



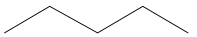
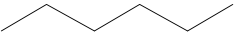
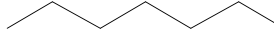
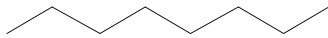
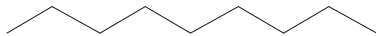

Chemistry 1110 – Organic Chemistry

IUPAC Nomenclature

Of the approximately 32 million unique chemical compounds presently known, over 95% of them can be classified as organic; i.e., containing carbon. The IUPAC system of nomenclature was established at the end of the 19th century in order for chemists to have a common method of naming compounds. Most introductory chemistry courses have a small section on simple organic molecules and naming is usually restricted to hydrocarbons. This summary contains an introduction to the recognition and naming of the various functional classes organic compounds, as well as the relationship between compounds that have the same molecular formula (**isomers**) that you will be exposed to in CHEM 1110. We hope that you will find it a useful supplement to the material in your textbook. Your particular instructor will also provide you with additional information and problem-solving techniques involving organic molecules.

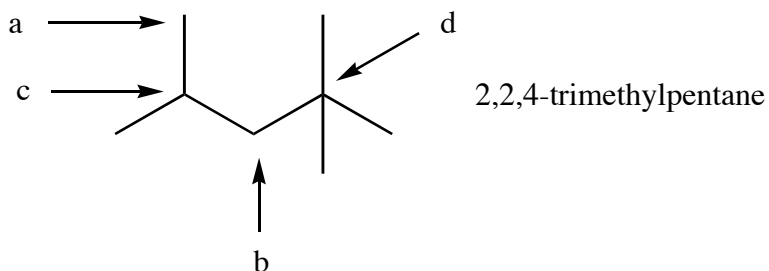
The following table contains a listing of the names and structures of the first 10 members of the alkane family of hydrocarbons.

Homologous Series of Alkanes

methane	CH_4	ethane	CH_3CH_3	propane	$\text{CH}_3\text{CH}_2\text{CH}_3$	
butane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$		pentane	$\text{CH}_3(\text{CH}_2)_3\text{CH}_3$		
hexane	$\text{CH}_3(\text{CH}_2)_4\text{CH}_3$		heptane	$\text{CH}_3(\text{CH}_2)_5\text{CH}_3$		
	octane	$\text{CH}_3(\text{CH}_2)_6\text{CH}_3$				
	nonane	$\text{CH}_3(\text{CH}_2)_7\text{CH}_3$				
	decane	$\text{CH}_3(\text{CH}_2)_8\text{CH}_3$				

You may initially find the above convention for drawing organic compounds confusing, but it saves time and you will soon become more comfortable using it. Your classroom instructor will also show you other methods to represent the structures of organic compounds.

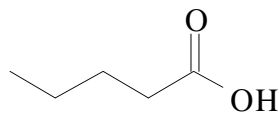
It is very important at this time to stress that since carbon must always have four covalent bonds in a neutral compound, the number of hydrogen atoms present at any carbon atom may simply be obtained by subtracting the number of bonds from four. Using this method, for the molecule 2,2,4-trimethylpentane (shown below), carbon a is connected to three hydrogen atoms, carbon b is connected to two hydrogen atoms, carbon c is connected to one hydrogen atom and carbon d is connected to no hydrogen atoms.



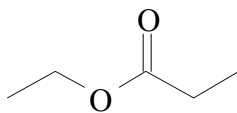
Carbon a is classified as being **primary** as it is attached to only one other carbon atom, and the hydrogen atoms bonded to carbon a are known as primary hydrogen atoms. Extending this concept leads to the designation of **secondary** for carbon b, **tertiary** for carbon c and **quaternary** for carbon d. You should be able to quickly determine that the compound above contains fifteen primary hydrogen atoms, two secondary hydrogen atoms and one tertiary hydrogen atom.

The next page contains examples of compounds containing the thirteen common functional groups that you will be responsible for knowing in CHEM 1110. The page after that contains the priority listing of all the prefixes and suffixes to be used for naming organic molecules containing these functional groups.

