3 Molecular Structure and Nomenclature

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Learning Goals and Reading Recommendations

- names of compound classes and functional groups
- interconvert IUPAC names and structure formulae

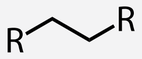
- differentiate identical/different compounds and types of isomers
- assign the type of isomeric relationship between two molecules
- understand stereochemical notation in structure formulae
- name geometric isomers, enantiomers, diastereomers

3.1 Basic Rules of Nomenclature

Overview of Compound Classes and Functional Groups

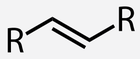
hydrocarbons

alkanes



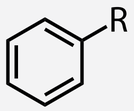
cycloalkanes

alkenes (olefins)



alkynes (acetylenes)

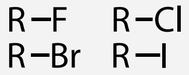
arenes (aromatics)



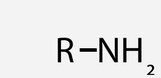
functionalized molecules

monovalent

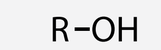
haloalkanes (halogenides)



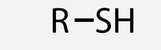
alkanamines (amines)



alkanols (alcohols)

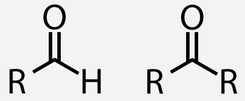


alkanthiols (mercaptans)

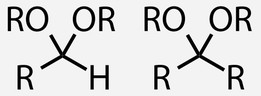


divalent

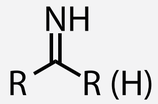
aldehydes & ketones



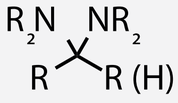
acetals & ketals



imines

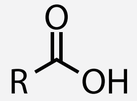


aminals

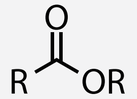


trivalent

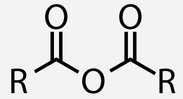
carboxylic acids (acids)



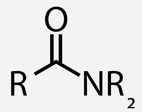
carboxylic esters (esters)



carboxylic anhydrides (anhydrides)

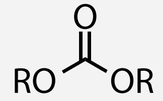


carboxylic amides (amides)

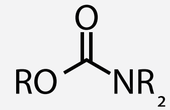


tetravalent

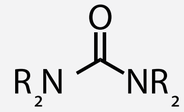
carbonates



urethanes (carbamates)

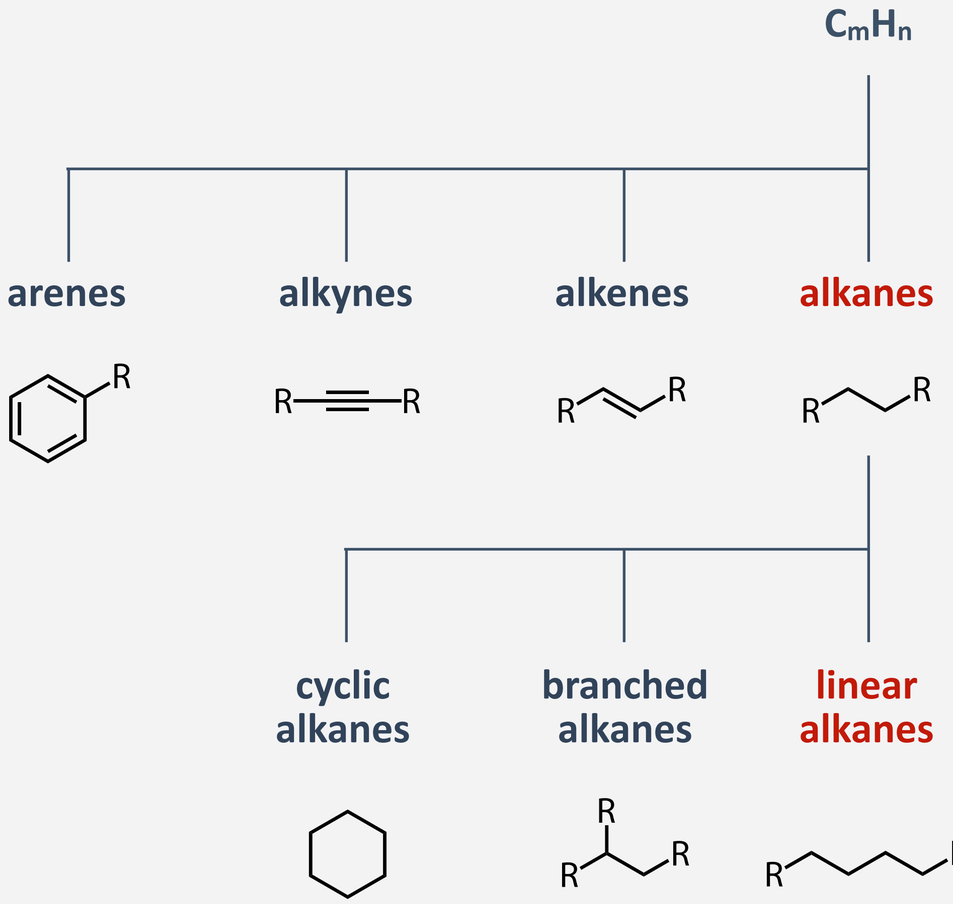


ureas



Hydrocarbons

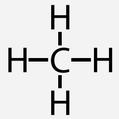
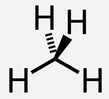
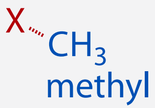
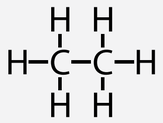
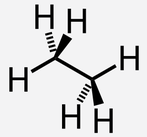
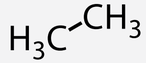
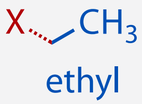
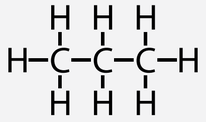
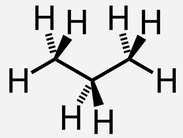
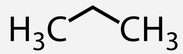
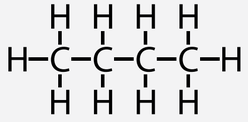
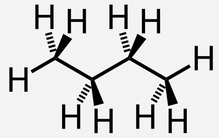
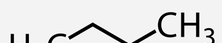
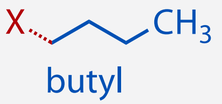
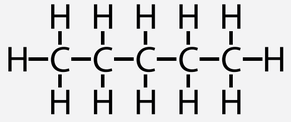
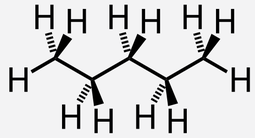
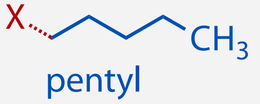
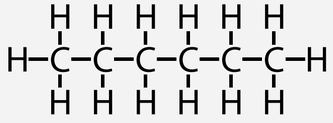
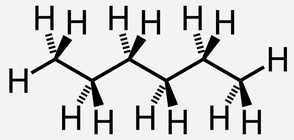
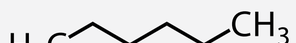
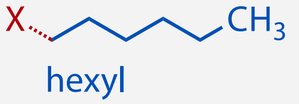
hydrocarbons compounds that only contain C and H



