CHAPTER 12. DECODING ORGANIC STRUCTURES: THE FUNCTIONAL GROUPS

Functional Groups: The Key To Understanding Organic Molecules

Since life on this planet is based on compounds of the element carbon, the study of these compounds, called organic chemistry, is an important area of chemistry. As we have seen in Chapter 10, the ability of carbon to form single or multiple covalent bonds with itself to form chains of varying length, and even rings of varying size, leads to great versatility in the size and shape of carbon-based molecules. In this chapter we consider the bonds carbon forms with other elements, further expanding the number and types of possible compounds. The number of compounds formed by carbon is so great that it far exceeds the number of all the compounds formed by all the other elements. Some of these compounds contain thousands of atoms. How are we to begin to understand this myriad of complex molecules?
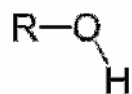
The backbone of any organic compound is its carbon structure, whether in long chains, branched chains, rings, or some combination of these. In nature only a few elements other than carbon are found in most organic compounds: oxygen and nitrogen are the most common of these, along with sulfur and phosphorous. These tend to be found most commonly in only a few arrangements called **functional groups**. When the structure of an organic compound is drawn, frequently the carbon backbone is indicated only by a structural skeleton, with symbols for the carbon atoms left out. Usually hydrogen atoms attached to carbon atoms are left out, too. Only the atoms and bonds belonging to the functional groups are shown in detail. Represented in this way, the structure of the organic compound is simpler and easier to draw. Highlighting the functional groups in this way also helps us in understanding how the molecule reacts with other molecules, because the functional groups are by far the most reactive parts of an organic molecule.

This chapter lists and describes the functional groups, along with the type of reactivity that is characteristic of each one. Then we can use our knowledge of the functional groups to look at the structure of some common organic molecules. What seems at first to be a complex molecule can be easily understood if its structure is interpreted in terms of a carbon backbone to which are attached familiar functional groups. Using these decoding skills, we will be able in later chapters to examine the structures of the molecules of drugs, foods, and cleaning products, as well as the molecules of our own bodies, and to understand how these molecules behave based on their molecular structures and functional groups. Table 12-1 lists the most common functional groups found in organic compounds.
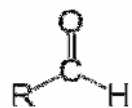
Table 12-1. *Common functional groups in organic molecules.*
R denotes the rest of the molecule; R' and R" can be different from R.

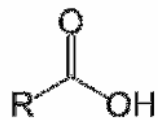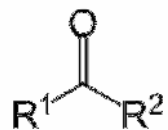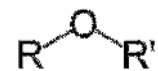| Structure	Name of Functional Group	Structure	Name of Functional Group

R—X
where X= F, Cl, Br or I   Halide

R—N with R" and R'   **Amine**
where R' or R" or both may be H

R—O H   **Hydroxyl (Alcohol)**

Amide structure   **Amide**
where R' or R" or both may be H

Aldehyde structure   **Aldehyde**

Carboxylic acid structure   **Carboxylic acid**

Ketone structure R^1 R^2 **Ketone**
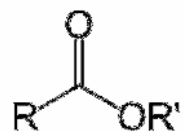
Ether structure R—O—R'   **Ether**

Ester structure R—O—OR'   **Ester**
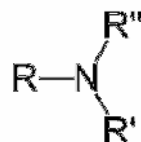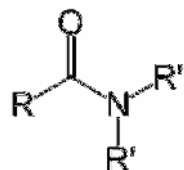
The Halide Group, -X

Perhaps the simplest functional group in organic molecules is the halide group: one of the halogen atoms (F, Cl, Br, or I) attached to a carbon in place of one of the hydrogens of a hydrocarbon. The halocarbons are low in polarity, mixing well with nonpolar substances, but not with water. These compounds are not normally found in nature, but can be synthesized in the laboratory, and have found wide commercial applications, including uses as solvents, refrigerants, and pesticides. Though useful in many commercial applications, many of the halocarbons have proven to cause adverse effects to health or the environment. Carbon tetrachloride, once used commonly in households and dry cleaning plants as a cleaning solvent, has been shown to cause cancer. DDT, once useful as a pesticide, built up in the environment and endangered the survival of birds. The CFC compounds, halocarbons which feature chlorine and fluorine atoms and were once used as refrigerants, rise to the stratosphere where they reduce the ozone which protects the earth from ultraviolet rays.

The chlorine compounds of methane are among the simplest organohalides. There are four possible chlorinated methane derivatives, in which one, two, three, or all four of the methane hydrogens are replaced by chlorine atoms. The structures of these compounds and their names are shown in Fig. 12-1.

Fig. 12-1. *Chemical structures of the four chlorine derivatives of methane.*

Large numbers of different chlorofluorocarbons are possible, since varying numbers of both chlorine and fluorine atoms can be present. Three chlorofluorocarbons are shown in Fig.12-2. The chlorofluorocarbons, most often referred to as CFC's, are chemically unreactive under normal conditions, and for that reason they became popular during the 1950's and 1960's for a variety of uses, including use as a propellant in aerosol cans and as refrigerant gas in refrigerators and air conditioners. Not until the late 1960's did scientists begin to suspect that when the CFC's floated into the upper levels of the atmosphere, their reactions with ozone molecules depleted the natural levels of ozone which screened out harmful UV radiation from reaching the earth's surface. (See Chapter 16 for more information about depletion of the ozone layer.) In 1978 as a result of the international agreement the Montreal Protocol the use of CFC's as aerosol propellants was banned, and their use as in refrigerant was banned in the United States effective in 1997. Nevertheless, CFC's still remaining in the atmosphere will continue to exert their effect for years to come.

Fig. 12-2. *Chemical structures of three chlorofluorocarbons.*
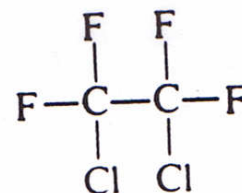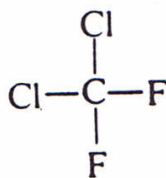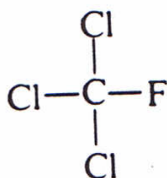
The Hydroxyl Group, -OH

Alcohols are an important class of compounds featuring the **hydroxyl group –OH**. Because the hydroxyl group features a hydrogen atom attached to an oxygen atom, it gives the capability for hydrogen bonding to a molecule to which it is attached. Table 12-2 shows the compounds that result when a hydroxyl group is substituted for a hydrogen for each of the first three alkanes, methane, ethane, and propane, to form methanol, ethanol, and propanol, as well as some other commonly used alcohol compounds.

