Isomerism

CH_4 C_2H_6 C_3H_8

C_4H_{10}

C_5H_{12}

Constitutional isomers ...

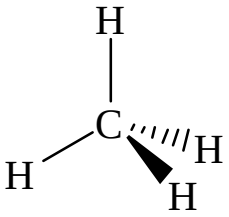
C_3H_8O

Positional isomers ...

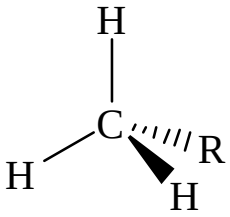
Functional isomers...

How many constitutional isomers are there for the formula C_4H_8O?

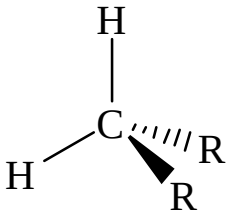
Carbon atoms are often classified as primary (1°), secondary (2°), tertiary (3°), and quaternary (4°)...



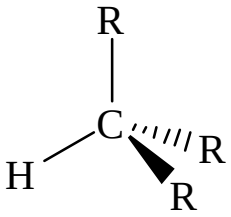
methane



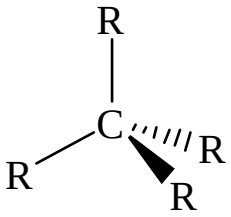
1°



2°



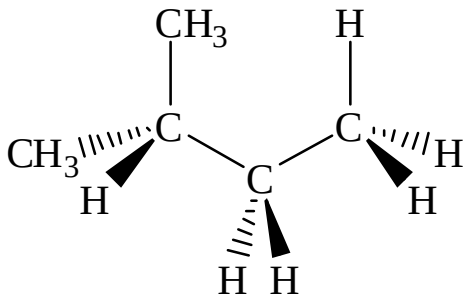
3°



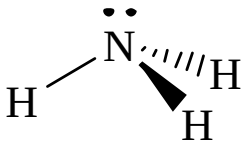
4°

Remember, these labels only pertain to carbon atoms with *four single bonds*.

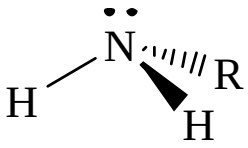
Label the carbon atoms in the following molecule as 1°, 2°, 3°, or 4°.



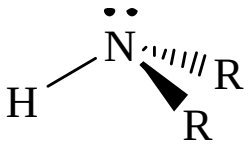
This terminology also applies to amines...



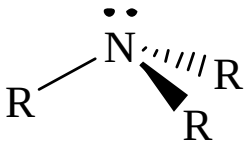
ammonia



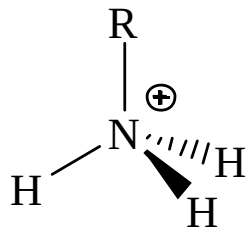
1°



2°

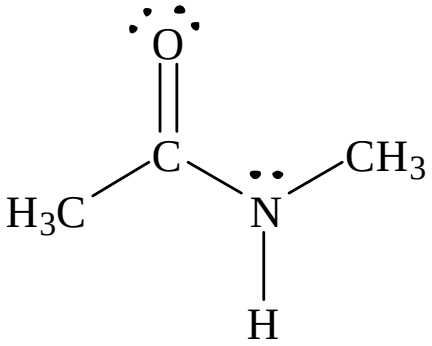


3°

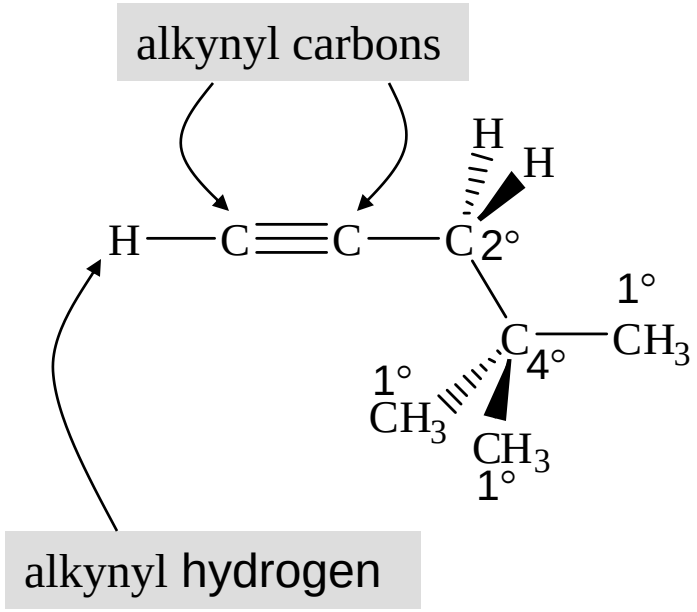


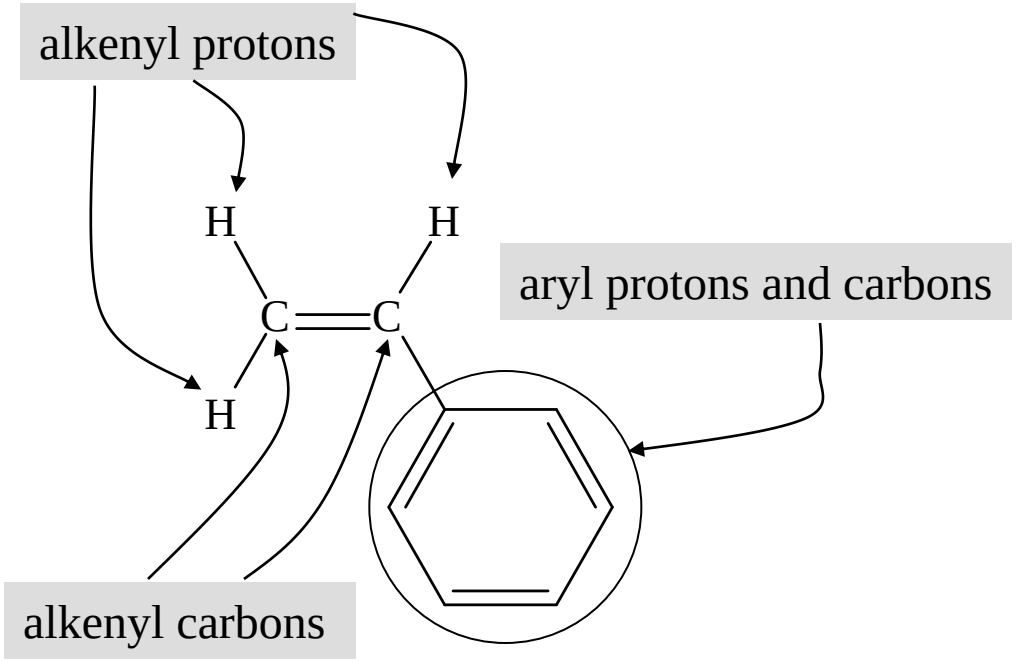
4°

and amides...



