

3

Molecular Structure and Nomenclature

Table of Contents

1. Introduction (2 h)

- 1.1. Organic Chemistry and Soft Matter Research
- 1.2. Carbon as the Basis of Organic Chemistry

2. The Nature of the Covalent Bond (6 h)

- 2.1. Atomic Orbitals and Hybridisation
- 2.2. Formation of Single Bonds
- 2.3. Formation of Multiple Bonds
- 2.4. Electron Delocalization & Resonance Structures

3. Molecular Structure and Nomenclature (4 h)

- 3.1. Basic Rules of Nomenclature
- 3.2. Isomerism

4. Mechanisms of Organic Reactions (10 h)

- 4.1. Reaction Thermodynamics & Kinetics
- 4.2. Reaction Types and Intermediates
- 4.3. Nucleophilic Substitutions

- 4.4. Nucleophilic Reactions on Carbonyl Carbons
- 4.5. Electrophilic Additions
- 4.6. Electrophilic Substitutions
- 4.7. Elimination Reactions
- 4.8. Radical Reactions
- 4.9. Orbital-Controlled Reactions

5. Polymer Chemistry (6 h)

- 5.1. Introduction to Polymer Science
- 5.2. Step-Growth Polyreactions
- 5.3. Chain-Growth Polymerizations
- 5.4. Living and Controlled Polymerizations
- 5.5. Molecular Weight Determination

6. Other Examples of Organic Materials (2 h)

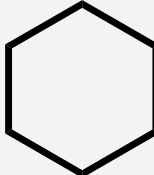
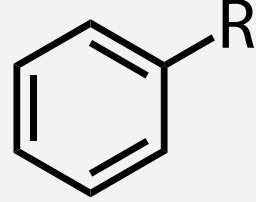
- 6.1. Chemical Technology
- 6.2. Surfactants
- 6.3. Organic Dyes and Semiconductors

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 conformers, geometric isomers, enantiomers, diastereomers

3.1 Basic Rules of Nomenclature

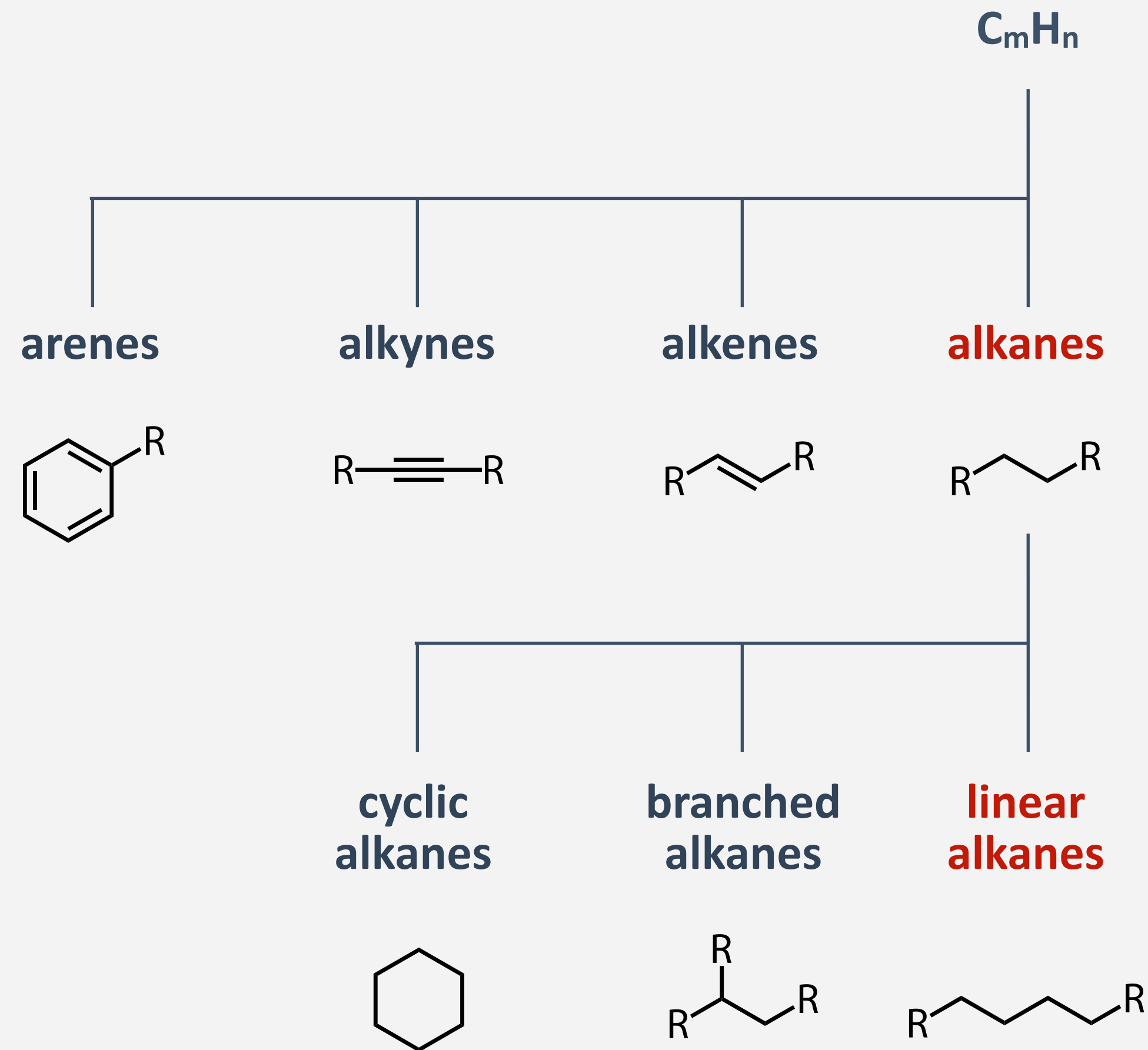
Overview of Compound Classes and Functional Groups