Table 12-2. **Some Common Alcohols**

Alcohol	Formula	Boiling Point (degrees Celsius))	Common name, uses
Methanol	CH_3OH	64	Wood alcohol; fuel
Ethanol	C_2H_5OH	78	Beverage alcohol
Isopropanol	$CH_3CHOHCH_3$	82	Rubbing alcohol
Ethylene glycol	CH_2OH_2OH	198	Antifreeze
Glycerol (glycerin)	$CH_2OHCH_2OHCH_2OH$	290 (decomposition)	Moisturizer

When an -OH group is added to the simplest hydrocarbon, methane, the alcohol called methanol or methyl alcohol is formed. Methanol is sometimes called wood alcohol because it can be made by heating wood in a closed container and collecting the vapors that form. Methanol is highly toxic. Drinking it can cause blindness and death, and too frequently this does happen when people confuse it with or substitute it for drinking alcohol, which is ethanol. Ethanol, or ethyl alcohol, has the structure of ethane with an -OH group substituted for one of the hydrogens. This alcohol, found in alcoholic beverages, is often called grain alcohol because it can be made by fermenting grains. Actually, any starchy or sugary food can be fermented to make alcoholic beverages. Grapes and apples when allowed to ferment, for example, can form wine and hard cider.

Formulas like those in Table 12-2 are very limited in representing molecules. Pictures of three-dimensional models give a somewhat clearer picture of the shapes of the molecules, but not the way the atoms can rotate around their bonds to form different shapes. For example, it makes no difference where the -OH is placed on the diagram of ethanol because all the positions are equivalent. This fact, which becomes evident when a three-dimensional model is examined, is not at all clear from a diagram like the one in Table 12-2. It is not difficult, however, to see from Table 12-2 that there are two possible isomers, or different structures using the same atoms, of the alcohol formed by adding an -OH group to the three carbon chain of propane. The alcohol group can either be placed on an end carbon, forming propanol or propyl alcohol, or it can be placed on the middle carbon, forming isopropanol, or isopropyl alcohol. Most rubbing alcohol sold in pharmacies is isopropanol, which is not drinkable.

All the alcohols shown in Table 12-2 are miscible with water, because the alcohol molecules and the water molecules are mutually attracted by hydrogen bonding forces. Molecules with larger hydrocarbon groups (containing six or more carbons) have much lower solubility in water, since the nonpolar hydrocarbon end of the molecule does not have these attractive forces. Nevertheless, the part of a molecule, even a very large one, that features an -OH group will exhibit hydrogen bonding forces, and these can be important in interactions of that molecule with other molecules.

Antifreeze for auto radiators is the alcohol ethylene glycol, with two alcohol groups and two carbon atoms. Having two alcohol groups means that the hydrogen bonding forces in ethylene glycol are especially strong. It is much higher-boiling than the alcohols in Table 12-2 with only one -OH group because of these strong intermolecular forces, so it does not evaporate when a radiator heats up the way these other alcohols would do. Glycerine, with three carbon atoms and three -OH groups, has an even higher boiling point, and a viscous texture. Mixed with water, it is often used as a component in hand creams and other cosmetic products. By attracting and holding water molecules with hydrogen bonding, it keeps the skin from drying out.

The Ketone Group, C=O

Like the alcohol group, the **ketone** group contains an oxygen. The oxygen of the ketone group, however, is double-bonded to a carbon. This carbon must be attached to two other carbons in the organic molecule. Acetone, used as a solvent for fingernail polish and other organics, is one of the more common ketones around the home (Fig. 12-2).

Fig. 12-3. *Structures of acetone and cyclohexanone.*

$$CH_3-C-CH_3$$
$$\overset{\|}{O}$$

Acetone
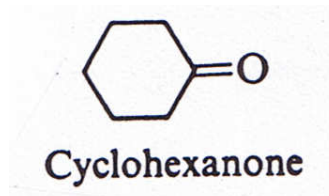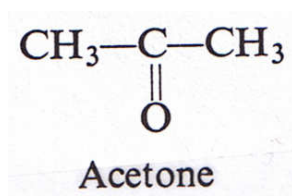
Cyclohexanone

Notice how the structure of the cyclic ketone, cyclohexanone, is represented in Fig. 12-2. In the structure on the left, all the atoms in the molecule are indicated by their element symbols. In the structure on the right, none of the six carbon atoms in the ring is labeled, and all of the hydrogen atoms are omitted from the structure drawing. Only the doubly bonded oxygen of the ketone group is shown. This type of structure drawing is very common for more complex drawings. Understanding the identity of the "hidden" atoms in a drawing like this is important in decoding these chemical structure drawings.

The Aldehyde Group,

The **aldehyde** functional group is similar to the ketone group in that each has a carbon double-bonded to an oxygen; this C=O pair is often called a **carbonyl** group. In the aldehyde group, however, the carbonyl carbon is also bonded to a hydrogen. Since carbon forms only four covalent bonds, and the double bond to the oxygen plus the single bond to the hydrogen make three, the aldehyde group bonds to only one carbon, unlike the ketone group, which appears between two carbons. Structures of some common aldehydes are shown in Fig. 12-4.

Fig. 12-4. *Chemical structures of some common aldehydes*

Benzaldehyde
(Oil of bitter almond)

Cinnamaldehyde
(Oil of cinnamon)
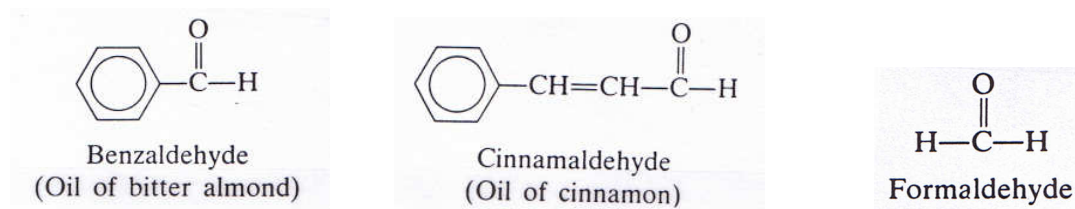
Formaldehyde

Aldehydes are often associated with pleasant fragrances. Benzaldehyde is the artificial fragrance and flavor associated with maraschino cherries; cinnamaldehyde, with cinnamon. The simplest compound with an aldehyde group is formaldehyde, used as a cadaver preservative and known for its unpleasant odor. Formaldehyde also sees wide use in cosmetic products as a preservative and in building products, for example in plywood adhesives. Formaldehyde has been linked with cancer, and for that reason insulation products which emit formaldehyde into the home environment have been banned. Traces of formaldehyde, however, are found in almost all foods, and we constantly form and use small amounts of formaldehyde in our own bodies in normal biochemical processes.