Unsaturated Carbon Classification...

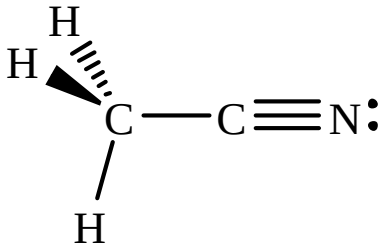


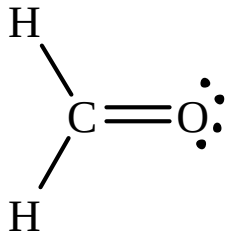


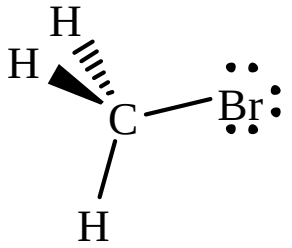
For more examples, see the textbook, page 23.

Until you hear otherwise, the terms primary, secondary, tertiary and quaternary shall apply to saturated carbons. So, if asked for a molecule that contains only 3° carbons, benzene would not be a correct answer.

Functional Groups: "Reactive" centers that contain heteroatoms or multiple carbon-carbon bonds.

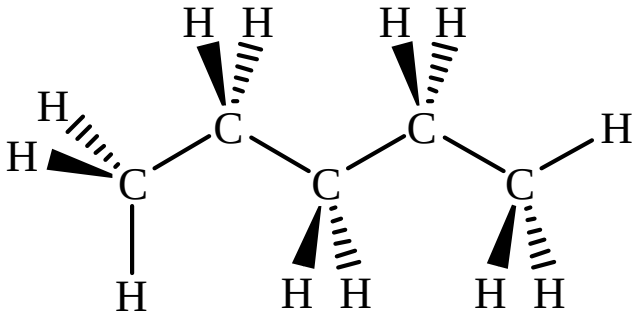




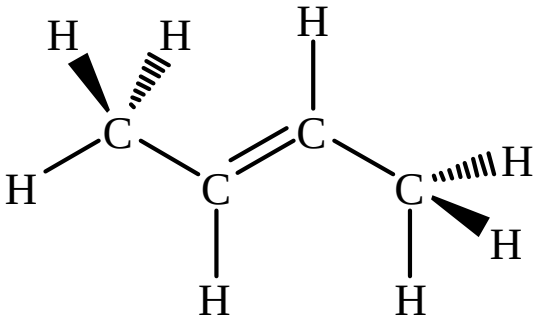


Heteroatom: atoms other than carbon or hydrogen. Typically N, O, Si, P, S, Se, F, Cl, Br, I.

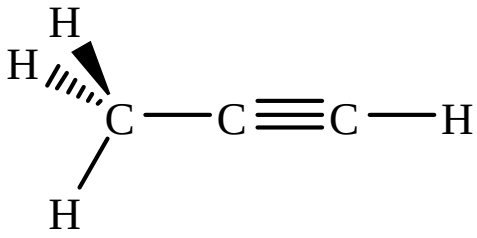
multiple carbon-carbon bonds: unsaturation.



alkanes



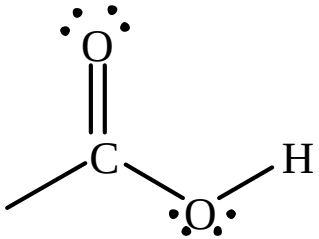
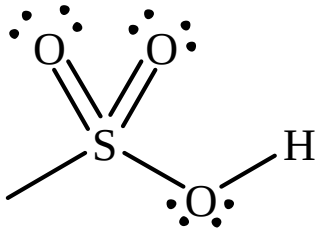
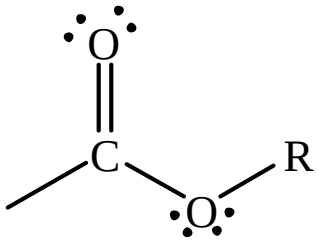
alkenes

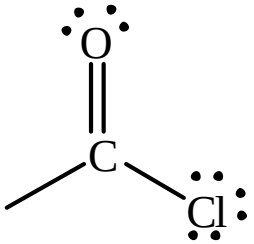
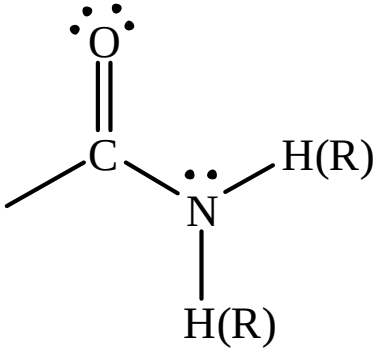
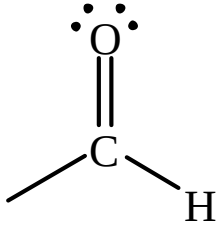
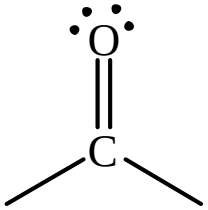