alkanes "saturated" hydrocarbons that only contain single bonds

linear alkanes alkanes with a single carbon backbone without branching points

Nomenclature of Linear Alkanes and Alkyl Residues

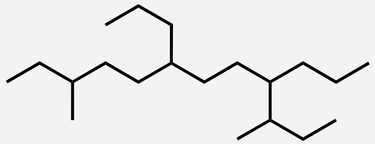
methane méthane	CH_4				
ethane éthane	CH_3CH_3				
propane propane	$CH_3CH_2CH_3$				
butane butane	$CH_3(CH_2)_2CH_3$				
pentane pentane	$CH_3(CH_2)_3CH_3$				
hexane hexane	$CH_3(CH_2)_4CH_3$				

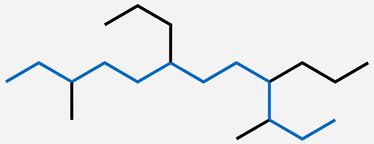
analogous for the higher alkanes: heptane, octane,nonane, decane, undecane, dodecane, tridecane, tetradecane, pentadecane, hexadecane, heptadecane, octadecane, nondecane, eicosane ($C_{20}H_{42}$), heneicosane ($C_{21}H_{44}$), docosane ($C_{22}H_{46}$), tricosane ($C_{23}H_{48}$) ... tricontane ($C_{30}H_{62}$), ... tetracontane ($C_{40}H_{82}$) ...

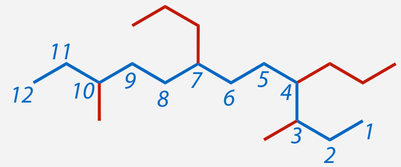
Basic Rules of Nomenclature of Branched Alkanes

1. identify the parent chain or principal chain, i. e., the longest carbon chain in the molecule

- if two chains are equally long, choose the one that has more substituents
- assign position numbers to main chain atoms starting at end closest to first (second …) substituent



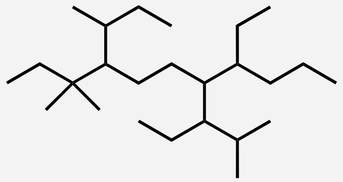


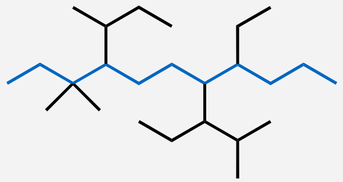


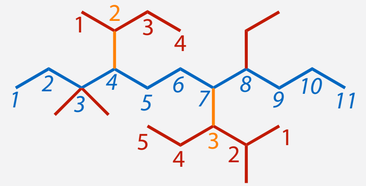
3,10-dimethyl-3,7-dipropyldodecane

2. name all alkyl residues attached to this parent chain, place them before main chain

- assign position numbers and put the substituents into alphabetic order
- if multiple substituents of same type, assemble using a Greek number prefix (di, tri, tetra, etc.)
- for branched side chains, find the longest carbon chain connected to the main chain (iterative)
- assign position numbers to substituent atoms starting at end closest to connected atom
- if not terminally attached insert position number of the connecting atom into the suffix “anyl”

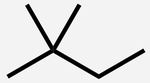


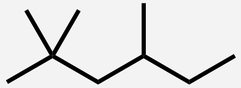


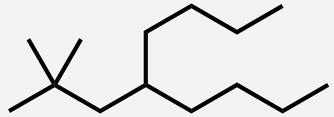


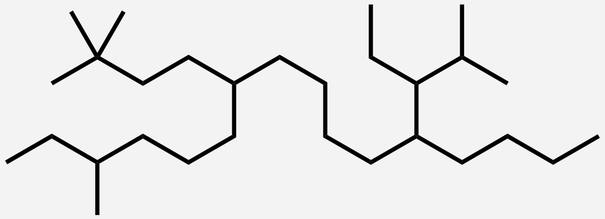
4-(butan-2-yl)-8-ethyl-3,3-dimethyl-7-(2-methylpentan-3-yl)undecane

Examples for the Nomenclature of Branched Alkanes

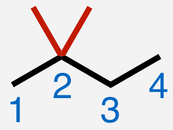




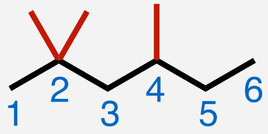




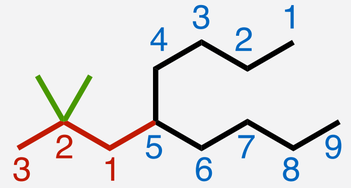
Examples for the Nomenclature of Branched Alkanes



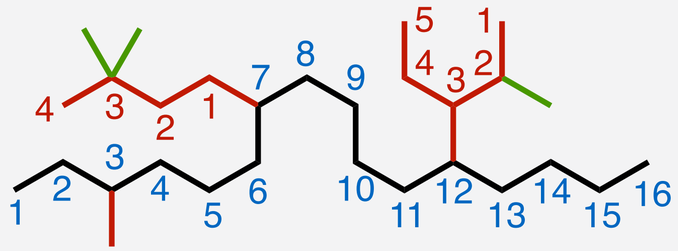
2,2-dimethylbutane



2,2,4-trimethylhexane

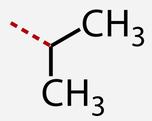


5-(2,2-dimethylpropyl)nonane

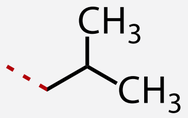


7-(3,3-dimethylbutyl)-3-methyl-
12-(2-methylpentan-3-yl)hexadecane

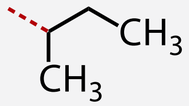
Trivial Names of Alkyl Groups



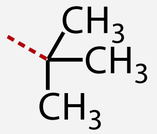
isopropyl (propan-2-yl)



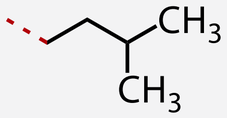
isobutyl (2-methylpropyl)



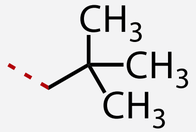
sec.-butyl (1-methylpropyl)



tert.-butyl (2-methylpropan-2-yl)

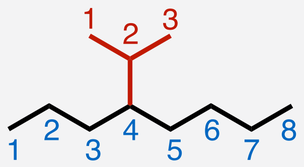


isopentyl (3-methylbutyl)