The Carboxylic Acid Group

The **carboxylic acid group** features both a carbonyl group like the ketone and aldehyde groups and a hydroxyl group like the alcohol group. Like the alcohol group, the carboxylic acid group gives a molecule the ability to form hydrogen bonds. The most important property, however, that appears when both -OH and =O are attached to the same carbon, is that the hydrogen atom becomes acidic because of the combined electronegative effect of the two oxygens, pulling away electron density from the bond between the hydrogen and the oxygen to which it is bonded. Carboxylic acids, like other weak acids, give up this weakly attached proton to base molecules and form aqueous solutions of pH lower than 7. Unlike inorganic acid molecules, organic acid molecules usually have a number of hydrogen atoms. Only the hydrogen on the carboxylic acid group, however, is acidic.

Organic acid formulas can appear written in several different ways, which can potentially cause some confusion in identifying them. Figure 12-5 shows the structure of acetic acid, along with several ways of writing the formula for this compound. In each of the formulas in the figure the acidic hydrogen is identified. The formal chemical name for acetic acid is ethanoic acid.

Fig. 12-5: *The chemical formula for the common acid acetic acid can be written several ways, with the acidic hydrogen appearing at the beginning or the end of the formula:*

$$HC_2H_3O_2$$

$$CH_3COOH$$

$$CH_3CO_2H$$
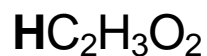
The chemical compound we know as vinegar is a dilute solution of acetic acid. Naturally occurring microorganisms turn grape juice to wine vinegar and apple juice to cider vinegar. Acetic acid can also be made by chemical synthesis starting with acetylene or ethanol. A few of the many common organic acids are shown in Fig. 12-6.

Fig. 12-6: *Formulas of some common organic acids.*
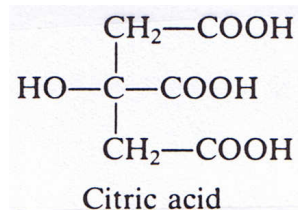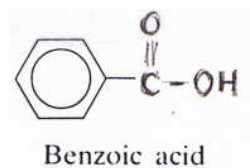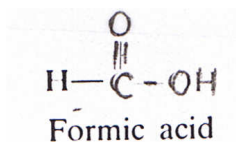
Citric acid is another naturally occurring acid; it gives citrus fruits their tang. Benzoic acid is used as a food preservative. Formic acid is the chemical that makes an ant bite sting.

The Ester Group

$$R \overset{O}{\underset{}{\parallel}} C \diagdown OR'$$

When a carboxylic acid reacts with an alcohol, an **ester** is formed, along with a molecule of water. Fig. 12-9 shows an example of this reaction the reaction of acetic acid with ethyl alcohol to make the ester ethyl acetate. Ester formation is an example of a dehydration reaction since water is produced as a product. It is catalyzed by the addition of sulfuric acid. An interesting example of this reaction occurs when the carboxylic acid butyric acid reacts with the alcohol **n**-butanol to form water and the ester butyl butanoate. One of the reactants, butyric acid, has a notable stench (it is the chemical compound responsible for the odors of rancid butter and smelly feet), while the ester which is the reaction product is responsible for the pleasant characteristic odor of the pineapple. Butyl butanoate made by this chemical reaction is the component responsible for the pineapple flavor and fragrance of most pineapple-flavored candies. Fragrance is a characteristic of many esters, as noted in the list of some common esters in Fig. 12-8.

Fig. 12-8. *Some common esters. Ethyl formate is an artificial rum flavor. Methyl butyrate is in apples, and ethyl butyrate is in pineapples. Isopentyl acetate is banana oil, used as a solvent and in flavoring, while benzyl alcohol is oil of jasmine, used in perfumes.*
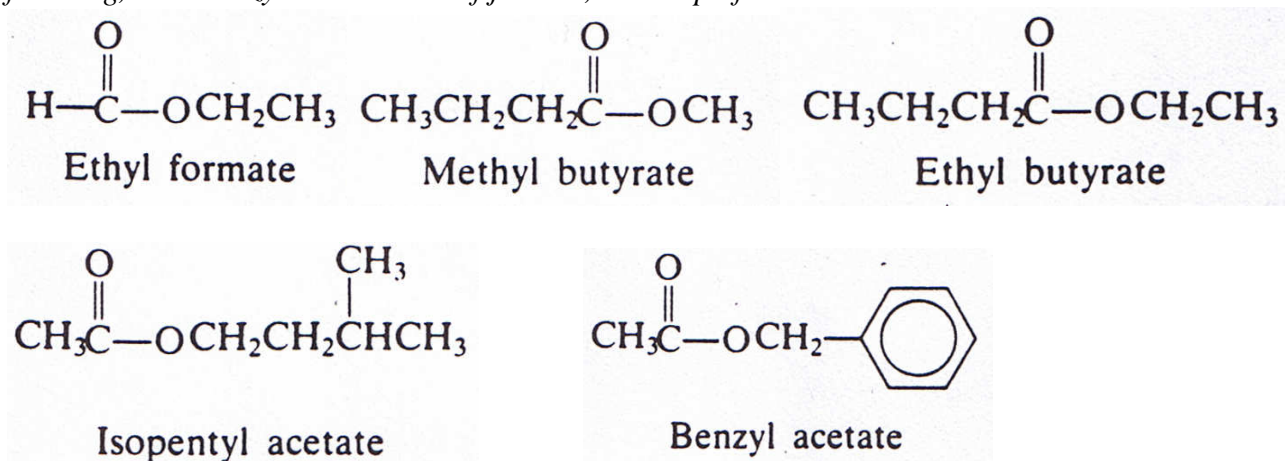