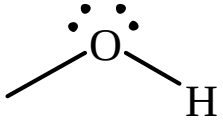
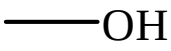
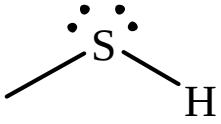
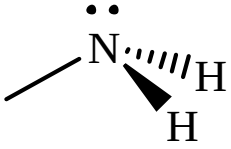
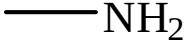
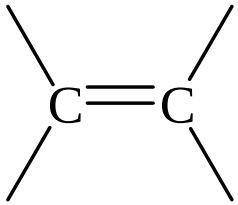
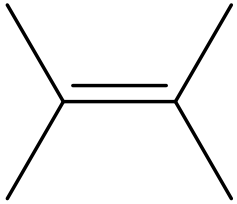
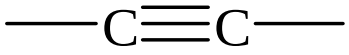
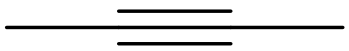
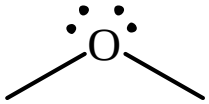
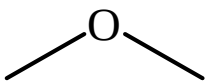
alkynes

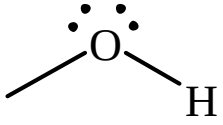
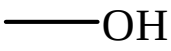
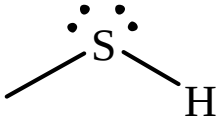
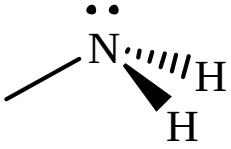
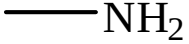
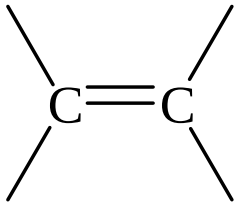
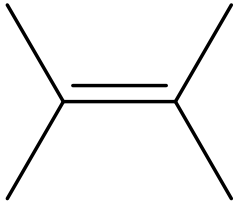
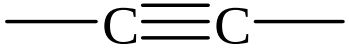
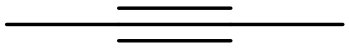
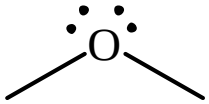
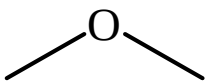
The Functional Groups

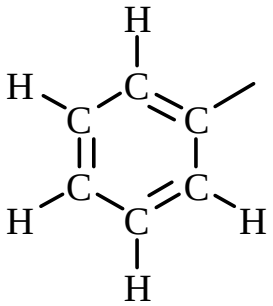
(Table 1.1 page 4)

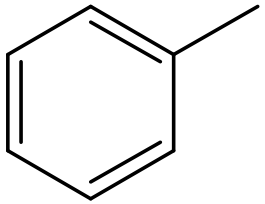
Structure	Condensed Structure	Name	Nomenclature suffix
	—CO_2H or —COOH	Carboxylic acid	-oic acid
	—SO_3H	Sulfonic acid	-sulfonic acid
	—CO_2R or —COOR	Ester	-oate

	—COCl	Acid chloride	-oyl chloride
	—$CONH_2(R)_2$	Amide	-amide
	—CN	Nitrile	-nitrile
	—CHO	Aldehyde	-al
	—CO—	Ketone	-one

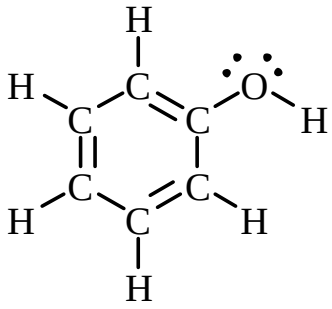
		Alcohol	-ol
		Thiol	-thiol
		Amine	-amine
		Alkene	-ene
		Alkyne	-yne
		Ether	N/A

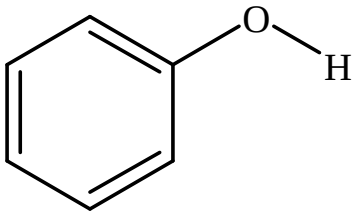
		Alcohol	-ol
		Thiol	-thiol
		Amine	-amine
		Alkene	-ene
		Alkyne	-yne
		Ether	N/A





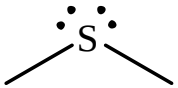
Arene N/A



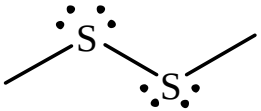


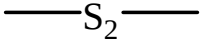
Phenol N/A

other common functional groups…

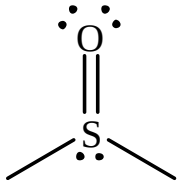


Sulfide N/A

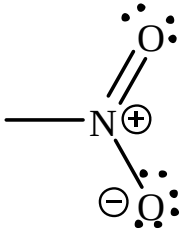


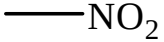


Disulfide N/A



Sulfoxide N/A

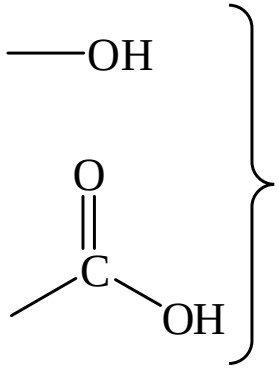




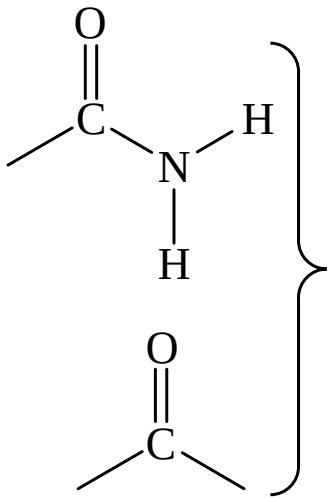
Nitro N/A

Things to watch for...

…common structural elements.



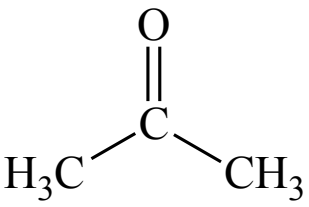
Both of these contain the *hydroxyl group(-OH)* but they represent different functional groups.