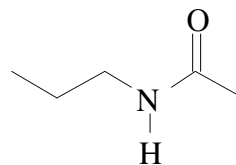
Functional Groups



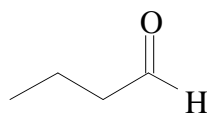
pentanoic acid
(carboxylic acid)



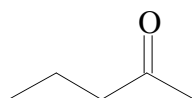
ethyl propanoate
(ester)



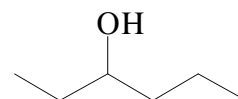
N-propyl ethanamide
(amide)



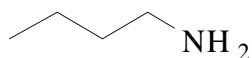
butanal
(aldehyde)



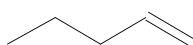
2-pentanone
(ketone)



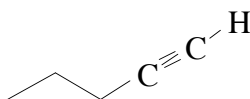
3-hexanol
(alcohol)



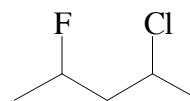
butylamine
or 1-butanamine
(amine)



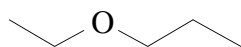
1-pentene
(alkene)



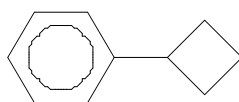
1-pentyne
(alkyne)



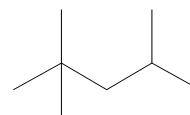
2-chloro-4-fluoropentane
(alkyl halide)



ethyl propyl ether
or 1-ethoxypropane
(ether)



cyclobutylbenzene
or phenylcyclobutane
(alkyl benzene)



2,2,4-trimethylpentane
(alkane)

Functional Group Priorities & Prefixes/Suffixes

GROUP ONE

Functional Group	Prefix	Suffix
carboxylic acid		oic acid
ester		oate
amide		amide

GROUP TWO

Functional Group	Prefix	Suffix
aldehyde	oxo	al
ketone	oxo	one
alcohol	hydroxy	ol
amine	amino	amine
alkene	enyl	ene
alkyne	ynyl	yne

SUBORDINATE GROUPS

Functional Group	Prefix	Suffix
alkyl halide	halo	
ether	oxy	ether
alkyl benzene	phenyl	benzene
alkane	yl	ane

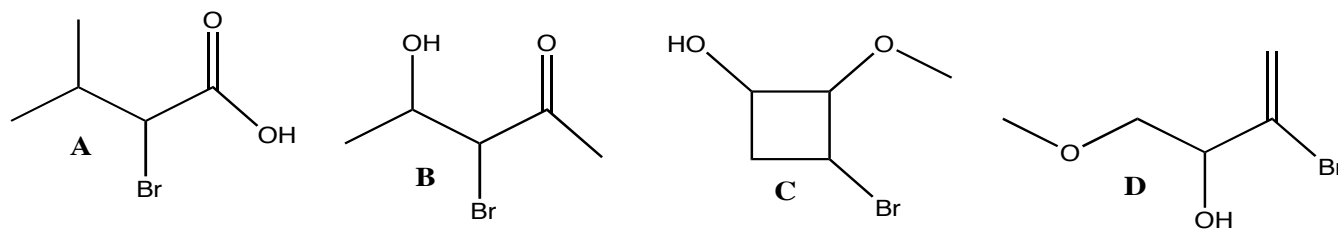
Principal functional groups are listed in decreasing priority.

Subordinate functional groups have no established priority.

The functional group at the top of the list (**carboxylic acid**) has the highest priority for naming, while the functional group at the bottom of the list (**alkane**) has the lowest priority for naming. A compound that contains several functional groups can be named by finding the functional group with the highest priority and completing the name with the appropriate suffix. The presence of the other functional groups can be indicated by using the appropriate prefixes.

If your instructor brings molecular models to class, you may get to work in small groups to build organic molecules using the same molecular formula, draw the structures, and then provide the corresponding

IUPAC names. This process can be illustrated on the next page by considering four isomeric compounds (A, B, C and D), all having the same molecular formula $C_5H_9BrO_2$.



Compound A has a **carboxylic acid** as part of a longest chain of four carbon atoms with a Br atom connected to carbon number 2 and a methyl group connected to carbon number 3. The complete IUPAC name for the compound would be:

2-bromo-3-methylbutanoic acid

Compound B has an **alcohol** and a **ketone** in addition to the Br atom. According to the priority listing of functional groups, the ketone is more important than the alcohol. Using the same procedure as above, the complete IUPAC name for the compound would be:

3-bromo-4-hydroxy-2-pentanone

Compound C has an **alcohol**, an **ether** and a ring in addition to the Br atom. The alcohol group has the highest priority, and therefore must receive the lowest number. Using the same procedure as above, the complete IUPAC name for the compound would be:

3-bromo-2-methoxy-1-cyclobutanol

Compound D has an **alcohol**, an **alkene** and an **ether** in addition to the Br atom. The alcohol group has the highest priority, and therefore must receive the lowest number when deciding where to begin naming the compound. The complete IUPAC name for the compound would be:

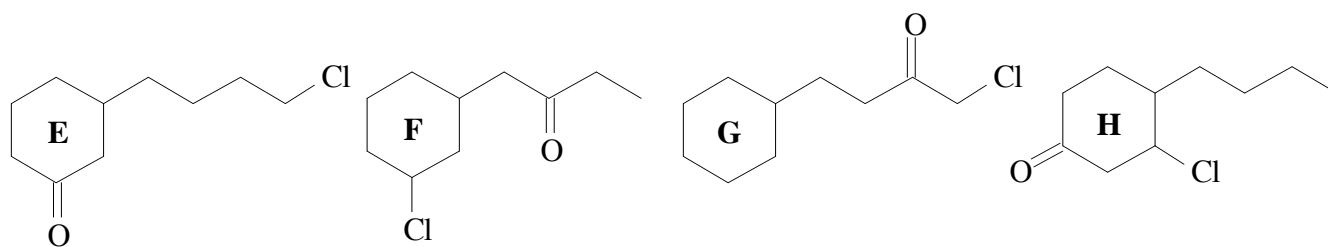
3-bromo-1-methoxy-3-butene-2-ol

At this point you may wonder why compound D was not named **3-bromo-1-methoxy-3-enyl-2-butanol**? The prefix enyl is used in cases where the alkene functional group is not part of the longest chain containing the functional group of highest priority. This can be illustrated by considering the following isomeric compounds X and Y.



The complete IUPAC name for compound X will be: **2-(3-butenyl)-1-cyclopentanol** while the complete IUPAC name for compound X will be: **1-cyclopentyl-3-butene-1-ol**

You will quickly discover that making small changes in the structure of a molecule will produce compounds with very different IUPAC names. This can be illustrated by considering the following four isomeric compounds E, F, G and H (all $C_{10}H_{17}ClO$).



The names of the four compounds must all end in “one” as the **ketone** functional group is the most important. As the highest priority functional group, the ketone must also receive the lowest possible number. The use of brackets will be required to separate two substituent numbers for compounds E and F as the two functional groups are on different parts of the molecule; i.e., one on the cyclohexyl portion and the other one on the butyl group.

In compound E, carbon number one is where the ketone group is located. At carbon number three on the ring we have a butyl group attached. The first carbon atom out from the ring is numbered as one, the chlorine atom is therefore attached to carbon number four. The use of a set of brackets for the butyl side chain will result in the following IUPAC name: **3-(4-chlorobutyl)-1-cyclohexanone**

In compound F, carbon number one is where the four-carbon chain is attached to the six-membered ring. The chlorine atom on the ring is attached to carbon number three as the point of attachment to the higher priority butyl chain must occur at carbon number one. The use of a set of brackets for the cyclohexyl side chain will result in the following IUPAC name: **1-(3-chlorocyclohexyl)-2-butanone**

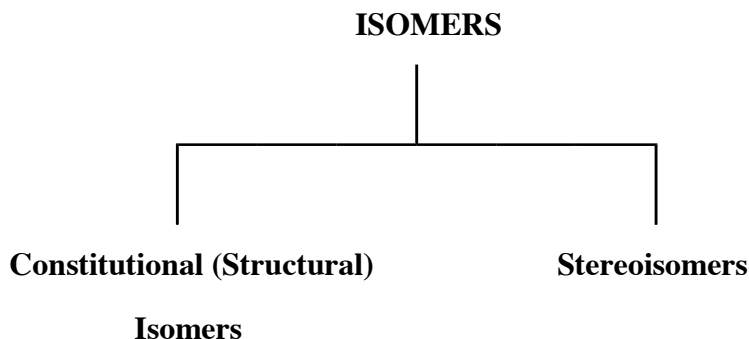
The naming process for compounds G and H can be done in the same way, resulting in the following IUPAC names:

Compound G: **1-chloro-4-cyclohexyl-2-butanone**

Compound H: **4-butyl-3-chloro-1-cyclohexanone**

With the examples presented above as a guide and using the provided tables of information, you should now be capable of naming hundreds of different organic molecules. Once you become proficient at recognizing functional groups and providing IUPAC names for compounds, it is time to move on to determining the exact relationship between two isomeric compounds. There are several different

