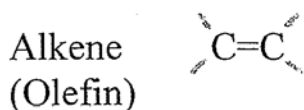


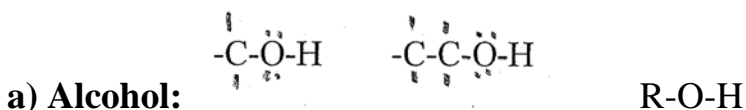
1.7 FUNCTIONAL GROUPS

Certain combinations of bonds show up repeatedly in organic chemistry and organic chemists give those bonding combinations specific names. It is very useful to know the names of those specific types of bonds. Examples are shown below and you should make flash cards and learn them by heart. There can be (and frequently are) multiple functional groups in one organic molecule.

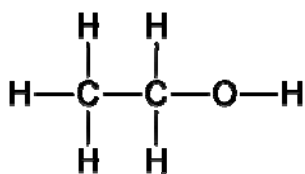
1.61 Functional groups containing only C atoms:



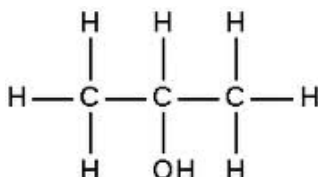
1.62 Functional groups containing one (or more) single bonded O atoms



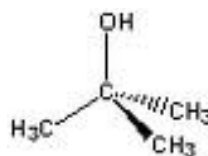
We can write a more generalized formula for a molecule with an alcohol functional group as R-O-H where R is the symbol organic chemists commonly use to indicate a C chain without specifying the exact length. Alcohols are often labeled more specifically based on the number of C atoms bonded to the C with the O-H.



Primary alcohol



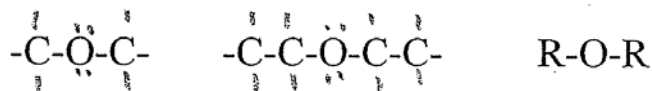
Secondary alcohol



Tertiary alcohol

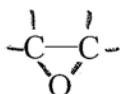
Primary alcohols have 1 C bonded to the C with the OH group. Secondary alcohols have 2 C atoms bonded to the C with the OH. Tertiary alcohols have 3 C atoms bonded to the C atom with the OH.

b) Ether:



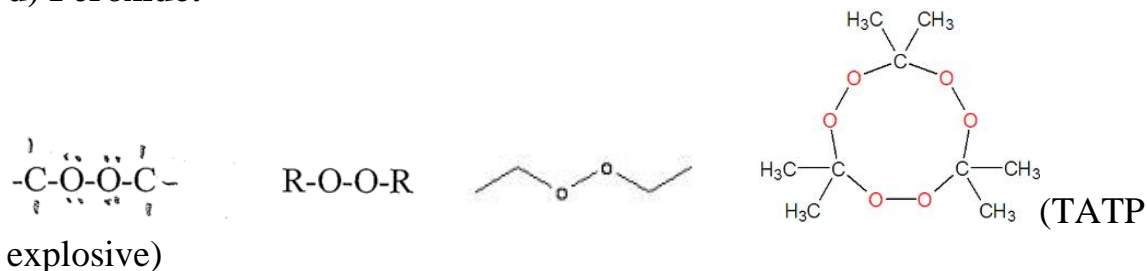
We might also write $\text{R}_1-\text{O}-\text{R}_2$ to indicate that R_1 and R_2 are not the same

c) Epoxide:

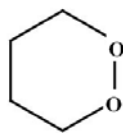
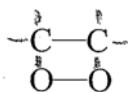


An epoxide is a special type of ether functional group in a 3-membered ring.

d) Peroxide:

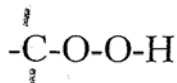


e) Endoperoxide:

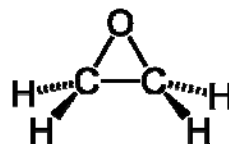
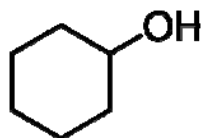
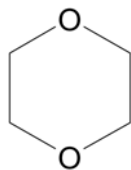
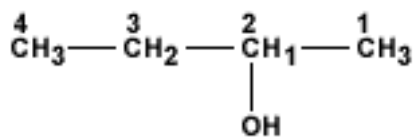
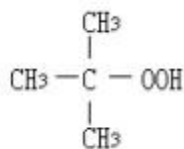
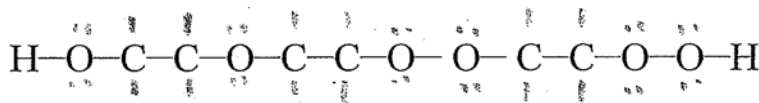
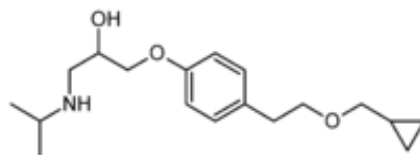
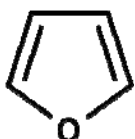
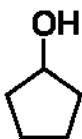
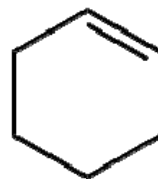
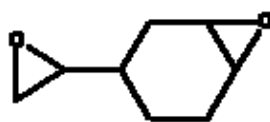
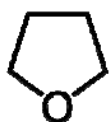
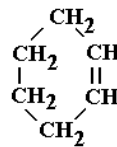
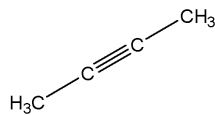
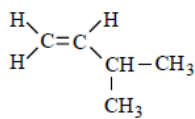
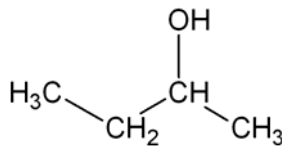
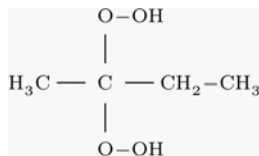
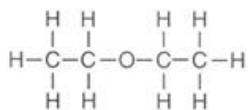


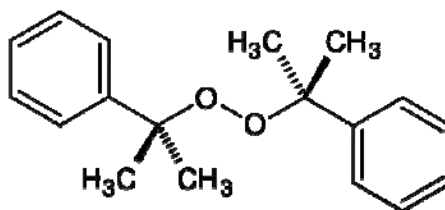
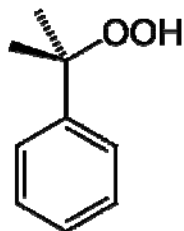
A peroxide group within a ring is called an endoperoxide.

f) Hydroperoxide:

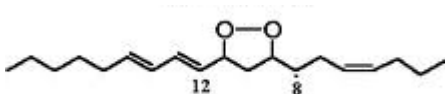
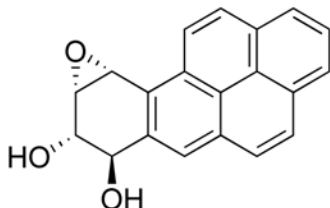


Circle and label the functional groups in the following molecules:





(6-membered rings containing 3 alternating double bonds are very common in organic chemistry and are called benzene rings.)



In the above structure explain the significance of the wedges and dashes.

1.63 Functional groups containing a C=O (carbonyl) group

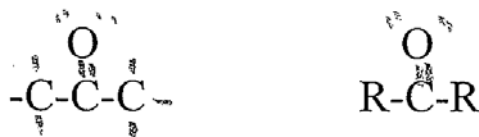
1) An **aldehyde** has a **carbonyl group (C=O)** bonded to (at least) one H atom, as shown below

Aldehyde:

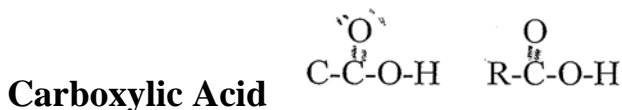


2) In a **ketone** the two additional bonds of the C of the **carbonyl group (C=O)** are both bonded to C atoms

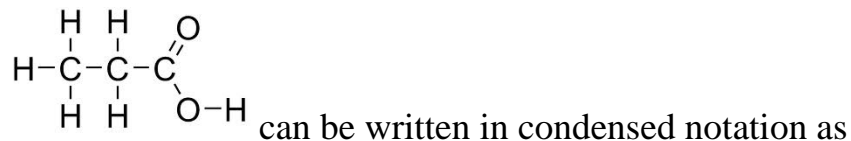
Ketone:



3) A **carboxylic acid** has the C atom of the **carbonyl group (C=O)** bonded to an OH group, as shown below. Even though you would be tempted to label the OH on the carbonyl group as an alcohol, the presence of the C=O completely changes the chemical properties of the OH and it does not have the properties of an alcohol group and is not labeled as such.



