INTERNATIONAL COLLEGE OF PHARMACEUTICAL INNOVATION
国际创新药学院

Fundamentals of Medicinal and Pharmaceutical Chemistry

FUNCHEM.13 Introduction to Organic Chemistry I
functional groups, isomers (geometric structural & optical)

Professor Dan Wu

DATE: 6th November 2024

Learning outcomes

At the end of this lecture, the learner will be able to

- Identify the following functional groups (alkane, alkene, alkyne, alcohol, thiol, ether, sulphide, aldehyde, ketone, carboxylic acid, amine, amide, ester, acid halide, aromatic).
- Identify and describe aliphatic and aromatic hydrocarbons.
- Describe and identify examples of structural, geometric and optical isomers.
- Interpret and construct Lewis structures, condensed structures and line structures of organic compounds.
- Identify and describe structural geometry and bonding present in organic compounds according to valence bond theory.
- Compare properties of organic and inorganic compounds.

Recommended reading

- Organic chemistry with biological application (John McMurry)
- Chapter 3, section 3.1 Functional groups
- Chapter 6: an overview of organic reactions

Introduction

What is organic chemistry about?

'The Chemistry of Carbon Compounds'

Carbon Compounds:

Provides Constituents of Living Matter, e.g. DNA, Proteins, Carbohydrates

Provides Energy by Conversion to CO_2

Gasoline, Oil as an Industrial Feedstock etc etc….

Why Carbon?

Less than 1% of the earth's crust! ….compare with Si (~28%), O (~50%), Fe (5%)

Ability to form chains of atoms — linear, branched & cyclic

Combines with H, N, O (98% of living tissue is derived from these 4 elements)

Enormous variety of structures available (3-dimensional)

Introduction

Organic Compounds:

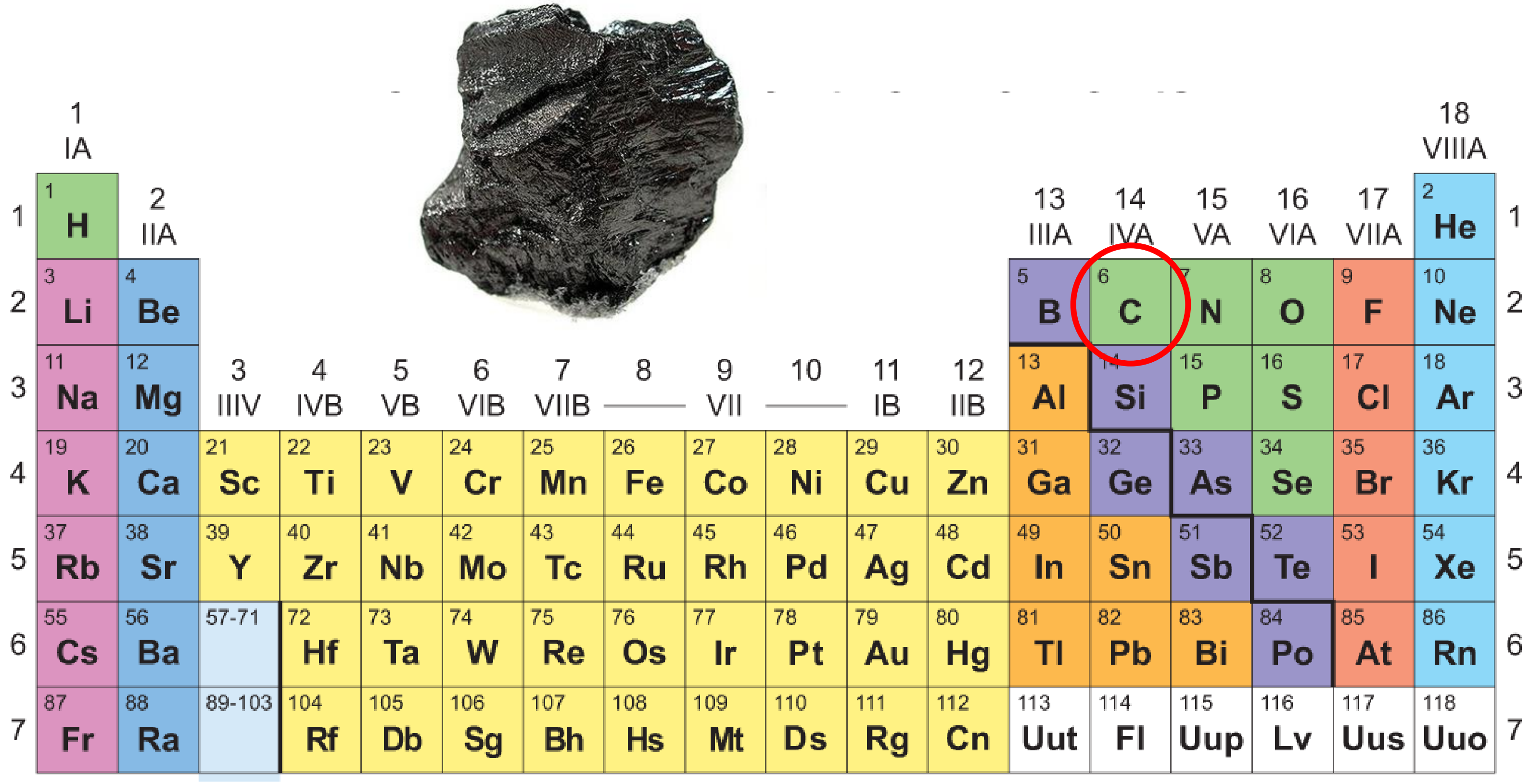
Compounds made of carbon atoms covalently bonded to each other and to other non-metal atoms, such as H, O, N, S and halogens.