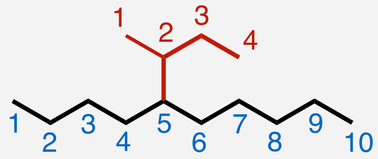


neopentyl (2,2-dimethylpropyl)

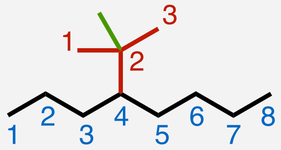
Examples Using Trivial Names of Alkyl Groups



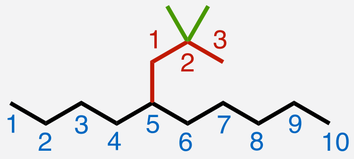
4-(propan-2-yl)octane
or 4-isopropyloctane



5-(butan-2-yl)decane
or 5-(*sec.*-butyl)decane



4-(2-methylpropan-2-yl)octane
or 4-(tert.-butyl)octane

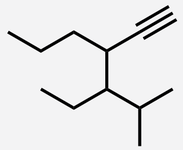


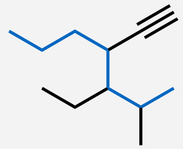
5-(2,2-dimethylpropyl)decane
or 5-neopentyldecane

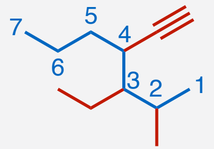
Basic Rules for the Nomenclature of Alkenes and Alkynes

1. name the longest carbon chain, irrespective of the presence of double or triple bonds

- molecule may contain double/triple bonds but these have *no priority*
- follow all rules for naming and position number assignment of and within substituents



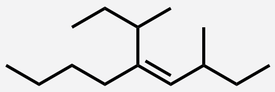


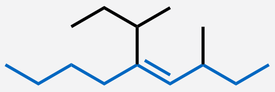


3-ethyl-4-(ethyn-1-yl)-2-methylheptane

2. name all double or triple bonds in the parent chain, using suffix “ene” or “yne” (replacing “ane”)

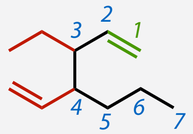
- name double/triple bonds in substituents using “enyl”/“ynyl”
- assign the position number of the carbon atom of the double/triple bond closer to the end
- put double/triple bonds into alphabetic order if both present
- for multiple double/triple bonds, suffix is preceded with a Greek number prefix (di, tri, tetra, etc.)



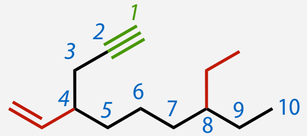


5-(butan-2-yl)-3-methylnon-4-ene

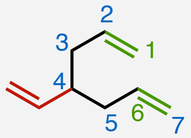
Advanced Examples of Branched Alkenes and Alkynes



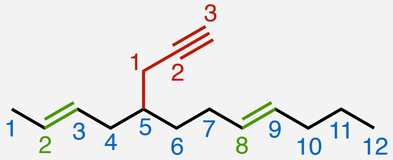
3-ethyl-4-(eth-1-enyl)hept-1-ene



8-ethyl-4-(eth-1-enyl)dec-1-yne



4-(eth-1-enyl)hepta-1,6-diene



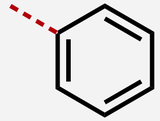
5-(prop-2-ynyl)dodeca-2,8-diene

- **priority rules: double and triple bonds have no priority (and alkane = alkene = alkyne)**
  - always search the longest carbon chain, even if it contains less or even no double or triple bonds
  - if >2 alkenes/alkynes are in different chains of equal length, priority for maximum number of alkenes
- **proceed with branches containing double and triple as before, but use suffixes “enyl” or “ynyl”**

Trivial Names of Alkenyl, Alkynyl, and Aromatic Substituents

vinyl
(ethen-1-yl)

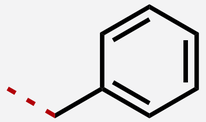
ethynyl
(ethyn-1-yl)



phenyl

allyl
(propen-2-yl)

propargyl
(propyn-2-yl)

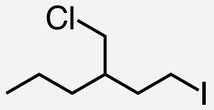


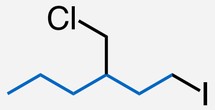
benzyl
(1-phenylmethyl)

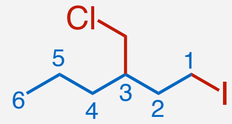
Nomenclature of Haloalkanes

1. name the longest carbon chain, irrespective of the presence of double or triple bonds

- molecule may contain halogen atoms but these have *no priority*
- follow all rules for naming and position number assignment of and within substituents



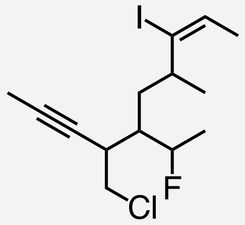


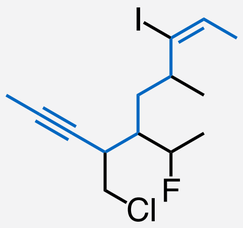


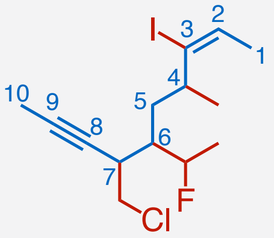
3-(chloromethyl)-1-iodohexane

2. name all halogens in the parent chain and subsitutents, using prefixes fluoro, chloro, bromo, iodo

- assign the position number (if no other substituents choose number closer to the end)
- put halogens into alphabetic order if different ones present
- for multiple halogens of the same type, assemble with a Greek number prefix (di, tri, tetra, etc.)

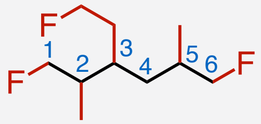




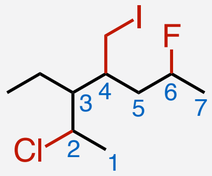


7-(chloromethyl)-6-(1-fluoroethyl)-3-iodo-4-methyldec-2-en-8-yne

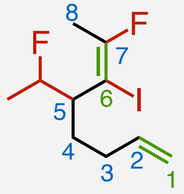
Advanced Examples of Haloalkanes and Multifunctional Compounds



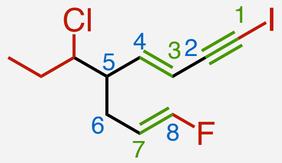
1,6-difluoro-3-(2-fluoroethyl)-2,5-dimethylhexane