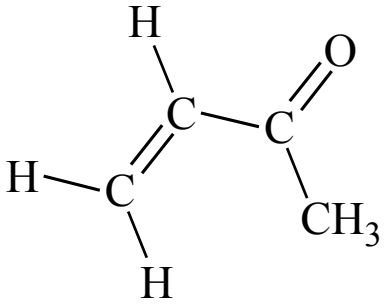
Both of these contain the *carbonyl group(C=O, pronounced carbon-eel group)* but they represent different functional groups.

IMPORTANT: the carbonyl group by itself *is not* a functional group. It is part of many functional groups depending on what is attached to it.

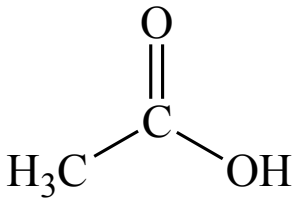
The "open" bond in these structures is attached to a carbon...



Ketone

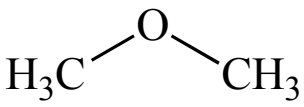


Ketone

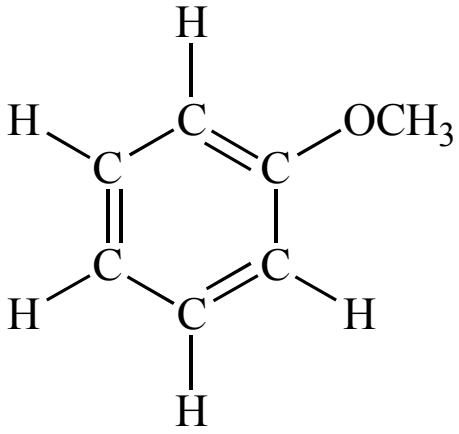


Not a ketone

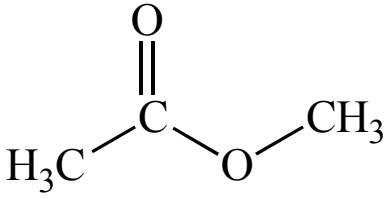
and, with the exception of alkene/alkyne/arene, this carbon is usually not part of another functional group...



Ether



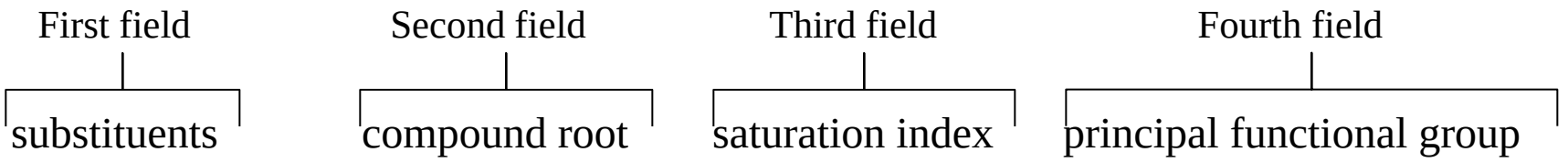
Ether



Not an ether

Organic Nomenclature

Systematic IUPAC Nomenclature – Compound names have four fields.

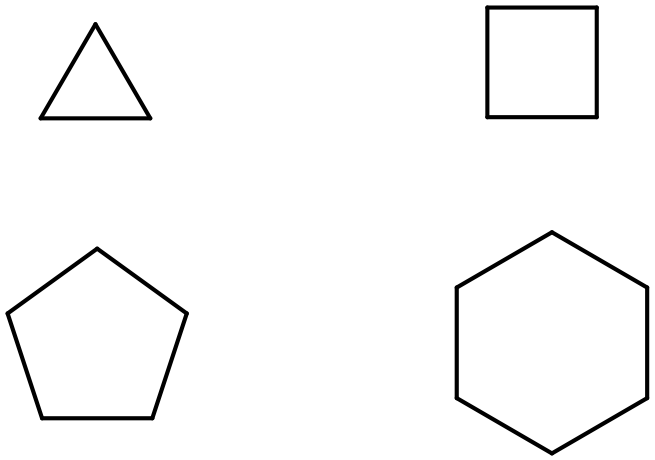


Compound Root – Second Field

The compound root name is based on the number of carbon atoms in the longest continuous chain or ring.

n	C_nH_{2n+2}	alkane
1	CH_4	meth-ane
2	CH_3CH_3	eth-ane
3	$CH_3CH_2CH_3$	prop-ane
4	$CH_3(CH_2)_2CH_3$	but-ane
5	$CH_3(CH_2)_3CH_3$	pent-ane
6	$CH_3(CH_2)_4CH_3$	hex-ane
7	$CH_3(CH_2)_5CH_3$	hept-ane
8	$CH_3(CH_2)_6CH_3$	oct-ane
9	$CH_3(CH_2)_7CH_3$	non-ane
10	$CH_3(CH_2)_8CH_3$	dec-ane

For cyclic molecules, the prefix ‘cyclo’ is added before the compound root prefix.



Saturation Index – Third Field

The presence of multiple bonds is indicated by “ene” (carbon-carbon double bonds) and/or “yne” (carbon-carbon triple bonds) in the third field of the name

When a *principal* functional group is not present, number the chain to give the multiple bond the lowest number. If there are multiple multiple bonds, add the prefix di, tri, tetra, etc to indicate the number of double or triple bonds in the molecule and give a number to indicate its position.

Substituents – First Field

- 5-chloro-1-hexene (or 5-chlorohex-1-ene)

- 4,5-dichloro-5-fluoro-1-hexene (or 4,5-dichloro-5-fluorohex-1-ene)

Principal Functional Groups – Forth Field

Functional Group	Suffix
Carboxylic acid	-oic acid
Sulfonic acid	-sulfonic acid
Ester*	-oate
Acid Chloride	-oyl chloride
Amide*	-amide
Nitrile	-nitrile
Aldehyde	-al
Ketone	-one
Alcohol (including phenol)	-ol
Thiol	-thiol
Amine	-amine

Note that certain functional groups are never considered as a principal functional group and are always treated as a substituent. These include the halogens, ethers, and nitro groups.

