

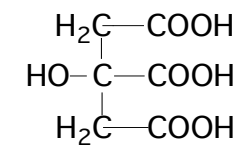
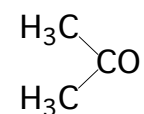
# ESSENTIAL OIL CHEMISTRY

1

## Introduction

NaCl

NaOCl

CaCO<sub>3</sub>C<sub>2</sub>H<sub>5</sub>OHC<sub>12</sub>H<sub>22</sub>O<sub>11</sub>CH<sub>3</sub>COOH

2

## Introduction

### ◇ Element

- A substance that cannot be separated into simpler substances by ordinary chemical methods

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## Introduction

Element	Symbol
Silver	Ag
Gold	Au
Carbon	C
Chlorine	Cl
Iron	Fe
Hydrogen	H
Sodium	Na
Oxygen	O

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## Introduction

### ◇ Element

- A substance that cannot be separated into simpler substances by ordinary chemical methods

### ◇ Compound

- Two or more different elements joined together

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## Introduction

Negative electrons



Positive protons



**ATOMS**

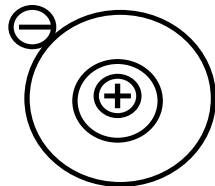


Neutral neutrons

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## Introduction

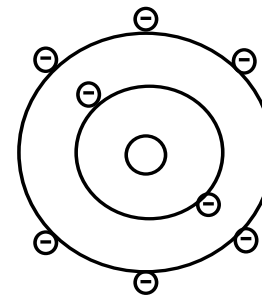
Hydrogen



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## Introduction

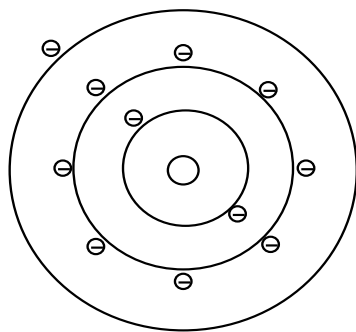
Oxygen



8

## Introduction

Sodium



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## Introduction

Filling orbitals

Inner shell	two electrons
Next two shells	eight electrons in each
Other shells	2 x 18: 2 x 32

10

## Introduction

Element	Electron arrangement
Hydrogen	1
Helium	2
Carbon	2,4
Oxygen	2,6
Neon	2,8
Sodium	2,8,1
Argon	2,8,8
Krypton	2,8,8,18

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## Introduction

✧ Molecule

- Two or more atoms held together strongly enough so as to behave as a unit

✧ Chemical bond

- The force holding any two atoms together

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## Introduction

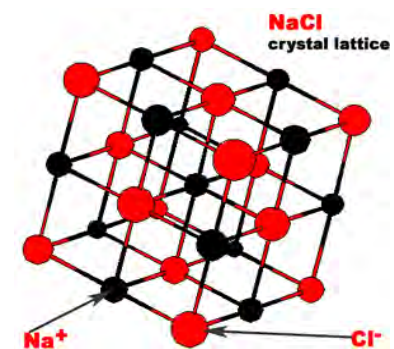
### Ionic/Electrovalent bonding

Sodium atom	2,8,1	Na
Chlorine atom	2,8,7	Cl
Sodium ion	2,8	Na <sup>+</sup>
Chlorine ion	2,8,8	Cl <sup>-</sup>

Sodium chloride Na<sup>+</sup>Cl<sup>-</sup>

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## Introduction



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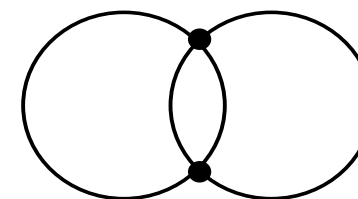
## Introduction