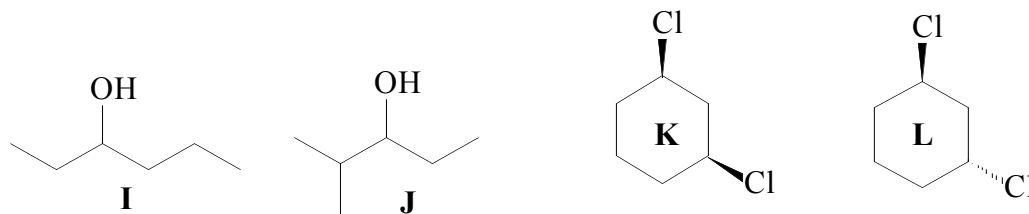
classification schemes to be found in the various textbooks on the market (including Petrucci et al); however, the scheme described below is based upon asking yourself a series of questions when presented with structural representations of several compounds that have the same molecular formula.



The first question is: **Based upon your understanding of the rules for IUPAC naming to this point, do the two compounds appear to have the same IUPAC name?**

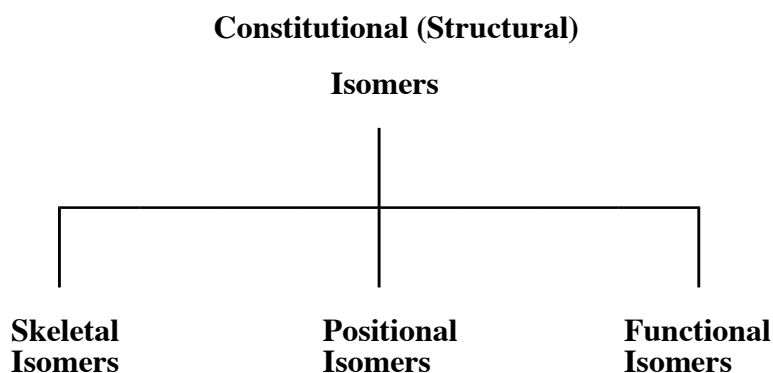
If the answer is YES, then the compounds are **stereoisomers** of each other. If the answer is NO, then the compounds are **constitutional isomers** of each other. The term **structural isomers** was originally used to describe these compounds, but was replaced several years ago.

The following compounds can be used to illustrate these types of isomers.



The name of compound I is 3-hexanol, the name of compound J is 2-methyl-3-pentanol. These compounds are constitutional isomers of each other since they have different IUPAC names. Since compounds K and L both have the same name; i.e., 1,3-dichlorocyclohexane, they must be stereoisomers of each other since they differ only in the way that the two Cl atoms are connected to the cyclohexane ring. Stereoisomers will be examined in greater detail later in this summary.

If we now consider constitutional isomers in greater detail, you find that there are three possible ways that isomers may have different names. You will now have to ask, exactly how are the two compounds different?



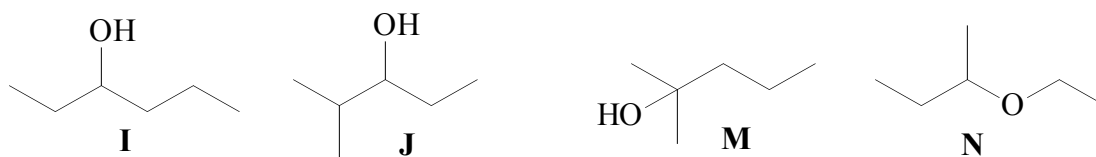
The next question is: **Do the two constitutional isomers contain different functional groups?**

If the answer is YES, then the compounds are **functional isomers** of each other. If the answer is NO, then you must ask another question.

The next question is: **Do the two constitutional isomers (which contain the same functional group) contain the same number of carbon atoms in the longest chain?**

If the answer is YES, then the two constitutional isomers are **positional isomers** of each other. If the answer is NO, then the two constitutional isomers are **skeletal isomers** of each other.

We can illustrate the three terms by providing additional constitutional isomers to consider.