2-chloro-3-ethyl-6-fluoro-4-(iodomethyl)heptane



7-fluoro-5-(1-fluoroethyl)-6-iodoocta-1,6-diene



5-(1-chloropropyl)-8-fluoro-1-iodooct-3,7-dien-1-yne

- **priority rules: alkane alkene, alkyne and halogens have *no priority***
  - always search the longest carbon chain, even if it contains less or even no double or triple bonds
  - halogens are always labeled with a prefix, the remaining nomenclature is as usual

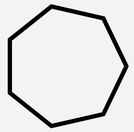
Nomenclature of Cyclic Alkanes

cyclopropane

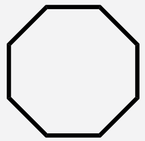
cyclobutane

cyclopentane

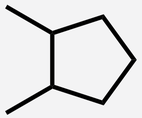
cyclohexane



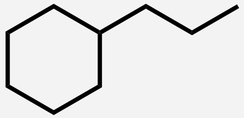
cycloheptane



cyclooctane



1,2-dimethylcyclopentane

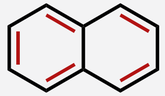


propylcyclohexane

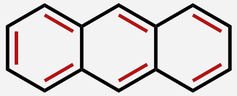
Nomenclature of Aromatic Compounds

benzene

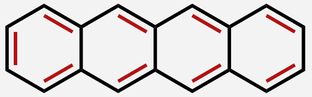
naphthalene



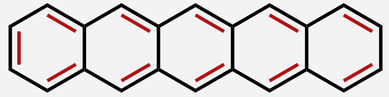
anthracene



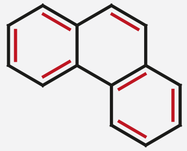
tetracene



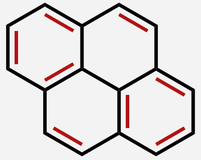
pentacene



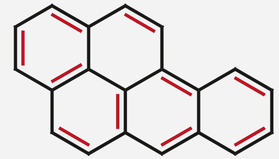
phenanthrene



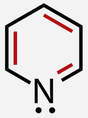
pyrene



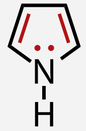
benzopyrene



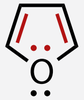
pyridine



pyrrol

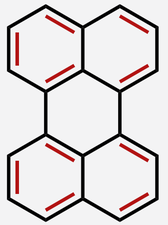


furan



thiophene

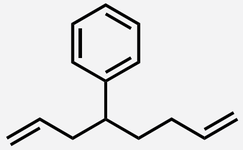
perylene

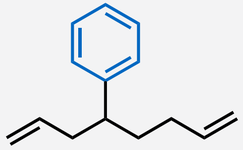


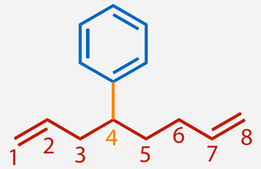
Nomenclature of Cyclic and Aromatic Compounds

1. in compounds containing only C, H, and halogens, the cycle is always considered the parent chain

- name all residues attached to the cycle as “alkyl” residues
- follow all previous rules for naming and position number assignment of and within substituents



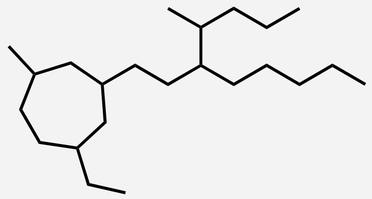


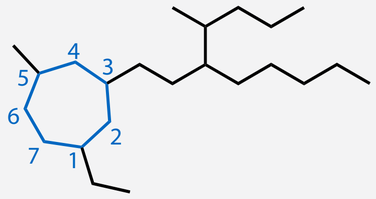


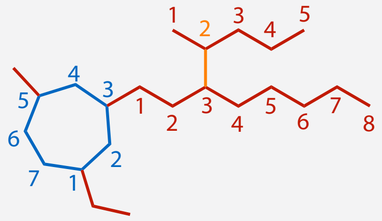
(octa-1,7-dien-4-yl)benzene

2. name and assign position numbers to the cycle

- number the atoms of the cycle starting at the carbon that is attached to first substituent
- if two substituents, alphabetic order decides
- if two identical substituents, next substituents along the cycle decide (iterative)

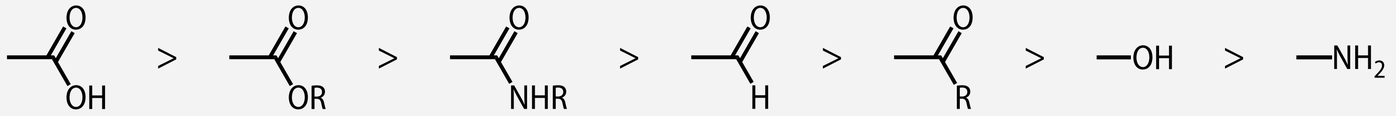






1-ethyl-5-methyl-3-(3-(pentan-2-yl)octyl)cycloheptane

Summary of the Priority Rules on Following Slides



group	acid	ester	amide	aldehyde	ketone	alcohol	amine
suffix	-oic acid	-oate	-amide	-al	-one	-ol	-amine
prefix	carboxy-	oxycarbonyl-	carbamoyl-	oxo-	oxo-	hydroxy-	amino-

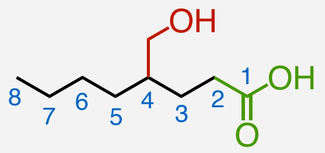
no priority

(alkene, alkyne)	halide
(-ene, -yne)	–
(en-, yn-)	halo-

- **alkanes, alkenes, alkynes and halogen do not possess *any* priority**
- **functional group with the highest priority is the principal characteristic group**
- **principal characteristic group the naming of the parent chain (using the suffix)**
- **functional group with a lower priority treated as a substituent (using prefix nomenclature)**
- **alkene/alkyne are concatenated with other suffixes (also with “yl” when in side groups)**

Rules for Parent Chain Determination in Molecules with Functional Groups

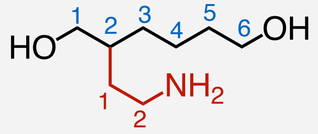
1. identify the longest chain that contains the principal characteristic group (highest priority)



4-(hydroxymethyl)octanoic acid

- if more than one type of functional group, the one with higher priority decides
- carboxylic acid is principal characteristic group because higher in priority than alcohol
- parent chain is longest carbon chain containing carboxylic acid

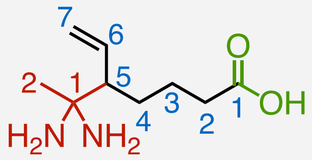
2. identify the chain that has the maximum number of principal characteristic groups