### Covalent bonding

Electrons are neither gained nor lost but shared between two nuclei

15

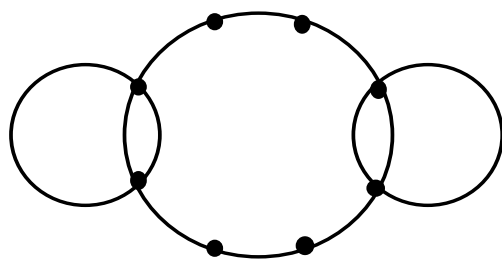
## Covalent bonding



H-H    H<sub>2</sub>    Hydrogen

16

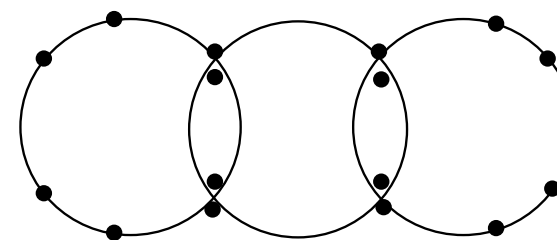
## Covalent bonding



H-O-H    H<sub>2</sub>O    Water

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## Covalent bonding



O=C=O    CO<sub>2</sub>    Carbon dioxide

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## Introduction

Organic chemistry:

The chemistry of living things or things which once lived

19

## Introduction

NaCl

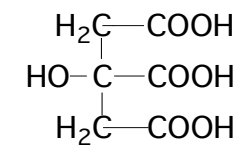
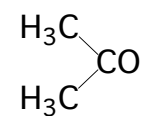
NaOCl

CaCO<sub>3</sub>

C<sub>2</sub>H<sub>5</sub>OH

C<sub>12</sub>H<sub>22</sub>O<sub>11</sub>

CH<sub>3</sub>COOH



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## Introduction

Organic chemistry:

The chemistry of living things or things which once lived

Or...

The chemistry of the compounds of carbon ie any compound based on a carbon skeleton

21

Salt

22

Salt  
Sugar

inorganic

23

Salt  
Sugar  
Bleach

inorganic

organic

24

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	

25

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	

26

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	

27

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	organic
Acetone	

28

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	organic
Acetone	organic
Petrol	

29

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	organic
Acetone	organic
Petrol	organic
Plastics	

30

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	organic
Acetone	organic
Petrol	organic
Plastics	organic
Rust	

31

Salt	inorganic
Sugar	organic
Bleach	inorganic
Chalk	inorganic
Alcohol	organic
Vinegar	organic
Acetone	organic
Petrol	organic
Plastics	organic
Rust	inorganic

32

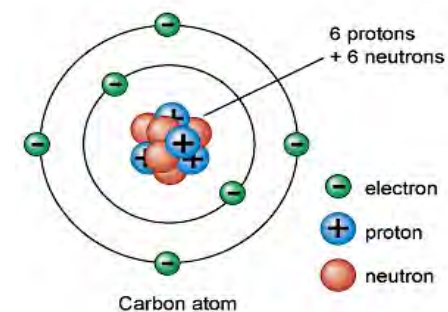


Essential oils are...

# Organic

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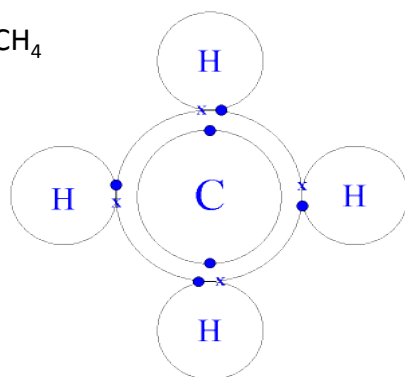
## Organic chemistry



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## Organic chemistry

Methane – CH<sub>4</sub>



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## Organic chemistry

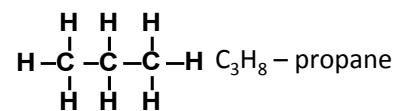
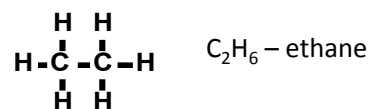
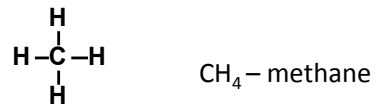
Methane – structure



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## Organic chemistry

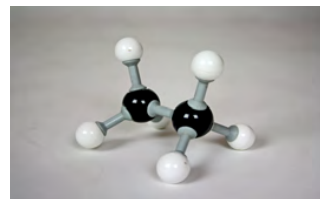
Carbon skeleton



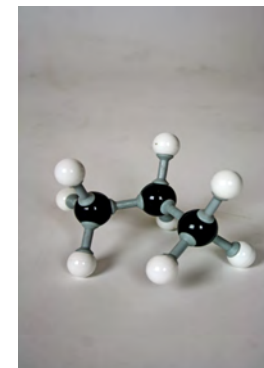
37

## Organic chemistry

Carbon chains



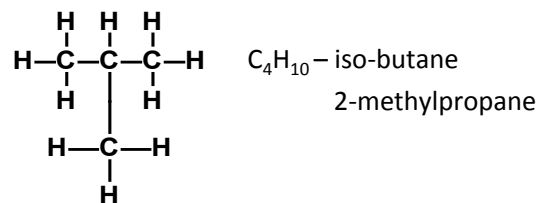
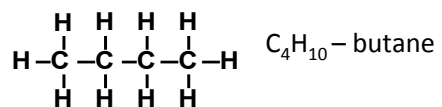
Ethane