Principal Functional Groups – Forth Field

- 5-chloro-1-hexen-3-ol (or 5-chlorohex-1-en-3-ol)

- 2-chloro-5-hexen-1-ol (or 2-chlorohex-5-en-1-ol)

- 2-chloro-4-hydroxy-5-hexenal (or 2-chloro-4-hydroxyhex-5-enal)

Note that no number is necessary for principal functional groups that must be terminal because they include the first carbon atom of the main chain.

Substituent List

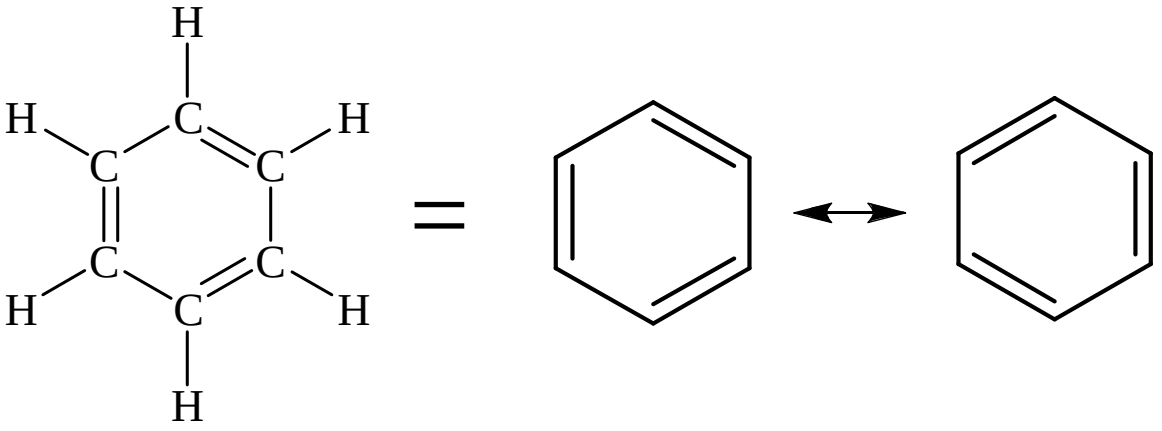
	Name
$-CH_3$	methyl
$-CH_2CH_3$	ethyl
$-CH_2CH_2CH_3$	propyl
$-CH_2CH_2CH_2CH_3$	butyl
etc.	
$-CH(CH_3)_2$	isopropyl
$-CH_2CH(CH_3)_2$	isobutyl
$-CH(CH_3)CH_2CH_3$	*s*-butyl
$-C(CH_3)_3$	*t*-butyl
$-C_6H_5$	phenyl
$-CH_2C_6H_5$	benzyl

	Name
$-OCH_3$	methoxy
$-OCH_2CH_3$	ethoxy
$-OCH_2CH_2CH_3$	propoxy
$-OCH_2CH_2CH_2CH_3$	butoxy
etc.	
$-OCH(CH_3)_2$	isopropoxy
$-OCH_2CH(CH_3)_2$	isobutoxy
$-OCH(CH_3)CH_2CH_3$	*s*-butoxy
$-OC(CH_3)_3$	*t*-butoxy
$-OC_6H_5$	phenoxy
$-OCH_2C_6H_5$	benzoxy

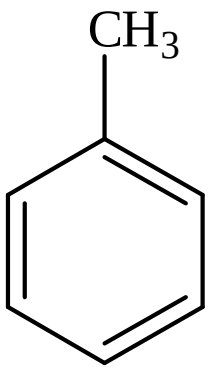
	Name
-F	fluoro
-Cl	chloro
-Br	bromo
-I	iodo
$-NH_2$	amino
$-NO_2$	nitro
-CN	cyano
-OH	hydroxy
=O	oxo
-SH	mercapto

Other names you need to know...

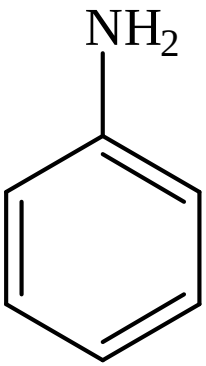
Benzene



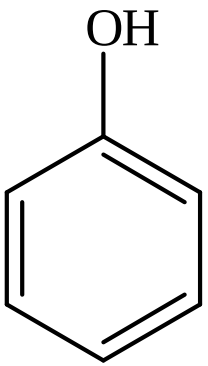
Molecules with this substructure are treated as a class – arenes.



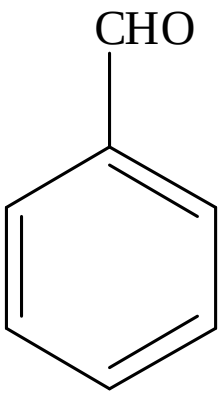
toluene*



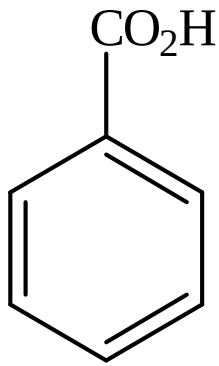
aniline*



phenol



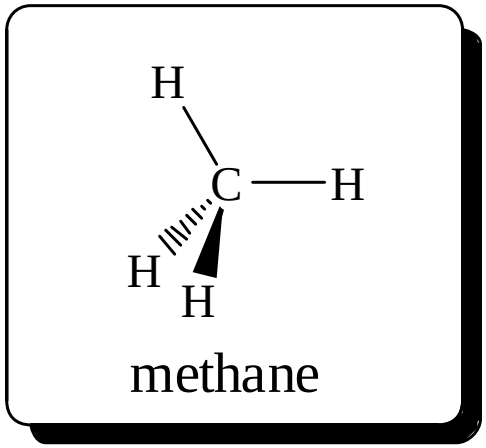
benzaldehyde

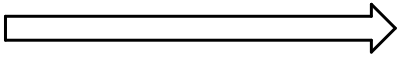


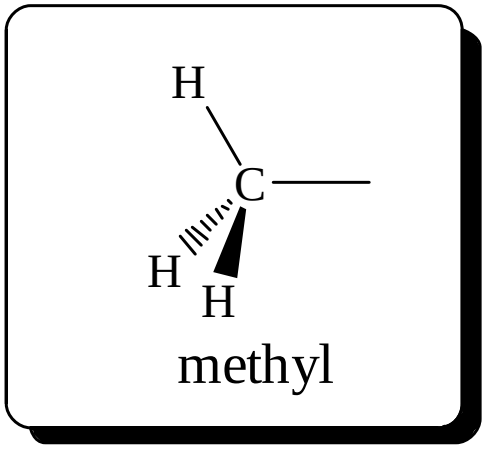
benzoic acid

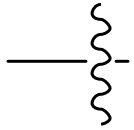
*these are not IUPAC names but common names that you should know.

