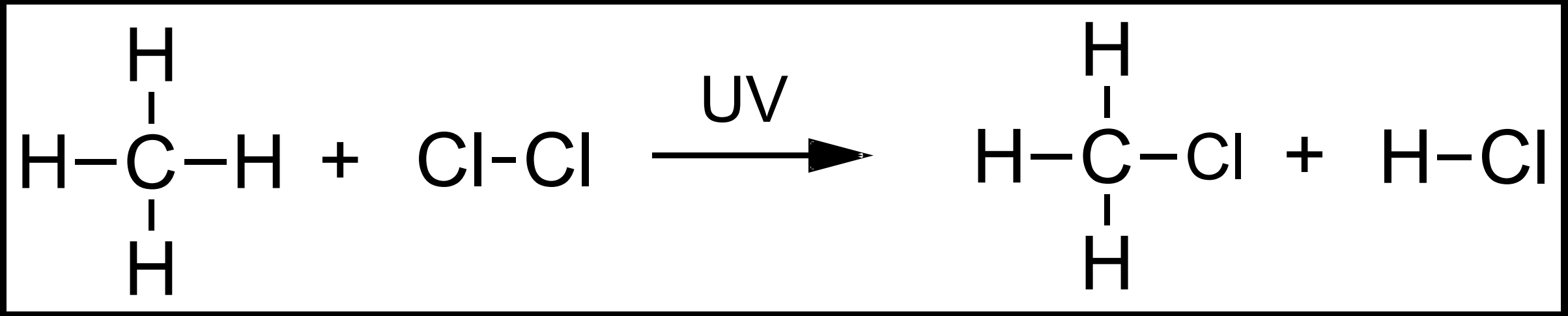
Reactions of the alkanes

Free radical substitution reactions occur in 3 steps; initiation, propagation and termination. Alkanes (CH_4 and C_2H_6) react with halogens (Cl_2 and Br_2) to form halogenoalkanes (CH_3Cl) and dihalogenoalkanes (CH_2Cl_2).

$$CH_{4(g)} + Cl_{2(g)} \xrightarrow{UV} CH_3Cl_{(g)} + HCl_{(g)}$$

Reactions of the alkanes

Free radical substitution reactions occur in 3 steps; initiation, propagation and termination.



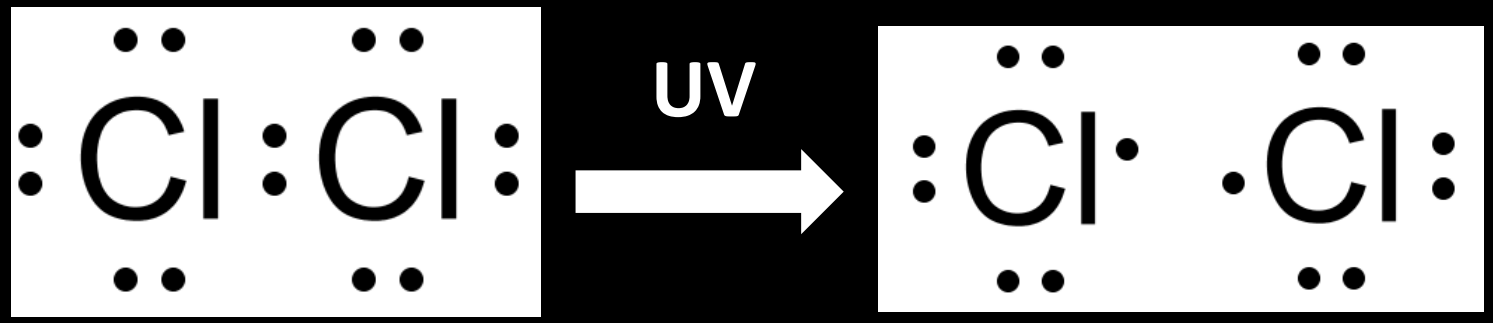
$$CH_{4(g)} + Cl_{2(g)} \xrightarrow{UV} CH_3Cl_{(g)} + HCl_{(g)}$$

Reactions of the alkanes

Initiation – occurs in the presence of UV light.

$$Cl_2 \xrightarrow{UV} 2Cl\bullet$$

Photochemical homolytic fission – the bond between the chlorine atoms is broken by UV light with each chlorine atom taking one electron.



Reactions of the alkanes

Propagation – these reactions keep the chain reaction going.

$$CH_4 + Cl\bullet \rightarrow \bullet CH_3 + HCl$$

$$\bullet CH_3 + Cl_2 \rightarrow CH_3Cl + Cl\bullet$$

Reactions of the alkanes

Termination – these reactions remove the free radicals from the system.

$$Cl\cdot + Cl\cdot \rightarrow Cl_2$$

$$\cdot CH_3 + \cdot CH_3 \rightarrow C_2H_6$$

$$\cdot CH_3 + Cl\cdot \rightarrow CH_3Cl$$

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Combustion reactions of the alkanes

Reactions of the alkanes

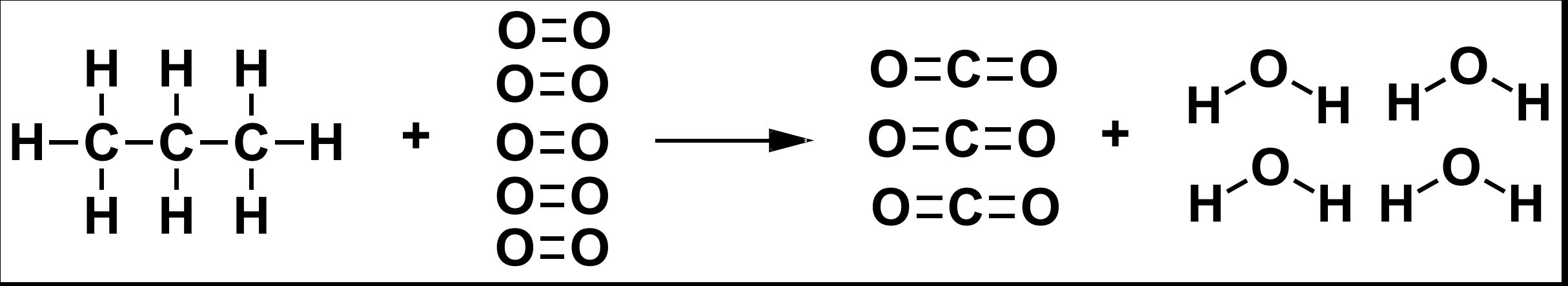
Alkanes react with oxygen in combustion reactions, usually producing carbon dioxide and water.

Alkanes make very good fuels as they release large amounts of heat when they burn (exothermic reactions).

Alkane	$\Delta H^{\ominus}_c$ (kJ mol^{-1})
Methane	- 891
Ethane	- 1561
Propane	- 2219
Butane	- 2878
Pentane	- 3509

Reactions of the alkanes

$$C_3H_{8(g)} + 5O_{2(g)} \rightarrow 3CO_{2(g)} + 4H_2O_{(l)}$$



2 × 346 kJ	5 × 498 kJ	6 × 804 kJ	8 × 463 kJ
8 × 414 kJ			
4004 kJ	2490 kJ	4824 kJ	3704 kJ

$$\Delta H = 6494 - 8528 = -2034 \text{ kJ mol}^{-1}$$

Reactions of the alkanes

Complete combustion (excess of oxygen):

$$C_3H_{8(g)} + 5O_{2(g)} \rightarrow 3CO_{2(g)} + 4H_2O_{(g)}$$

Incomplete combustion (lack of oxygen):

$$C_3H_{8(g)} + 3\tfrac{1}{2}O_{2(g)} \rightarrow 3CO_{(g)} + 4H_2O_{(g)}$$

$$C_3H_{8(g)} + 2O_{2(g)} \rightarrow 3C_{(s)} + 4H_2O_{(g)}$$

Reactions of the alkanes

Which equations represent the incomplete combustion of methane?

I. $CH_4(g) + 2O_2(g) \rightarrow CO_2(g) + 2H_2O(g)$

II. $CH_4(g) + 1\frac{1}{2}O_2(g) \rightarrow CO(g) + 2H_2O(g)$

III. $CH_4(g) + O_2(g) \rightarrow C(s) + 2H_2O(g)$

A. I and II only

B. I and III only

C. II and III only

D. I, II and III

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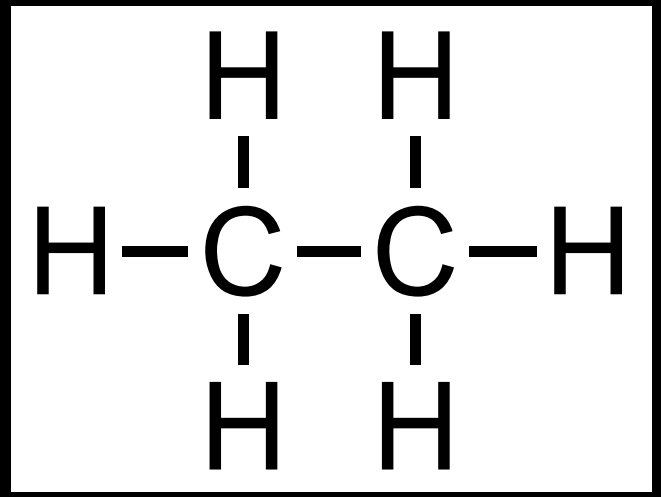
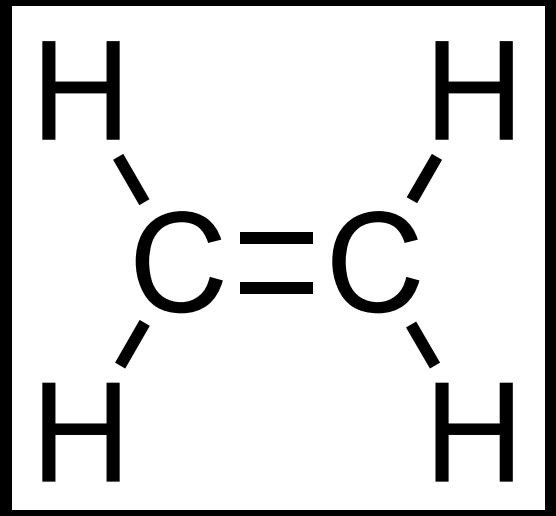
Test for unsaturation

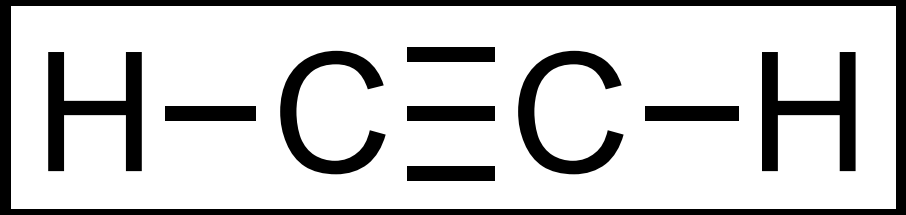
Test for unsaturation

Saturated molecules have carbon to carbon single bonds.

Unsaturated molecules have carbon to carbon double or triple bonds (multiple bonds).