hydrocarbons		functionalized molecules			
		monovalent	divalent	trivalent	tetravalent
alkanes	alkenes (olefins)	haloalkanes (halogenides)	aldehydes & ketones	carboxylic acids (acids)	carbonates
$\text{R}-\text{CH}_2-\text{CH}_2-\text{R}$	$\text{R}-\text{CH}=\text{CH}-\text{R}$	$\begin{matrix} \text{R}-\text{F} & \text{R}-\text{Cl} \\ \text{R}-\text{Br} & \text{R}-\text{I} \end{matrix}$	$\begin{matrix} \text{O} & \text{O} \\ \parallel & \parallel \\ \text{R}-\text{C}-\text{H} & \text{R}-\text{C}-\text{R} \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{OH} \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{RO}-\text{C}-\text{OR} \end{matrix}$
cycloalkanes	alkynes (acetylenes)	alkanamines (amines)	acetals & ketals	carboxylic esters (esters)	urethanes (carbamates)
	$\text{R}-\text{C}\equiv\text{C}-\text{R}$	$\text{R}-\text{NH}_2$	$\begin{matrix} \text{RO} & \text{OR} & \text{RO} & \text{OR} \\ & \diagdown \diagup & & \diagdown \diagup \\ & \text{C} & & \text{C} \\ & \diagup \diagdown & & \diagup \diagdown \\ \text{R} & & \text{R} & \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{OR} \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{RO}-\text{C}-\text{NR}_2 \end{matrix}$
	arenes (aromatics)	alkanols (alcohols)	imines	carboxylic anhydrides (anhydrides)	ureas
		$\text{R}-\text{OH}$	$\begin{matrix} \text{NH} \\ \parallel \\ \text{R}-\text{C}-\text{R} \text{ (H)} \end{matrix}$	$\begin{matrix} \text{O} & \text{O} \\ \parallel & \parallel \\ \text{R}-\text{C}-\text{O}-\text{C}-\text{R} \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{R}_2\text{N}-\text{C}-\text{NR}_2 \end{matrix}$
		alkanthiols (mercaptans)	aminals	carboxylic amides (amides)	
		$\text{R}-\text{SH}$	$\begin{matrix} \text{R}_2\text{N} & \text{NR}_2 \\ & \diagdown \diagup \\ & \text{C} \\ & \diagup \diagdown \\ \text{R} & \text{R} \text{ (H)} \end{matrix}$	$\begin{matrix} \text{O} \\ \parallel \\ \text{R}-\text{C}-\text{NR}_2 \end{matrix}$	