Propane

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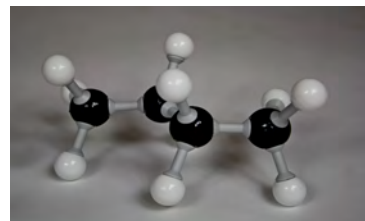
## Organic chemistry



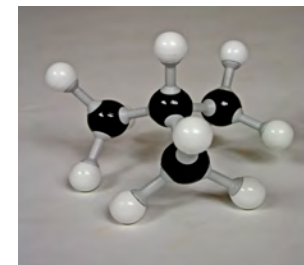
39

## Organic chemistry

Carbon – branched chains



Butane

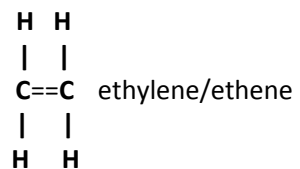
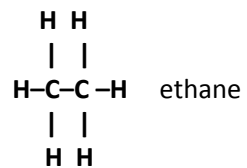


Iso-butane

40

## Organic chemistry

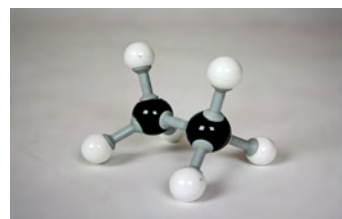
Carbon – double bonds



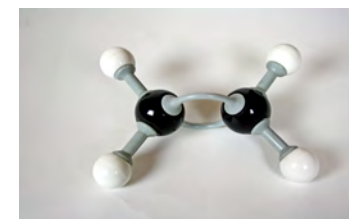
41

## Organic chemistry

Carbon – double bonds



Ethane



Ethylene

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## Organic chemistry

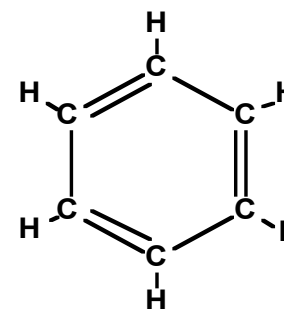
Classification of carbon compounds

Chains – linear or branched → aliphatic

Rings – 6 carbon atoms/3 double bonds → aromatic

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## Organic chemistry



benzene – C<sub>6</sub>H<sub>6</sub>

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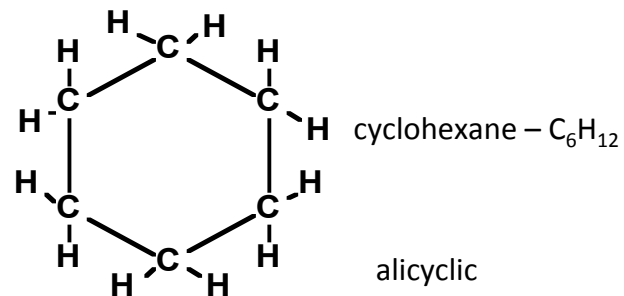
## Organic chemistry

Aromatic nucleus



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## Organic chemistry



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## Organic chemistry

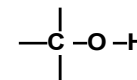
Functional groups

- ✧ A particular atom
- ✧ Or a group of atoms in a particular bonding arrangement
- ✧ Or a type of bond