2-(2-aminoethyl)hexane-1,6-diol

- if multiple instances of principal characteristic group, maximum number decides
- alcohol is the principal characteristic group
- chain with two alcohols is parent chain, even though a longer chain can be identified

3. identify the chain that contains a double or triple bond

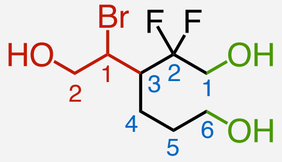


5-(1,1-diaminoethyl)hept-6-enoic acid

- if no decision on parent possible based on previous rules …
- identify the chain that has a double/triple bond
  - if two of same length, decide based on which one has more double/triple bonds
  - if still two, decide based on which one has closer first double/triple bond
  - if still two, decide based on following rules

Rules for Parent Chain Determination in Molecules with Functional Groups

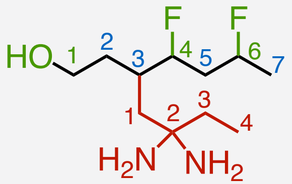
4. identify the chain that has the maximum number of substituents



2,2-difluoro-3-(1-bromo-2-hydroxy ethyl)hexan-1,6-diol

- if no decision based on previous rules …
- identify chain with maximum number of substituents in total
- alcohol is the principal characteristic group,
- but two equally long chains with two hydroxy groups
- chain with difluoro substituents takes priority over bromo substituent

5. lowest locant (position number) for the closest substituent



4,6-difluoro-3-(2,2-diaminobutyl) heptan-1-ol

- if no decision based on previous rules …
- identify chain lowest position number for closest substituent
- if the same, go to next substituent (iterative)
- alcohol is the principal characteristic group
- 4-fluoro wins against what would be 5-amino

Monovalent Functional Groups

R–F

R–Cl

R–Br

R–I

haloalkanes

R–OH

alkanols
alcohols
(hydroxy)

$R–NH_2$

alkanamines
amines
(amino)

R–SH

alkanthiols
mercaptans
(sulfanyl)

$R–PH_2$

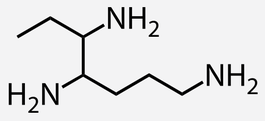
alkanphosphines
phosphanes
(phosphino)

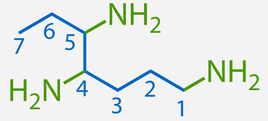
- **monovalent functional groups have a carbon single-bonded to a heteroatom (not C, H)**
- **we have already seen haloalkanes (no priority)**

Nomenclature of Amines

1. identify the longest chain to which the amine is attached (if principal characteristic group)

- identify the longest possible chain that has the maximum number of amines attached
- molecule may contain longer chains, but principal characteristic group always takes precedence!
- follow all previous rules for naming and position number assignment of and within substituents

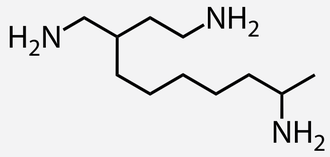


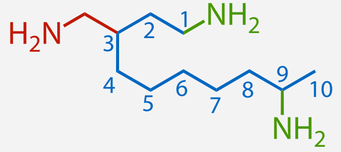


heptane-1,4,5-triamine

2. name the parent chain appending the suffix “amine” (if principal characteristic group)

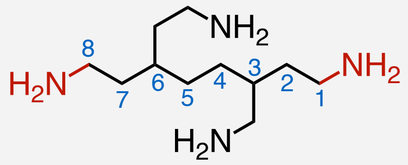
- assign the position numbers (choose number closer to the end)
- for multiple amines, suffix is preceded with a Greek number prefix (di, tri, tetra, etc.)
- if amine in side branch (or higher priority groups present), use prefix “amino”



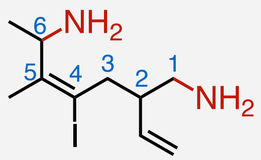


3-(aminoethyl)decane-1,9-diamine

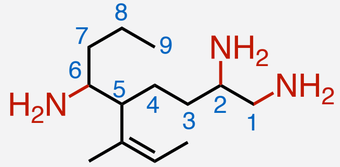
Advanced Examples of Amines and Multifunctional Compounds



3-(2-aminoethyl)-6-(aminomethyl)octane-1,8-diamine



4-iodo-5-methyl-2-(eth-1-enyl)hept-4-ene-1,6-diamine



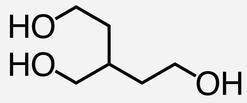
5-(but-2-en-2-yl) nonane-1,2,6-triamine

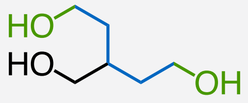
- **priority rules: amine > (arene, alkene, alkyne, halogen)**
  - always search the longest chain that contains the amine (if principal characteristic group)
  - chain with maximum number of amines takes precedence, even even if longer chains present
  - suffixes of alkenes/alkynes and amines can be combined if on the same chain
  - use prefix names for all other functions with lower priority
  - if higher priority groups present or amine is in a side branch, use instead prefix “amino”

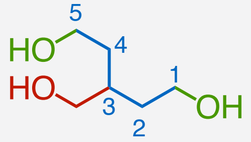
Nomenclature of Alcohols and Thiols

1. identify the longest chain to which the alcohol/thiol is attached (if principal characteristic group)

- identify the longest possible chain that has the maximum number of alcohols/thiols attached
- molecule may contain longer chains, but principal characteristic group always takes precedence!
- follow all previous rules for naming and position number assignment of and within substituents



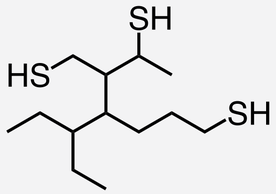


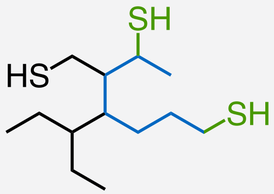


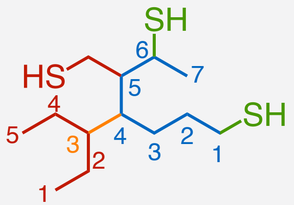
3-(hydroxymethyl)pentane-1,5-diol

2. name the parent chain appending the suffix "ol"/"thiol" (if principal characteristic group)

- assign the position numbers (choose number closer to the end)
- for multiple alcohols/thiols, suffix is preceded with a Greek number prefix (di, tri, tetra, etc.)
- if alcohol/thiol in side branch (or higher priority group present), use prefixes "hydroxy"/"sulfanyl"