Hydrocarbons

hydrocarbons

compounds that only contain C and H



“saturated” hydrocarbons that only contain single bonds

alkanes with a single carbon backbone without branching points

Nomenclature of Linear Alkanes and Alkyl Residues

methane méthane	CH_4					CH ₃ methyl
ethane éthane	CH_3CH_3			$\text{H}_3\text{C}-\text{CH}_3$		CH ₃ ethyl
propane propane	$\text{CH}_3\text{CH}_2\text{CH}_3$			$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_3$		CH ₃ propyl
butane butane	$\text{CH}_3(\text{CH}_2)_2\text{CH}_3$			$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_3$		CH ₃ butyl
pentane pentane	$\text{CH}_3(\text{CH}_2)_3\text{CH}_3$			$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_3$		CH ₃ pentyl
hexane hexane	$\text{CH}_3(\text{CH}_2)_4\text{CH}_3$			$\text{H}_3\text{C}-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_2-\text{CH}_3$		CH ₃ hexyl

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

Basic Rules of Nomenclature of Branched Alkanes

1. find the longest carbon chain in the molecule (parent chain or principal chain)

- if two chains are equally long, choose the one that has more substituents

2. name all residues attached to this main chain as “alkyl” residues and put them as prefix

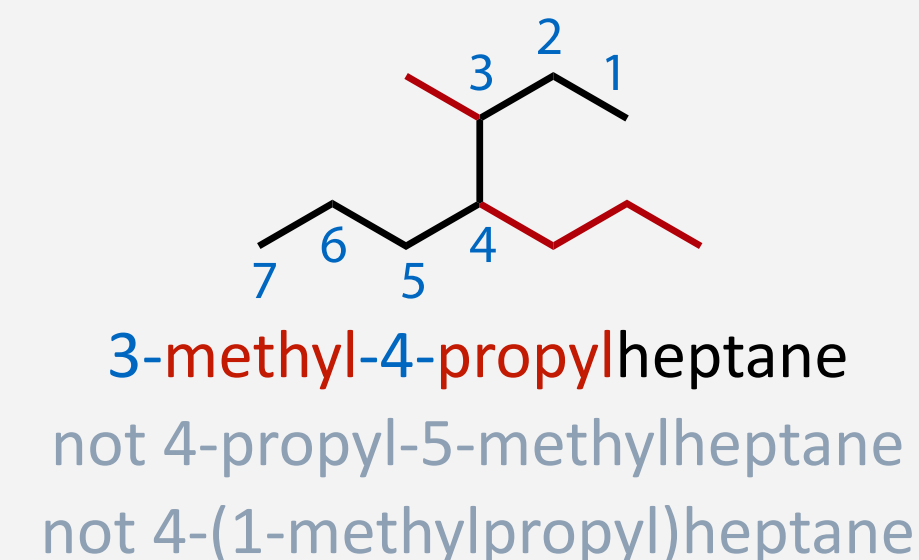
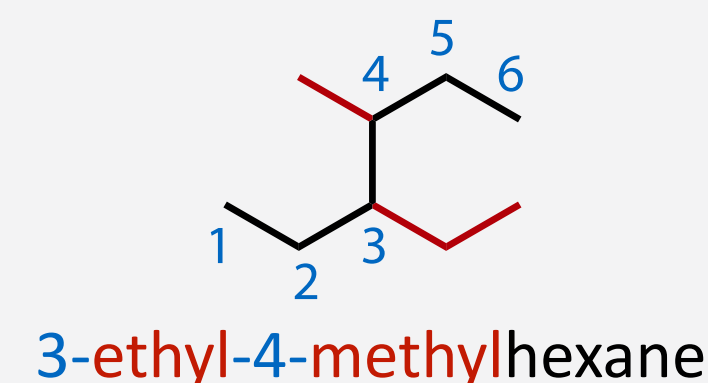
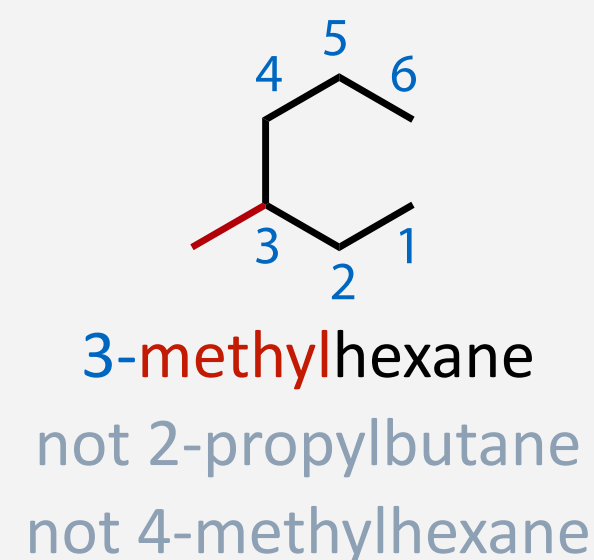
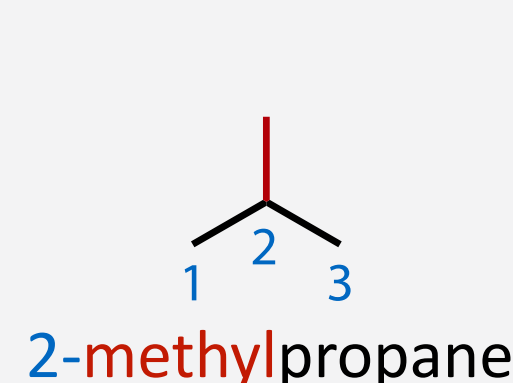
- if side chains are branched, apply the same rules iteratively: find the longest carbon chain, etc.