Fig. 12-9. *Formation of an ester from a carboxylic acid and an alcohol.*

The Ether Group

In the **ether** functional group, an oxygen atom is single-bonded to two of the carbon atoms of the molecule. Examples of some simple molecules containing the ether group are dimethyl ether CH_3OCH_3 and diethyl ether $CH_3CH_2OCH_2CH_3$. Diethyl ether is the original ether used in anesthesia to produce unconsciousness. It has been replaced by methyl propyl ether, also called neothyl, which has fewer side effects.
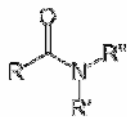

The Amine Group
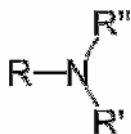
The amine group is related to the compound ammonia, NH_3, which we have already encountered as a common weak base. One of the hydrogens of the ammonia molecule can be replaced by an organic group, forming a primary amine like methyl amine, CH_3NH_2. If two of the hydrogens of the ammonia molecule are replaced by organic groups, a secondary amine like dimethyl amine, $(CH_3)_2NH$ is formed. All three of the ammonia hydrogens can be replaced by organic groups, forming a tertiary amine like trimethyl amine, $(CH_3)3N$. Like ammonia, the amines are weak bases. Some representative organic compounds containing the amine functional group are listed in Fig. 12-10.

Fig. 12-10. *Some common amines*
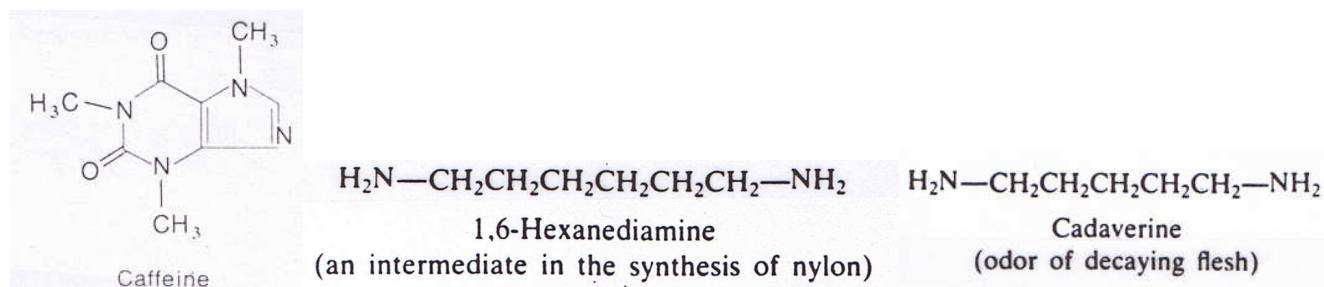
Amines are known for foul odors, as may be noted from some of the amines listed in Fig. 12-10; the stench of decaying flesh is largely due to amines. "Fish and guests smell after three days" because of the buildup of amines. When lemon juice, tomato sauce, or other acidic materials are added to fish in cooking, the basic amines react with the acid, forming nonvolatile salts, hence reducing the "fishy" odor.

The Amide Group

Just as alcohols can react with carboxylic acids to form esters, primary or secondary amines can react with carboxylic acids to form the **amide** group. For example, dimethyl amine reacts with acetic acid to form the amide linkage as shown in Fig. 12-11.

Fig. 12-11. Reaction of a carboxylic acid with an amine to form an amide.
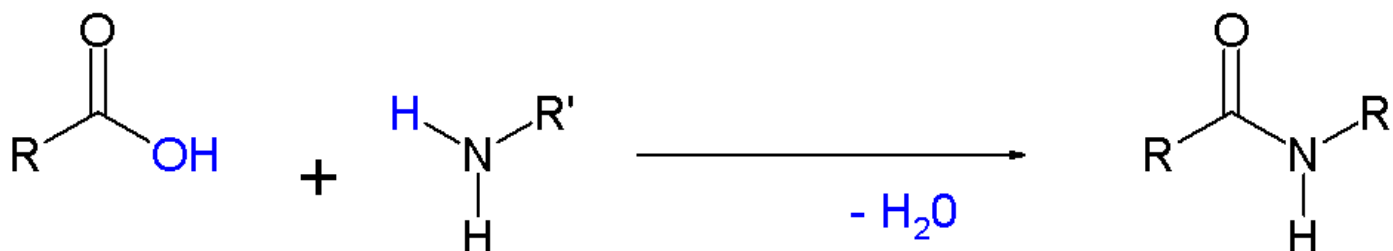
The amide linkage is important in the formation of proteins, which form much of our body tissue. In a protein molecule the amide linkage is referred to as the **peptide** linkage. Protein molecules are natural polymers held together by peptide linkages, and are discussed in Chapter 13.

**Decoding the Structures of Organic Molecules**

The concept of the organic functional groups is a tool which can be used to understand the structure and reactivity of even the most complex organic molecules. Using this concept to decode molecular structures is a skill gained with practice.

For simple molecules containing only a few carbons and one or two functional groups, it is relatively simple to predict some properties of the molecule by identifying the functional groups, as we have seen in earlier examples in this chapter. A molecule with an amine group, for example, is very likely to be foul-smelling. An ester group in many cases, but not all, may indicate a fragrant substance. Alcohols with fewer than six carbons are water soluble because of hydrogen bonding.

For larger molecules, we need to examine both the carbon "backbone" and the functional groups, and to compare these with other molecules in attempting to predict patterns of reactivity. Often chemists have to make guesses about how changing a molecule's structure will change its reactivity. For example, cortisone is a powerful hormone with a remarkable ability to reduce inflammation. Its antiinflammatory properties are valuable in the treatment of serious disorders like rheumatoid arthritis, lupus, leukemia, ulcerative colitis, and transplant rejection. Cortisone has serious side effects, however, due to its potent actions on the immune system and other body

functions. New drugs have been created with chemical structures slightly different from cortisone in an attempt to produce the therapeutic effects of cortisone without the unwanted side effects. Many of these new compounds have been very successful. Hydrocortisone, for example, has proven to be so safe and effective that it is now available in low dosages as a non-prescription cream for treating inflammation due to insect bites and skin rashes.