The carboxylic acid group is often abbreviated COOH or CO₂H when shorthand notation is being used. Example:

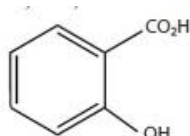


CH₃CH₂COOH or CH₃CH₂CO₂H. One has to be careful not to confuse this shorthand notation with a hydroperoxide group, which would have the shorthand notation: CH₃CH₂CH₂OOH. Note the extra H₂ in the formula.

Examples:

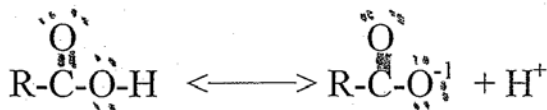


has a carboxylic acid group, not a hydroperoxide group, because there are not 2 H atoms on the C of the COOH.



In the CO₂H group is a carboxylic acid group, not a hydroperoxide group, which would be abbreviated CH₂OOH.

By definition, an acid is a substance which produces H⁺. Carboxylic acids produce H⁺ ions by ionizing the H on the carboxylic acid group.



The resulting negative ion is called a **carboxylate ion**. The dissociation of the carboxylic acid is reversible and so carboxylic acids are **weak acids**.

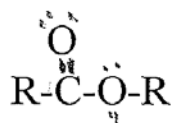
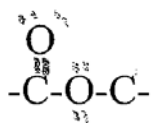


The carboxylate ion structure is often condensed to COO⁻¹ or CO₂⁻¹.

Example: CH₃(CH₂)₄COO⁻¹ or (CH₂)₄CO₂⁻¹.

When a C=O is covalently bonded to an O-C linkage, it is called an **ester** functional group. Examples

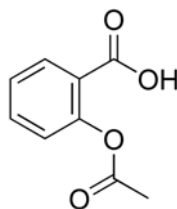
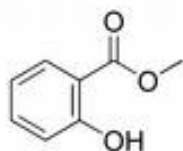
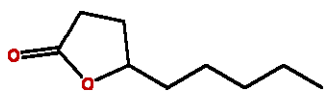
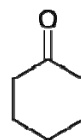
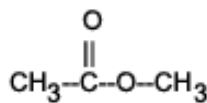
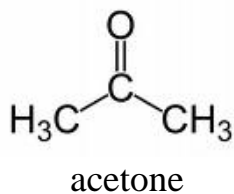
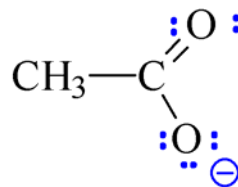
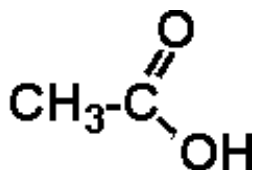
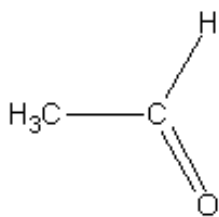
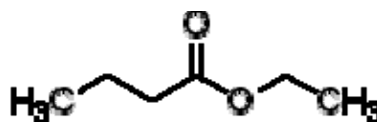
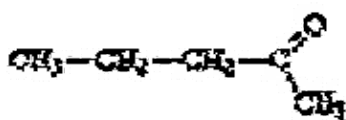
5) Ester:



In shorthand notation esters may be abbreviated COOC, although this can easily be confused with a peroxide bond. Usually keeping track of the number of bonds and H atoms on each C will help you tell the difference.