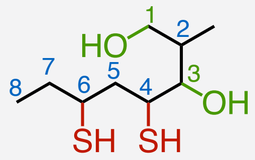




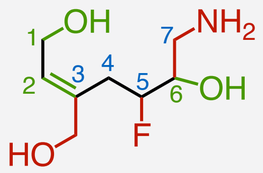


4-(pentan-3-yl)-5-(sulfanilmethyl)heptane-1,6-dithiol

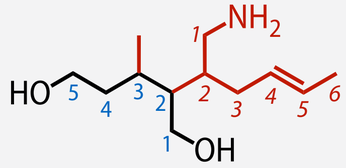
Advanced Examples of Alcohols/Thiols and Multifunctional Compounds



4,6-disulfanyl-2-methyloctane-1,3-diol



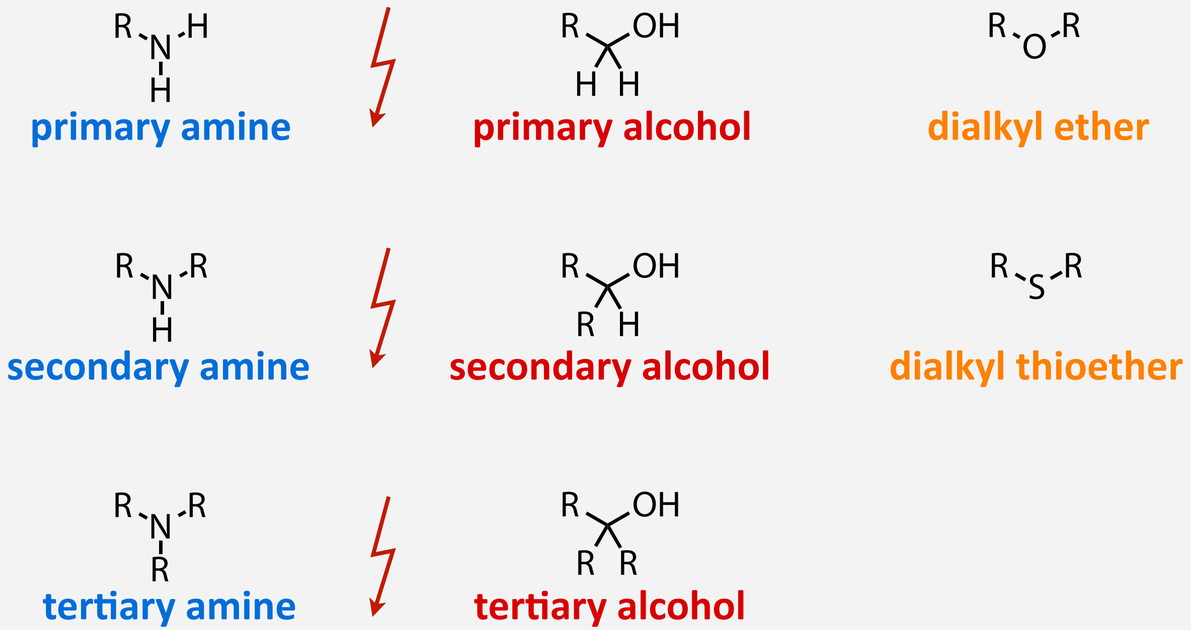
7-amino-5-fluoro-3-(hydroxymethyl)hept-2-ene-1,6-diol



4-(1-aminohex-4-en-2-yl)-3-methyl-pentane-1,5-diol

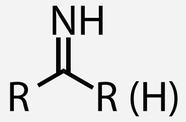
- **priority rules: alcohol > thiol > amine > (arene, alkene, alkyne, halogen)**
  - always search the longest chain that contains the alcohol/thiol (if principal characteristic group)
  - chain with maximum number of alcohols/thiols takes precedence, even if longer chains present
  - suffixes of alkenes/alkynes and alcohols/thiols can be combined if on the same chain
  - use prefix names for all other functions with lower priority
  - if higher priority groups present or alcohol/thiol is in a side branch, use prefix “hydroxy”/“sulfanyl”

Categorization of Amines and Alcohols

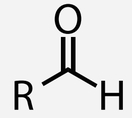


- in primary/secondary/tertiary amines, nitrogen has one/two/three alkyl residues
- in primary/secondary/tertiary alcohols, oxygen is bonded to a primary/secondary/tertiary carbon
- primary/secondary/tertiary carbons have one/two/three alkyl residues
- oxygen/sulfur with two alkyl residues is called ether/thioether

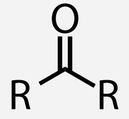
Divalent Functional Groups



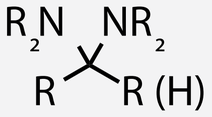
imine



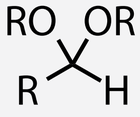
aldehyde
alkanal



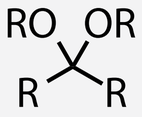
ketone
alkanone



aminal



acetal



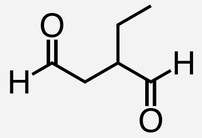
ketal

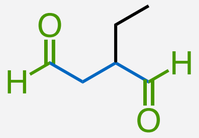
- in divalent functional groups, carbon has two bonds connected to heteroatom(s)
- the C=O group is called “carbonyl” group

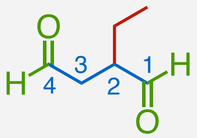
Nomenclature of Ketones and Aldehydes

1. identify the longest chain containing the ketone/aldehyde (if principal characteristic group)

- identify the longest possible chain that has the maximum number of ketones/aldehydes
- molecule may contain longer chains, but principal characteristic group always takes precedence!
- if ketone and aldehyde are present, aldehyde is principal characteristic group
- follow all previous rules for naming and position number assignment of and within substituents



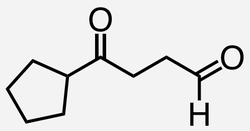


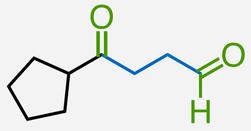


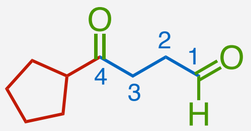
2-ethyl-1,4-butanedial

2. name the parent chain appending the suffix “one”/“al” (if principal characteristic group)

- assign the position numbers (choose number closer to the end)
- for multiple ketones/aldehydes, suffix is preceded with a Greek number prefix (di, tri, tetra, etc.)
- if ketone/aldehyde in side branch (or higher priority group present), use prefix “oxo” (both)

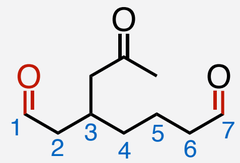




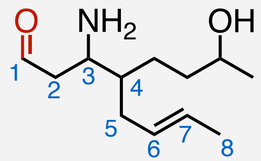


4-cyclopentyl-4-oxobutanal

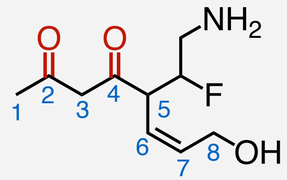
Advanced Examples of Ketones/Aldehydes and Multifunctional Compounds