Naming Carbon-Based Substituents

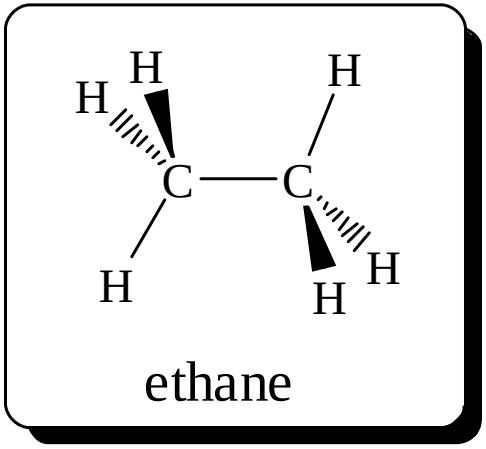


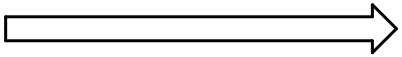


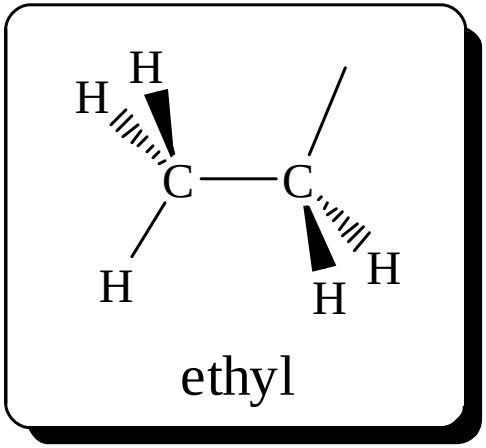




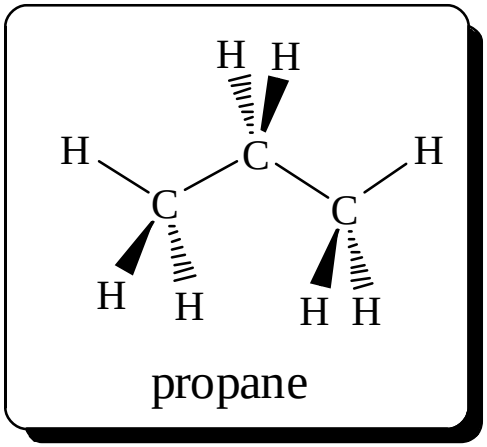
methyl group

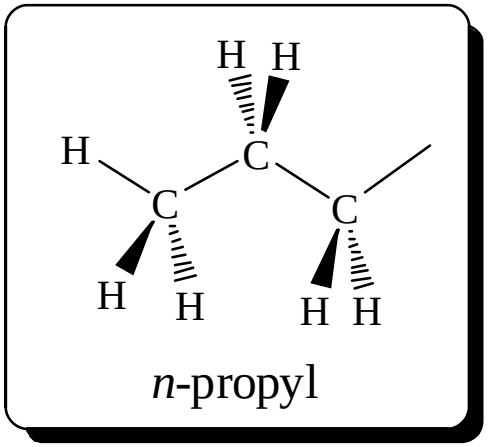


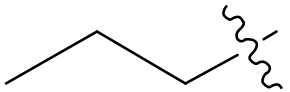




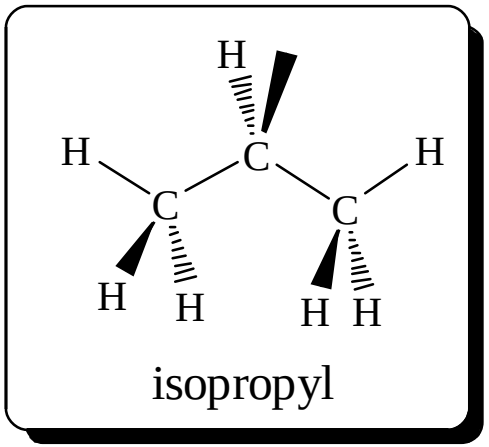
ethyl group

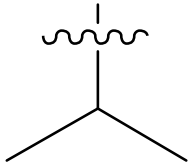






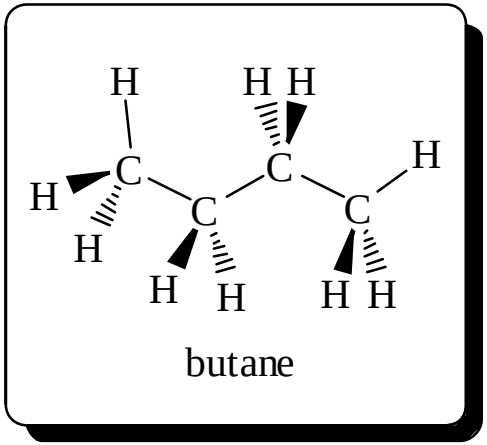
The *n*-propyl or propyl group. ("n" stands for normal i.e. straight chain)

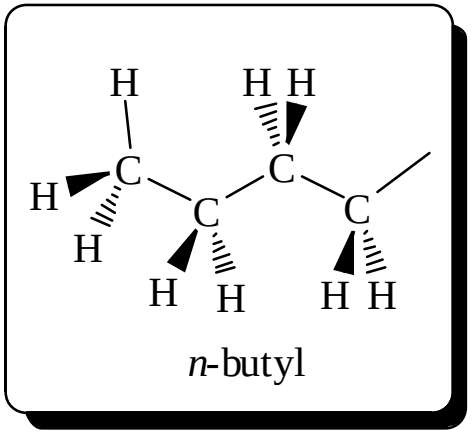


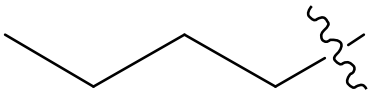


The 2-propyl or isopropyl group.