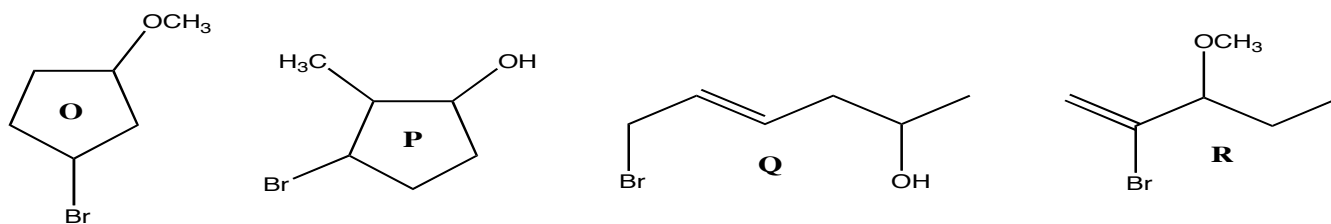


Compound I (**3-hexanol**) and compound J (**2-methyl-3-pentanol**) are skeletal isomers of each other as the longest chain containing the alcohol functional group is different for the two molecules. Compound J and compound M (**2-methyl-2-pentanol**) are positional isomers as the position of the OH group has changed, but the length of the longest chain containing the functional group is the same. Compound N (**2-ethoxybutane**) is a functional isomer of the other three constitutional isomers I, J and M.

You should now be ready to move on to the concept of **degrees (units) of unsaturation** and see how it applies to the above discussion of isomeric structures. It is important to realize that a molecule

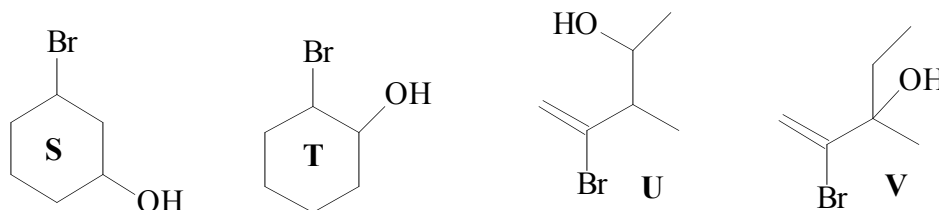
containing one degree of unsaturation does not necessarily have to be unsaturated (you will learn more about this topic from your instructor in the classroom). A saturated compound is one that contains only single bonds while an unsaturated compound is one that contains at least one multiple bond; i.e., a double or a triple bond.

Let us suppose that we wish to consider some of the possible structures for the molecular formula $C_6H_{11}BrO$. The compounds will all contain one degree of unsaturation, but they could either be saturated or unsaturated. The following four compounds would represent two sets of functional isomers, one set in which both compounds are saturated and one set in which both compounds are unsaturated.



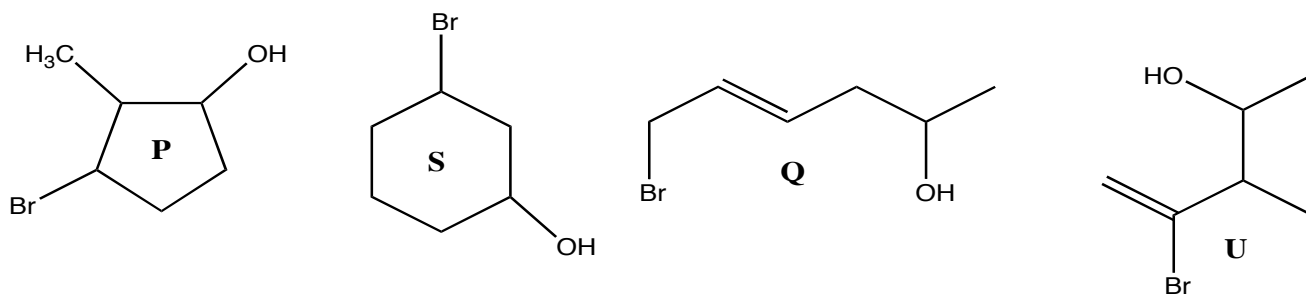
Compound O (**3-bromo-1-methoxycyclopentane** or **1-bromo-3-methoxycyclopentane**) and compound P (**3-bromo-2-methyl-1-cyclopentanol**) are saturated functional isomers of each other. Compound Q (**6-bromo-4-hexene-2-ol**) and compound R (**2-bromo-3-methoxy-1-pentene**) are unsaturated functional isomers of each other.

We can repeat the above process for a consideration of positional isomers.



Compound S (**3-bromo-1-cyclohexanol**) and compound T (**2-bromo-1-cyclohexanol**) are saturated positional isomers of each other. Compound U (**4-bromo-3-methyl-4-pentene-2-ol**) and compound V (**4-bromo-3-methyl-4-pentene-3-ol**) are unsaturated positional isomers of each other.