3-(2-oxopropyl)heptane-1,7-dial



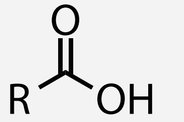
3-amino-4-(3-hydroxybutyl)oct-6-enal



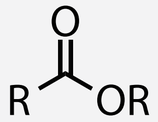
5-(2-amino-1-fluoroethyl)-8-hydroxyoct-6-ene-2,4-dione

- **priority rules: aldehyde > ketone > alcohol > thiol > amine > (arene, alkene, alkyne, halogen)**
  - always search the longest chain that contains the ketone/aldehyde (if principal characteristic group)
  - chain with maximum number of ketones/aldehydes takes precedence, even over longer chains
  - suffixes of alkenes/alkynes and ketones/aldehydes can be combined if on the same chain
  - use prefix names for all other functions with lower priority
  - if higher priority groups present or ketone/aldehyde is in a side branch, use prefix “oxo” (both)

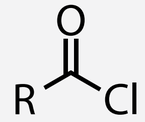
Trivalent Functional Groups



carboxylic acid



carboxylic acid ester



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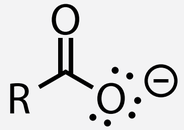
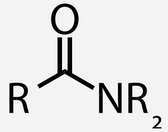
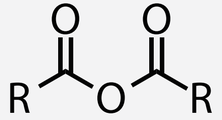


carboxylate



carboxylic acid amide



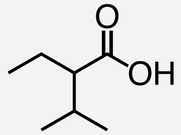
carboxylic acid anhydride

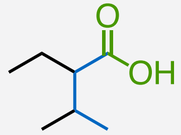
- in trivalent functional groups, carbon has three bonds connected to heteroatom(s)
- the C(O)O fragment is generically called “carboxyl group”

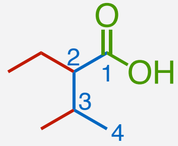
Nomenclature of Carboxylic Acids

1. identify the longest chain containing the carboxylic acid (if principal characteristic group)

- identify the longest possible chain that has the maximum number of carboxylic acids
- molecule may contain longer chains, but principal characteristic group always takes precedence!
- follow all previous rules for naming and position number assignment of and within substituents



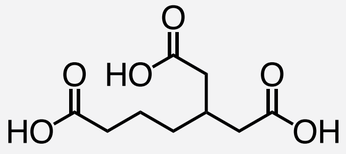


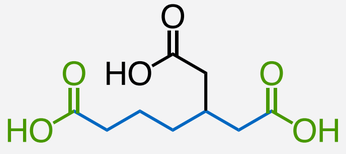


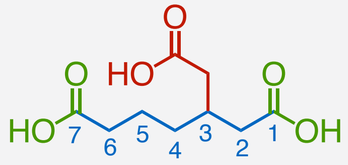
2-ehtyl-3-methylbutanoic acid

2. name the parent chain appending the suffix “oic acid” (if principal characteristic group)

- no need to assign position numbers
- for two carboxylic acids, suffix is preceded with a Greek number prefix (di)
- if carboxylic acid is in side branch (or higher priority group present), use prefix “carboxy”

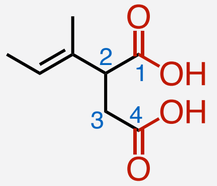




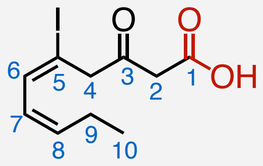


3-(carboxymethyl)heptanedioic acid

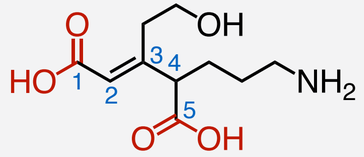
Advanced Examples of Carboxylic Acids and Multifunctional Compounds



2-(but-2-en-2-yl)butanedioic acid



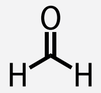
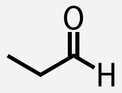
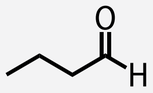
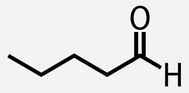
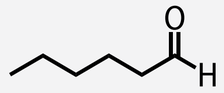
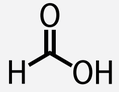
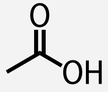
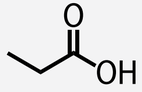
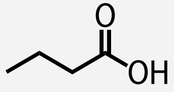
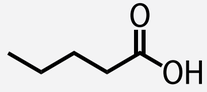
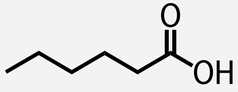
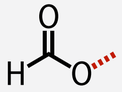
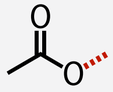
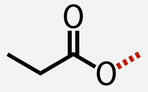
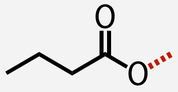
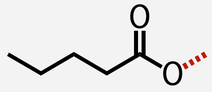
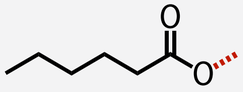
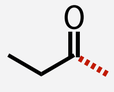
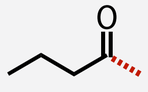
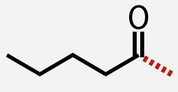
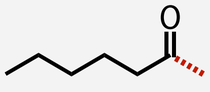
5-iodo-3-oxodeca-5,7-diennoic acid



4-(3-aminopropyl)-3-(2-hydroxyethyl)pent-2-enedioic acid

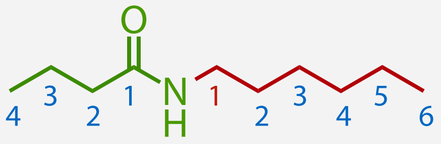
- **priority rules: acid > ester > amide > aldehyde > ketone > alcohol > thiol > amine > …**
  - always search the longest chain that contains the carboxylic acid (if principal characteristic group)
  - chain with maximum number of carboxylic acids takes precedence, even if longer chains present
  - suffixes of alkenes/alkynes and carboxylic acids can be combined if on the same chain
  - use prefix names for all other functions with lower priority
  - if higher priority groups present or carboxylic acid is in a side branch, use prefix “carboxy”