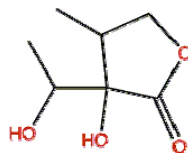
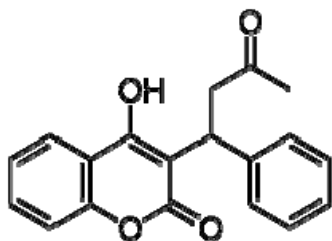
CH₃COOCH₃ is an ester. CH₃CH₂OOCH₃ is a peroxide.

Identify the functional groups in the following molecules:

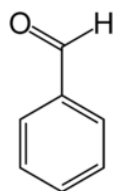
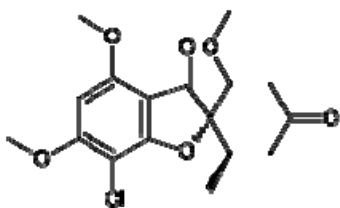


wintergreen

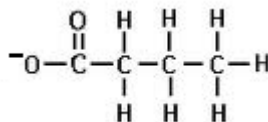
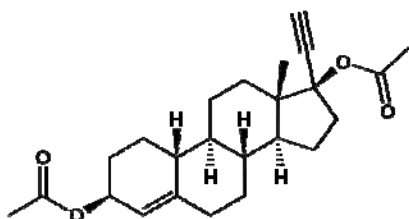
aspirin



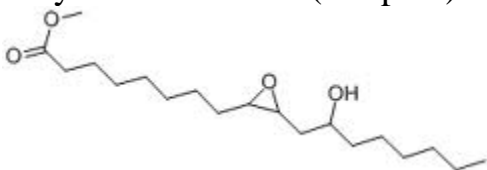
Warfarin(Coumadin), structure shown above on left, is a very commonly used anticoagulant



Griseofulvin



Ethynodiol diacetate(BC pills)



1.64 Compounds with S atoms:

a)Sulphydryl



Sulphydryl groups are also sometimes referred to as thiol or mercaptan groups.

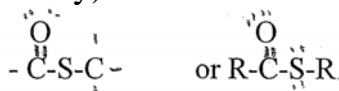
Sulfide(do not confuse with the inorganic sulfide ion S⁻²)



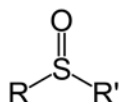
Disulfide:



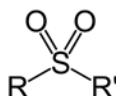
Thioester: (notice similarity to regular ester; important in metabolic biochemistry)



Sulfoxide:

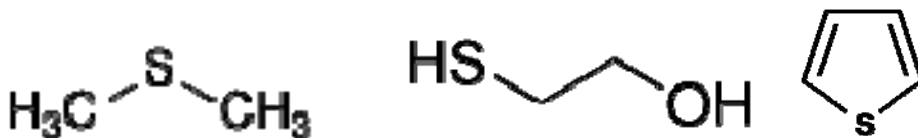


Sulfone:

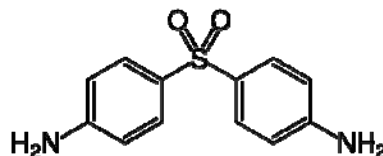
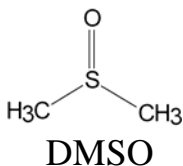
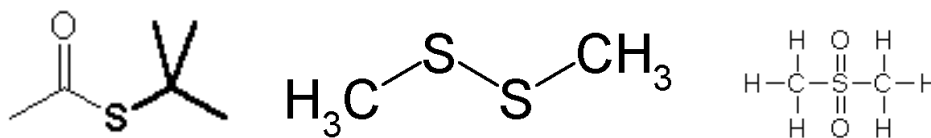


Note that in sulfoxides and sulfones, the S atom has more than 2 bonds.

Identify the functional groups in the structures shown below:



(cooked cabbage smell)



dapsone (antibiotic for leprosy and other conditions)

1.65 Functional groups containing N

1) Amines are molecules in which a N is single bonded to one or more C atoms. Their chemistry is similar to that of ammonia, NH₃, except that there are one or more C atoms bonded to the N atom.