We can repeat the above process for a consideration of skeletal isomers using some of the compounds from above.



Compound P and compound S are saturated skeletal isomers of each other, while compound Q and compound U are unsaturated skeletal isomers of each other. There are obviously many more possible compounds for the same formula $C_6H_{11}BrO$.

We will now return for a more detailed discussion of stereoisomers. Most students (with a little practice) easily comprehend the relationship between constitutional isomers; i.e., compounds which have different IUPAC names. Many students; however, have much greater difficulty with two molecules that initially appear to have the same IUPAC name. Compounds that fall into this category have the same connectivity of all the atoms, but they differ in the way in which the atoms are arranged in space. A stereochemical prefix must precede the IUPAC name to indicate the exact location (in three-dimensional space) of all the atoms. These compounds are classified as **stereoisomers** of each other and can be broadly classified as to whether they are **chiral** or **achiral**; i.e., containing an internal plane of symmetry or not. A chiral molecule can be either right or left-handed; however, a detailed discussion of this aspect of stereochemistry will not be presented in this summary.

Asking questions will again form part of the analysis. We can consider the structures of two isomeric compounds; i.e., compounds having the same molecular formula, and ask the question:

Do these compounds appear to have the same IUPAC name?

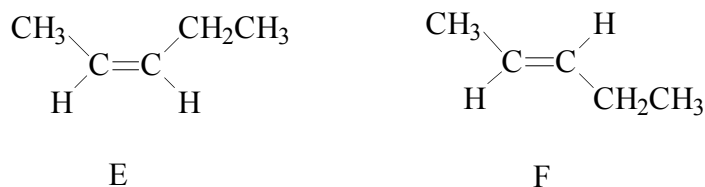
If the answer is YES, then the two compounds are **stereoisomers** of each other. If the answer is NO, then the two compounds are **constitutional isomers** of each other.

We will now consider the situation where the two compounds initially appear to have the same IUPAC name and see how to determine the exact relationship between the two stereoisomers.

The new question is: **Can the structures be inter-converted by simple bond rotation?**

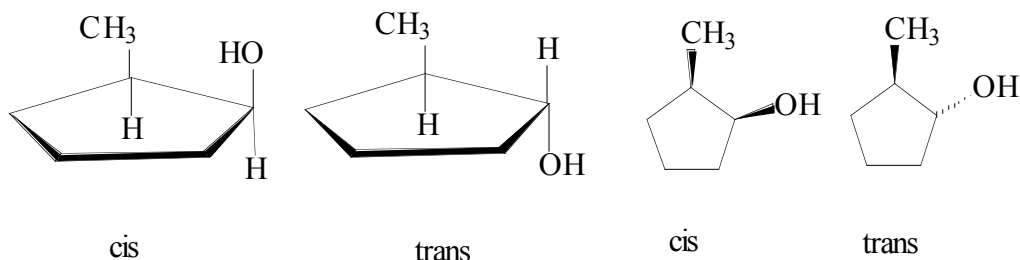
If the answer is YES, then the two compounds are **conformational isomers** of each other. You will learn more about this particular class of isomers if you continue on to take CHEM 2320.

If the answer to the above question is NO, then the two compounds are **configurational isomers** of each other. The compounds are also often referred to as **geometric isomers** of each other. The only way that the structures can be inter-converted is by breaking covalent bonds; the isomerism is a result of restricted rotation. One example is shown below for the compound **2-pentene**.



Both compounds have four groups attached to the carbon atoms of the alkene portion of the molecule. In compound E, the two hydrogen atoms are located on the same side of the molecule, while in compound F the two hydrogen atoms are located on opposite sides of the molecule. The prefix **cis** is used for identical groups that are on the same side, while the prefix **trans** is used for groups that are on opposite sides. The complete IUPAC name for compound E is **cis-2-pentene**, while **trans-2-pentene** is the IUPAC name for compound F.

Geometric isomers are also possible for cyclic compounds. These can be drawn in several ways; two of them are shown below for **cis-2-methyl-1-cyclopentanol** and **trans-2-methyl-1-cyclopentanol**.



It is important to remember that the prefixes **cis** and **trans** must always refer to identical groups (H atoms in the examples above). If the molecule does not contain two identical groups, a different set of prefixes must be used. You will learn more about this aspect of stereochemistry if you continue on to take CHEM 2320.