Important Trivial Names for Aldehydes, Acids, Esters, and Acyl Residues

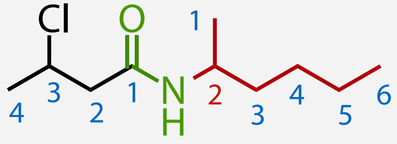
aldehydes						
	formaldehyde methanal	acetaldehyde ethanal	propionaldehyde propanal	butyraldehyde butanal	valeraldehyde pentanal	capronaldehyde hexanal
carboxylic acids						
	formic acid methanoic acid	acetic acid ethanoic acid	propionic acid propanoic acid	butyric acid butanoic acid	valeric acid pentanoic acid	caproic acid hexanoic acid
esters						
	formate methanoate	acetate ethanoate	propionate propanoate	butyrate butanoate	valerate pentanoate	caproate hexanoate
acyl residues						
	formyl methanoyl	acetyl ethanoyl	propionyl propanoyl	butyryl butanoyl	valeryl pentanoyl	caproyl hexanoyl

Nomenclature of Carboxylic Acid Amides

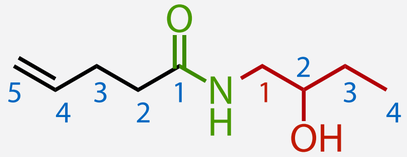
1. identify the longest chain to which the amide C=O is attached, name it, append suffix “amide”
2. prepend the name with the remaining residue, ended by “yl” (use number prefix if necessary)
3. carboxylic acid amide(s) always terminal, no number needed
4. if two carboxylic acid amides attached to same chain, use number prefix (di)



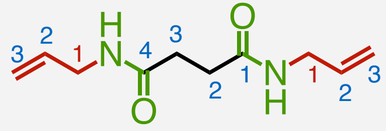
hexyl butanamide
old: butanoic acid
hexyl amide



1-methylpentyl 3-chlorobutanamide
old: 3-chlorobutanoic acid
2-hexyl amide



2-hydroxybutyl pent-4-enamide
old: 4-pentenoic acid
2-hydroxybutyl amide

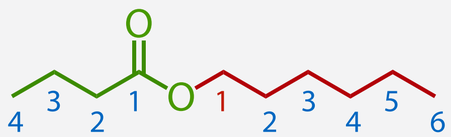


di(2-propenyl) butandiamide
or diallyl butandiooate
old: butandioic acid
di(2-propenyl) amide

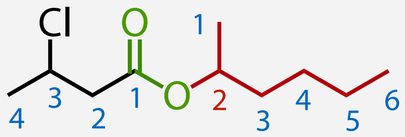
- alternatively, name like a carboxylic acid, append residue ended by “yl”, append “amide”
- naming of compounds with >2 amides (i.e., in side chains) complex but rarely needed

Nomenclature of Carboxylic Acid Esters

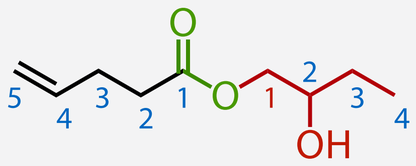
1. identify the longest chain to which the ester C=O is attached, name it, append suffix “oate”
2. prepend the name with the remaining residue, ended by “yl” (use number prefix if necessary)
3. carboxylic acid ester(s) always terminal, no number needed
4. if two carboxylic acid esters attached to same chain, use number prefix (di, more impossible)



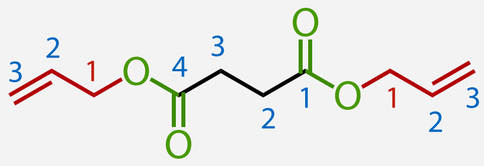
hexyl butanoate
old: butanoic acid
hexyl ester



Hexane-2-yl 3-chlorobutanoate
old: 3-chlorobutanoic acid
2-hexyl ester



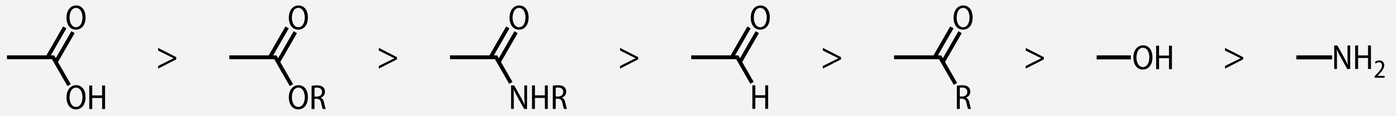
2-hydroxybutyl pent-4-enoate
old: 4-pentenoic acid
2-hydroxybutyl ester



di(2-propenyl) butandioate
or diallyl butandioate
old: butandioic acid
di(2-propenyl) ester

- alternatively, name like a carboxylic acid, append the residue ended by “yl”, append “ester”
- naming of compounds with >2 esters (i.e., in side chains) complex but rarely needed

Summary of the Priority Rules on Following Slides



group	acid	ester	amide	aldehyde	ketone	alcohol	amine
suffix	-oic acid	-oate	-amide	-al	-one	-ol	-amine
prefix	carboxy-	oxycarbonyl-	carbamoyl-	oxo-	oxo-	hydroxy-	amino-

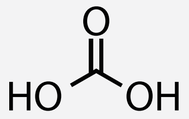
no priority

(alkene, alkyne)	halide
(-ene, -yne)	–
(en-, yn-)	halo-

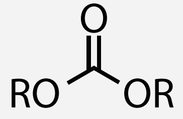
- **alkanes, alkenes, alkynes and halogen do not possess *any* priority**
- **functional group with the highest priority is the principal characteristic group**
- **principal characteristic group the naming of the parent chain (using the suffix)**
- **functional group with a lower priority treated as a substituent (using prefix nomenclature)**
- **alkene/alkyne are concatenated with other suffixes (also with “yl” when in side groups)**

Naming of Simple Compounds with Tetravalent Functional Groups

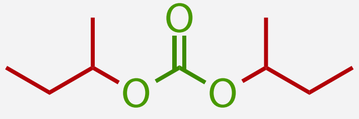
- in tetravalent functional groups, carbon has four bonds connected to heteroatom(s)



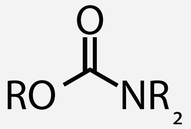
carbonic acid



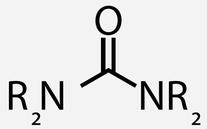
carbonate



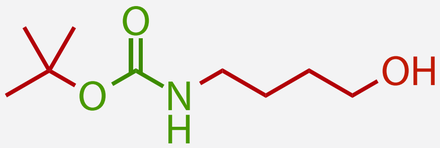
di(butan-2-yl) carbonate



urethane (carbamate)



urea



N-(4-hydroxybutyl) *O*-*tert.*-butyl urethane

- **tetravalent functions are relevant in polymers (polycarbonates, polyurethanes, polyureas)**

Learning Outcomes

- names of compound classes and functional groups
- some trivial names
- convert IUPAC names into structure formulae
- convert structure formulae into IUPAC names