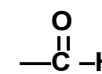
47

## Functional groups

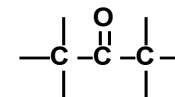
Alcohol/Phenol



Aldehyde



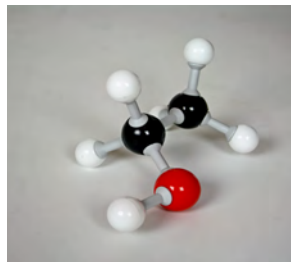
Ketone



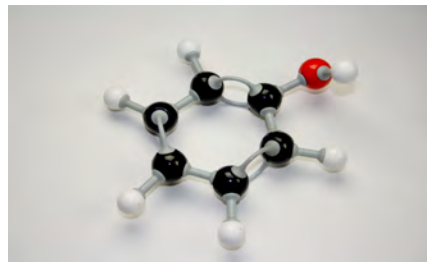
48

## Alcohols/Phenols

Alcohol

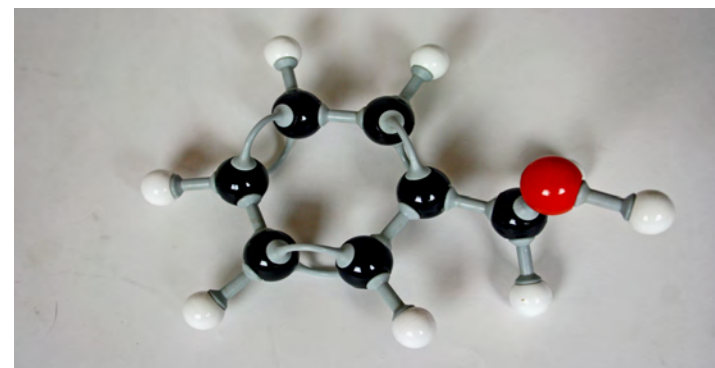


Phenol



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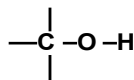
## Alcohol or Phenol?



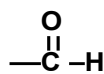
50

## Functional groups

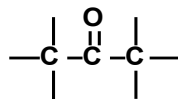
Alcohol/Phenol



Aldehyde



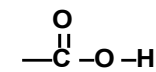
Ketone



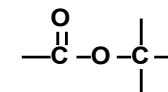
51

## Functional groups

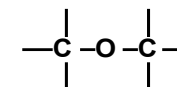
Carboxylic acid



Ester



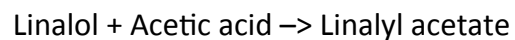
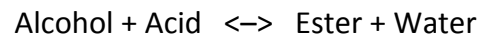
Ether



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## Organic chemistry

### Formation of esters



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## Organic chemistry

### Isomers

#### ✧ Structural

- differ in the order in which atoms are attached to one another ie connectivity

#### ✧ Stereo

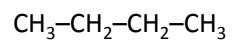
- differ in configuration in space

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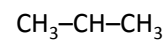
## Structural isomers

### 1. Different carbon structures

$\text{C}_4\text{H}_{10}$  molecular formula



butane



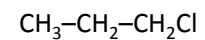
2-methylpropane

55

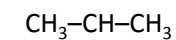
## Structural isomers

### 2. Same arrangement of carbon atoms but functional group in different position

$\text{C}_3\text{H}_7\text{Cl}$  molecular formula



1-chloropropane



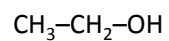
2-chloropropane

56

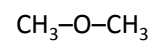
## Structural isomers

### 3. Different functional groups

$C_2H_6O$  molecular formula



ethanol

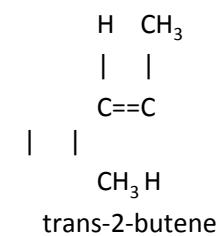
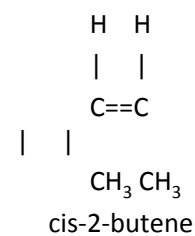


dimethyl ether

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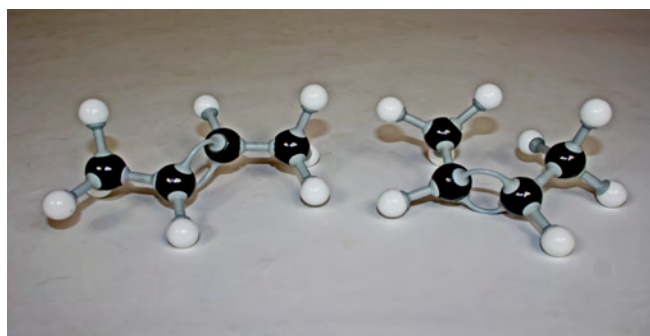
## Stereoisomers