(All other compounds are inorganic compounds).

Organic Chemistry:
The study of the structures, properties and syntheses of organic compounds.

Organic Molecules	Inorganic Molecules
a. Covalent bonds	a. Ionic bonds
b. Usually are poorly soluble in water	b. Usually are very soluble in water
c. Relatively low melting and boiling points	c. Relatively high melting and boiling points

Carbon



Group 4 element

Can share 4 valence electrons

Can form 4 strong covalent bonds

Carbon Summary

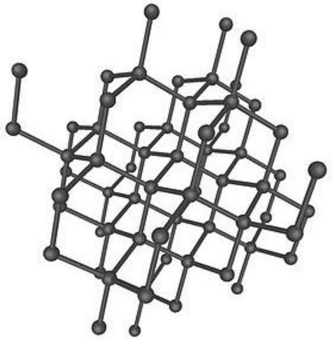
Atomic number = 6

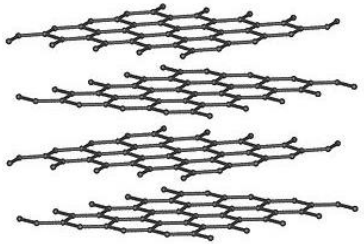
Has 6 electrons to be divided into shells (and corresponding orbitals)

Lowest energy electron configuration: $1s^2\ 2s^2\ 2p_x^{\ 1}\ 2p_y^{\ 1}$

Four valence electrons (the electrons in the outermost shell)

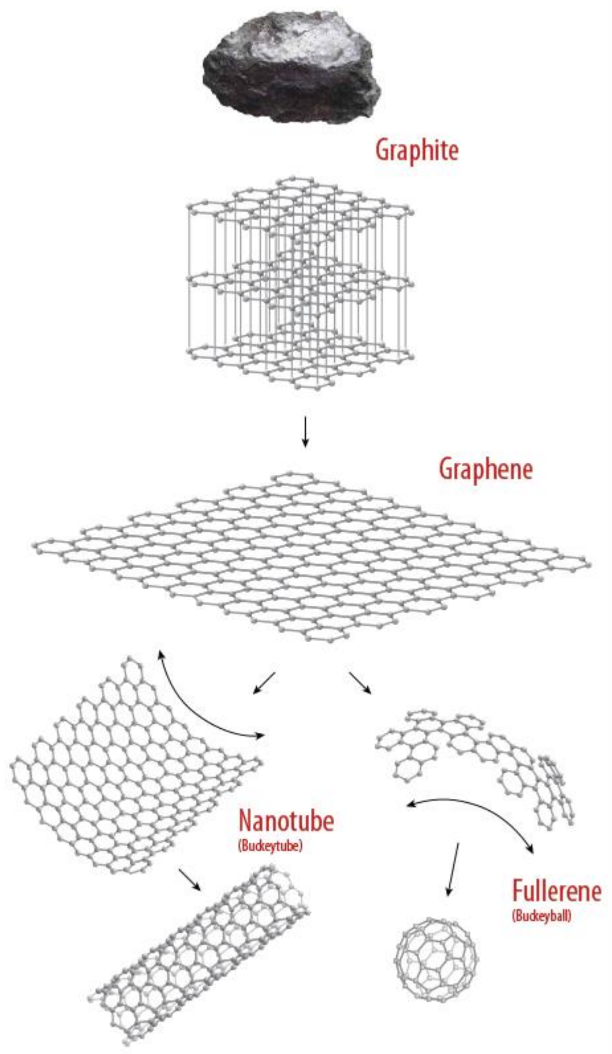
Neither strongly electropositive nor strongly electronegative with an electronegativity value of 2.5