3. number the atoms of the main chain starting with the end that is closest to first substituent

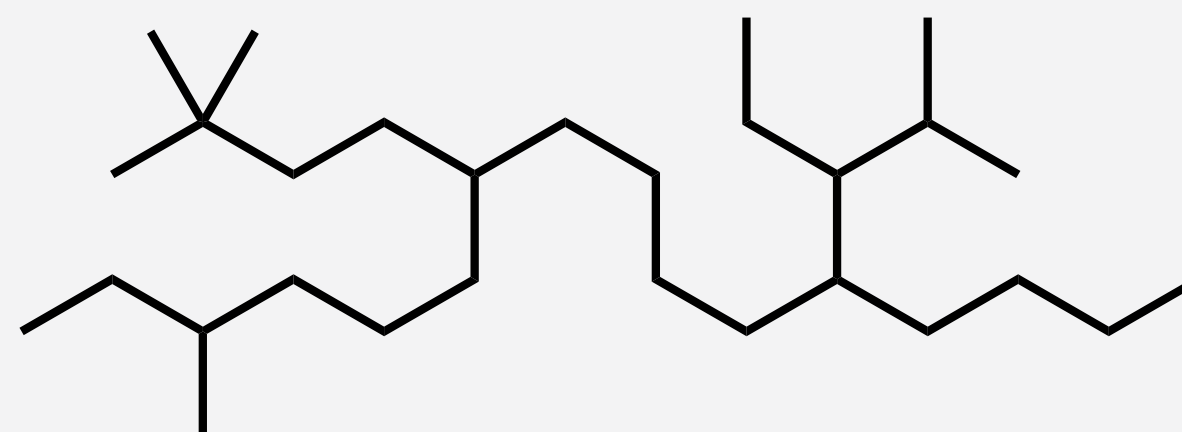
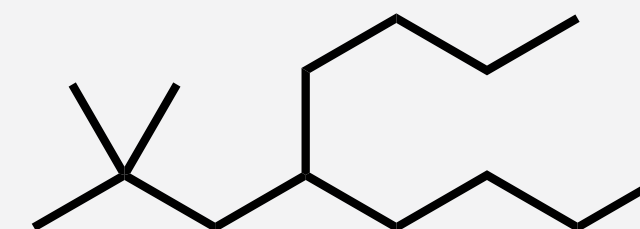
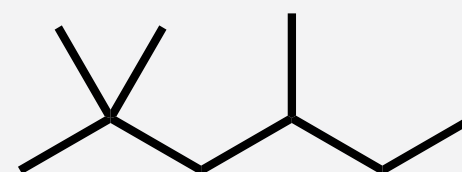
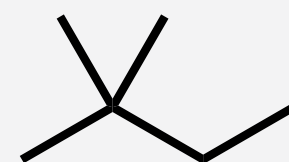
- if two substituents at same distance, alphabetic order of these substituents decides
- if identical substituents at same distance, next substituents along the chain decide (iterative)
- number atoms in substituents starting with the first atom attached to the main chain