### 1. Geometric – difference relative to a double bond or ring



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## Geometric Isomers



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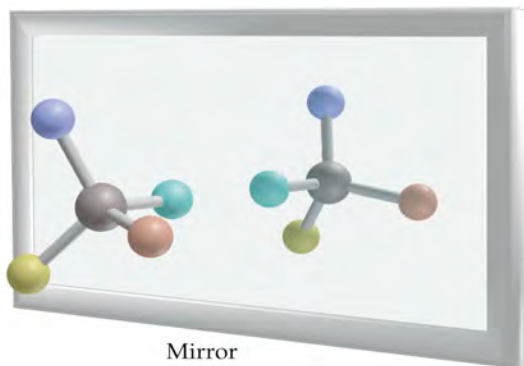
## Stereoisomers

### 2. Optical/Enantiomers

- ✧ Alike in all respects
- ✧ Non-superimposable mirror images
- ✧ Exhibit optical activity

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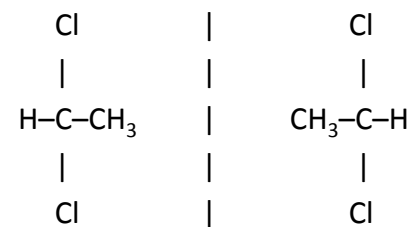
## Mirror Images



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## Stereoisomers

Superimposable mirror images



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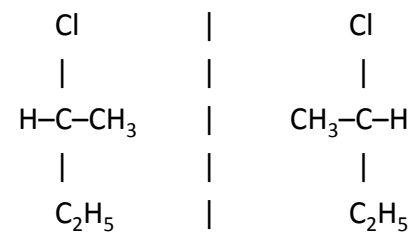
## Superimposable Mirror Images



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## Stereoisomers

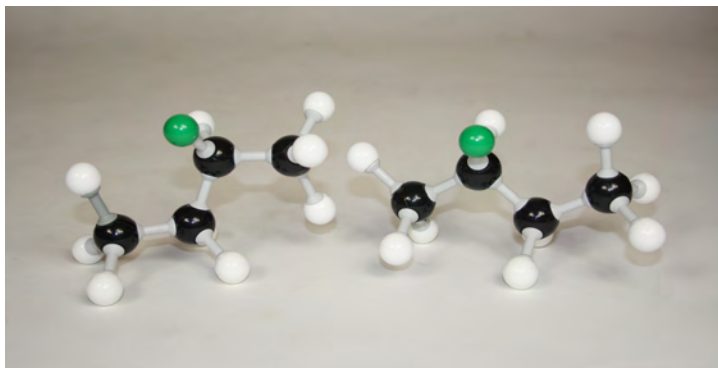
Non-superimposable mirror images



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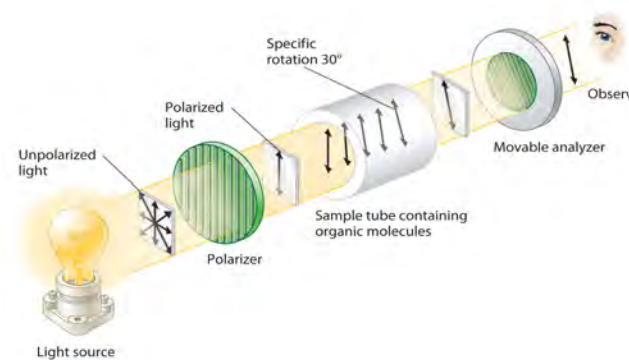


## Non-superimposable Mirror Images



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## Optical rotation



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## Enantiomers

- ✧ Optically active – rotate the plane of plane-polarised light
- ✧ Each enantiomer rotates the light by same amount but in opposite directions
  - Clockwise – indicated by placing (+) or *d*- before name
  - Anticlockwise – indicated by placing (-) or *l*- before name

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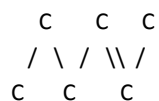
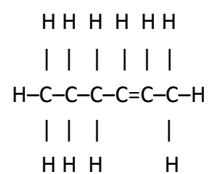
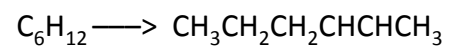
## Enantiomers

As shape is different – odour will be different

<i>d</i> -limonene	citrus essential oils
<i>l</i> -limonene	turpentine
<i>d</i> -carvone	caraway essential oil
<i>l</i> -carvone	spearmint essential oil