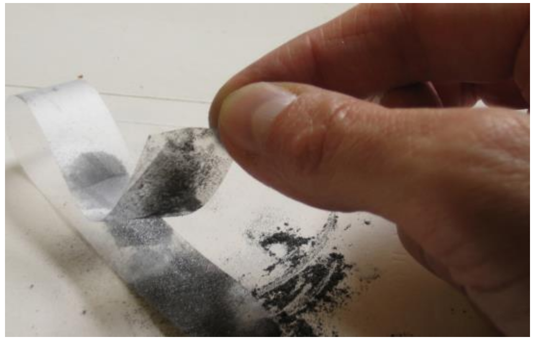




Graphene

Andre Geim and Konstantin Novoselov, 2010 Nobel Laureates in Physics





Graphene's properties are contradictory it is flexible like plastic but is stronger than diamond; it conducts electricity like a metal but is transparent to light like glass.

See: http://www.newdestinymining.com/?attachment_id=206

Covalent Bonding

Atoms approach each other in such a way that their atomic orbitals can *overlap* to form a bond.

Sigma (σ) Bond

A sigma (σ) bond is a covalent bond formed by head-on overlap of two atomic (sp^3 hybrid) orbitals on adjacent atoms

pi (π) Bond

A pi (π) bond is a covalent bond formed by sideways overlap of two atomic (p) orbitals on adjacent atoms

e.g. carbon-carbon double bonds contain one sigma bond and one pi bond

A pi bond can only form after a sigma bond has already formed. It is always part of a double or triple bond.

Reminder

An orbital is a region of space around the nucleus where electrons are located

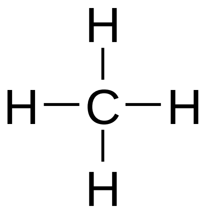
Covalent Bonding

A covalent bond is the interaction that arises from sharing a pair of valence electrons between two adjacent atoms

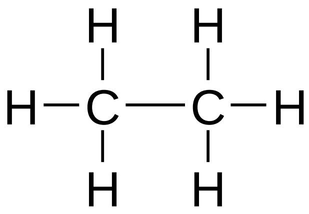
Symbolised by a line connecting the two atoms e.g. H–H

A covalent bond generally represents a stabilisation of the molecule relative to the separated atoms

By sharing electrons each atom can achieve a stable octet configuration analogous to that of the noble gases

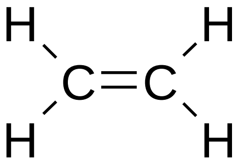


Methane



Ethane

Two atoms may share more than one pair of electrons with each other to give multiple bonds



Ethene

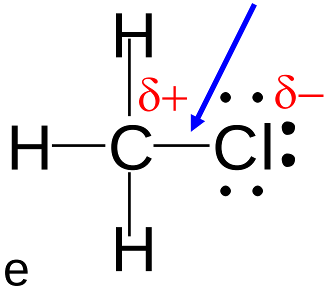
Ethyne

Covalent Bonding

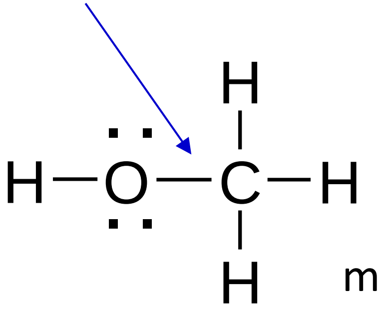
Polar covalent bond:
a covalent bond where electron pair is not shared equally between the atoms

Electronegativity:
is a measure of the tendency of an atom to attract a bonding pair of electrons

Polar Covalent Bond



chloromethane



methanol

Electronegativity values
C = 2.5
Cl = 3.1

Electronegativity values
C = 2.5
O = 3.5

Electronegativity determines bond polarization
(unequal sharing of electrons in covalent bond).

Note: C (2.5) and H (2.2) have very close electronegativity values.