4. put the substituents into alphabetic order

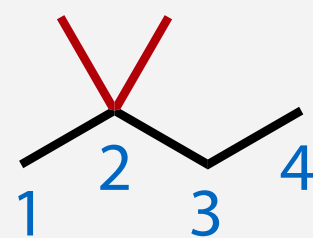
- substituents preceded with number indicating the atom of the main chain they are attached to
- if multiple substituents of same type, name is preceded with a prefix (di-, tri-, tetra-, etc.)



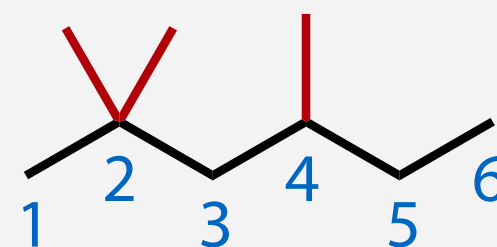
Examples for the Nomenclature of Branched Alkanes



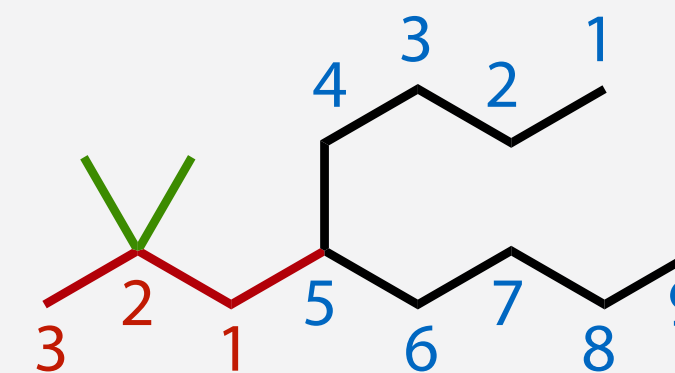
Examples for the Nomenclature of Branched Alkanes



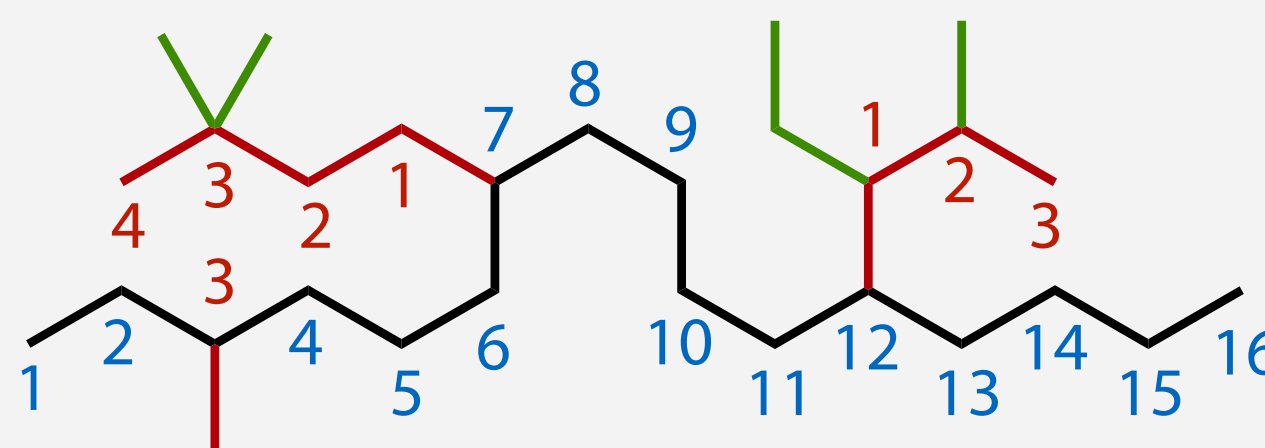
2,2-dimethylbutane



2,2,4-trimethylhexane

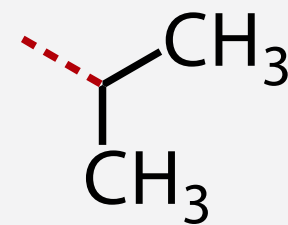


5-(2,2-dimethylpropyl)nonane

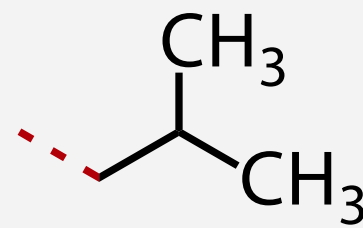


7-(3,3-dimethylbutyl)-
12-(1-ethyl-2-methylpropyl)-3-methylhexadecane

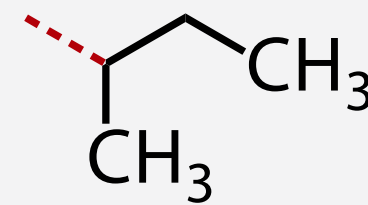
Trivial Names of Alkyl Groups



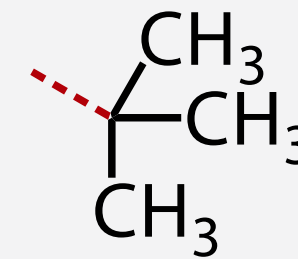
isopropyl (1-methylethyl)



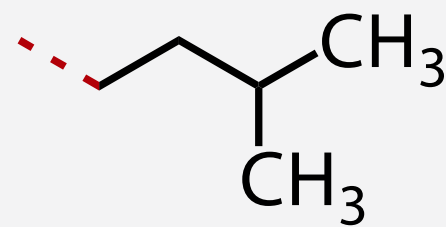
isobutyl (2-methylpropyl)



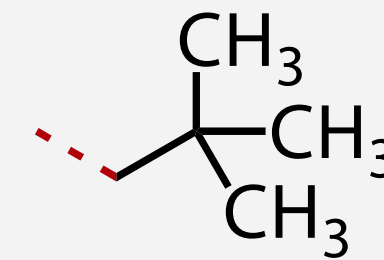
sec.-butyl (1-methylpropyl)



tert.-butyl (1,1-dimethylethyl)

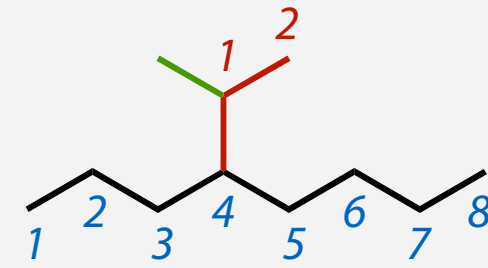


isopentyl (3-methylbutyl)

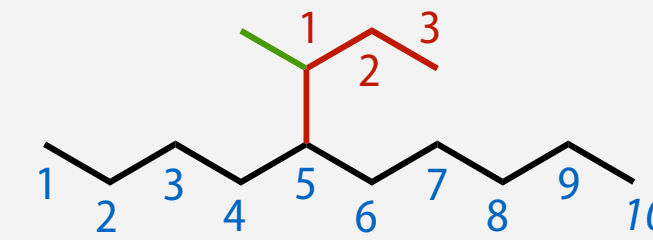


neopentyl (2,2-dimethylpropyl)

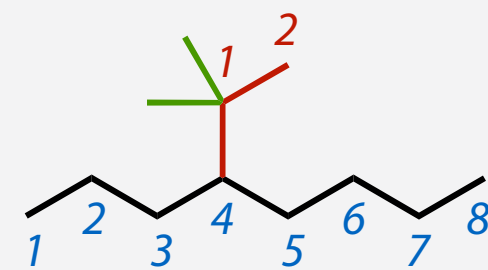
Examples Using Trivial Names of Alkyl Groups



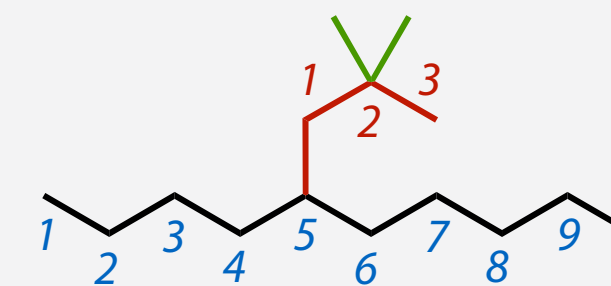
4-(1-methylethyl)octane
or 4-isopropyloctane



5-(1-methylpropyl)decane
or 5-(sec-butyl)decane



4-(1,1-dimethylethyl)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 multiple bonds**

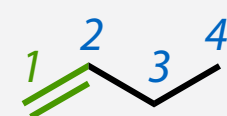
- molecule may contain double bonds or triple bonds, but priority for determining the parent chain is simply the longest carbon chain

2. indicate the position of the double/triple bond

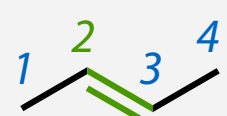
- give the number of the carbon atom of the double/triple bond closer to the end of the chain

3. replace the suffix “ane” by “ene” or “yne” (sort alphabetically if both present)

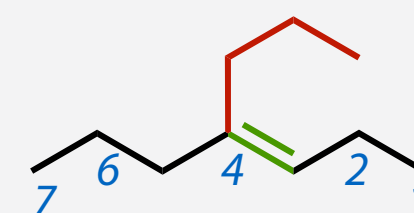
- for multiple double/triple bonds, suffix is preceded with a number prefix (di-, tri-, tetra-, etc.)