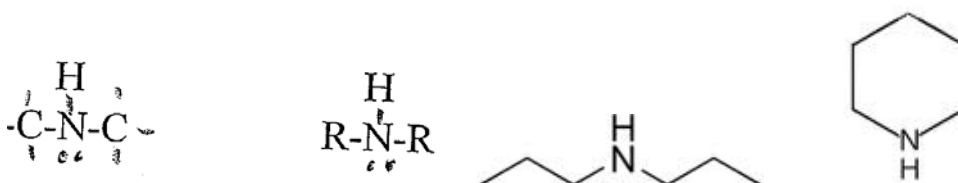
a) A **primary amine** is a functional group that has a N atom with one C atom bonded to it by a single bond.

Primary amine



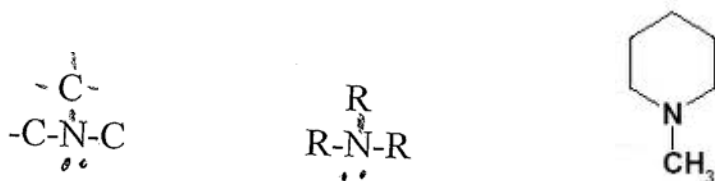
b) A **secondary amine** is a N atom that has two C atoms bonded to it by single bonds.

Secondary amine



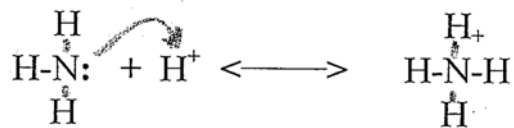
c) A **tertiary amine** is a N atom that has three C atoms bonded to it by single bonds.

Tertiary amine



2) Ammonium ions

The non-bonding pair of electrons in **ammonia** (NH₃) can react with a H⁺ (from an acid such as HCl) to form an **ammonium** ion, NH₄⁺.

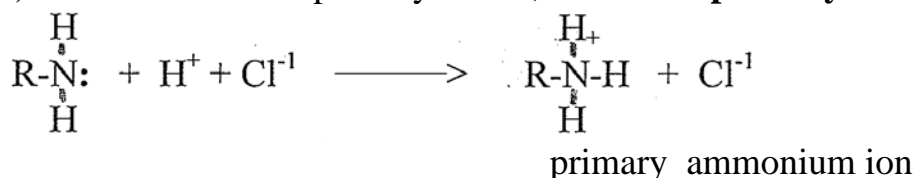


This reaction can occur because the H⁺ needs a pair of electrons to have a full n=1 shell and the N atom has a pair of electrons which it is not sharing (a non-bonding pair of electrons). When the neutral NH₃ combines with the positively charged H⁺, the resulting ammonium ion has a positive charge. (Another way of looking at it: when the N atom shares the fourth pair of

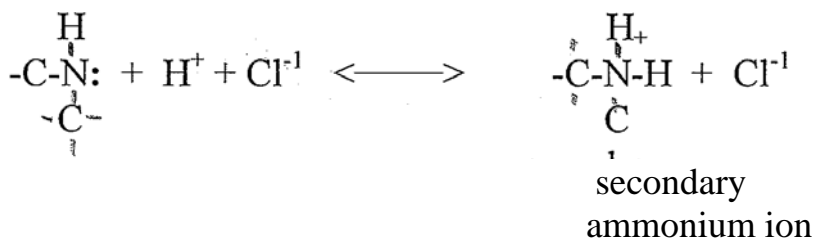
electrons, it is sharing more electrons than normal and this is equivalent to giving one electron away, putting a positive charge on the N atom.)

A very similar reaction occurs if we add an acid (containing H^+) to an amine the non-bonding pair of electrons of the N can bond to the H^+ and we can form an alkyl **ammonium ion**.

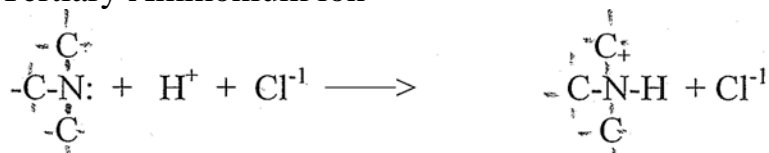
a) If we add acid to a primary amine, we form a **primary ammonium ion**.