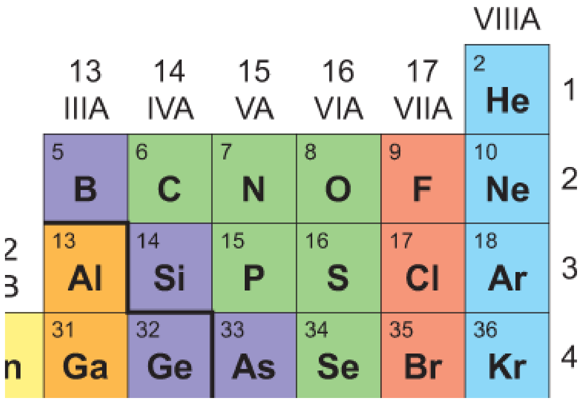
Covalent Bonding

From left to right within a given period in periodic table, the elements become *more* electronegative, owing to increasing charge on the nucleus;

From top to bottom of the table within a given group, the elements become *less* electronegative because the valence electrons are shielded from the nucleus by an increasing number of inner-shell electrons.

Biologically relevant examples:

$\overset{\delta+}{C}-\overset{\delta-}{N}$ $\overset{\delta+}{C}-\overset{\delta-}{O}$ $\overset{\delta+}{H}-\overset{\delta-}{O}$ $\overset{\delta+}{C}-\overset{\delta-}{Cl}$ $\overset{\delta+}{C}-\overset{\delta-}{F}$



δ+ is partial positive charge; δ- is partial negative charge

Lewis Structures

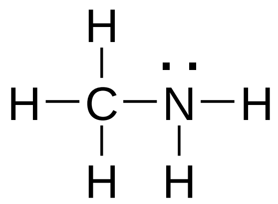
Gilbert N. Lewis 1916

Lewis symbolism for the illustration of molecular structures

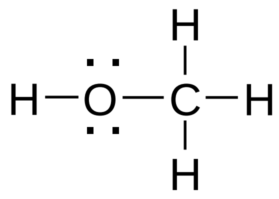
Every valence electron must be shown

Valence electrons in covalent bonds (single, double or triple) are symbolised by one or more lines between atoms

Unshared valence electrons are symbolised as dots on the atoms to which they belong



Methylamine



Methanol

Unshared electrons that are paired are called lone pairs.

Note: when lone pairs are not shown they are understood to be present

Organic Molecules

Carbon and other common elements including

hydrogen, oxygen, nitrogen, sulphur and halogens

A functional group is an atom or group of atoms within a molecule that

shows a characteristic set of physical and chemical properties

The chemical reactivity of every organic molecule, regardless of complexity

or size, is determined by the functional groups it contains

Hydrocarbons

A hydrocarbon is a compound which contains only carbon and hydrogen

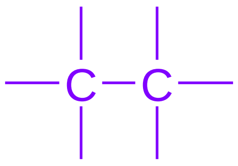
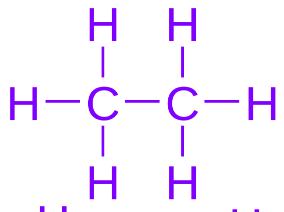
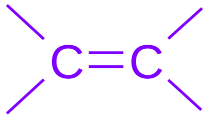
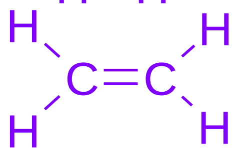
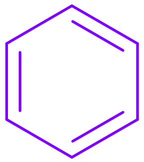
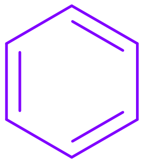
An aliphatic hydrocarbon is a non-aromatic hydrocarbon