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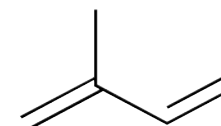
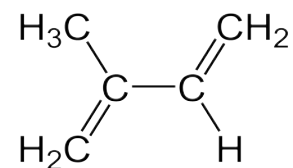
## Structural formulae



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## Terpenes

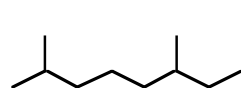
Isoprene



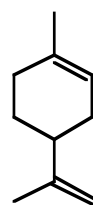
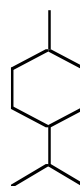
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## Terpenes

Monoterpenes



-α ring structure



limonene

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## Monoterpenes

Limonene	citrus, fennel, pine, neroli
Pinene	pine, lemon, frankincense
Cymene	lemon, thyme, sage, tea tree
Ocimene	basil, sweet marjoram
Myrcene	juniper, black pepper
Camphene	rosemary, citronella, valerian

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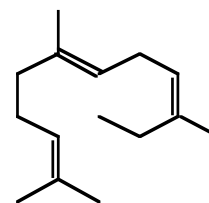
## Monoterpenes

### Properties

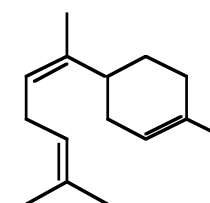
- Antiseptic
- Analgesic – slight
- Expectorant
- Useful for skin hygiene
- *Stimulate adrenal glands*
- ✗ Can be irritating to the skin – especially mucous membrane

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## Sesquiterpenes



Sesquictronellene

 $\alpha$ -bisabolene

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## Sesquiterpenes

$\alpha$ -bisabolene	lemon, black pepper, sandalwood
$\beta$ -caryophellene	black pepper, clove, clove bud
Cadinene	lemongrass, cypress, patchouli
Farnesene	ylang ylang, German chamomile
Aromadendrene	niaouli, tea tree, patchouli
Chamazulene	German chamomile, yarrow

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## Sesquiterpenes

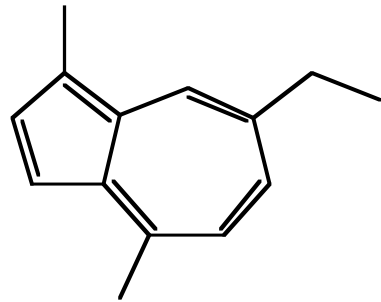
### Properties

- Calming
- Hypotensive – slightly
- Antiseptic
- Antibacterial
- Anti-inflammatory – chamazulene

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## Sesquiterpenes

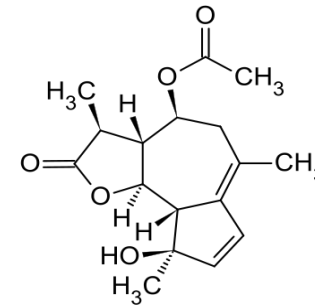
Chamazulene



77

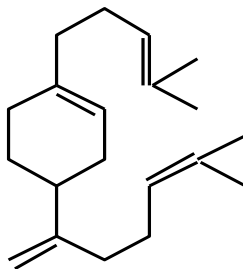
## Sesquiterpenes

Matricin



78

## Diterpenes

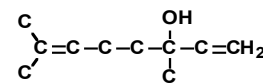


$\alpha$ -camphorene

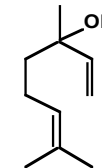
79

## Alcohols

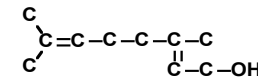
Monoterpenols



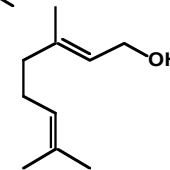
or



linalol



or



geraniol

80

## Monoterpenols

Linalol	lavender, bergamot, coriander
Geraniol	rose, geranium, palmarosa
Borneol	citronella, rosemary, lavandin
Menthol	peppermint, spearmint
Citronellol	citronella, Eucalyptus citriodora
Terpinen-4-ol	tea tree, sweet marjoram, juniper