Fig. 12-12: *The chemical structures of cortisone and hydrocortisone.*

Cortisone   Hydrocortisone
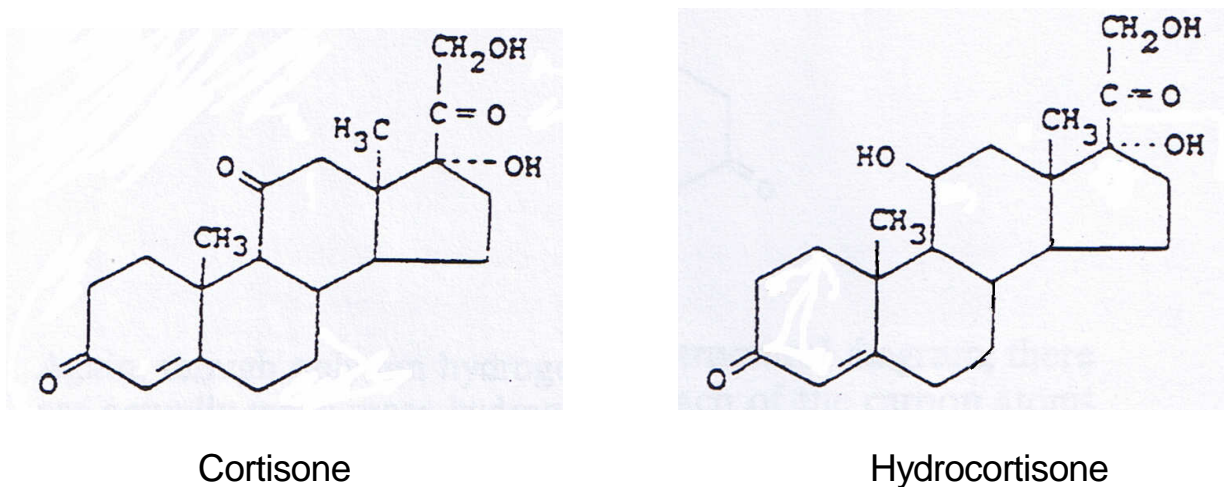
Comparing the structures of cortisone and hydrocortisone (Fig. 12-12) shows how new drugs can be created by making changes in the molecule of a known chemical compound. The two molecules are alike except for one functional group, which is a ketone in cortisone, and an alcohol group in hydrocortisone; can you find it on the structure? The carbon backbone of four rings joined together is common to a number of substances manufactured in the body with important biochemical functions. These compounds, called **steroids**, will be discussed at greater length in later chapters. Examining these two molecules carefully can provide us with useful practice in decoding structural diagrams of organic molecules.

Problem example 12-1: How many carbon atoms are in the cortisone molecule?
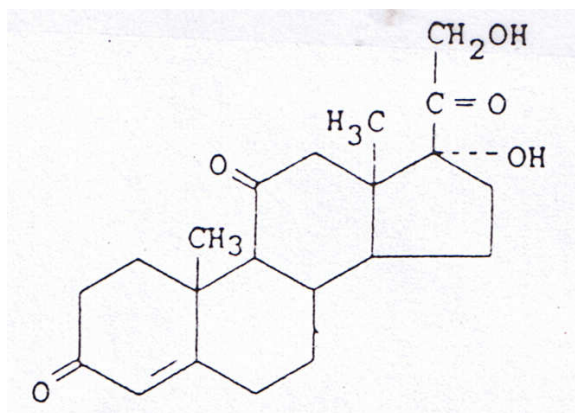
As frequently happens in structural diagrams of larger molecules, the carbon atoms in Fig. 12-12 are represented only by positions on the rings of the molecule's structure. This structural drawing is made easier to interpret by numbering these carbon positions. This numbering order is standard for steroid molecules, and is a great help to those chemists whose work involves synthesizing and discussing steroid molecules. Although only four carbon atoms appear as the element symbol in positions 18 through 21, adding to these the other carbons in the 17 numbered positions on the steroid rings gives a total of 21 carbon atoms in cortisone.
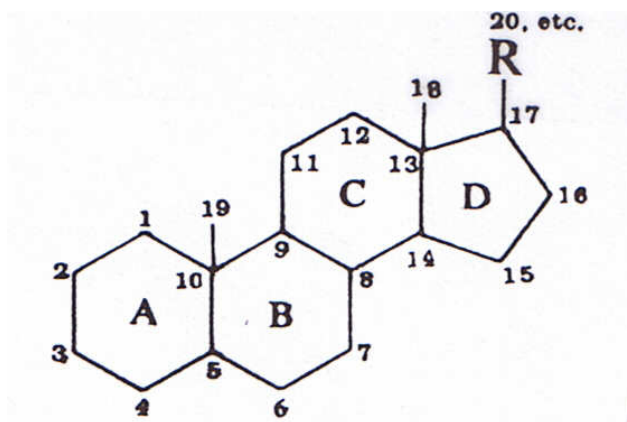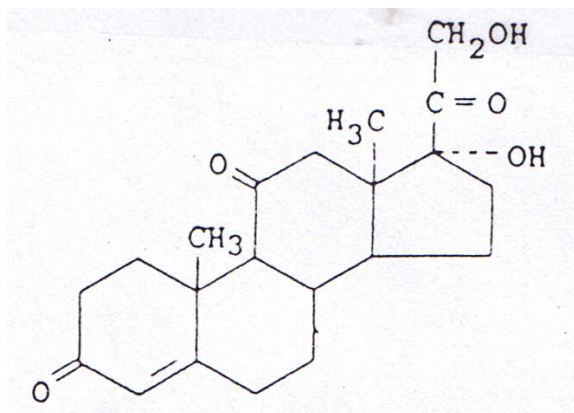

Fig. 12-13. *Numbered positions on the steroid ring.*

Problem example 21-2: How many hydrogen atoms are in the cortisone molecule?