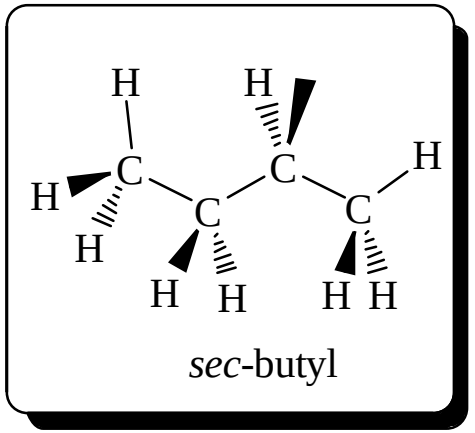
Notice that the only difference between n-propyl and isopropyl is the *point of attachment*.

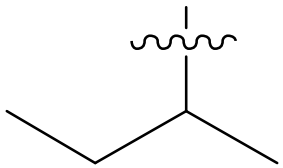






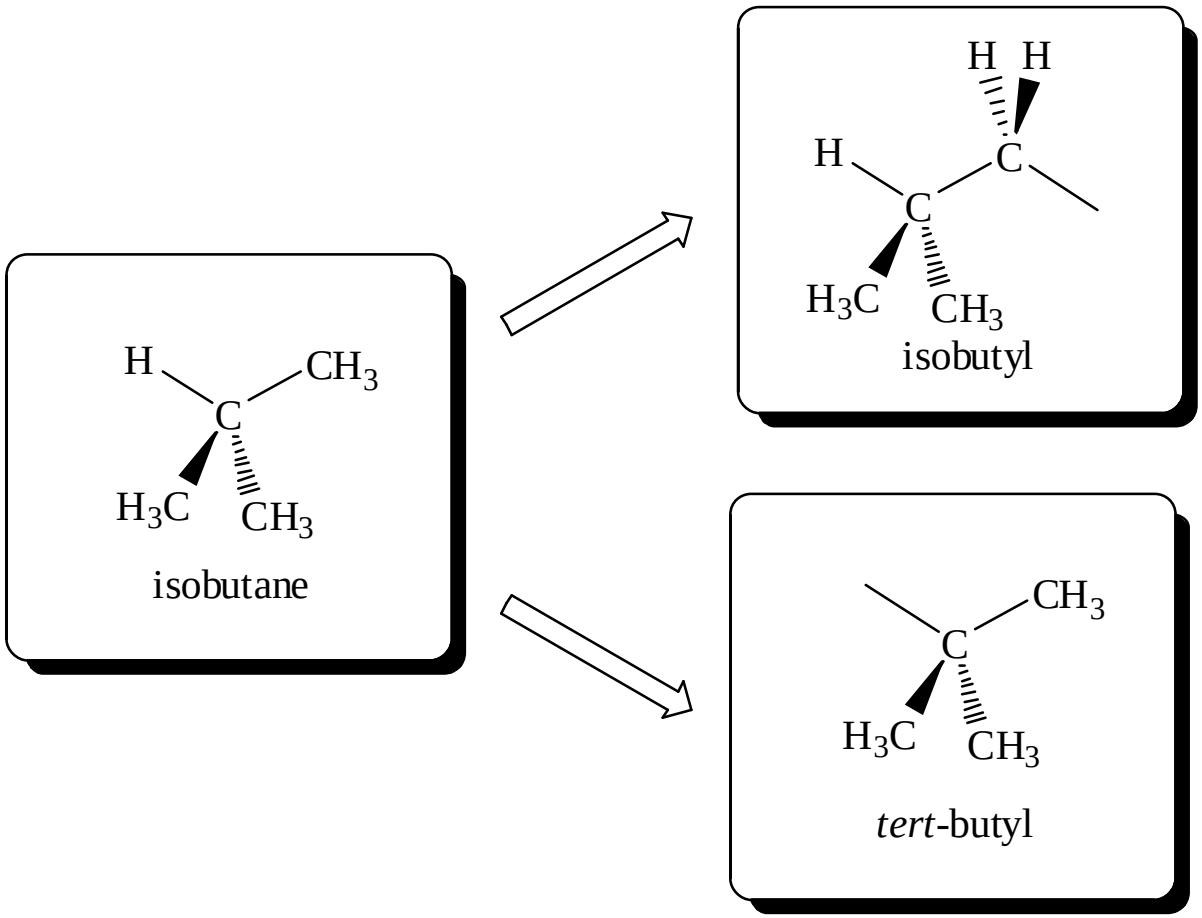
The *n*-butyl or butyl group.

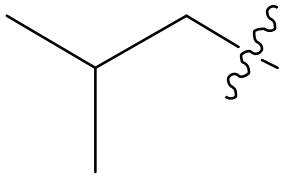




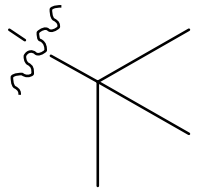
The 2-butyl, *sec*-butyl or *s*-butyl group.

Again, notice that the only difference is the *point of attachment*.



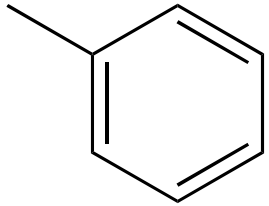


The isobutyl group.

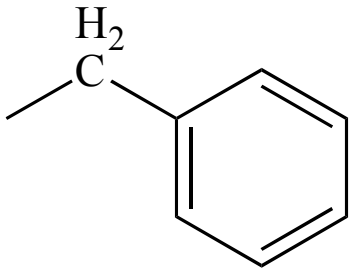


The 2-methyl-2-propyl, *tert*-butyl or *t*-butyl group.