Classification of Organic Compounds

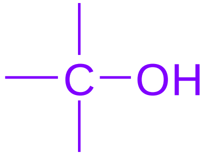
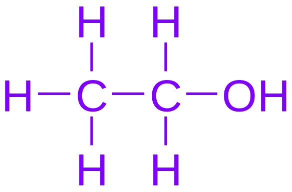
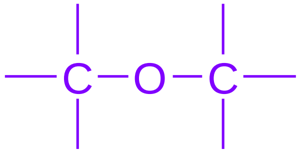
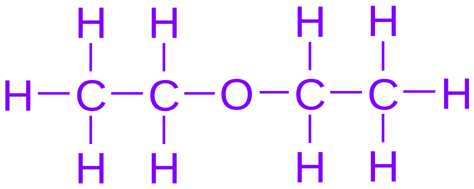
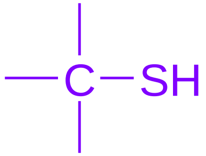
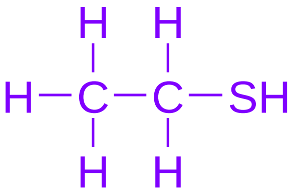
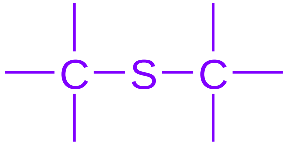
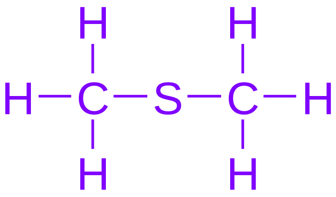
Functional groups are groups of atoms that have characteristic chemical properties regardless of the molecular framework to which they are attached

Molecules containing only carbon and hydrogen atoms are called hydrocarbons

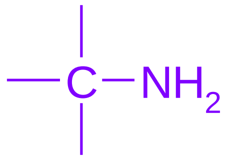
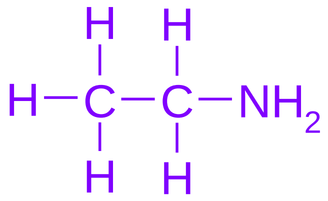
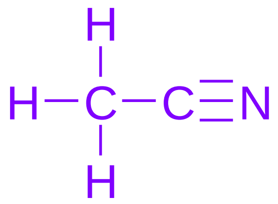
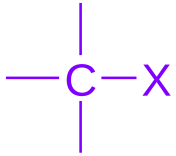
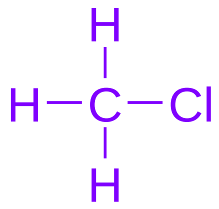
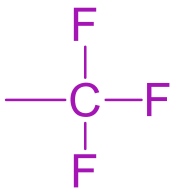
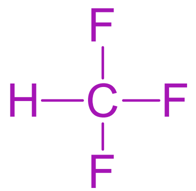
Functional Groups

Structure	Family Name	Simple Example	
	Alkane (contains only C-H & C-C bonds)		ethane
	Alkene		ethene (ethylene)
	Alkyne		ethyne (acetylene)
	Aromatic		benzene

Functional Groups

Structure	Family Name	Simple Example
	Alcohol	 ethanol
	Ether	 diethyl ether
	Thiol	 ethane thiol
	Sulfide (*or* thioether)	 dimethyl sulfide

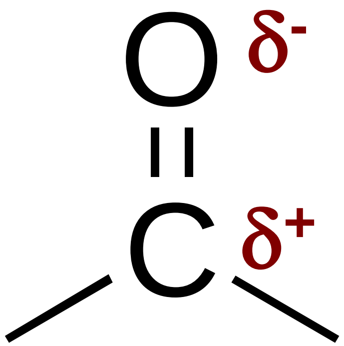
Functional Groups

Structure	Family Name	Simple Example	
	Amine		ethylamine
	Nitrile		acetonitrile
 (X = Cl, Br, or I)	Halide		chloromethane
	Trifluoromethyl		trifluoromethane

Carbonyl Functional Groups

The most important functional group in organic chemistry

Polarised covalent carbon – oxygen double bond



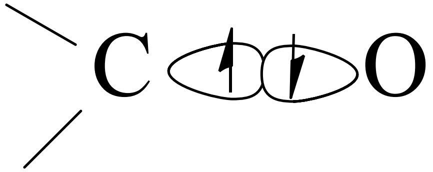
Electronegativity values
C = 2.5
O = 3.5

There are many different types of carbonyl compounds

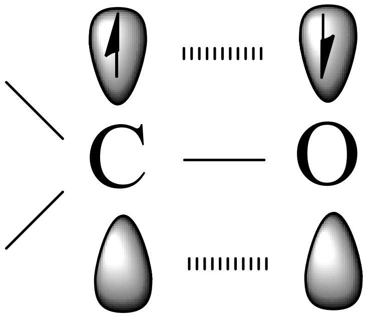
Covalent Bonding of the Carbonyl Group

The carbon-oxygen double bond consists of one sigma (δ) and one π bond.

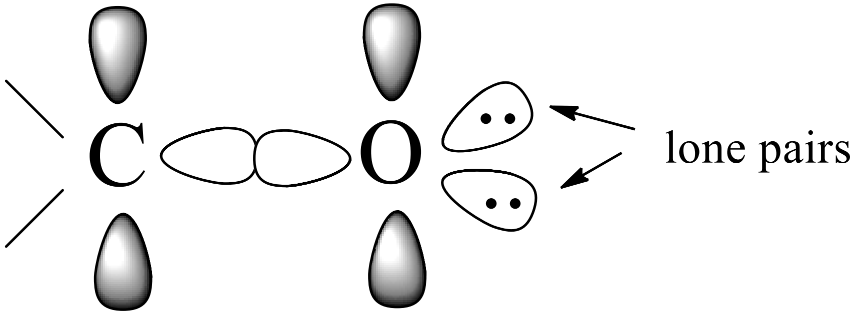
Sigma bond (δ):
Overlap of sp^2 orbital on carbon
and sp^2 orbital on oxygen



π bond:
Overlap of p-orbital on carbon
and p-orbital on oxygen

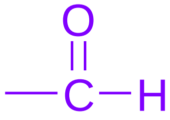
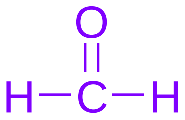
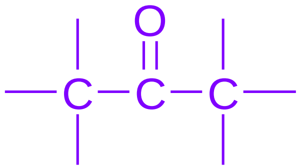
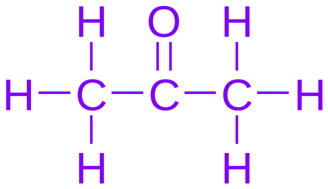
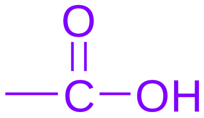
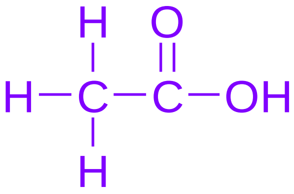
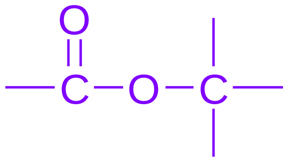
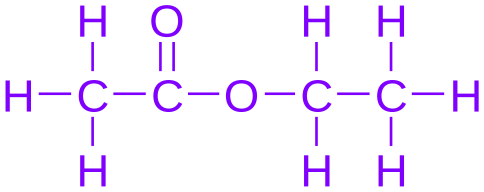


Overall bonding picture

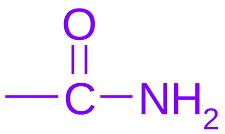
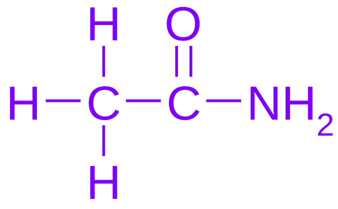
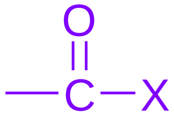
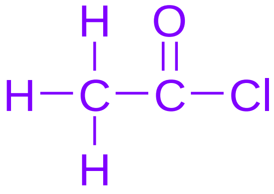
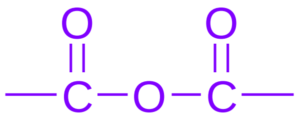
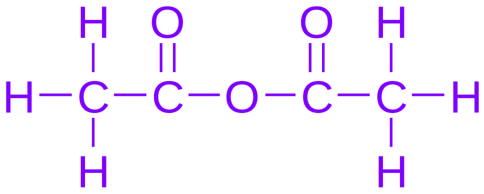
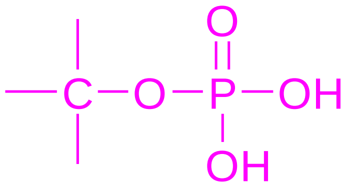
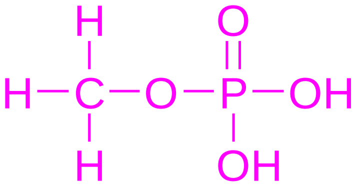


The oxygen atom also has two nonbonding pairs of electrons,
which occupy its remaining two orbitals

Functional Groups: Carbonyls

Structure	Family Name	Simple Example
	Aldehyde	 formaldehyde
	Ketone	 propan-2-one (acetone)
	Carboxylic acid	 ethanoic acid (acetic acid)
	Ester	 ethyl acetate

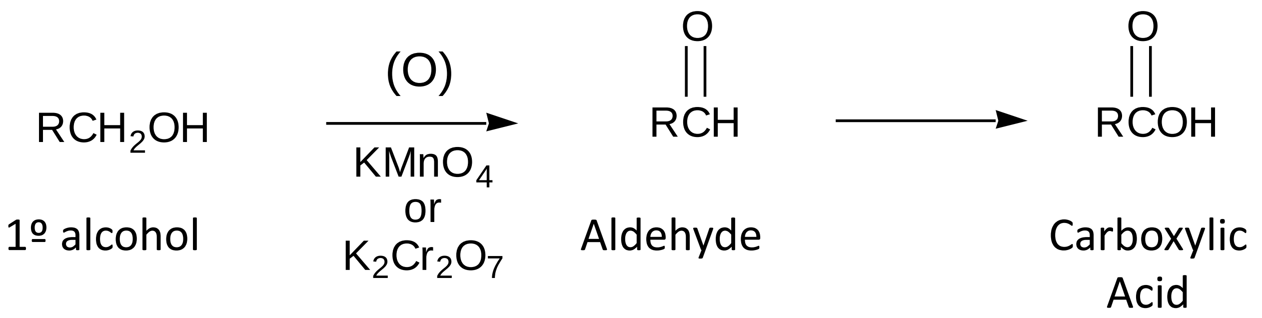
Functional Groups: Carbonyls

Structure	Family Name	Simple Example	
	Amide		acetamide
	Acyl halide (X = Cl or Br)		acetyl chloride
	Carboxylic acid anhydride		acetic anhydride
	Ester of Phosphoric Acid		methyl monophosphate

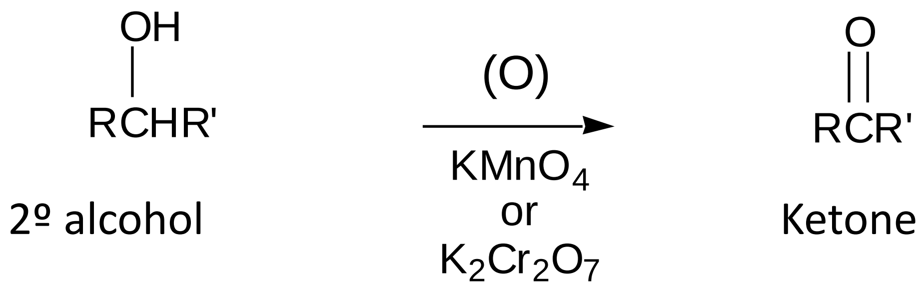
Functional Group Inter-conversion

e.g. alcohols

1º alcohols are oxidised first to aldehydes and, if sufficient oxidising agent, they are further oxidised to carboxylic acids.

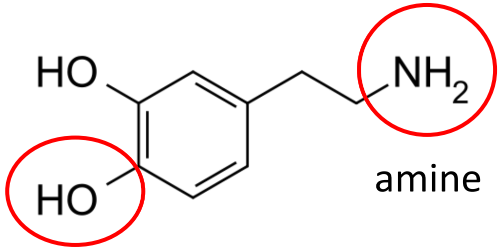


2º alcohols are oxidised to ketones and no further.



Note: the symbol for oxidation is (O)

Identify the Functional Groups

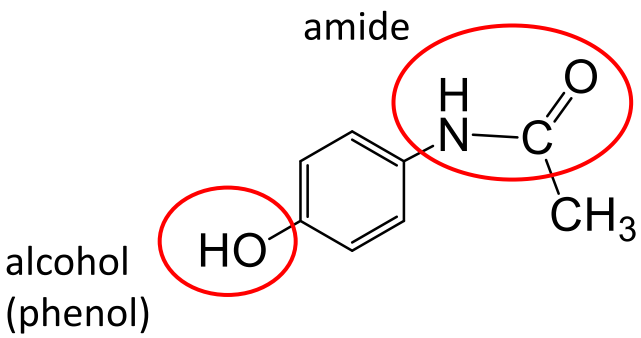


amine

alcohol
(phenol)