Again, though only eight hydrogen atoms are shown on the structural diagram, there are actually many more hydrogen atoms in the molecule. Only the hydrogens on the alcohol functional groups and the two methyl groups that project from the rings are usually drawn in. (The dotted lines to one of the alcohol groups are there to indicate that that group is pointing away from the viewer in the three-dimensional molecule.) Each of the carbon atoms in the molecule forms four covalent bonds. Hence, you can figure out how many "invisible" hydrogens there must be. The number of hydrogen atoms on each carbon atom can be deduced by subtracting from four the number of bonds formed from the carbon atom to other atoms. To the newcomer to organic chemistry this may seem to be a mystifying process, identifying carbon and hydrogen atoms, all of which appear to be invisible on the structural diagram. In practice, however, the process is quite simple. Carbon number 1, for example, is bonded to two other carbon atoms, carbon 2 and carbon 18. Since carbon forms a total of four bonds, carbon number 1 must be bonded to two hydrogen atoms. Carbons number 2, 6, 7, 15, 16, and 12 are bonded to two hydrogen atoms also. Carbon number 3 is bonded to two carbon atoms. Its double bond to the oxygen atoms counts as two bonds. The structural diagram, then shows a total of four bonds to this carbon, two to carbons and two to oxygen. Since carbon can form only four bonds, there must be no hydrogen atoms bonded to this carbon. Similarly, carbon number 11 and carbon number 20 are not bonded to any hydrogen atoms. Carbon number 4 is bonded to two other carbon atoms; one of these bonds is a single bond, and one is a double bond. The total number of bonds formed with other carbon atoms by carbon number 4 is three; it must be bonded to one hydrogen as well. Carbon number 5 is bonded to three other carbon atoms; two of these are single bonds, and one, a double bond. The total number of bonds formed to other carbon atoms is four, and so carbon 5 is not bonded to any hydrogen atoms. The carbon atoms numbered 10 and 13 each form single bonds to four other carbon atoms, so they bond to no hydrogens. Carbons numbered 8, 9, and 14 are each bonded to three other carbon atoms; one hydrogen is attached to each of them. Carbon number 17 is attached to three carbon atoms and one oxygen, so it has no hydrogens. The total number of hydrogen atoms in the molecule is 28.

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Problem example 12-3: Identify the functional groups on the cortisone molecule.
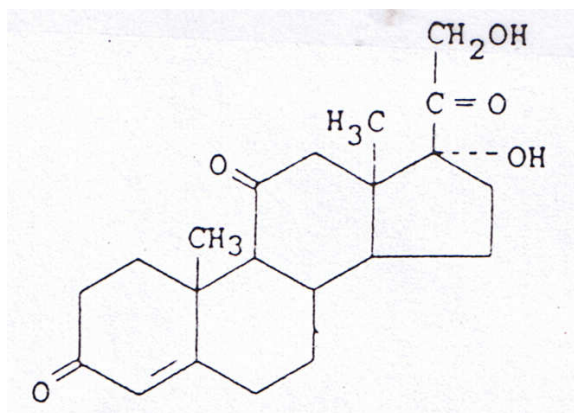
Cortisone has three ketone groups, recognizable as C=O, or simply as =O attached to the "invisible" carbon on the ring. Can you find them? There are two alcohol, or hydroxyl, groups, -OH. One of them is attached to the 5-carbon ring structure, and the other is two carbons away.

Problem example 12-4: Identify the functional groups on the hydrocortisone molecule.
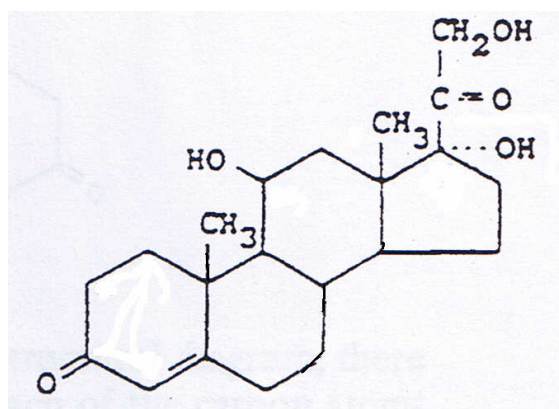
Hydrocortisone has two ketone groups; can you find them? One is on the ring and therefore the carbon does not appear, but you can see the =O. There are three alcohol, or hydroxyl, groups –OH. Can you find them all?

Problem example 12-5: How many carbon atoms are in the caffeine molecule, with the structure shown below:


Caffeine

Each position on the two rings not occupied by a nitrogen atom is occupied by a carbon atom. Five ring carbons plus the three carbons on the methyl groups add up to a total of eight carbon atoms.

Problem example 12-6: How many hydrogen atoms are in the caffeine molecule?

Each carbon forms four covalent bonds, so only one of the ring carbons is attached to a hydrogen atom. (Which one?) This carbon atom, added to the nine carbon atoms on the methyl groups, add up to a total of ten.

Problem example 12-7: What functional groups are present in the caffeine molecule?

This molecule features two amide groups and two amine groups . Each of these functional groups is incorporated into the ring structure of the molecule.

Using Decoding Skills To Understand Molecular Structures of Important Organic Molecules

Interpreting structural diagrams, as demonstrated in the problem examples above, is a valuable tool for understanding complex molecules that have a powerful effect on the functioning of our own bodies. Cortisone and hydrocortisone molecules, we have seen, are very similar in their overall structure, determined by the carbon-carbon bonds within the molecule. This **steroid** structure of four rings fused together appears again in the problem set for this chapter in the molecules testosterone and progesterone, which function in the body as male and female sex hormones, respectively. Again in these compounds we see demonstrated both the potent effects a steroid molecule can have upon the body, and the great difference a change in just one functional group can have on the molecule's effect on the body.

The structures of the addictive drugs cocaine and nicotine are given in the problem set as well; these drugs exert a powerful effect on the central nervous system of the body. You may notice some similarities in the structures and functionalities of these two molecules. Notice, also, that ring structures of these molecules are very readily distinguishable from the steroid molecule structures.

Using Functional Groups To Understand the Solubility Properties of Organic Molecules

Whether an organic molecule is soluble in aqueous (water) or nonaqueous solutions is a very important characteristic. For example, if a water-soluble vitamin is consumed in greater quantities than the body consumes, the excess is excreted in the aqueous urine solution. Oil-soluble vitamins, in contrast, are stored in body fat, and can even build up to toxic levels if too great an excess is consumed.

Since water molecules are attracted to one another by the strong attractive forces of hydrogen bonds (Chapter 7), in order for a substance to dissolve in water to an appreciable degree, it must exert strong attractive forces on water molecules. Hydrocarbons are nonpolar molecules, so, if organic molecules are to dissolve in water, the functional groups must have attractive interactions with water molecules.

Alcohol and carboxylic acid functional groups feature hydrogen atoms bonded to oxygen atoms, so they exhibit hydrogen bonding, and enhance a molecule's solubility in water. Amine and amide groups, as shown in Table 12-1, may vary in the number of carbon atoms attached to the nitrogen group; some amines and amides feature a hydrogen attached to a nitrogen atom, and these functional groups will exhibit hydrogen bonding with water. As we have seen with the alcohol functional group, it may be taken as a general rule that one hydrogen-bonding functional group can result in aqueous solubility of a hydrocarbon chain of up to six carbons.