Aryl based Substituents



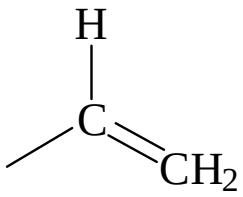
Phenyl —Ph or $-C_6H_5$



Benzyl —Bn or $-CH_2C_6H_5$

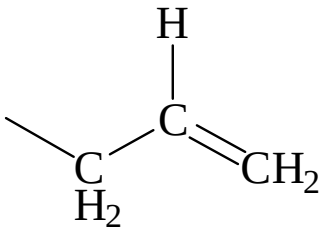
"benzylic"

Common Unsaturated Alkyl substituents

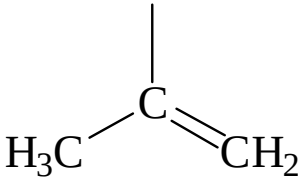


Vinyl or ethenyl

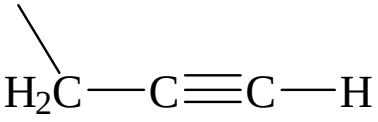
"allylic"



Allyl or propenyl



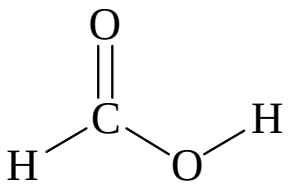
2-propenyl or isopropenyl



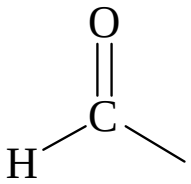
Propargyl

Yet more substituents...

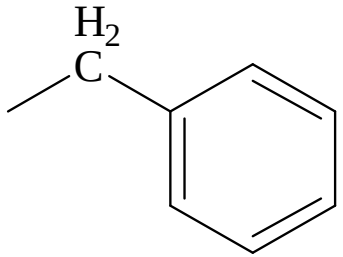
"Acyl" substituents...



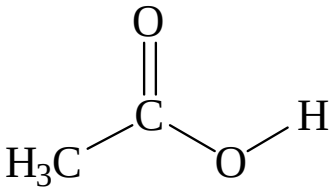
"Formic acid"



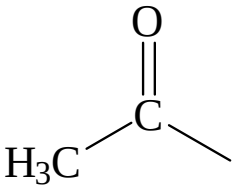
formyl



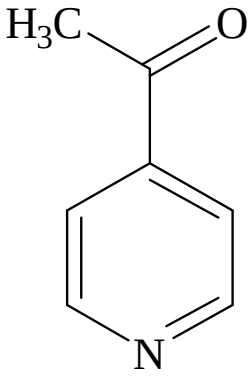
Benzyl



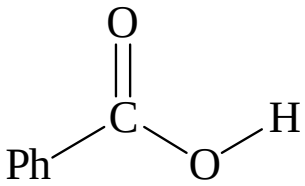
"Acetic acid"



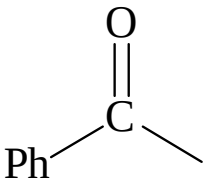
acetyl



4-acetylpyridine



Benzoic acid



benzoyl

Alkoxy substituents

CH_3OH

Methanol

H_3CO——

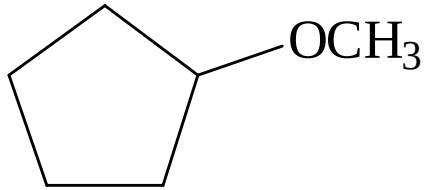
methoxy

CH_3CH_2OH

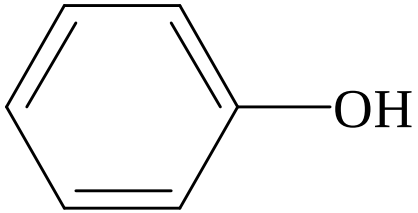
Ethanol

H_3CH_2CO——

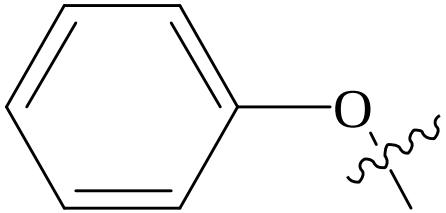
ethoxy



methoxycyclopentane



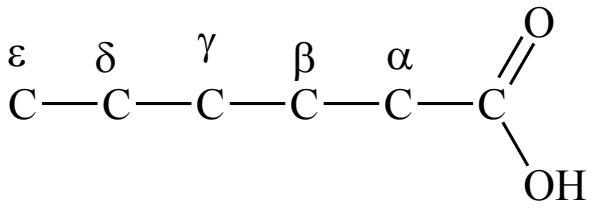
Phenol

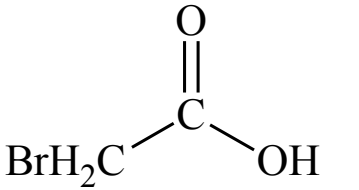


phenoxy

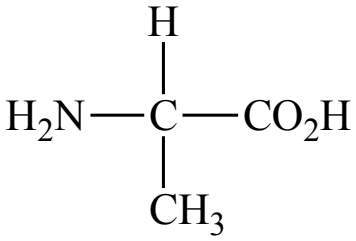
It's all Greek...

On occasion, greek letters are used to indicate the position of an atom relative to a functional group...

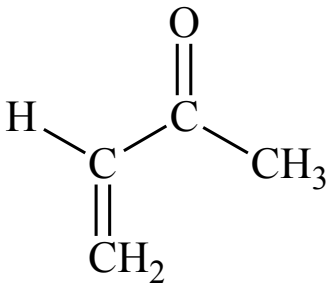




"α-bromoacetic acid"

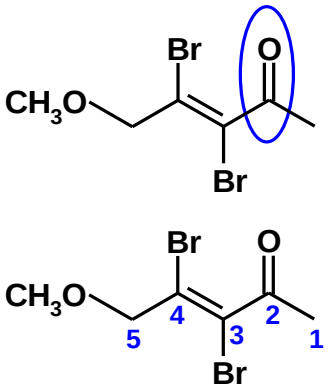


An α-amino acid.



An example of an α,β-unsaturated ketone.

Organic Nomenclature Summary:



Practice

Substituents	Root	Unsaturations	Functional Group