Dopamine

Identify the Functional Groups



Paracetamol

Practice Example

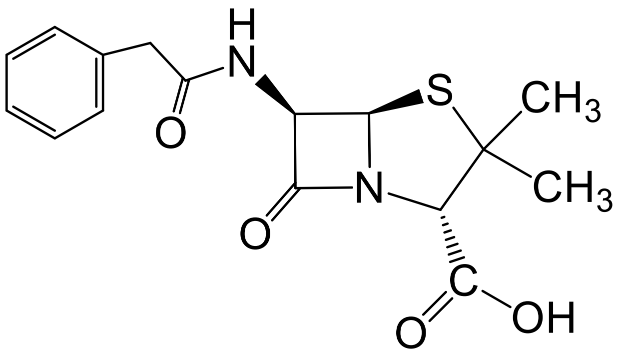
Penicillin G is a commonly use antibiotic, its structure is given below

a) Identify and name four of the functional group in penicillin

b) Redraw the structure, adding all unshared electron pairs

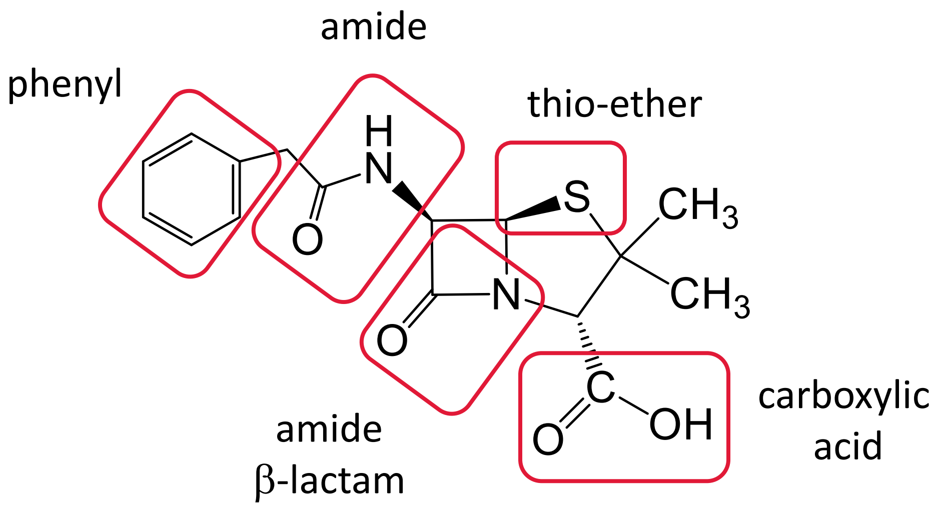
c) What is the molecular formula of penicillin ?

d) Identify the most polarised covalent bonds

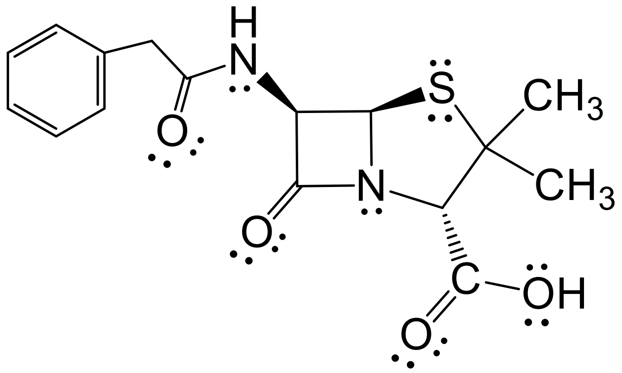


Example Answers

Functional Groups



Unshared electron pairs



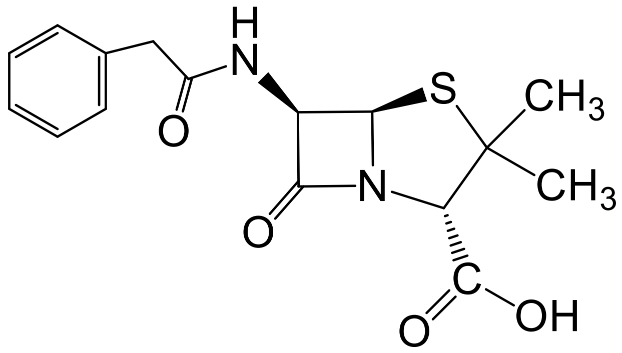
Molecular formula: $C_{16}H_{18}N_2O_4S$

Most polarised covalent bond are the C=O

Approach to Question Answering

b) Redraw the structure, adding all unshared electron pairs

memorise or understand ???



What do you need to understand ? (so you don't have to memorise)

What atoms have unshared electron pairs?

Oxygen has two sets of unshared electron pairs

Nitrogen has one set of unshared electron pairs

Sulphur has two sets of unshared electron pairs

Keep Up With Your Chemistry Studies !

Thank you

FOR MORE INFORMATION PLEASE CONTACT

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