A positive or negative charge on an organic molecule results in a strong attractive force toward water molecules, much like that exerted by the ions of salts like sodium chloride. Carboxylic acids can produce charged organic salts by reacting with bases, and, since amines are basic compounds, they can produce salts by reacting with bases.

Even in the absence of hydrogen bonding or positive or negative charges, it is possible for a polar organic molecule to exhibit some solubility in aqueous solution. In the caffeine molecule, for example (Problem example 12-5), the two electronegative oxygen atoms on the carbonyl (C=O) groups and the four electronegative nitrogen atoms in the rings result in a molecule of sufficient polarity that this eight-carbon molecule has appreciable solubility in water.

Problem example 12-8: Would you expect the cortisone molecule to be appreciably water-soluble?
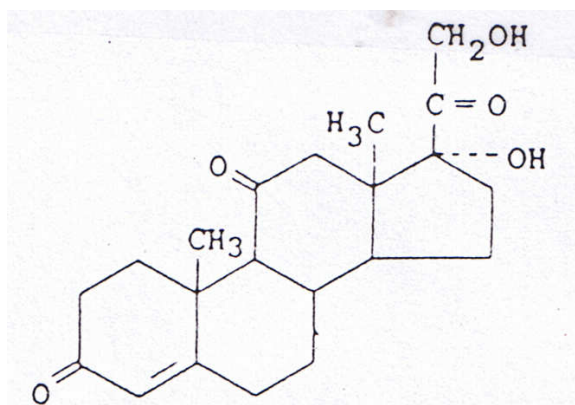
Identifying the two hydroxyl (or alcohol) functional groups, we expect hydrogen bonding interactions with water on this end of the molecule. However, since we have determined that this molecule has 21 carbon atoms, two hydogen-bonding functional groups are insufficient to result in appreciable water solubility of this large water molecule, one hydrogen bonding group would be required for each six carbons..

CONCEPTS TO UNDERSTAND FROM CHAPTER 12

Reactive groups of atoms called <u>functional groups</u> recur repeatedly in organic compounds. Understanding the chemistry of the functional groups is important in understanding the chemistry of organic molecules.

Organic compounds: acid, base, or neutral?

A *carboxylic acid group* makes the compound an *acid* (produces H^+ in aqueous solution); if this is the only functional group in the compound that affects pH, then the pH will be lower than 7 in aqueous solutions of this compound.

An *amine* group makes the compound a *base* (produces OH^- in aqueous solution); if this is the only functional group which affects pH, then the pH will be greater than 7 in aqueous solution.

These are the only functional groups we have studied that affect pH.
(Exception: if an -OH group (hydroxyl) is attached to a benzene ring, it is called a phenol and has an acidic hydrogen.)

Solubility of organic compounds

In order for compounds to mix together, they must be attracted to one another. Polar compounds (those with a positive and a negative end) are attracted to one another because of the electrostatic attraction between a + and a - charge.

Hydrocarbons are nonpolar compounds because C and H have similar electronegativities. They will mix with other nonpolar compounds, because of very weak attractive forces like dispersion forces. But they will not be able to attract polar compounds like water, and hence are not water soluble.

Water molecules are attracted to one another by a strong attractive force, hydrogen bonding. These will be more attracted to one another than to a nonpolar molecule, but they will be attracted to charged ions or to other polar molecules, particularly those that can form hydrogen bonds. Organic compounds that can mix with water usually have functional groups that exhibit hydrogen bonding. These functional groups can be recognized because they feature hydrogen atoms bonded to oxygen, nitrogen, or fluorine. *Each functional group which hydrogen bonds will be able to make an organic compound soluble in water with a hydrocarbon chain up to 6 carbons long.* Bigger organic molecules would need more H-bonded functional groups to make them water soluble.

A simple rule: "like attracts like" or nonpolar compounds like hydrocarbons mix together, while hydrogen-bonded compounds will also mix with each other and with other polar molecules.

So… will an organic compound be water soluble?Check the functional groups: can they form hydrogen bonds? (H bonded to O,N or F?) Is there at least one functional group that can hydrogen bond for every 6 carbons? Then it will dissolve in water!

FACTS TO LEARN FROM CHAPTER 12

It is useful to know the structures of the common functional groups listed in Table 12-1.

DECODING SKILLS TO LEARN FROM CHAPTER 12

After finishing this chapter you should be able to determine from the structural diagram of a complex organic molecule the number of carbons, the number of hydrogens, and the functional groups.

By examining the functional groups and the number of carbons in the molecule, you should be able to predict whether or not an organic compound will be soluble in water.

By examining the functional groups you should be able to find if there is an acidic group (carboxylic acid) or basic group (amine).

Name _____ **CHAPTER 12 PROBLEMS** *Date* _____

12-1. The chemical structure below is that of vanillin, the compound responsible for the flavor and fragrance of vanilla. The circle inside a hexagon represents the structure of a benzene ring. You can draw in alternating double and single bonds in the ring to help count the number of bonds to each carbon correctly.
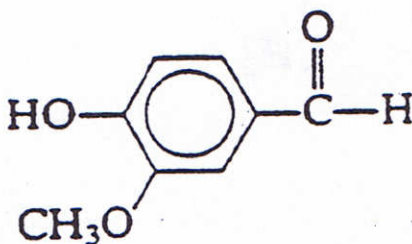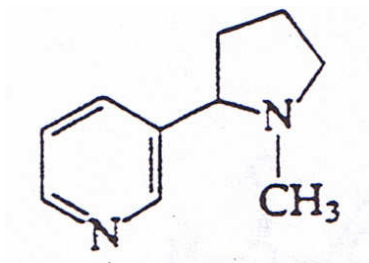

     a. Identify all functional groups in this molecule by circling and labeling each one.

     b. Can you "see" all the carbons? Sketch a C on top of all the "invisible" carbon positions on the ring. How many carbons are in this molecule?