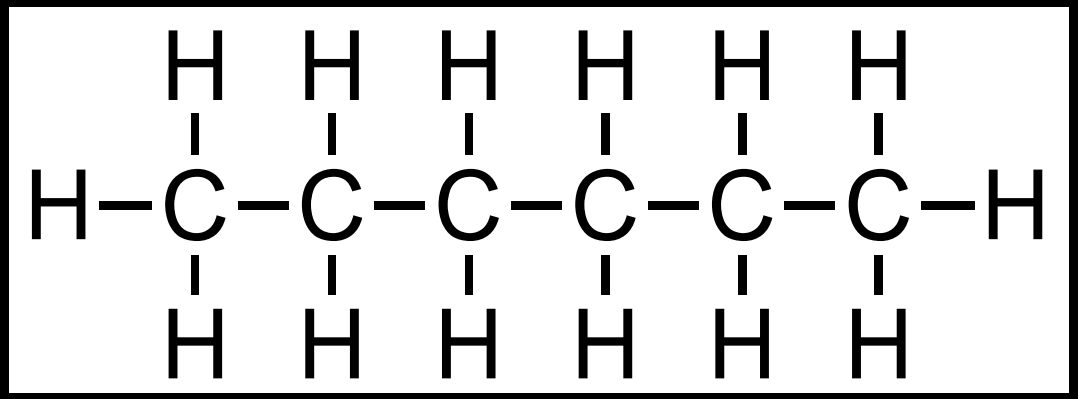


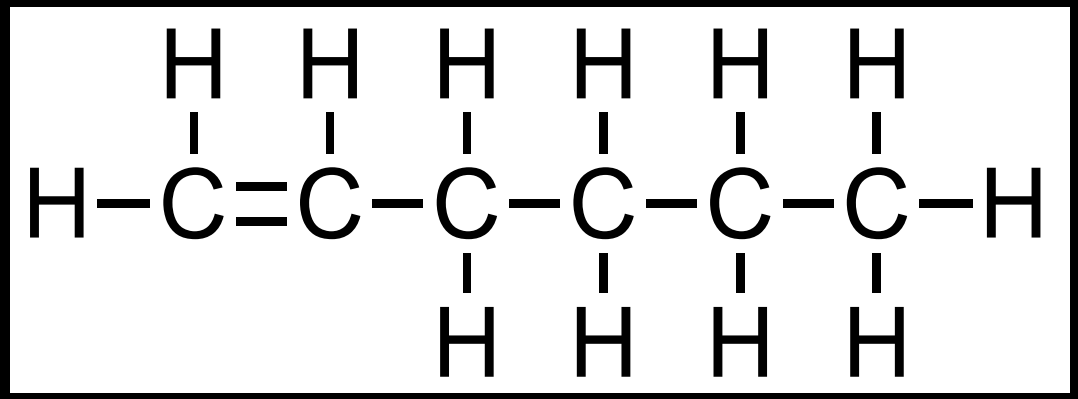
Test for unsaturation

Bromine water, $Br_{2(aq)}$, can be used to distinguish between an alkane and an alkene.

Bromine water is a brown-coloured solution. When added to an alkene, the bromine water is decolourised (brown to colourless). This indicates the presence of carbon to carbon double bonds in the molecule. When added to an alkane, there is no colour change.

Test for unsaturation





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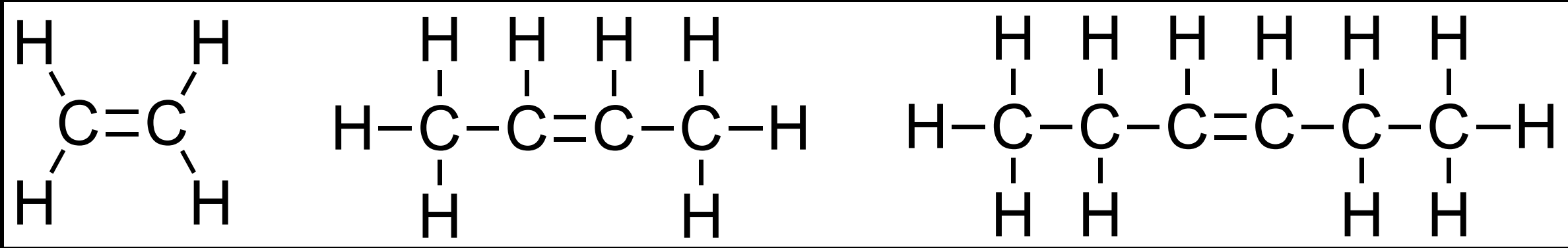
Addition reactions of the alkenes

Addition reactions of the alkenes

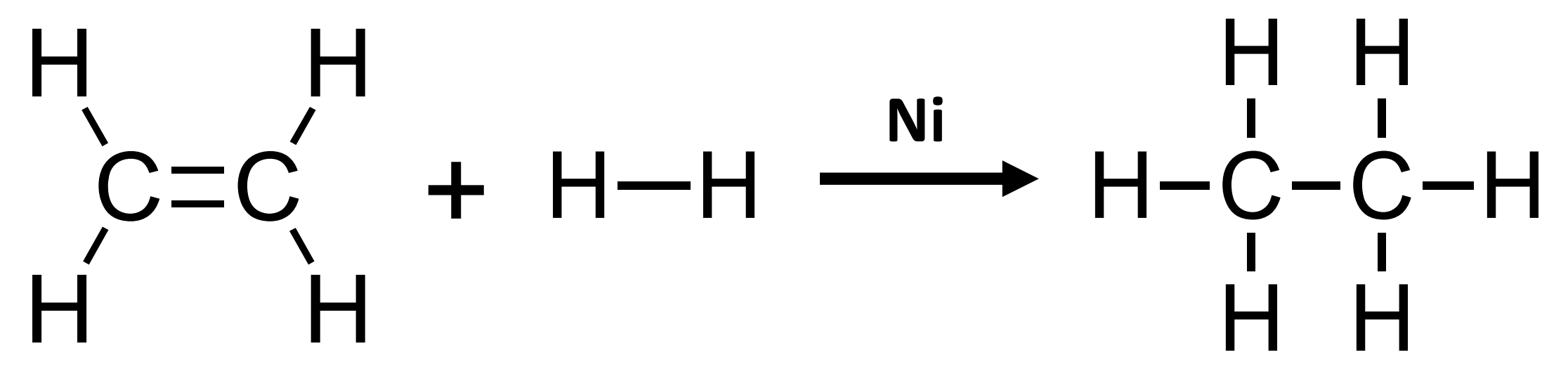
Alkenes are reactive molecules due to the presence of a carbon to carbon double bond (alkenyl group). They undergo electrophilic addition reactions in which two molecules combine to produce a larger molecule.



Ethene But-2-ene Hex-3-ene

Addition reactions of alkenes

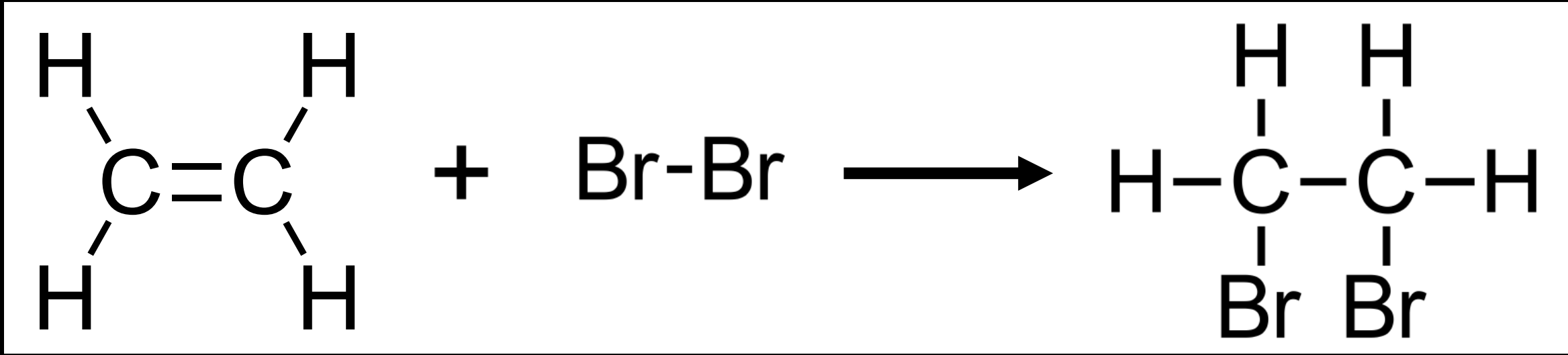
Hydrogenation – an alkene reacts with hydrogen to form an alkane.



$$C_2H_{4(g)} + H_{2(g)} \xrightarrow{Ni} C_2H_{6(g)}$$

Addition reactions of alkenes

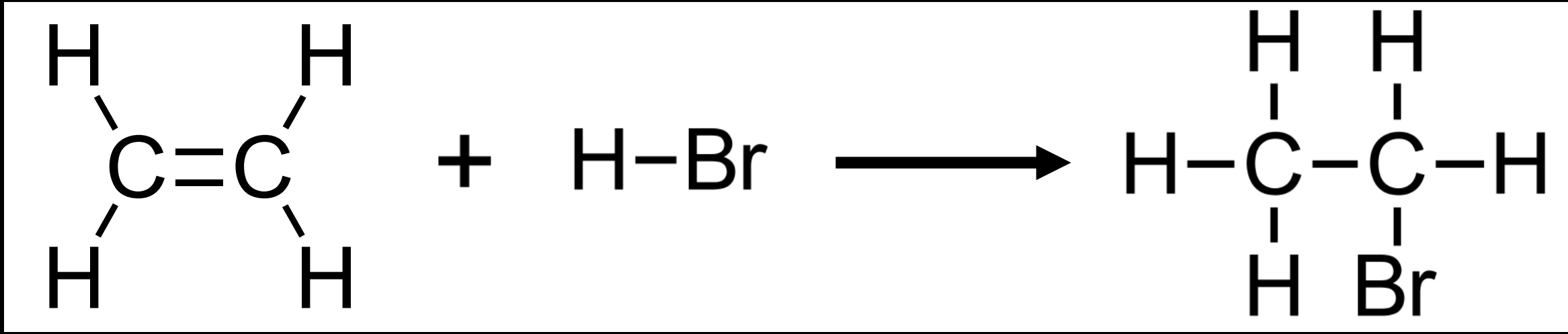
Halogenation – alkenes react with halogens to produce dihalogeno compounds.



$$C_2H_{4(g)} + Br_{2(g)} \longrightarrow CH_2BrCH_2Br_{(g)}$$

Addition reactions of alkenes

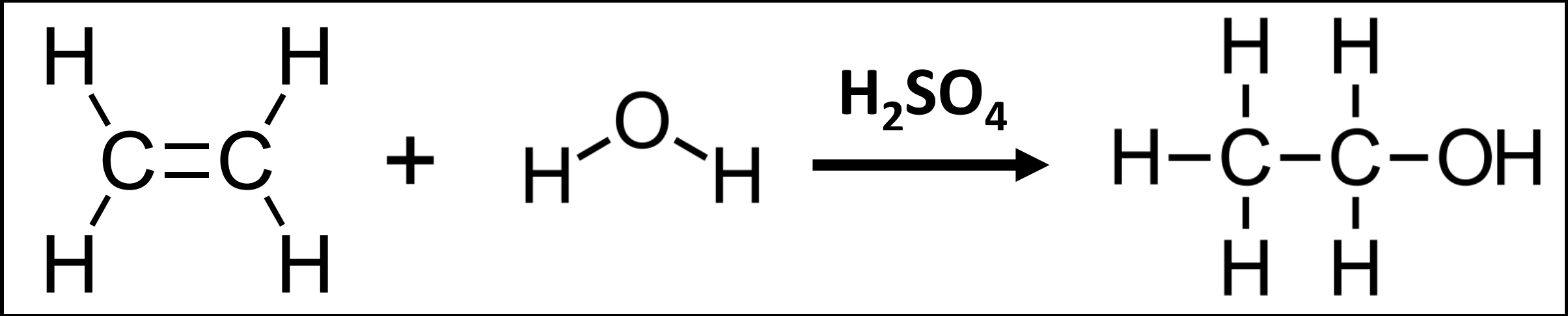
Alkenes react with hydrogen halides (HCl, HBr or HI) to produce halogenoalkanes.



$$C_2H_{4(g)} + HBr_{(g)} \longrightarrow CH_3CH_2Br_{(g)}$$

Addition reactions of alkenes

Hydration – an alkene reacts with steam to form an alcohol.



$$C_2H_{4(g)} + H_2O_{(g)} \xrightarrow{H_2SO_4} CH_3CH_2OH_{(l)}$$

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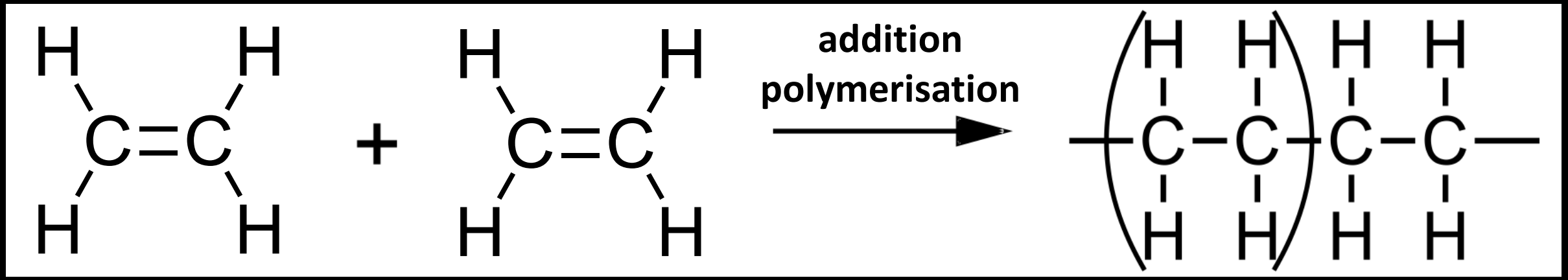
Addition polymerisation

Addition polymerisation

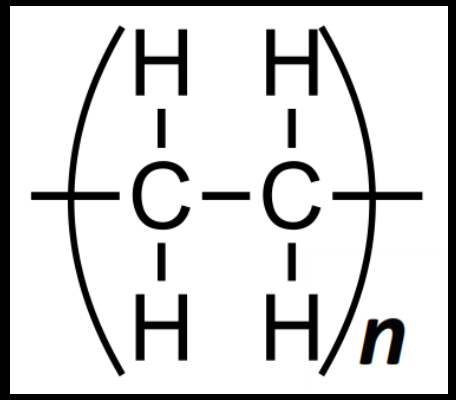
Addition polymers are formed when smaller unsaturated molecules (monomers) react together.



ethene monomers

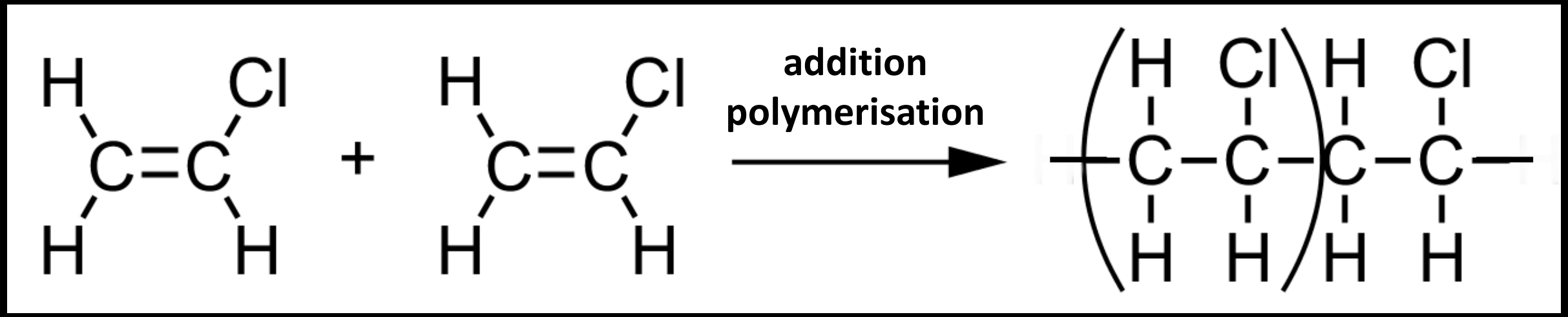
polymer polyethene

repeating unit

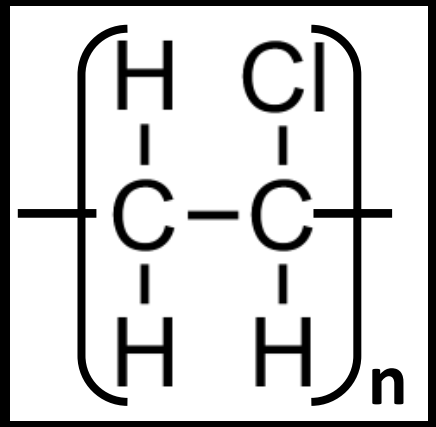


Addition polymerisation

PVC or poly(vinyl chloride) is a polymer made from the monomer unit chloroethene (vinyl chloride).

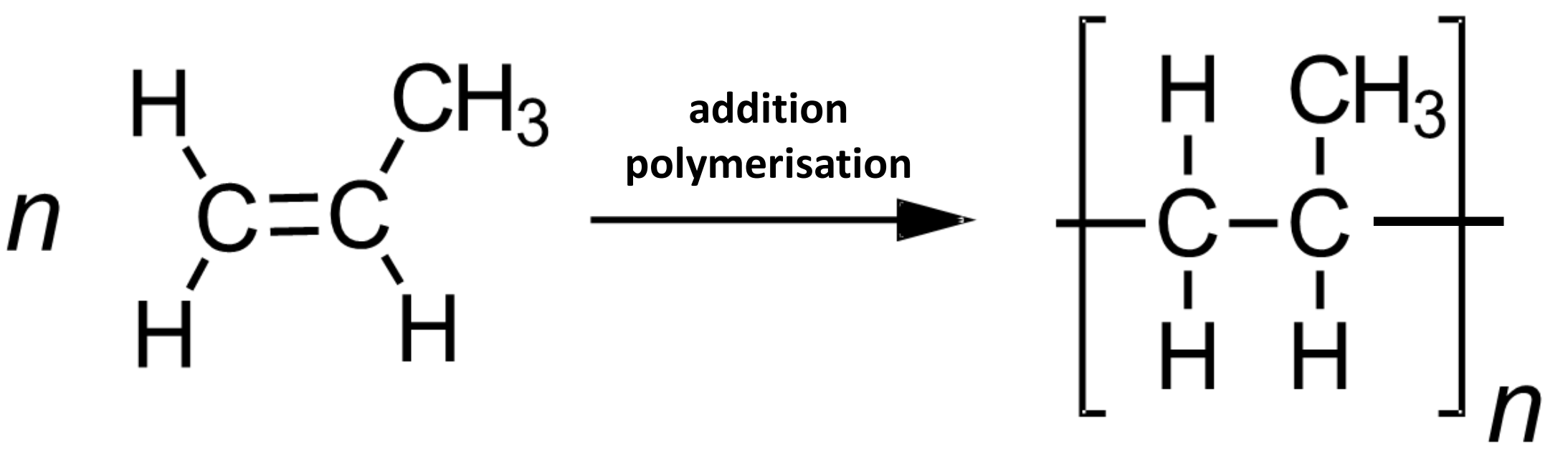


repeating unit



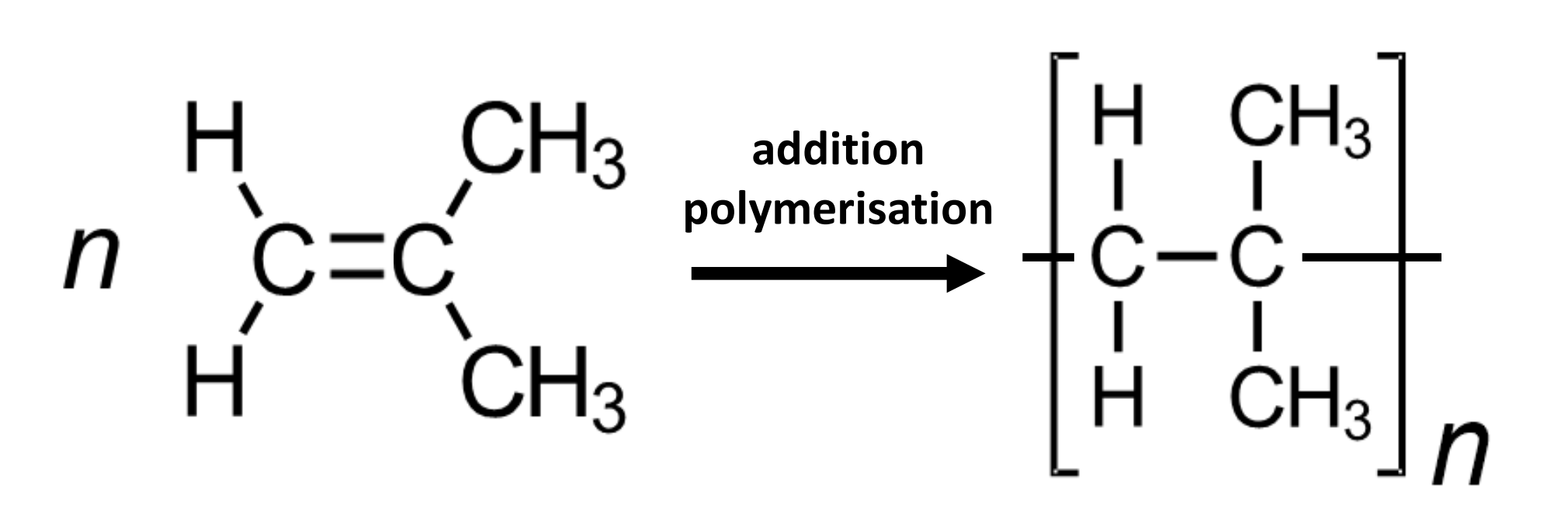
Addition polymerisation

Poly(propene) is an addition polymer made from the monomer unit propene.



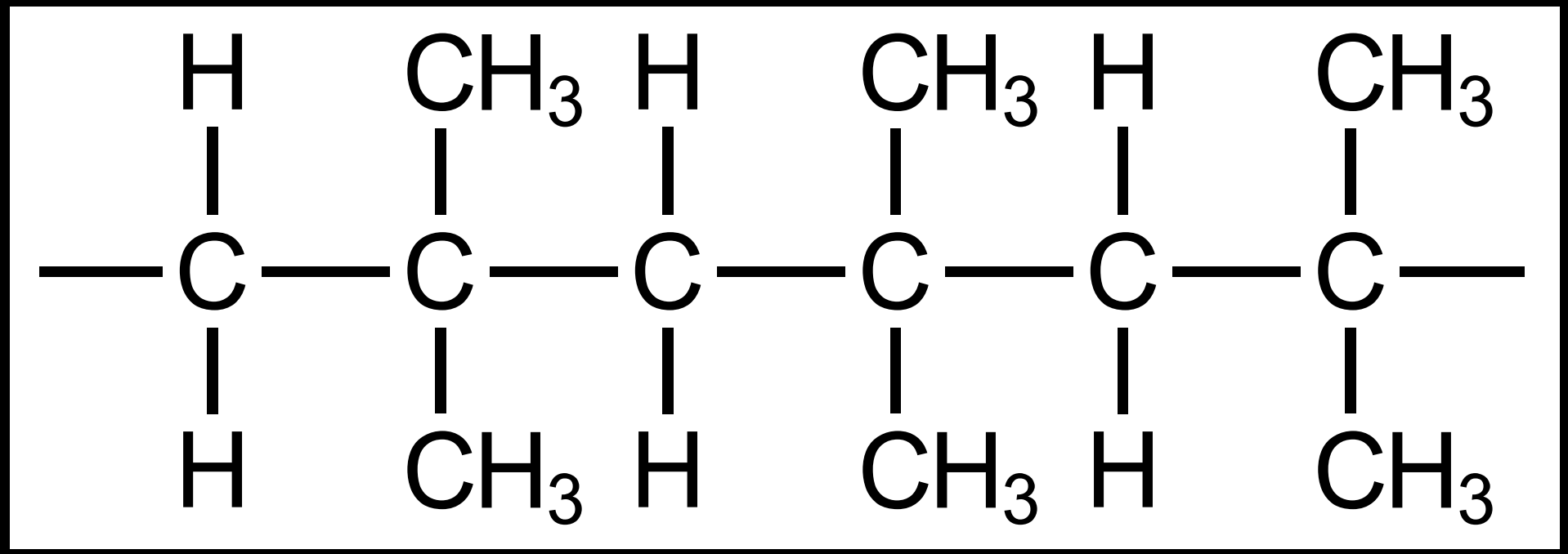
Addition polymerisation

The polymerisation of 2-methylpropene forms the polymer poly(2-methylpropene) or butyl rubber.



Addition polymerisation

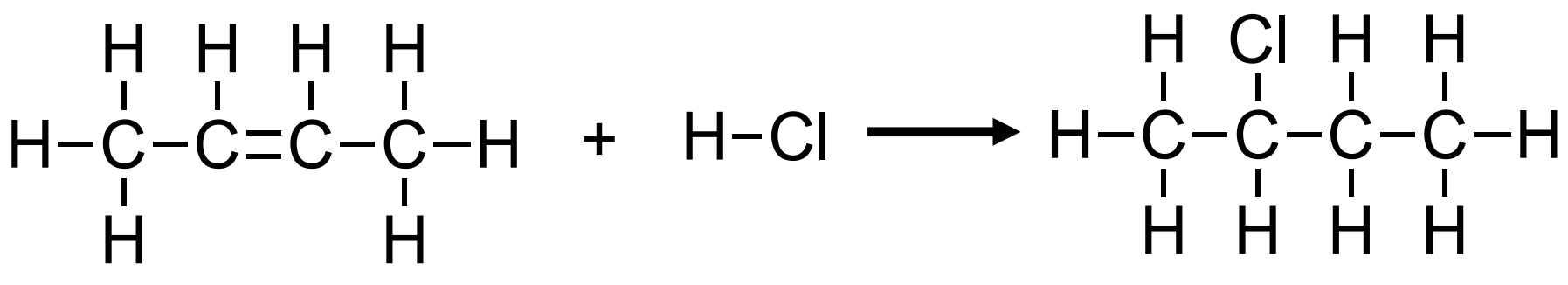
Draw the structure of the polymer made from three 2-methylpropene monomer units.

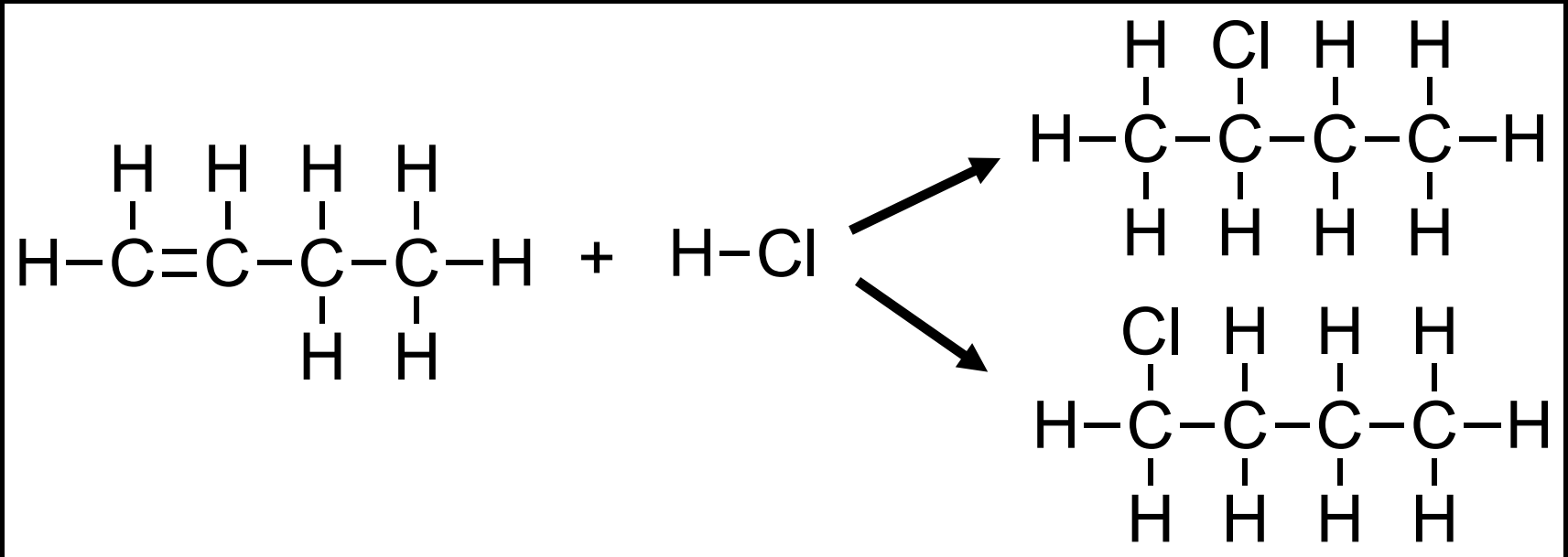


Every second carbon atom is bonded to two methyl (CH_3) groups.

Addition reactions of alkenes

The addition reactions of symmetrical alkenes produce only one possible product.





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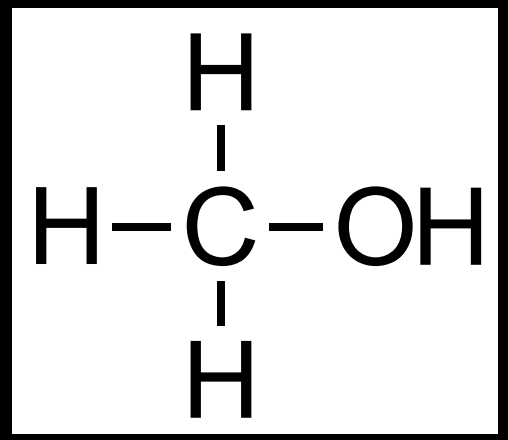
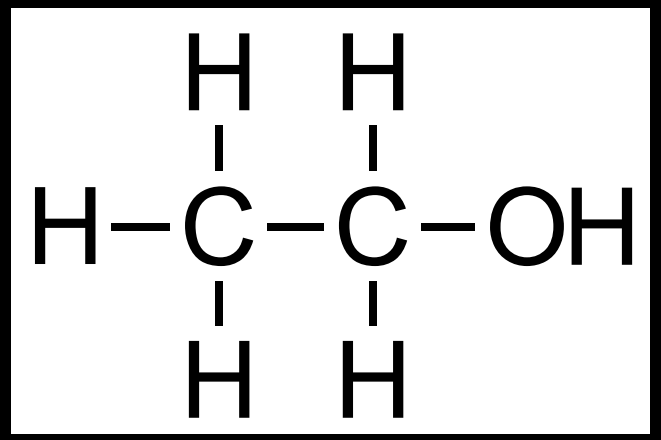
Combustion reactions of the alcohols

Reactions of the alcohols

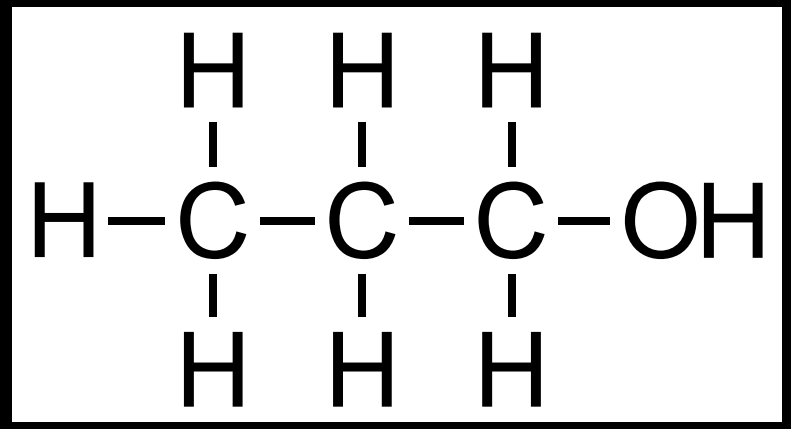
Alcohols are organic compounds composed of carbon, hydrogen and oxygen.



CH_3OH
Methanol



CH_3CH_2OH
Ethanol



$CH_3CH_2CH_2OH$
Propan-1-ol

Reactions of the alcohols

These $\Delta H^{\ominus}_c$ values can be found in section 13 of the IB chemistry data booklet.

Alcohol	$\Delta H^{\ominus}_c$ (kJ mol^{-1})
Methanol	- 726
Ethanol	- 1367
Propan-1-ol	- 2021
Butan-1-ol	- 2676

As the number of carbon atoms increases, the enthalpy change also increases.

Reactions of the alcohols

Alcohols undergo combustion in excess oxygen (complete combustion) to form carbon dioxide and water.

$$2CH_3OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 4H_2O_{(g)}$$

$$C_2H_5OH_{(l)} + 3O_{2(g)} \rightarrow 2CO_{2(g)} + 3H_2O_{(g)}$$

$$C_nH_{(2n+1)}OH_{(l)} + (2n+1)O_{2(g)} \rightarrow nCO_{2(g)} + (n+1)H_2O_{(l)}$$

Reactions of the alcohols

Alcohols undergo combustion in a limited supply of oxygen (incomplete combustion) to form carbon monoxide (CO) or carbon (C).

$$C_2H_5OH_{(l)} + 2O_{2(g)} \rightarrow 2CO_{(g)} + 3H_2O_{(g)}$$

$$C_2H_5OH_{(l)} + O_{2(g)} \rightarrow 2C_{(g)} + 3H_2O_{(g)}$$

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Oxidation reactions of the alcohols

Reactions of the alcohols

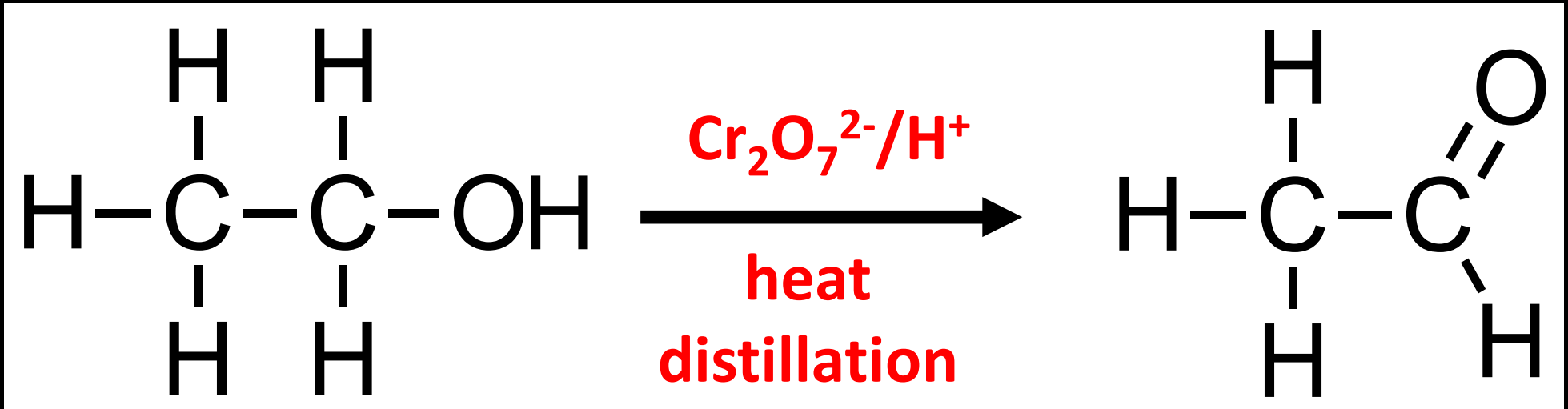
Alcohols undergo oxidation reactions when reacted with a suitable oxidising agent such as acidified potassium dichromate(VI), $H^+/Cr_2O_7^{2-}$

Colour change is orange to green ($Cr_2O_7^{2-}$ ion is reduced to the Cr^{3+} ion).

$$Cr_2O_7^{2-}{}_{(aq)} + 14H^+{}_{(aq)} + 6e^- \rightarrow 2Cr^{3+}{}_{(aq)} + 7H_2O_{(l)}$$

Reactions of the alcohols

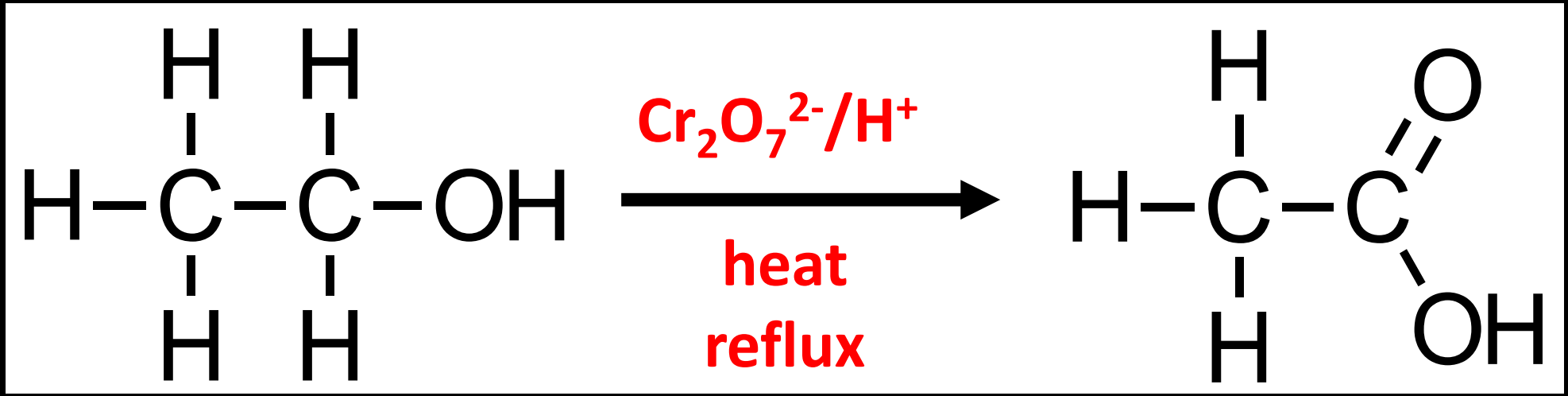
Primary alcohols undergo partial oxidation to form aldehydes.



An excess of alcohol is used in the reaction and the aldehyde is distilled off as it is produced.

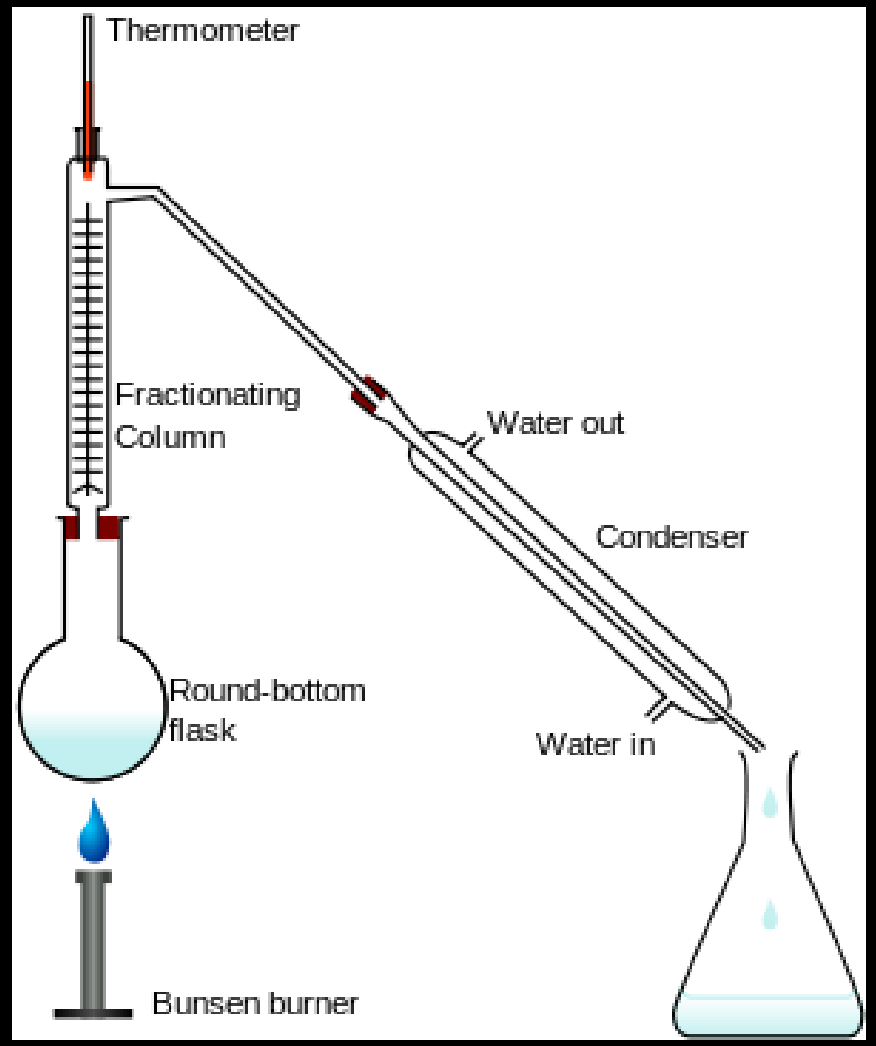
Reactions of the alcohols

Primary alcohols can also undergo complete oxidation to form carboxylic acids.



An excess of oxidising agent is used in the reaction.

Reactions of the alcohols

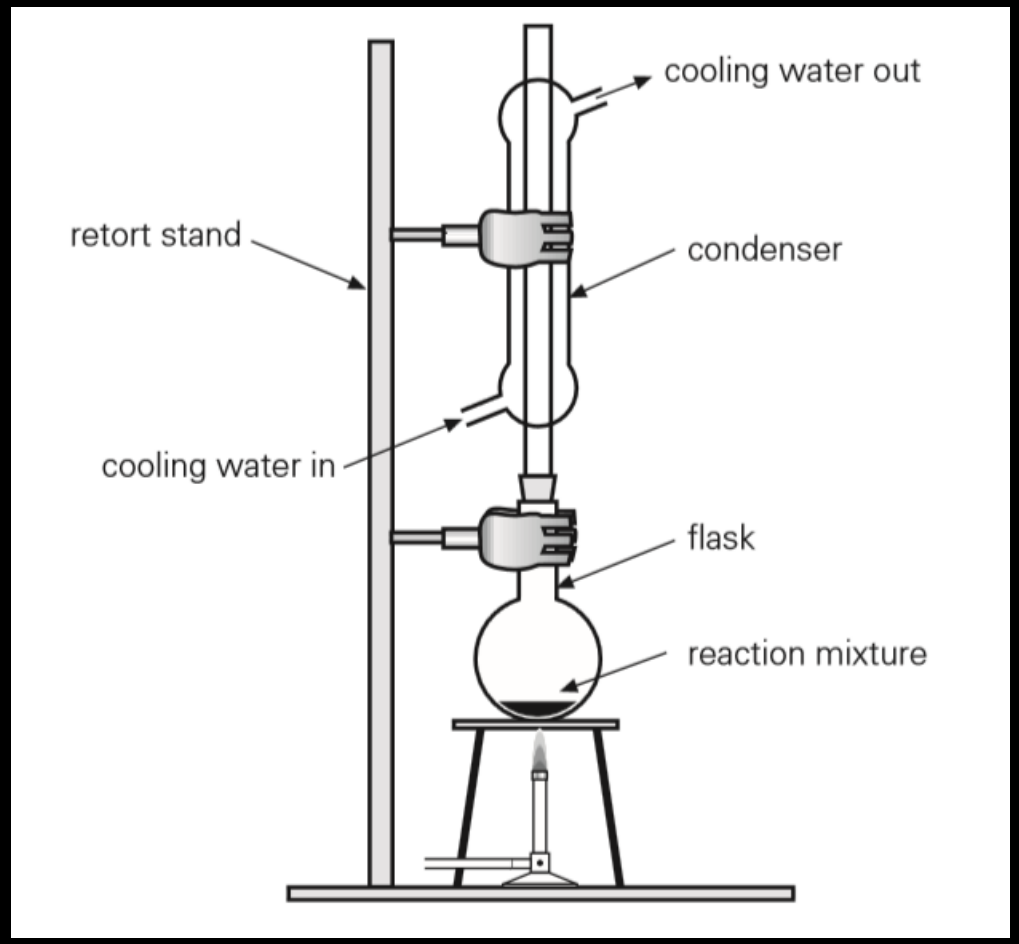


Distillation is used to separate the components of a mixture that have different boiling points.

Aldehydes, due to their weaker intermolecular forces, have lower boiling points than alcohols.

The aldehyde evaporates, rises up the fractionating column and condenses to form a liquid.

Reactions of the alcohols



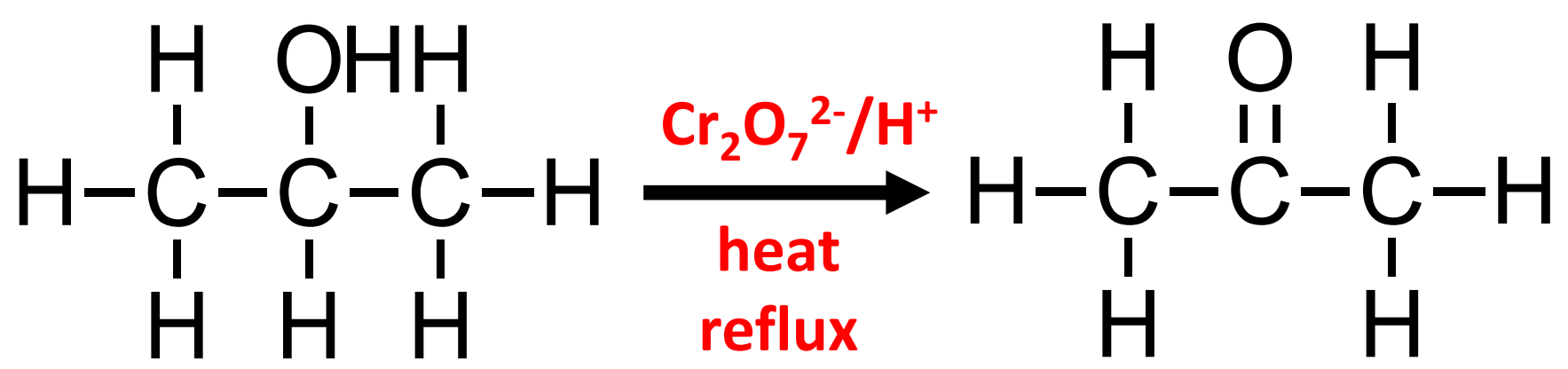
A reflux condenser is used to prevent the loss of a solvent from a mixture.

The vapours rise up the column, condense, and flow back down to the flask.

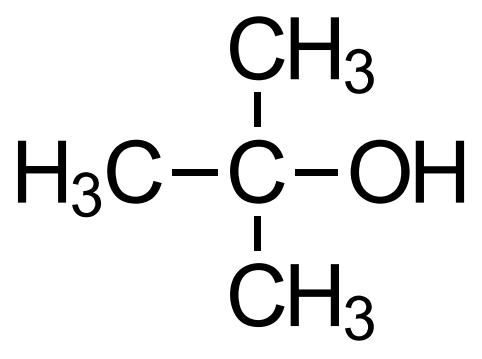
The reaction mixture and oxidising agent are kept in contact for a longer period of time.

Reactions of the alcohols

Secondary alcohols undergo oxidation to form ketones.



Tertiary alcohols do not undergo oxidation as there are no H atoms bonded directly to C-OH.



Reactions of the alcohols

	Oxidising agent	Conditions	Product
Primary alcohols	$H^+/Cr_2O_7^{2-}$ (orange to green)	Heat / distillation	Aldehyde
Primary alcohols	$H^+/Cr_2O_7^{2-}$ (orange to green)	Heat / reflux	Carboxylic acid
Secondary alcohols	$H^+/Cr_2O_7^{2-}$ (orange to green)	Heat / reflux	Ketone

An alternative oxidising agent is potassium manganate(VII).

$$MnO_4^-{}_{(aq)} + 8H^+{}_{(aq)} + 5e^- \rightarrow Mn^{2+}{}_{(aq)} + 4H_2O_{(l)}$$

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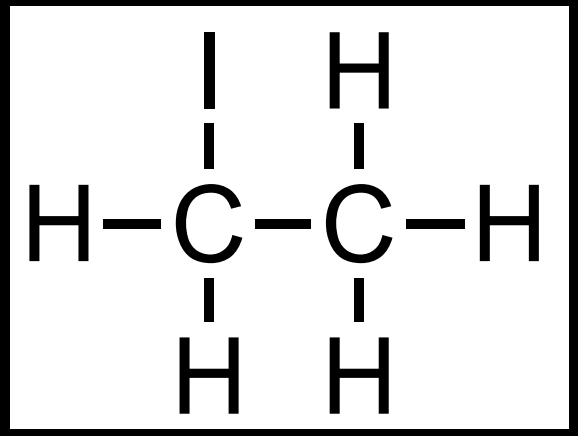
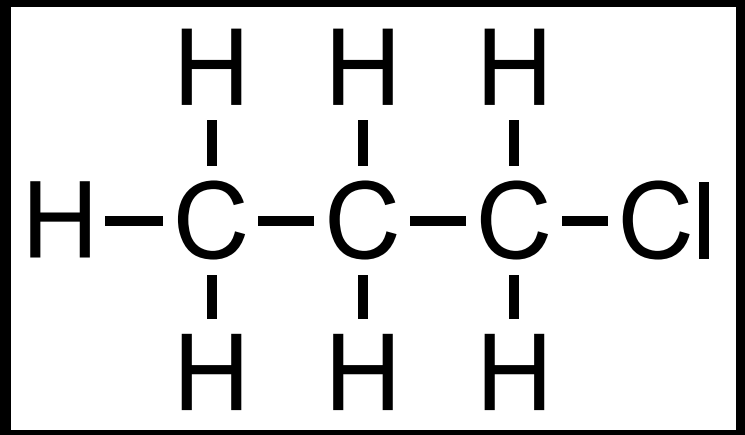
Reactions of halogenoalkanes

Halogenoalkanes

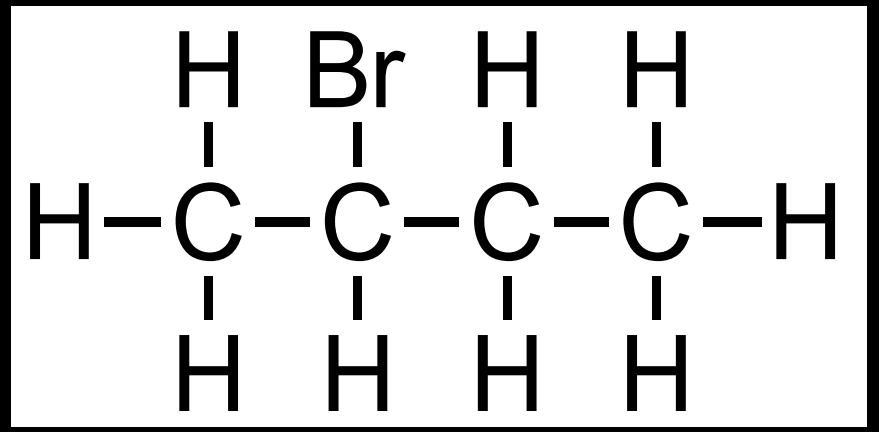
Halogenoalkanes contain an atom of fluorine, chlorine, bromine or iodine.



Iodoethane



1-chloropropane

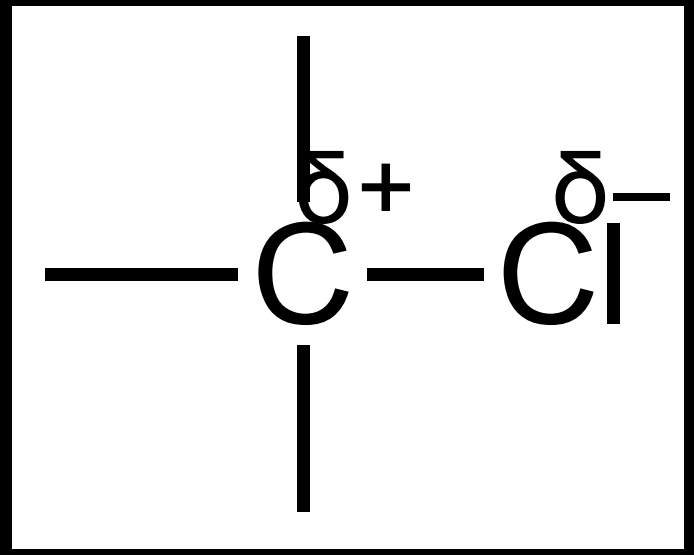


2-bromobutane

General formula: $C_nH_{2n+1}X$

Halogenoalkanes

Halogenoalkanes undergo nucleophilic substitution reactions (the replacement of one atom by another atom or group).

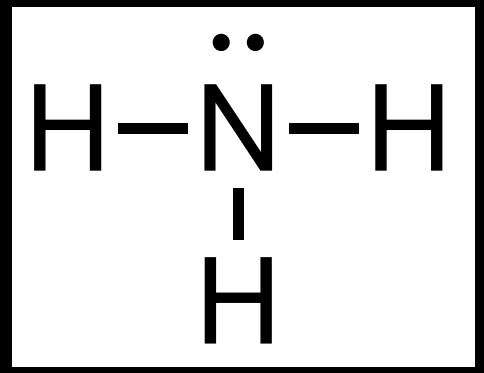


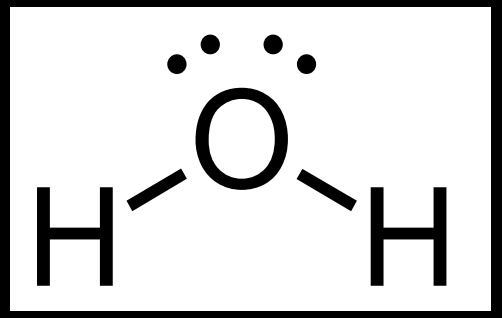
The halogen atom is more electronegative than the carbon atom forming a polar bond.
The halogen has a partial negative charge and the carbon has a partial positive charge (electron deficient).

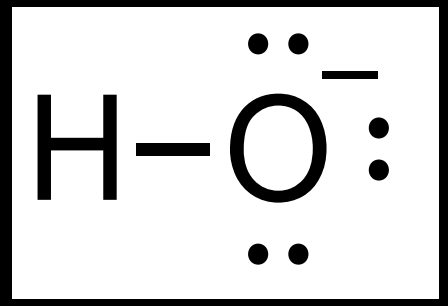
Nucleophiles

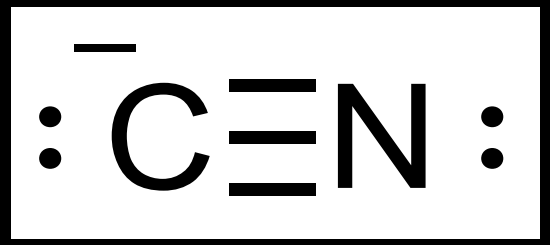
Nucleophiles are electron rich species that have lone pairs of electrons.

They are attracted to regions of positive charge.

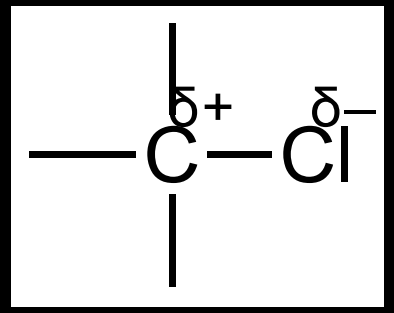






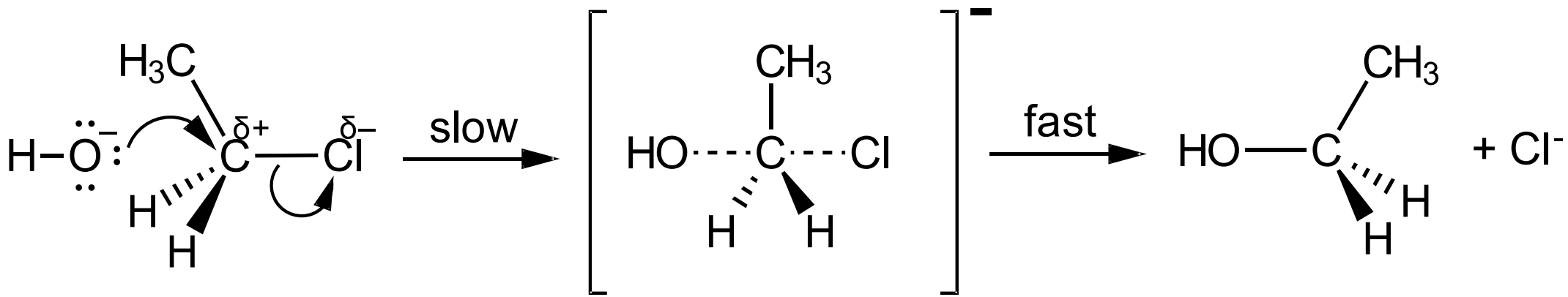


Nucleophiles are attracted to the electron deficient carbon in the halogenoalkane.



Halogenoalkanes

Halogenoalkanes react with aqueous sodium hydroxide to produce alcohols.



unstable transition state

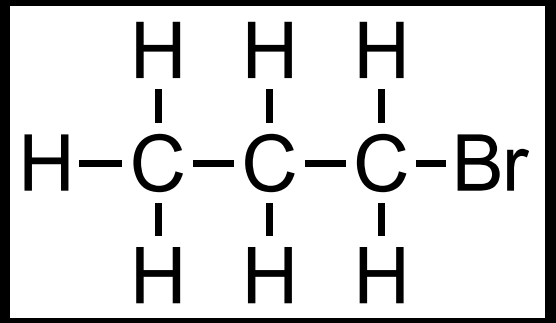
$$CH_3CH_2Cl_{(g)} + NaOH_{(aq)} \rightarrow CH_3CH_2OH_{(l)} + NaCl_{(aq)}$$

chloroethane **ethanol**

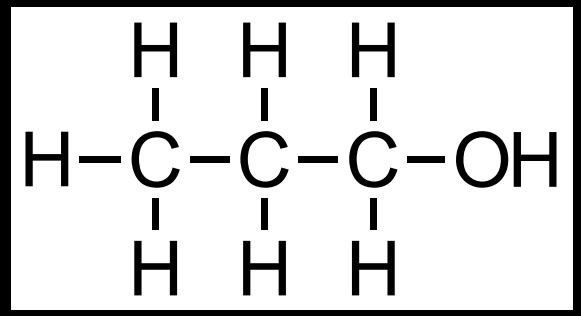
Halogenoalkanes

$$C_3H_7Br_{(l)} + NaOH_{(aq)} \rightarrow C_3H_7OH_{(l)} + NaBr_{(aq)}$$

1-bromopropane



propan-1-ol



Halogenoalkanes react with alkalis such as NaOH to form alcohols.

The hydroxide ion behaves as a nucleophile.

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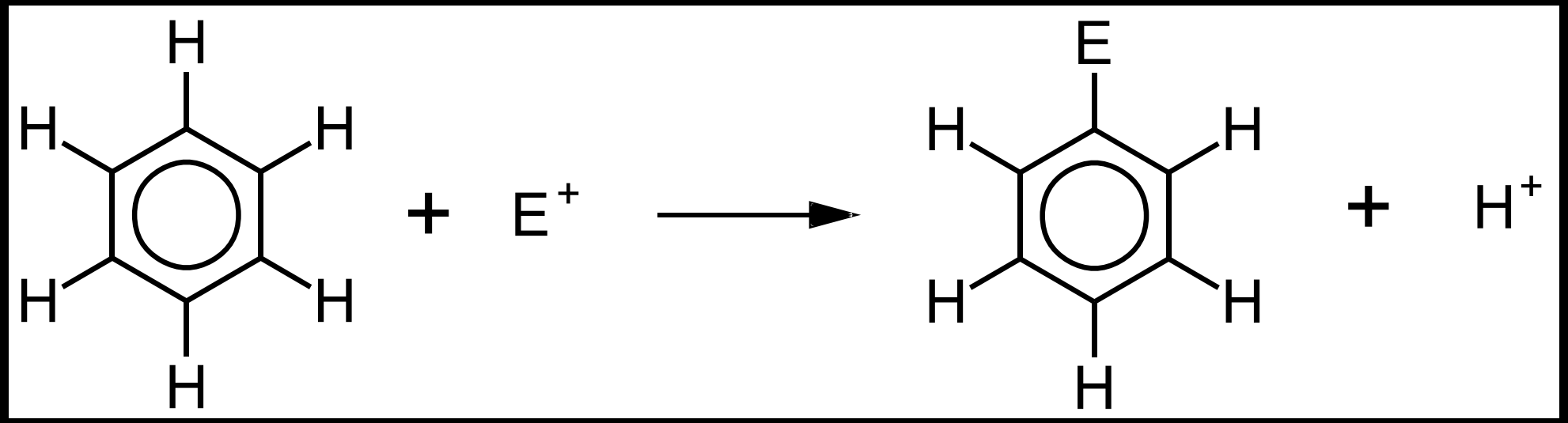
Reactions of benzene

Reactions of benzene

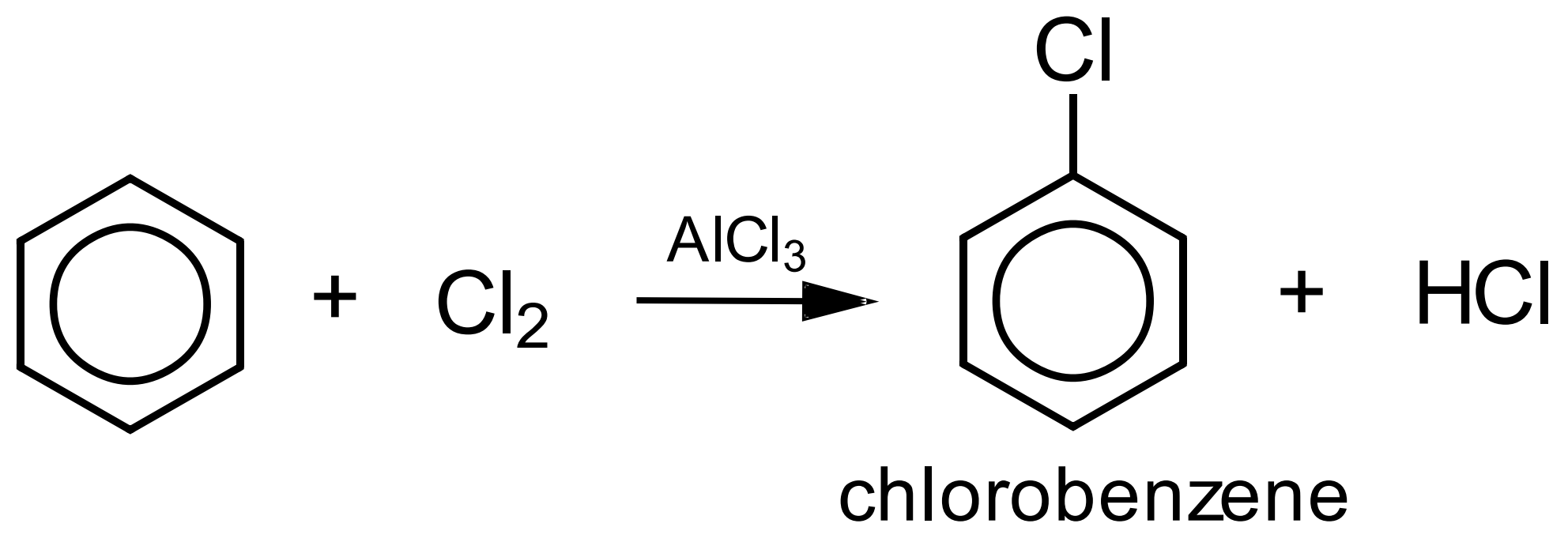
Benzene undergoes electrophilic substitution reactions in which a hydrogen atom is replaced by an incoming group.

An electrophile is a species which is electron deficient (either a positive ion or have a partial positive charge).



Reactions of benzene

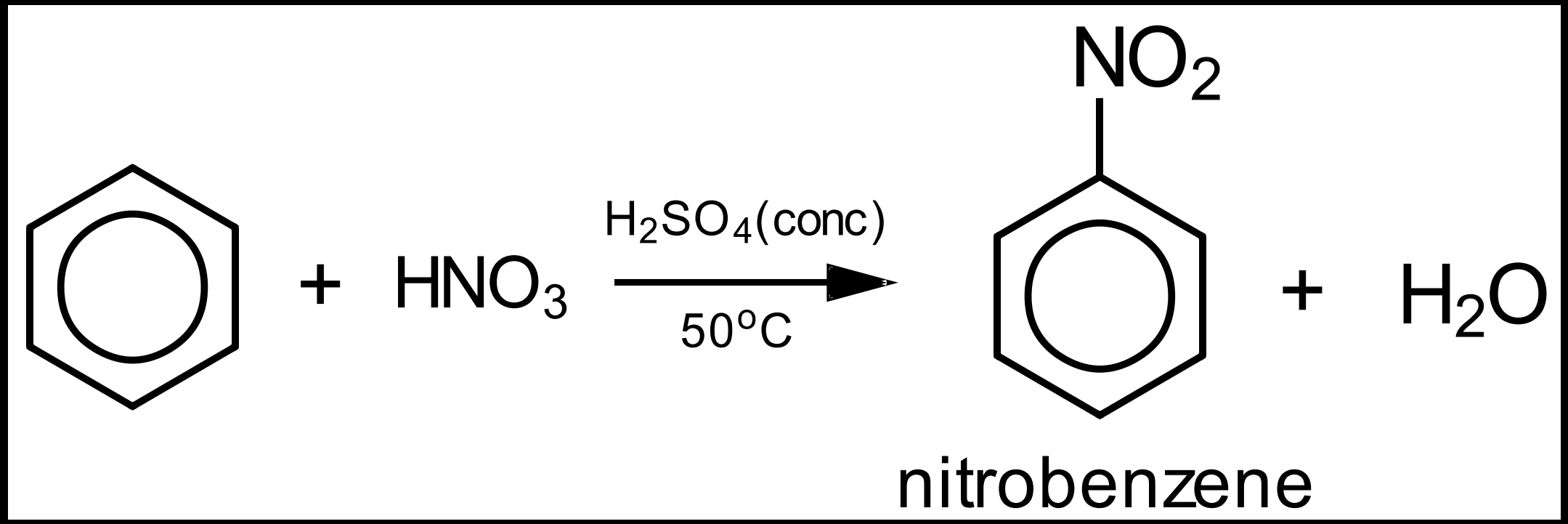
Benzene reacts with chlorine to form chlorobenzene.



$$C_6H_6 + Cl_2 \rightarrow C_6H_5Cl + HCl$$

Reactions of benzene

Benzene reacts with a nitrating mixture (conc. HNO_3 and conc. H_2SO_4) to form nitrobenzene ($C_6H_5NO_2$).



$$C_6H_6 + HNO_3 \rightarrow C_6H_5NO_2 + H_2O$$

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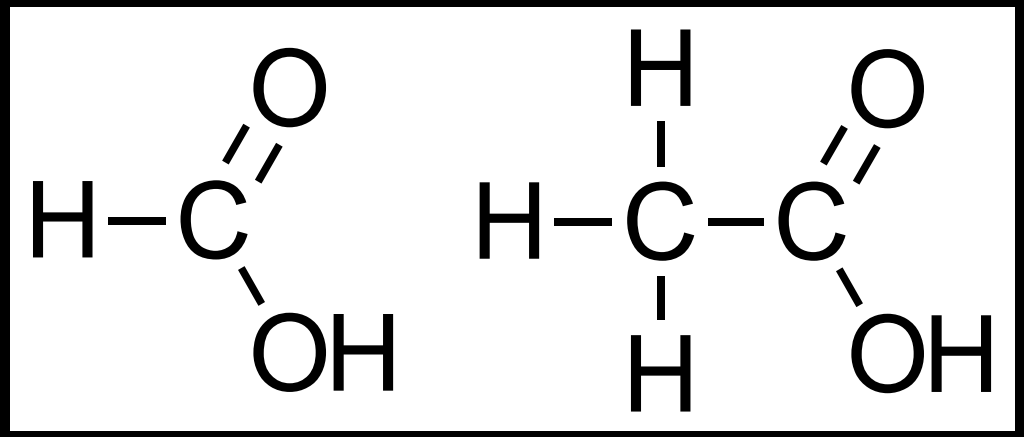
Tutorials for IB Chemistry

Organic acids and bases

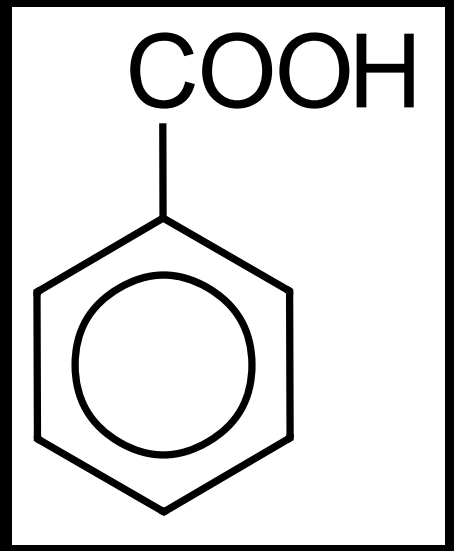
Organic acids and bases

Organic acids are organic compounds that have acidic properties.

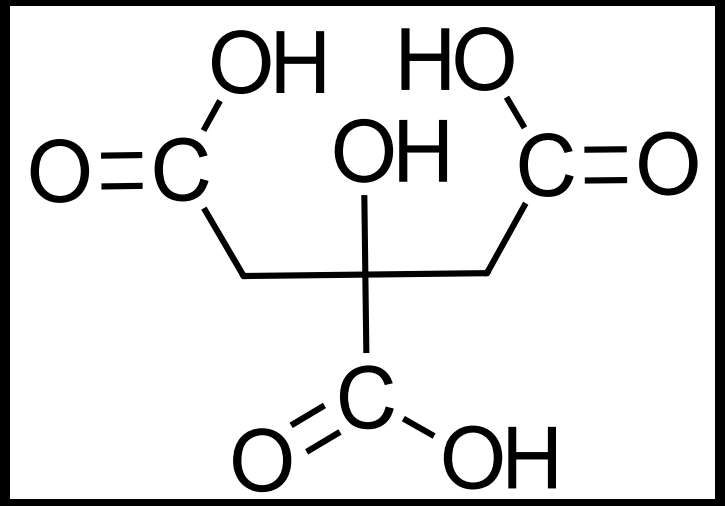


Methanoic acid
HCOOH

Ethanoic acid
CH_3COOH



Benzoic acid
C_6H_5COOH



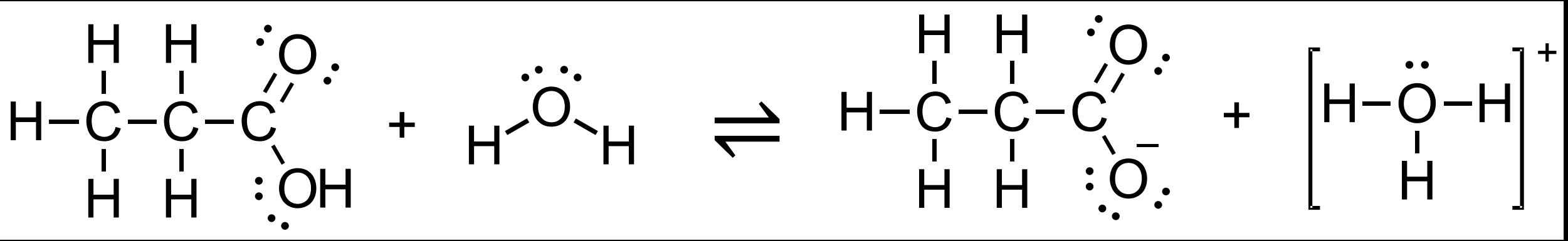
Citric acid
$C_6H_8O_7$

Organic acids and bases

Organic acid	pK_a (at 298 K)
Methanoic	3.75
Ethanoic	4.76
Propanoic	4.87
Benzoic	4.20
Chloroethanoic	2.87
Dichloroethanoic	1.35
Trichloroethanoic	0.66

Organic acids and bases

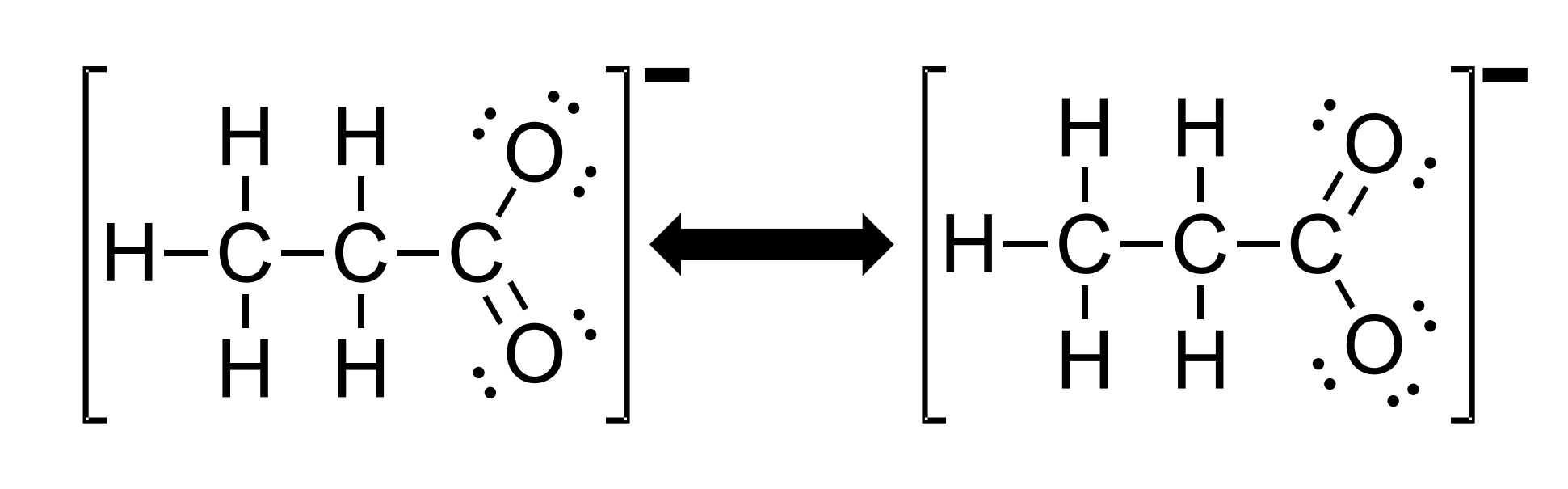
Organic acids react with water to form a carboxylate ion and a hydronium ion (H_3O^+).



$$CH_3CH_2COOH_{(aq)} + H_2O_{(l)} \rightleftharpoons CH_3CH_2COO^-_{(aq)} + H_3O^+_{(aq)}$$

The equilibrium position lies to the left because it is a weak acid (partially dissociates).

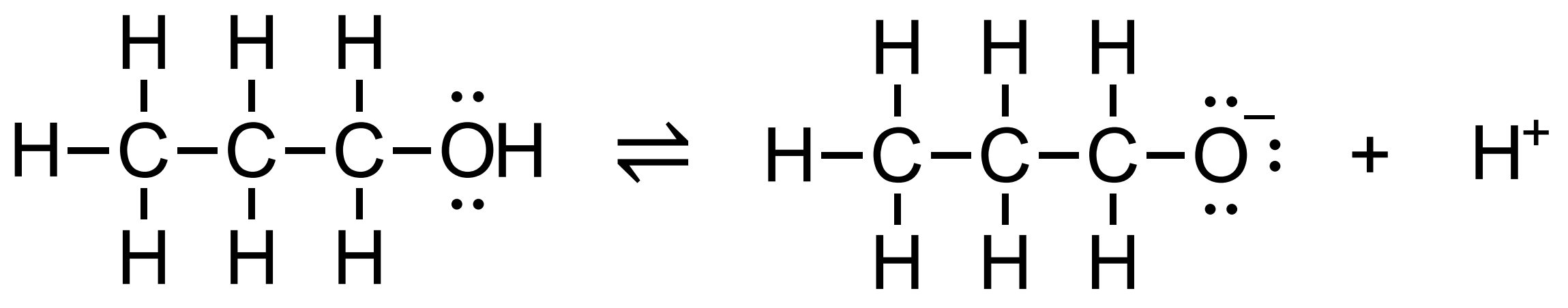
Organic acids and bases



The resonance form of the carboxylate ion is stabilised by delocalised electrons.

This explains why carboxylic acids are much stronger acids than alcohols such as ethanol.

Organic acids and bases

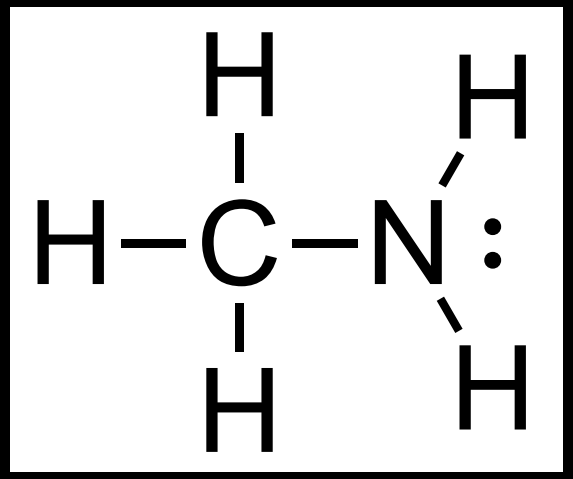


The negative charge on the alkoxide ion is localised on only one oxygen atom.

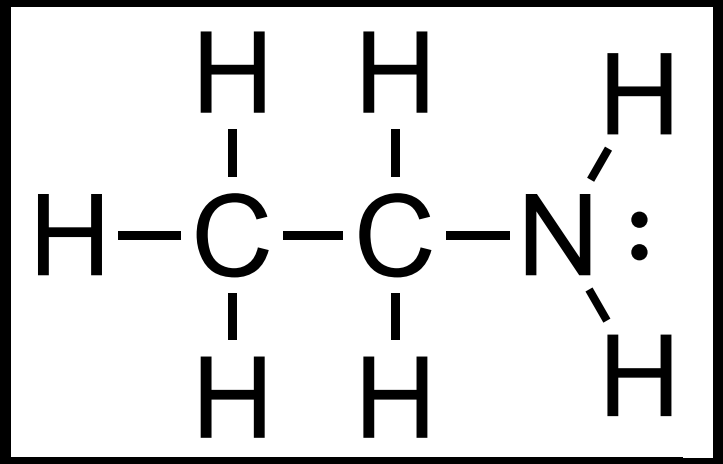
An alkoxide ion is less stable than a carboxylate ion, meaning that alcohols are weaker acids than carboxylic acids.

Organic acids and bases

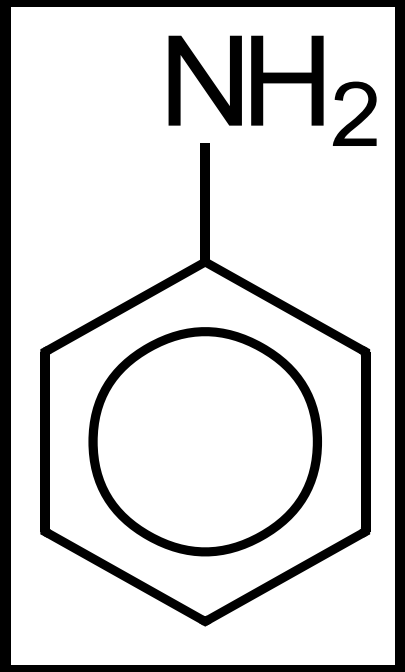
Organic bases are organic compounds that have basic properties.



Methanamine
CH_3NH_2



Ethanamine
$CH_3CH_2NH_2$



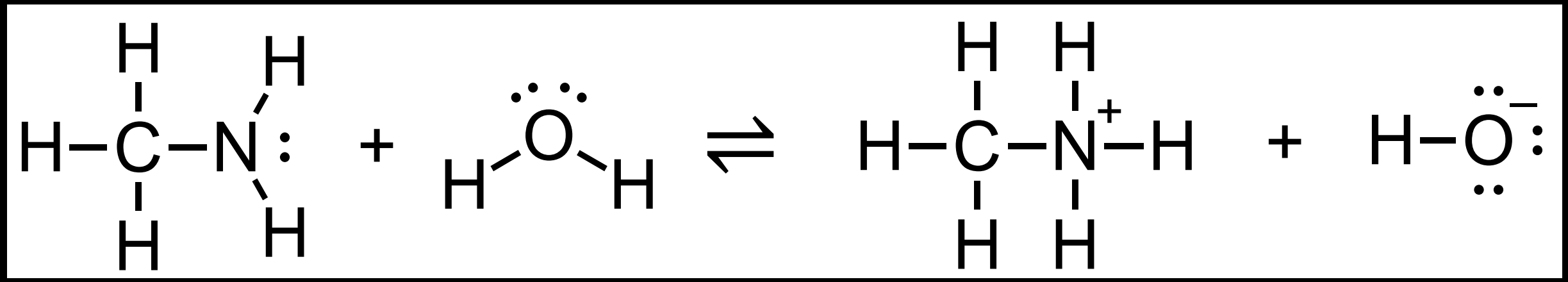
Phenylamine
$C_6H_5NH_2$

Organic acids and bases

Organic base	pK_b (at 298 K)
Ammonia	4.75
Methanamine (methylamine)	3.34
Ethanamine (ethylamine)	3.35
Phenylamine	9.13

Organic acids and bases

Amines react with water to form an ammonium ion and a hydroxide ion.

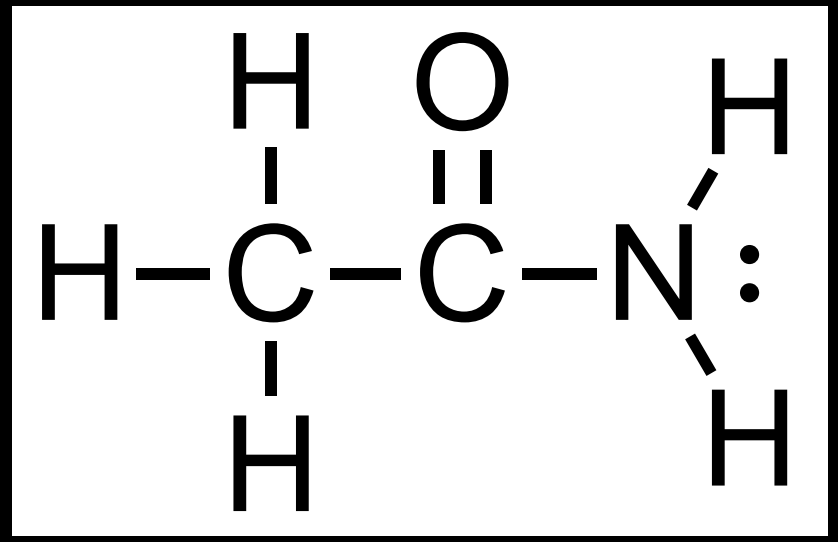


$$CH_3NH_{2\,(aq)} + H_2O_{(l)} \rightleftharpoons CH_3NH_3^+{}_{(aq)} + OH^-{}_{(aq)}$$

The equilibrium position lies to the left because it is a weak base (partially dissociates).

Organic acids and bases

Amides do not have basic properties – they do not react with acids and form neutral solutions with water.



The lone pair of electrons on the nitrogen atom are shared with the C=O π orbital.
Therefore, they are less available for bonding to a proton.

Organic acids and bases

Organic acids and bases are organic compounds that have acidic or basic properties.

Organic acids include carboxylic acids such as ethanoic acid (CH_3COOH).

Organic bases include amines such as methanamine (CH_3NH_2).

Organic acids and bases are weak, meaning that they only partially dissociate.