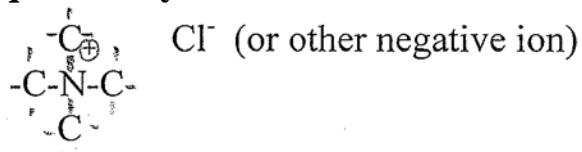
b) We can add acid to a secondary amine and form a **secondary ammonium ion**:



c) We can add acid to a tertiary amine and form a **tertiary ammonium ion**:
Tertiary Ammonium ion

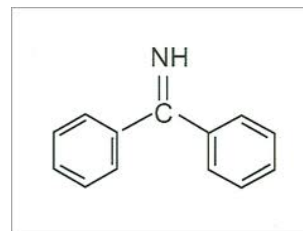
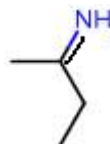
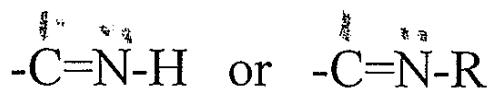


d) We can also have a N atom with 4 C atoms bonded to it, which is called a **quaternary ammonium ion**.



3) Imines

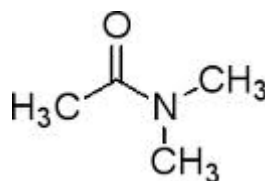
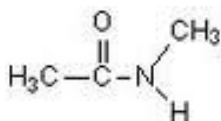
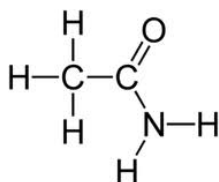
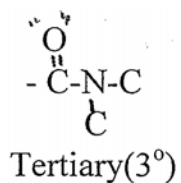
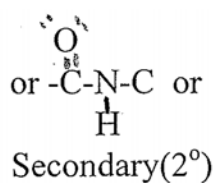
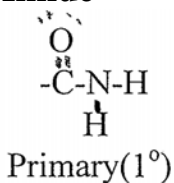
A N atom which has a **double bond** to a C atom is called an **imine**.



4) Amides

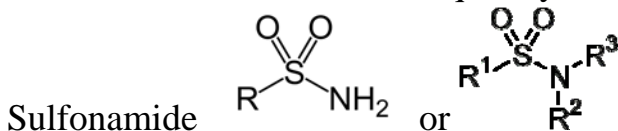
A N atom which is bonded to a C=O (carbonyl) group is called an **amide**. Amides are called primary amides if the N is bonded to one C atom, secondary amides if the N is bonded to two C atoms, or tertiary amides if the N atom is bonded to 3 C atoms.

Amide

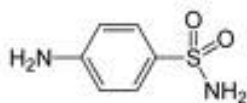


5) Sulfonamides

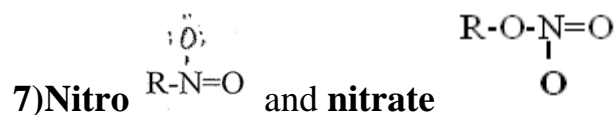
When a N atom is bonded to a O=S=O group, it is referred to as a sulfonamide. The sulfonamide drugs were one of the first effective antibiotic families and are frequently referred to as the “sulfa” drugs.



(Note S has more than two bonds in the sulfonamides.)

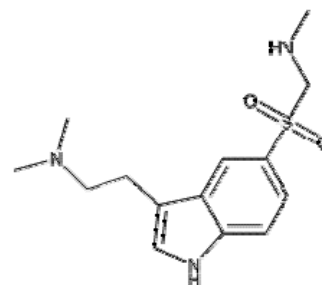
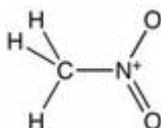
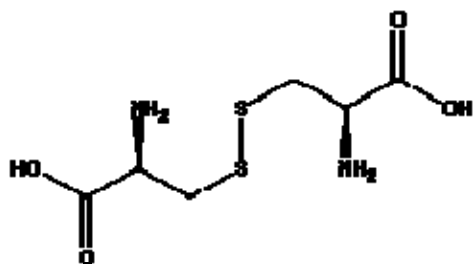
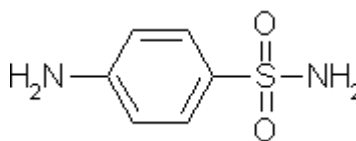
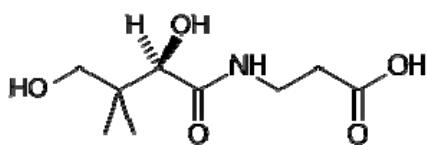