     c. How many hydrogens are in the vanillin molecule? To determine the number of hydrogens, remember that each carbon can form four bonds, then draw in all the "invisible" hydrogens with their bonds to each carbon.
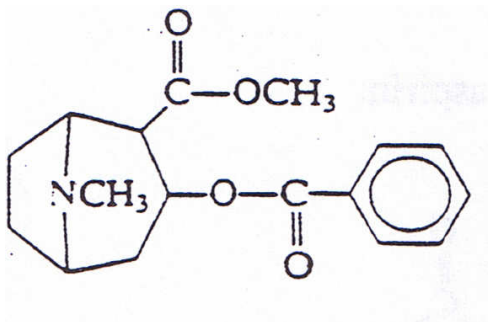
12-2. The chemical structure below is that of aspirin.
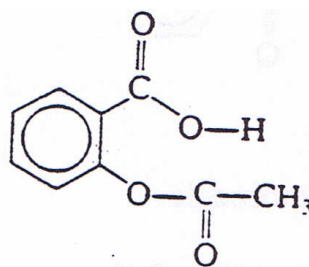
     a. Circle and label all functional groups in this molecule.

     b. How many carbons are in the aspirin molecule? Sketch them in on top of their positions.

     c. How many hydrogens are in the aspirin molecule? Sketch them in with their bonds to carbon.
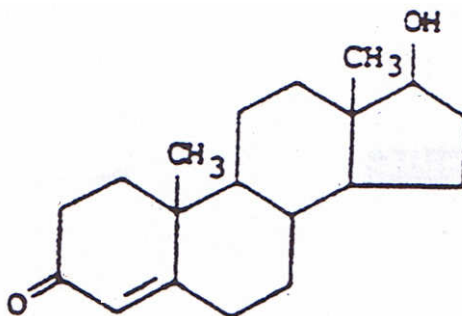
12-3. The chemical structure below is that of nicotine.

a. Circle and label all functional groups in this molecule.

b. How many carbons are in the nicotine molecule? Sketch them in.

c. How many hydrogens are in the nicotine molecule? Sketch them in, with their bonds to carbon.
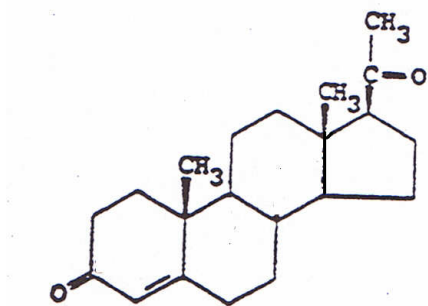
12-4. The chemical structure below is that of morphine.

a. Circle and label all functional groups in this molecule.

b. How many carbons are in the morphine molecule? Sketch them in.

c. How many hydrogens are in the morphine molecule? Sketch them in with their bonds to carbon.

d. Name some similarities between the morphine and nicotine structures.

12-5. The chemical structure below is that of testosterone, a male hormone.

    a. Identify all functional groups in this molecule.

    b. How many carbons are in the testosterone molecule? Sketch them onto their ring positions with a C.

    c. How many hydrogens are in the testosterone molecule? Sketch them in, attached with bonds to the appropriate carbons.

12-6. The chemical structure below is that of progesterone, a female hormone.

    a. Circle and label all functional groups in this molecule.

    b. How many carbons are in the progesterone molecule? Sketch them in.

    c. How many hydrogens are in the progesterone molecule? Sketch them in with their bonds to C..

    d. How is the progesterone structure similar to the testosterone structure? How do they differ?

12-7. Fill in the following table of organic compounds with two carbon atoms.

<table>
<tr><td><u>Name</u></td><td><u>Structure</u></td><td><u>Commercial Use</u></td></tr>
<tr><td>Ethane</td><td></td><td></td></tr>
<tr><td>Ethanol</td><td></td><td></td></tr>
<tr><td>Acetic acid (ethanoic acid)</td><td></td><td></td></tr>
</table>

12-8. Match the following chemical compounds with their commercial uses.

$CH_3OC_3H_7$ a. Cosmetic component

CH_3COOH b. Anesthetic

CH_3CH_2OH c. Refrigerant

CH_2OHCH_2OH d. Beverage component

$CH_2OHCHOHCH_2OH$ e. Antifreeze

$CFCl_3$ f. Vinegar

12-9. Which of the following compounds would you expect to be soluble in water? Circle them.

    a. CH_3OH

    b. CH_3Cl

    c. CH_3NH_2

    d. CH_3COOH

    e. $CFCl_3$

    f. CH_3CH_2OH

    g. $C_{17}H_{35}COOH$

12-10. Predict whether aqueous solutions of the following substances will have a pH equal to 7, greater then 7, or less than 7.

    a. C_6H_5COOH

    b. C_2H_5OH

    c. $C_2H_5NH_2$

    d. Aspirin

    e. CH_3COCH_3

12-12. Judging from the structures of vitamin A and vitamin C below, is vitamin A soluble in water? Is vitamin C soluble in water? Explain your reasoning. If a vegetable was cut into pieces and cooked in a large quantity of water, what would be the effect on the content of each of these vitamins in the food?
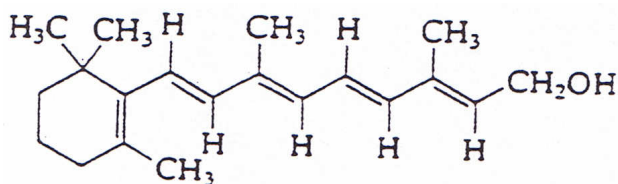
Vitamin A   Vitamin C
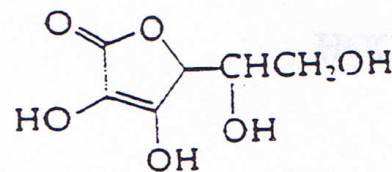
12-13. Match each compound with the appropriate chemical formula.

      1. Wood alcohol   A. C_2H_5OH

      2. Grain alcohol   B. $C_2H_5COCH_3$

      3. Phenol   O

      4. Methyl chloride   C. $C_2H2_5OC_2H_5$

      5. Carbon tetrachloride   D. $C_2H_5NH_2$

      6. Acetic acid   E. C_2H_5COH

      7. Benzoic acid

      8. Ethyl acetate   F. CH_3OH

      9. Ethyl ether   G. CH_3Cl

      10. Ethyl amine   H. C_6H_5OH

      11. Benzaldehyde   I. C_6H_5COH

                                        O

                           J. C_6H_5CH

                                        O

                          K. C_6H_5COH

                                        O