81

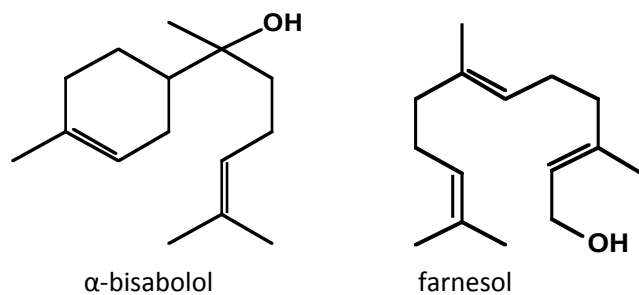
## Monoterpenols

### Properties

- Antiviral
- Antibacterial
- Antifungal
- Uplifting
- Immune system stimulants
- Good general tonic
- ✓ Free from hazard

82

## Sesquiterpenols



83

## Sesquiterpenols

Farnesol	rose, melissa, neroli, lemongrass
$\alpha$ -bisabolol	German chamomile
Santalol	sandalwood
Elemol	elemi, juniper, hyssop, melissa
Viridiflorol	tea tree, cajuput, niaouli, sage
Patchoulol	patchouli

84

## Sesquiterpenols

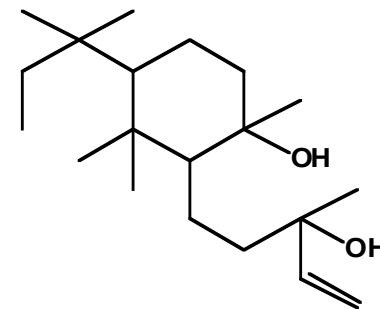
### Properties

- Anti-inflammatory                       $\alpha$ -bisabolol
- Anti-infectious                            santalol (urinary tract)
- Antibacterial                                farnesol (deodorants)
- Tonic
- Liver stimulant
- ✓ Free from hazard

85

## Diterpenols

### Sclareol



86

## Diterpenols

Sclareol	clary sage
Manool	cypress
Abienol	Norway spruce

87

## Diterpenols

### Properties

Said to have structural similarities to human steroid hormones

- Balancing effect on endocrine system?

88

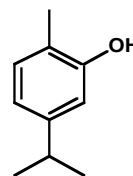
## Alcohols

Non-terpene-derived alcohols also found:

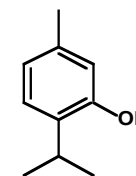
Aliphatic	hexenol – clary sage, lavender octenol – clary sage, hyssop decanol nonanol
Aromatic	benzyl alcohol – ylang ylang, neroli phenylethyl alcohol – rose, neroli

89

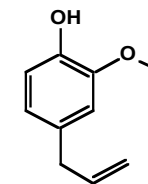
## Phenols



carvacrol



thymol



eugenol

90

## Phenols

Carvacrol	thyme, oregano (green), savory
Thymol	thyme, oregano (green), savory
Eugenol	cinnamon leaf, clove bud, bay (WI)
Cresol	myrrh
Isoeugenol	basil, ylang ylang, clove bud

91

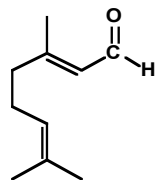
## Phenols

### Properties

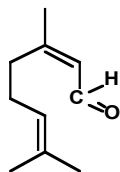
- Antiseptic
- Anti-infectious
- Bactericidal
- Stimulant to immune system
- Stimulant to nervous system
- ✗ Skin/mucous membrane irritants
- ✗ Toxic to the liver

92

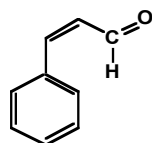
## Aldehydes



geranial



neral



cinnamaldehyde

93

## Aldehydes

Geranial	melissa, lemongrass, verbena
Neral	melissa, lemongrass, verbena
Citronellal	citronella, melissa, E citriodora
Vanillin	benzoin
Cinnamaldehyde	cinnamon bark, cassia
Benzaldehyde	niaouli, cajuput

94

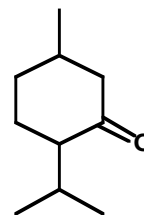
## Aldehydes

### Properties

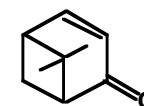
- Anti-inflammatory
- Anti-infectious
- Hypotensive
- Temperature reducing
- Calming to the nervous system
- ✗ Skin irritants
- ✗ Possible skin sensitisers

95

## Ketones



menthone



verbenone

96



## Ketones

Verbenone	rosemary, frankincense
Menthone	peppermint, pennyroyal, spearmint
Carvone	( <i>d</i> -) – dill, caraway: ( <i>l</i> -) – spearmint
Camphor	lavandin, rosemary, sage
Thujone	sage, tansy
Pulegone	pennyroyal

97

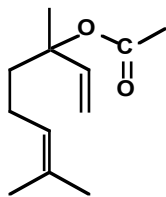
## Ketones

### Properties

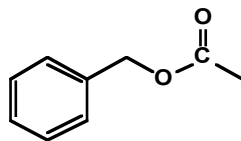
- Mucolytic
- Analgesic
- Calming and sedative
- Encourage wound healing
- ✗ Neurotoxic
- ✗ Abortifacient

98

## Esters



linalyl acetate



benzyl acetate

99

## Esters

Linalyl acetate	lavender, neroli, bergamot
Geranyl acetate	geranium, citronella, petitgrain
Terpinyl acetate	cajuput, niaouli, pine
Citronellyl formate	geranium
Benzyl acetate	jasmine, ylang ylang, neroli
Benzyl benzoate	benzoin, ylang ylang

100

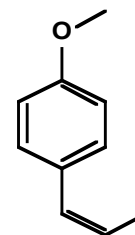
## Esters

### Properties

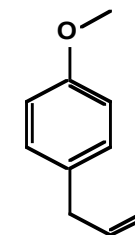
- Antispasmodic
- Anti-inflammatory
- Fungicidal
- Calming and tonic to nervous system
- Effective for skin rashes
- ✓ Gentle in action
- ✓ Free from hazard

101

## Ethers



anethole



estragole

102

## Phenyl ethers

Anethole	fennel, anise
Estragole	basil, fennel, tarragon
Methyl eugenol	nutmeg, tarragon
Elemicin	elemi, nutmeg
Myristicin	nutmeg, parsleyseed
Safrole	cinnamon leaf, ylang ylang, camphor

103

## Phenyl ethers

### Properties

- Antispasmodic
- Expectorant & mucolytic
- Sedative
- Antidepressant
- ✗ Abortifacient
- ✗ Neurotoxic
- ✗ Carcinogenic

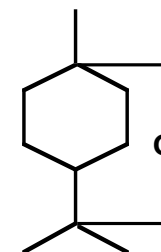
104

## Phenyl ethers

Ether	Essential oil	%
Anethole	fennel	52–86
	anise	80–90
Estragole	basil	5–87
	fennel	2–7
Eugenol	cinnamon leaf	70–90
	clove bud	70–95
Safrole	cinnamon leaf	0.7–1.0
	ylang ylang	0–0.3
	sassafras	85–90

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## Oxides



1,8-cineole

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## 1,8-cineole

Eucalyptus globulus	60–85%
Eucalyptus smithii	70–80%
Eucalyptus radiata	62–72%
Rosemary	30–55%
Spanish marjoram	41–75%
Tea tree	0.5–18%
Cajeput	50–75%
Niaouli	38–65%

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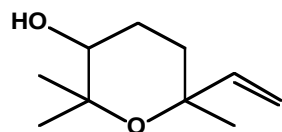
## 1,8-cineole

### Properties

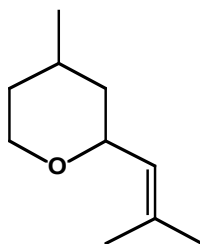
- Mucolytic
- Expectorant
- ✗ Skin irritant

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## Oxides



linalol oxide



rose oxide

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## Lactones

Alantolcatone

elecampane

Bergapten

bergamot, lime, lemon

Costuslactone

costus

Coumarin

hay, lavender

Bergamottin

bergamot, lemon

Umbelliferone

dill, fennel, lavender

110

## Lactones

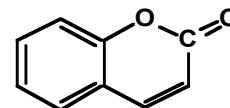
### Properties

- Mucolytic & expectorant
- Temperature reducing
- Sedative
- Hypotensive
- Anticoagulant

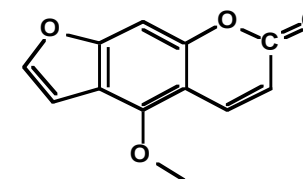
✗ Photosensitisers

111

## Coumarins



coumarin



bergapten

112

### Coumarins

Bergapten	bergamot	0.3–0.4%
	lime	0.1–0.3%
	lemon	0.15–0.25%
	orange	0.069–0.073%
	grapefruit	0.012–0.013%
Coumarin	lavender	0.04%

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### Essential Chemistry

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