6) Cyanide (nitrile)



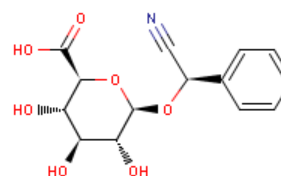
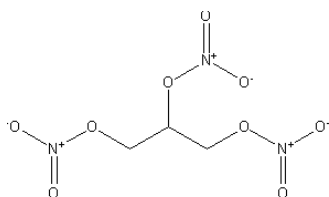
In the nitro group the N atom is directly bonded to the C, while in a nitrate group it is an O atom that connects the C and the N. Common names sometimes can be misleading in this regard however.

Identify the functional groups in the following biologically important molecules:



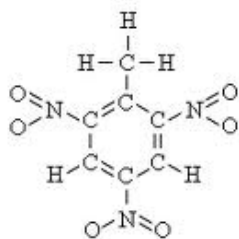
(Cystine)

Sumatriptan(Imitrex)

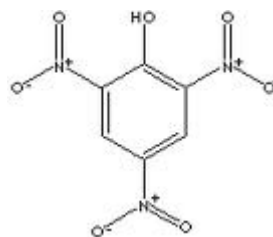


Nitroglycerin-what's wrong with this name?

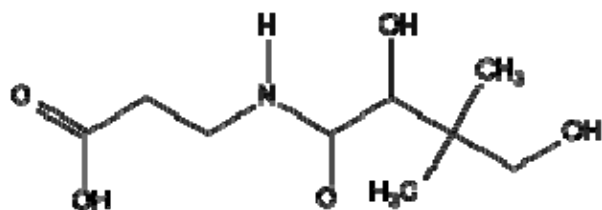
Amygdalin



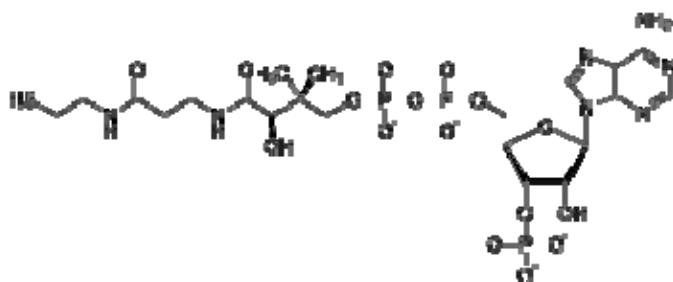
TNT(trinitrotoluene)



(picric acid)

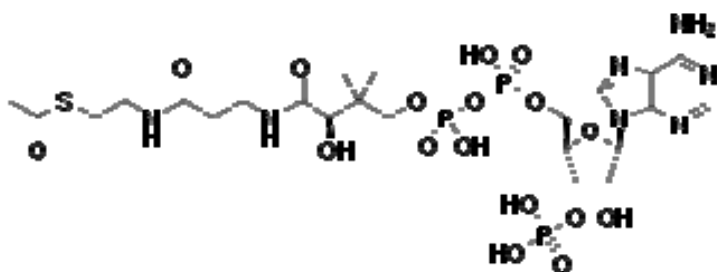


(pantothenic acid)



Coenzyme A

Can you find the pantothenic acid structure within the structure of coenzyme A?



acetyl Coenzyme A

What new functional group is in acetyl CoA that is not in coenzyme A itself?

For practice flash cards see: <http://www.flashcardmachine.com/1543843/i54f>

1.66 Additional Practice recognizing functional groups

Using the examples given above, identify the functional groups in the following molecules:

