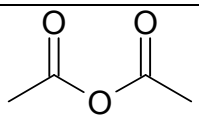
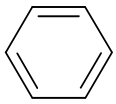
IUPAC NOMENCLATURE OF ORGANIC COMPOUNDS

IUPAC – International Union of Pure and Applied Chemistry

CLASSIFICATION OF FUCNTIONAL GROUPS FOR PURPOSES OF NOMENCLATURE

FUNCTIONAL GROUP	STRUCTURE	NAME WHEN USED AS SUFFIX (PARENT)	NAME WHEN USED AS PREFIX (SUBSTITUENT)
Principal Groups			
Carboxylic acid	-COOH	-oic acid	carboxy
	RING-COOH	-carboxylic acid	
Carboxylic anhydrides		-oic anhydride	
	RING-(C=O)-O-C(=O)-	-carboxylic anhydride	
Carboxylic esters	-(C=O)OR	-oate	alkoxycarbonyl
	RING-(C=O)OR	-carboxylate	
Acid halides	-(C=O)X	-oyl halide	halocarbonyl
	RING-(C=O)X	carbonyl halide	
Amides	-(C=O)NH_2	-amide	amido
	RING-(C=O)NH_2	-carboxamide	
Nitriles	-C≡N	-nitrile	cyano
	RING-C≡N	-carbonitrile	
Aldehydes	-(C=O)H	-al	oxo
	RING--(C=O)H	-carbaldehyde	formyl
Ketones	C=O	-one	oxo
Alcohols	-OH	-ol	hydroxy
Phenols	-OH	-ol	hydroxy
Thiols	-SH	-thiol	mercapto / sulfanyl
Amines	-NH_2	-amine	amino
Imines	=NH	-imine	imino
Benzene		-benzene	phenyl
Alkenes	C=C	-ene	alkenyl
Alkynes	C≡C	-yne	alkynyl
Alkanes	C-C	-ane	alkyl
Subordinate Groups			
Ethers	-OR		alkoxy
Sulfides	-SR		alkylthio
Halides	-F, -Cl, -Br, -I		halo
Nitro	-NO_2		nitro
Azides	N=N=N		azido
Diazo	=N=N		diazo

- The principal functional groups are listed in order of decreasing priority; subordinate functional groups have no established priority order.

COMPONENTS OF AN ORGANIC COMPOUND NAME

LOCANTS – PREFIXES – PARENT – SUFFIX

LOCANTS – numbers that tell where the substituents are located on the main chain or ring
PREFIX – parts that identify what substituents are located on the main chain or ring
PARENT – part that identifies the size of the parent chain
SUFFIX – part which identifies the principal functional group class to which the molecule belongs
Substituent – any other group attached to the carbon chain other than hydrogen

GENERAL STEPS AND RULES IN NAMING ORGANIC COMPOUNDS

1. Find the longest carbon chain containing the principal functional group and assign it as the parent chain. In case for a presence of two or more functional groups, the highest priority functional group will be chosen for the parent chain and the rest will simply be substituents.

2. Determine the type and number (quantity) of the substituents attached on the parent carbon chain.

3. Use prefixes di, tri, tetra, etc to indicate the number (quantity) of similar substituents.

4. Start assigning numbers for each carbon in the parent chain beginning at the terminal carbon nearest the principal functional group or the first branch point (in alkanes and alkyl halides). Make sure to assign the LOWEST possible numbers for all substituents. In case of ambiguity in numbering (i.e. same number at both terminal ends) assign the lowest number to the substituent which follows the alphabetical order.

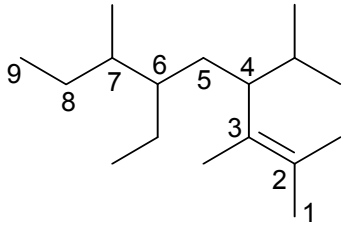
5. Determine the position (carbon number) of all the substituents in the main/parent chain.

6. Use comma to separate numbers and use dash/hyphen to separate numbers and words.

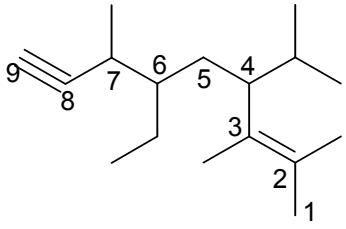
7. Arrange the names of the substituents in alphabetical order (excluding the prefixes like di, tri, tetra; sec and tert); only iso and neo are considered in alphabetization and they are not separated by a dash.

8. Write the name of the compound according to the format above.

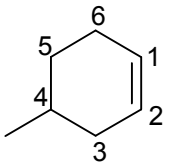
Example



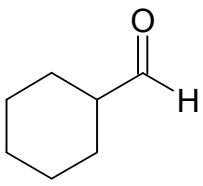
6-ethyl-4-isopropyl-7-methyl-2-nonene



6-ethyl-4-isopropyl-7-methyl-2-nonen-8-yne



4-methyl-1-cyclopentene

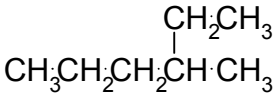


cyclohexanecarbaldehyde

A. NAMING ALKANES

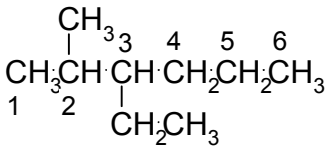
1. Find the parent carbon.

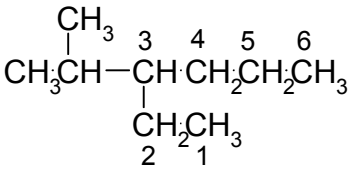
a. Find the longest continuous chain of carbon atoms and use the name of that chain as the parent name:



the longest chain has 6 carbons, so this is hexane

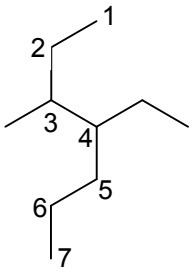
b. If two chains of equal length are present, choose the one with the greater number branch points as the parent:



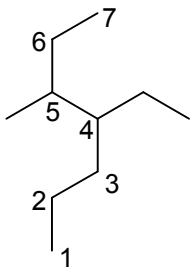


hexane with two substituents and NOT hexane with one substituent

2. Number the atoms in the main chain beginning at the end nearer the first branch point.

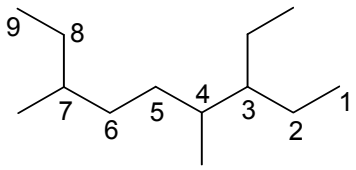


and NOT

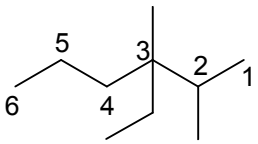


- C3 is the first branch point and not C4

3. Identify and number the substituents.

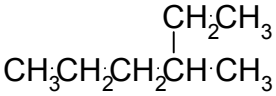


Substituents:
On C3, CH_2CH_3 (3-ethyl)
On C4, CH_3 (4-methyl)
On C7 CH_3 (7-methyl)

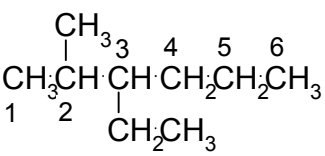


Substituents:
On C2, CH_3 (2-methyl)
On C3, CH_3 (3-methyl)
On C3, CH_2CH_3 (3-ethyl)

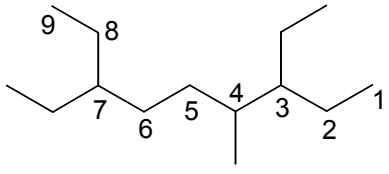
4. Write the name as a single word. Use hyphens to separate number-word prefixes and commas to separate numbers. If two or more different side chains are present, cite them in alphabetical order. If two or more identical side chains are present, use one of the prefixes di-, tri-, tetra-, and so forth. Do not use these prefixes in alphabetizing.



ethylhexane

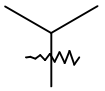
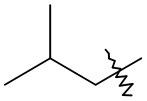
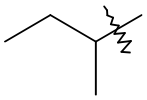
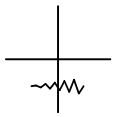
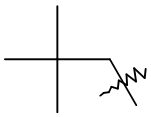
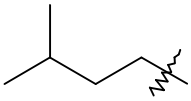


3-ethyl-2-methylhexane



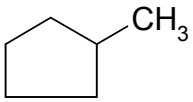
3,7-diethyl-4-methylnonane

SOME ALKYL GROUPS USED IN IUPAC NAMING

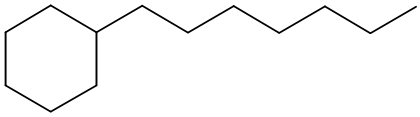
					
isopropyl	isobutyl	sec-butyl	tert-butyl	neopentyl	isopentyl

B. NAMING CYCLOALKANES

1. Count the number of carbon atoms in the ring, and add the prefix cyclo- to the name of the corresponding alkane. If a substituent is present on the ring, the compound is named as an alkyl-substituted cycloalkane. If the number of carbon in the chain is greater than the number of carbon in the ring, then, the compound has to be named as a cycloalkyl substituted alkane.

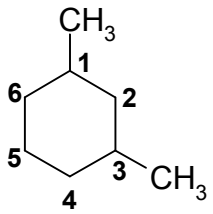


methylcyclopentane

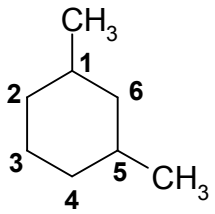


cyclohexylpentane

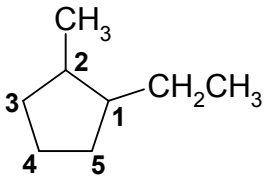
2. For substituted cycloalkanes, start at a point of attachment and number around the ring. If two or more substituents are present, begin numbering at the group that has alphabetical priority and proceed around the ring so as to give the second substituent the lowest number.



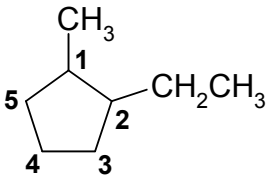
1,3-dimethylcyclohexane NOT



1,5-dimethylcyclohexane

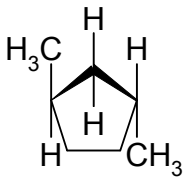


1-ethyl-2-methylcylcopentane NOT



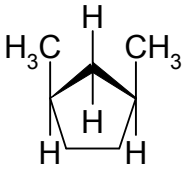
2-ethyl-1-methyl-cyclopentane

NAMING CIS AND TRANS ISOMERISM IN CYCLOALKANES



trans-1,3-dimethylcyclopentane

NOT EQUAL TO

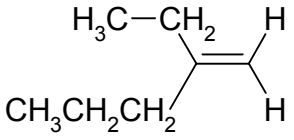


cis-1,3-dimethylcyclopentane

- cycloalkanes are isomers of alkenes
- cycloalkanes also has geometric isomers: cis and trans

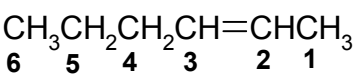
C. NAMING ALKENES

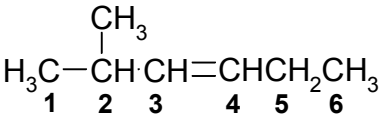
1. Name the parent carbon. It is the longest carbon chain containing the double bond and name the compound using the suffix –ene.



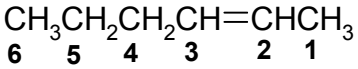
→ pentene and NOT hexane because the 6 C does not contain the double bond

2. Number the carbon atoms. Begin numbering at the end nearer the double bond. If the double bond is equidistant from the two ends, begin numbering at the end nearer the first branch point. This rule ensures that the double bond carbons receive the lowest numbers:

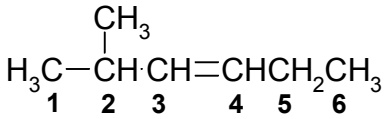




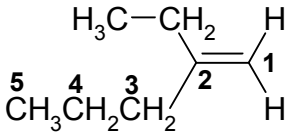
3. Write the full name. Number the substituents according to their position in the chain and list them alphabetically. Indicate the position of the double bond by giving the number of the first alkene carbon. If more than one double bond is present, give the position of each and use one of the suffixes –diene, -triene, and so on.



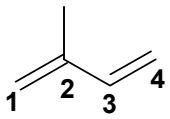
2-hexene
or hex-2-ene



2-methyl-3-hexene
or 2-methylhex-3-ene

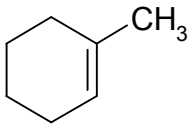


2-ethyl-1-pentene

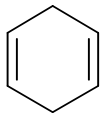


2-methyl-1,3-butadiene

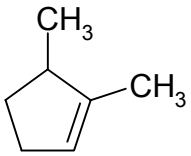
4. Cycloalkenes are named in similar way, but because there is no chain end to begin from, number the cycloalkenes so that the double bond is between C1 and C2 and so that the first substituent has a low number as possible. If there is only one double bond, it is not necessary to specify the position of the double bond in the name because it is always between C1 and C2:



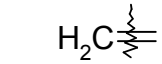
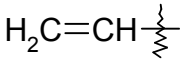
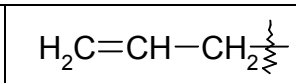
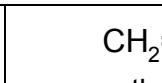
1-methylcyclohexene



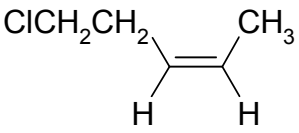
1,4-cyclohexadiene



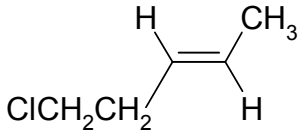
1,5-dimethylcyclopentene

 methylene group	 vinyl group	 allyl group	 ethylene

NAMING CIS AND TRANS IN ALKENES

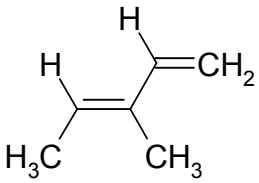


cis-5-chloro-2-pentene

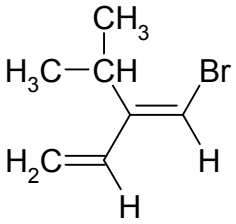


trans-5-chloro-2-pentene

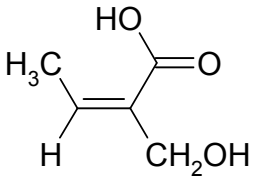
NAMING TRISUBSTITUTED AND TETRASUBSTITUTED ALKENES
The E,Z Designation: Cahn-Ingold-Prelog Rules



(3E)-3-methyl-1,3-pentadiene



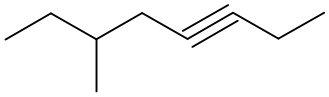
(3E)-1-bromo-2-isopropyl-1,3-butadiene



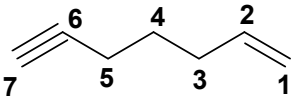
(2Z)-2-hydroxymethyl-2-butenoic acid

D. NAMING ALKYNES

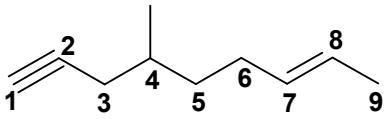
- Same rules in naming alkanes and alkenes apply in here, but using the suffix –yne.
- Compounds containing both double and triple bonds are called enynes (not ynenes). Numbering of the hydrocarbon chain starts from the end nearer the first multiple bond, whether double or triple. If there is a choice in numbering, double bonds receive lower numbers than triple bonds.



6-methyl-3-octyne

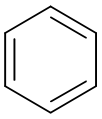
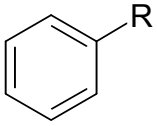
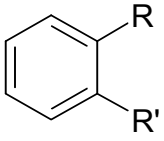
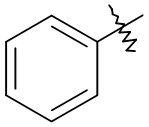
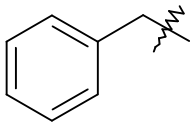


1-hepten-6-yne



4-methyl-7-nonen-1-yne

E. NAMING AROMATIC COMPOUNDS

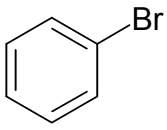
 benzene	 monosubstituted benzene	 disubstituted benzene	 phenyl group	 benzyl group

- phenyl and benzyl are used if benzene is considered as a substituent

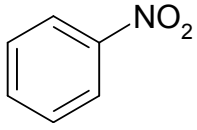
NAMING AROMATIC COMPOUNDS

1. Monosubstituted Benzene

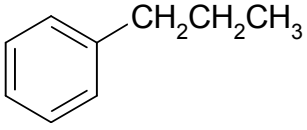
- same as naming a hydrocarbon except that benzene is the parent name



bromobenzene
benzylbromide



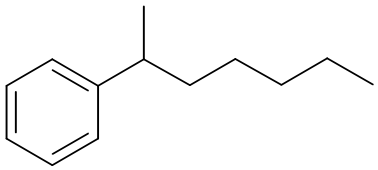
nitrobenzene



propylbenzene

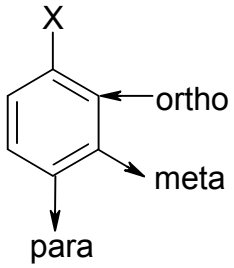
E. NAMING AROMATIC COMPOUNDS (cont)

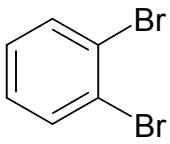
2. Alkyl substituted benzenes (arenes) depend on the size of the alkyl group. If the alkyl substituent has more than 6 carbons, the compound is named as phenyl-substituted alkane



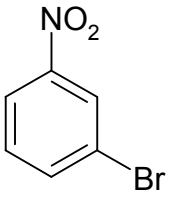
2-phenylheptane or heptan-2-ylbenzene

3. Disubstituted benzenes use:
   a. ORTHO (o): 1, 2 relationship
   b. META (m): 1, 3 relationship
   c. PARA (p): 1, 4 relationship





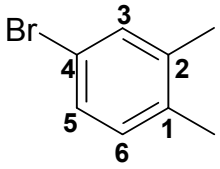
ortho-dibromobenzene



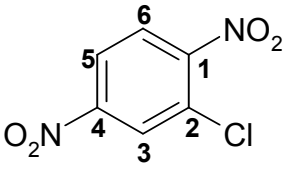
meta-bromonitrobenzene

para-dimethylbenzene

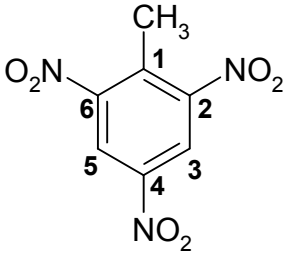
4. Benzenes with more than 2 substituents are named by numbering the position of each substituent so that the lowest possible numbers are used. The substituents are listed alphabetically.



4-bromo-1,2-dimethylbenzene

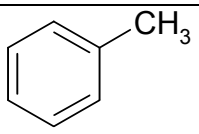
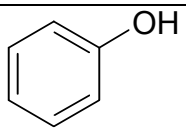
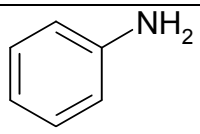
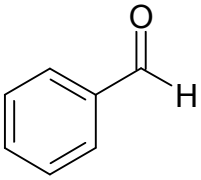
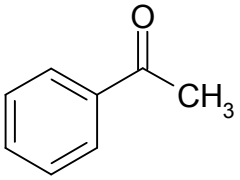
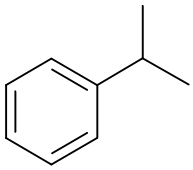


2-chloro-1,4-dinitrobenzene

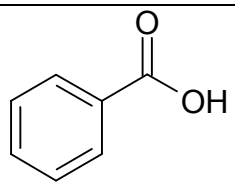
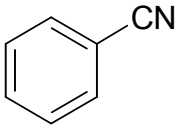
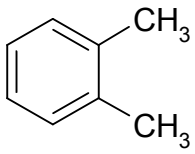
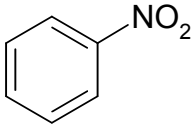
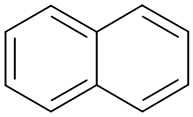
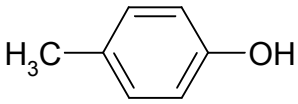


2,4,6-trinitrotoluene (TNT)

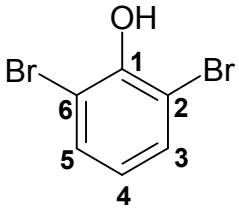
Common Names of Some Aromatic Compounds

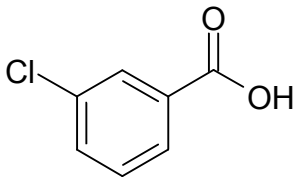
 toluene	 phenol	 aniline
 benzaldehyde	 acetophenone	 cumene

E. NAMING AROMATIC COMPOUNDS (cont)
Common Names of Some Aromatic Compounds

 benzoic acid	 benzonitrile	 ortho-xylene
 nitrobenzene	 naphthalene	 p-cresol

- The monosubstituted benzenes in the table can be used as parent name.

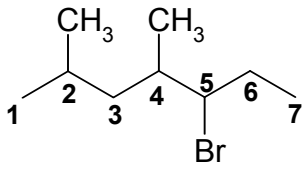

2,6-dibromophenol

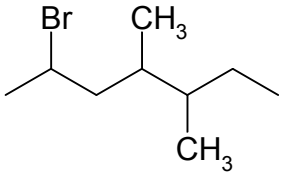

m-chlorobenzoic acid

F. NAMING ALKYL HALIDES

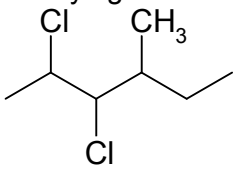
1. Find the longest carbon chain and name it as the parent. Treat the halogen as a substituent. If a multiple bond is present, the parent chain must contain it.

2. Number the carbons of the parent chain beginning at the end nearer the first substituent, regardless of whatever it is, alkyl or halo. Assign each substituent a number according to its position on the chain. If there are substituents that are equidistant, begin numbering at the end nearer the substituent with alphabetical priority.

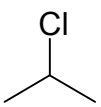

5-bromo-2,4-dimethylheptane

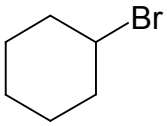

2-bromo-4,5-dimethylheptane

3. Write the name. List all substituents in alphabetical order and use one of the prefixes di-, tri-, and so forth if more than one of the same substituent is present. Many simple alkyl halides are also named by identifying first the alkyl group and then the halogen.


2,3-dichloro-4-methylhexane

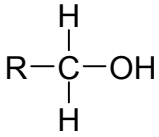
CH_3-I
methyl iodide
iodomethane

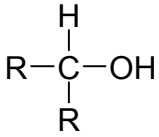

isopropyl chloride
2-chloropropane

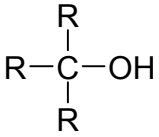

cyclohexyl bromide
bromocyclohexane

G. NAMING ALCOHOLS, PHENOLS, AND ETHERS

ALCOHOLS


primary ROH


sec ROH

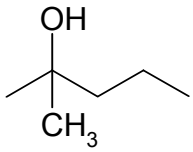

tert ROH

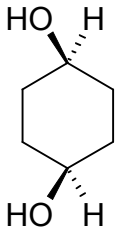
- Simple alcohols are named in the IUPAC system as derivatives of the parent alkane, using the suffix –ol.

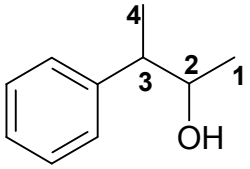
1. Select the longest carbon chain containing the hydroxyl group, and replace the –e ending of the alkane with –ol.

2. Number the carbons of the parent chain beginning at the end nearer the hydroxyl group.

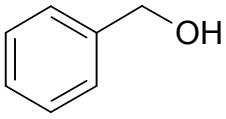
3. Number all the substituents according to their position on the chain, and write the name listing the substituents in alphabetical order.

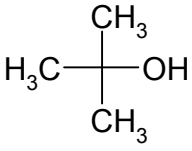

2-methyl-2-pentanol

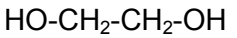

cis-1,4-cyclohexanediol

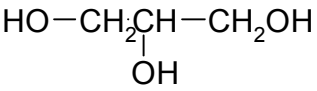

3-phenyl-2-butanol

Common Names of Some Alcohols


benzyl alcohol
(phenylmethanol)

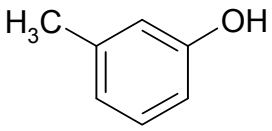

tert-butyl alcohol
(2-methyl-2-propanol)

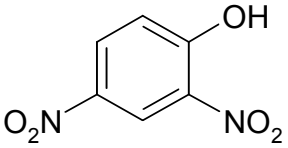

ethylene glycol
(1,2-ethanediol)


glycerol
(1,2,3-propanetriol)

PHENOLS

- The word phenol is used both as the name of a specific substance (hydroxyl benzene) and as the family name for all hydroxyl-substituted aromatic compounds. Phenols are named as substituted aromatic compounds according to the rules in Aromatic Compounds where –phenol is used as the parent name.

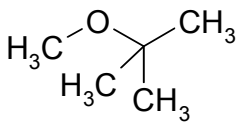

m-methylphenol
(m-cresol)


2,4-dinintrophenol

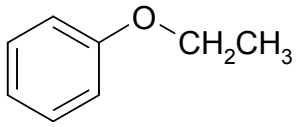
G. NAMING ALCOHOLS, PHENOLS, AND ETHERS (cont)

ETHERS

- Simple ethers that contain no other functional groups are named by identifying the two organic groups and adding the word ether.



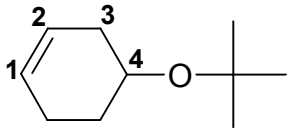
tert-butyl methyl ether
2-methoxy-2-methylpropane



ethyl phenyl ether
ethoxybenzene

- If more than one ether linkage is present, or if other functional groups are present, the ether part is named as an alkoxy substituent on the parent compound.

p-dimethoxybenzene
(Me = methyl group)

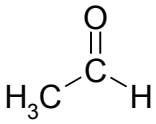


4-tert-butoxy-1-cyclohexene

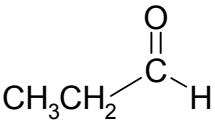
H. NAMING ALDEHYDES AND KETONES

ALDEHYDES

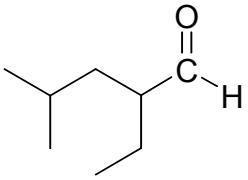
- Aldehydes are named by replacing the terminal –e of the corresponding alkane name with –al. The parent chain must contain the –CHO group, and the –CHO group is always numbered as carbon 1.



ethanol
(acetaldehyde)

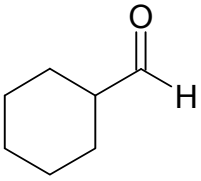


propanal
(propionaldehyde)

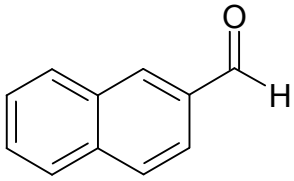


2-ethyl-4-methylpentanal

- Note that the longest chain in 2-ethyl-4-methylpentanal is a hexane, but this chain does not include the –CHO group and thus is not the parent.
- For more complex aldehydes in which the –CHO group is attached to a ring, the suffix –carbaldehyde is used:



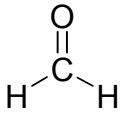
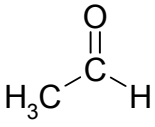
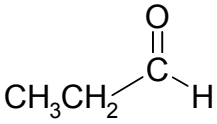
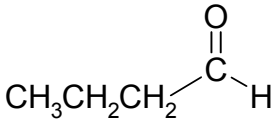
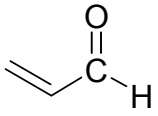
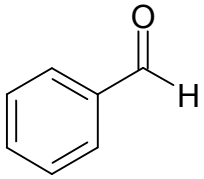
cyclohexanecarbaldehyde



2-napthalenecarbaldehyde
*naphthalene has restricted numbering

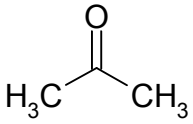
H. NAMING ALDEHYDES AND KETONES (cont)

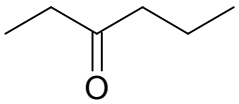
Common Names of Some Aldehydes

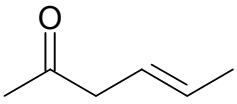
Structure	Common Name	Systematic Name
	formaldehyde	methanal
	acetaldehyde	ethanal
	propionaldehyde	propanal
	butyraldehyde	butanal
	acrolein	2-propenal
	benzaldehyde	benzenecarbaldehyde

KETONES

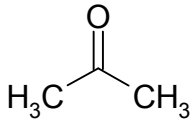
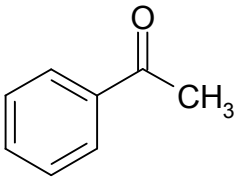
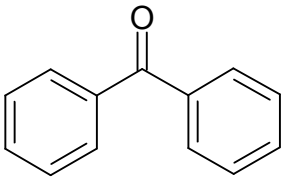
- Ketones are named by replacing the terminal –e of the corresponding alkane name with –one. The parent chain is the longest one that contains the ketone group, and numbering begins at the end nearer the carbonyl carbon.


propanone
(acetone)


3-hexanone

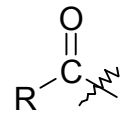
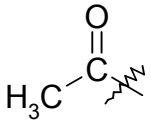
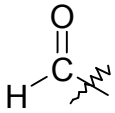
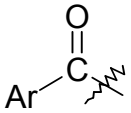
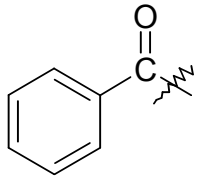

4-hexen-2-one

Ketones with Common Names

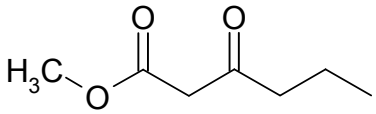
 acetone	 acetophenone	 benzophenone

H. NAMING ALDEHYDES AND KETONES (cont)

Substituent Naming in Aldehydes and Ketones

 acyl group	 acetyl	 formyl	 aroyl	 benzoyl

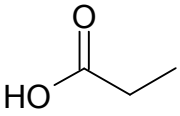
- Occassionally, the doubly bonded oxygen is considered a substituent, and the prefix oxo- is used.

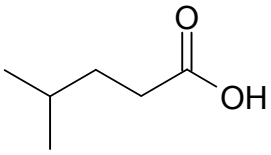

methyl-3-oxohexanoate

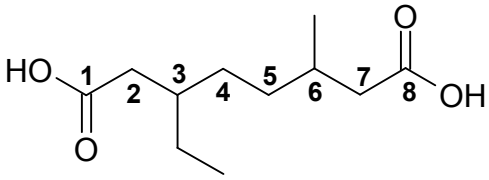
I. NAMING CARBOXYLIC ACIDS AND DERIVATIVES

CARBOXYLIC ACIDS: RCOOH

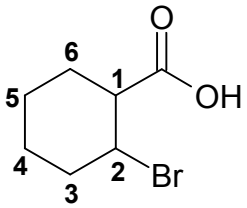
- Simple open-chain carboxylic acids are named by replacing the terminal –e of the alkane name with –oic acid. The –COOH carbon (carboxyl group carbon) is always numbered C1.

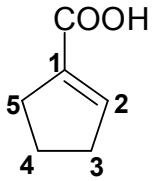

propanoic acid


4-methylpentanoic acid


3-ethyl-6-methyloctanedioic acid

- Alternatively, compounds that have a –COOH group bonded to a ring are named by using the suffix –carboxylic acid. In this alternative system, the carboxylic acid carbon is attached to C1 on the ring but is not itself numbered.


2-bromocyclohaxanecarboxylic acid

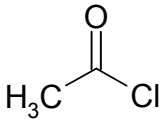

1-cyclopentenecarboxylic acid

- Carboxylic acids were among the first organic compounds to be isolated and purified, thus there are a large number of acids with common names. Systematic names must be used on most carboxylic acids but formic acid and acetic acid are already established names and are widely used.

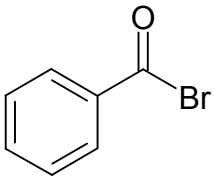
I. NAMING CARBOXYLIC ACIDS AND DERIVATIVES (cont)

ACID HALIDES: RCOX

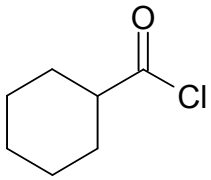
- Acid halides are named by identifying first the acyl group and then the halide. The acyl group name is derived from the acid name by replacing the –ic acid ending with –yl, or the –carboxylic acid ending with –carbonyl.



acetyl chloride



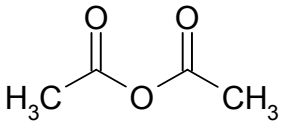
benzoyl bromide



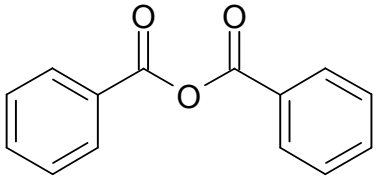
cyclohexanecarbonyl chloride

ACID ANHYDRIDES: RCOOCOR'

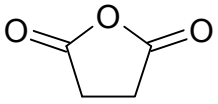
- Anhydrides from simple carboxylic acids and cyclic anhydrides from dicarboxylic acids are named by replacing the word acid with anhydride.



acetic anhydride



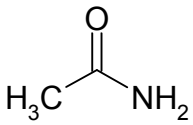
benzoic anhydride



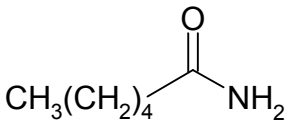
succinic anhydride

AMIDES: $RCONH_2$

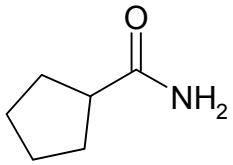
- Amides with an unsubstituted $–NH_2$ group are named by replacing the –oic acid or –ic acid ending with –amide, or by replacing the –carboxylic acid ending with –carboxamide.



acetamide

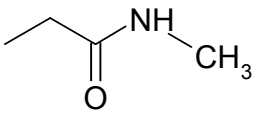


hexanamide

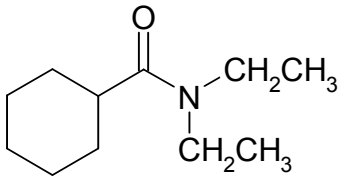


cyclopentanecarboxamide

- If the nitrogen atom is substituted, the amide is named by first identifying the substituent group and then the parent. The substituents are preceded by the letter N to identify them as being directly attached to nitrogen.



N-methylpropanamide

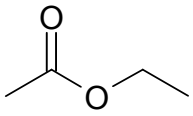


N,N-diethylcyclohexanecarboxamide

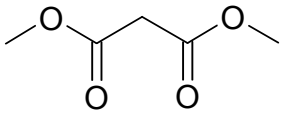
I. NAMING CARBOXYLIC ACIDS AND DERIVATIVES (cont)

ESTERS: RCOOR'

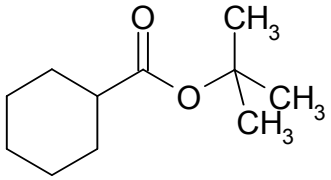
- Systematic names for esters are derived by first giving the name of the alkyl group attached to oxygen and then identifying the carboxylic acid, then, the –ic acid ending is replaced by –ate.



ethyl acetate
(ethyl ester of acetic acid)



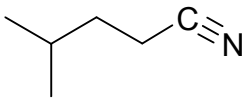
dimethyl malonate
(dimethyl ester of malonic acid)



tert-butylcyclohexanecarboxylate

NITRILES: R-C≡N

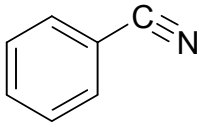
- Compounds containing the -C≡N functional group are called nitriles. Simple open chain nitriles are named by adding –nitrile as a suffix to the alkane name, with the nitrile carbon numbered C1.



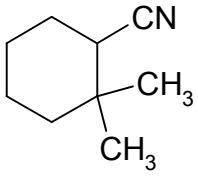
4-methylpentanenitrile

- More complex nitriles are named as derivatives of carboxylic acids by replacing the –ic acid or –oic acid ending with –onitrile, or by replacing the –carboxylic acid ending with –carbonitrile. In this system, the nitrile carbon atom is attached to C1 but is not itself numbered.

$CH_3C{\equiv}N$
acetonitrile

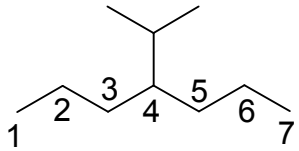
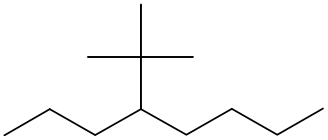


benzonitrile

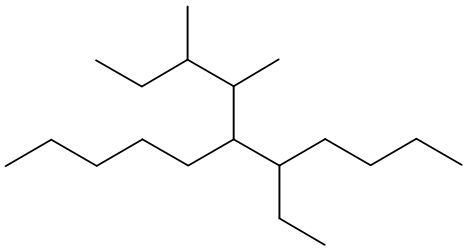
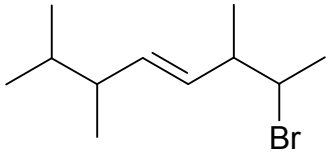
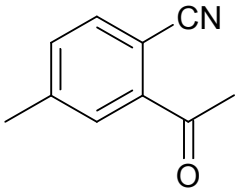
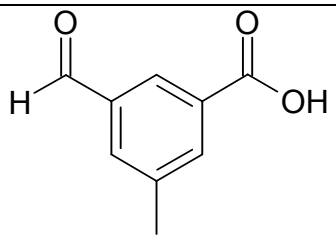
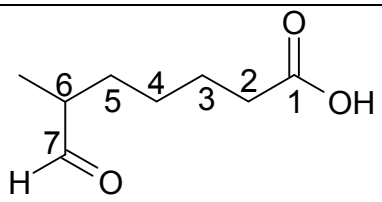
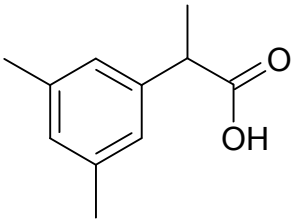
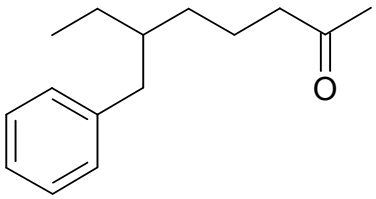


2,2-dimethylcyclohexanecarbonitrile

COMPLEX NOMENCLATURE

	4-(1-methylethyl)heptanes 4-isopropylheptane 4-(propan-2-yl)heptane
	4-(1,1dimethylethyl)octane 4-tert-butyloctane 4-(2-methylpropan-2-yl)octane

COMPLEX NOMENCLATURE

	**5-ethyl-6-(3-methylpentan-2-yl)undecane** **NOTE:** In the substituent at carbon 6, find the longest carbon chain alkyl group. The longest is a 5-carbon alkyl group with a methyl group at carbon 3 of the substituent. The 2-yl indicates that the hydrogen of the alkyl group has been removed from carbon 2 of the substituent.
	**2-bromo-3,6,7-trimethyl-2-octene** **NOTE:** The first substituents are ambiguous. They are both number 2 starting on either end. Remember if there is ambiguity in the numbering, assign the lowest number in alphabetical order.
	**2-acetyl-4-methylbenzonitrile** **NOTE:** Nitrile is the higher priority over ketone. Take note of the term acetyl (see table above in Naming Ketones)
	**3-formyl-5-methylbenzoic acid** **NOTE:** Carboxylic acid is the principal group. Take note of the term formyl (see table above in Naming Aldehydes)
	**6-methyl-7-oxoheptanoic acid** **NOTE:** The aldehyde is part of the chain, thus, instead of using formyl, oxo has been used.
	**2-(3,5-dimethylphenyl)propanoic acid** **NOTE:** The longest carbon chain contains the carboxylic acid and not the benzene ring. The ring is merely a substituent of the principal chain.
	6-benzyl-2-octanone