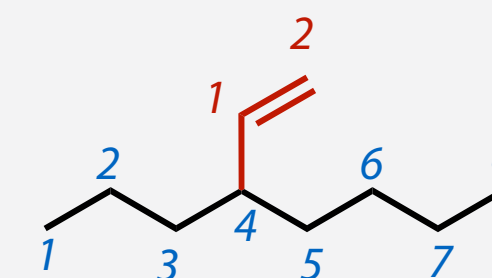
but-1-ene or butene
not 1-butene



but-2-ene
not 2-butene



4-propyl-hept-3-ene



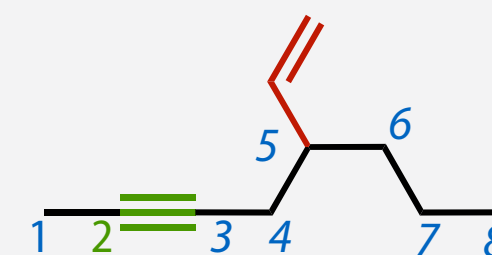
4-(eth-1-enyl)octane



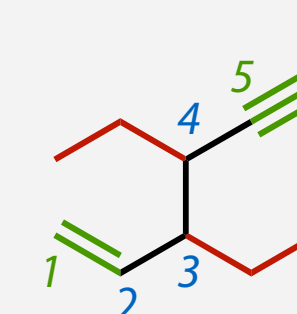
but-1-yne or butyne
not 1-butyne



but-2-yne
not 2-butyne

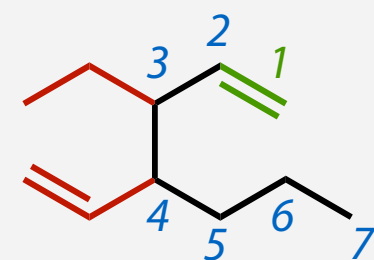


5-(eth-1-enyl)oct-2-yne

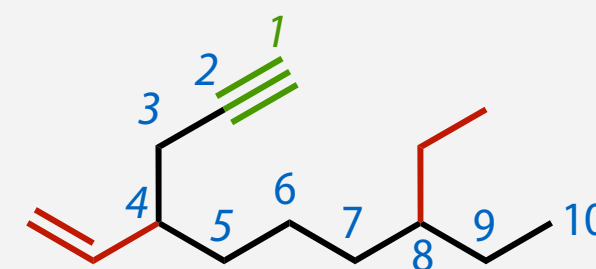


3,4-diethylhex-1-en-4-yne

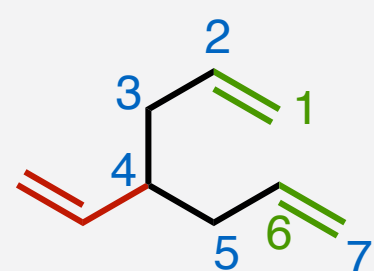
Advanced Examples of Branched Alkenes and Alkynes



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



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



4-(eth-1-enyl)-1,6-heptadiene



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

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

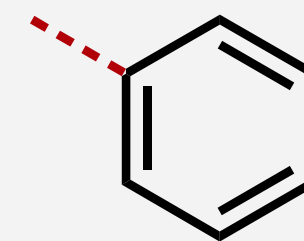
Trivial Names of Alkenyl, Alkynyl, and Aromatic Substituents



vinyl
(ethen-1-yl)



ethynyl
(ethyn-1-yl)



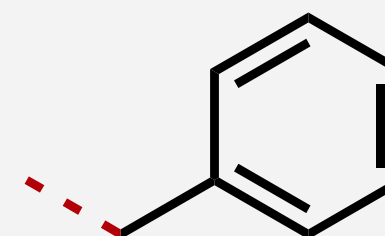
phenyl



allyl
(propen-2-yl)



propargyl
(propyn-2-yl)



benzyl
(1-phenylmethyl)

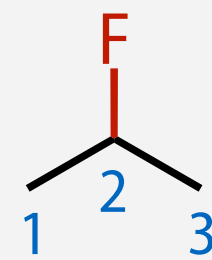


Nomenclature of Haloalkanes

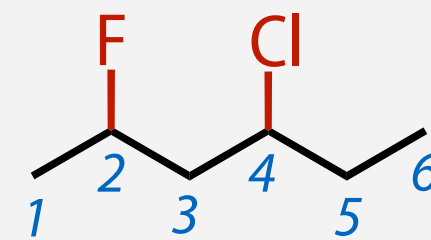
1. name the longest carbon chain, **irrespective of the presence of halogens**
 - other chains may contain (more) halogens, but the longest carbon chain has priority
2. indicate the position of the halogen atom
 - give the number of the carbon atom of the halogen atom that is closer to the end of the chain
3. if different halogen atoms attached to the same chain, sort alphabetically
4. if multiple halogen atoms of the same type at same chain, use number prefix (di, tri, tetra)



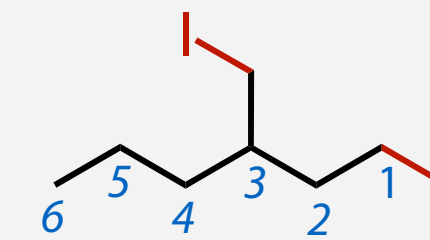
1-chloroethane



2-fluoropropane



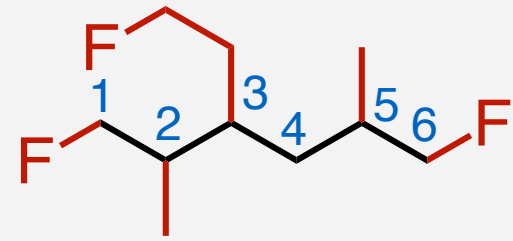
4-chloro-2-fluorohexane



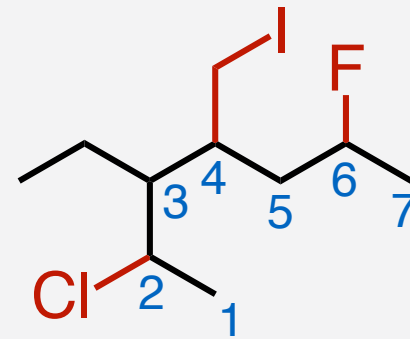
1-iodo-3-(iodomethyl)hexane

- **halogens have no priority; always labeled with a prefix, whether in main or side chain**

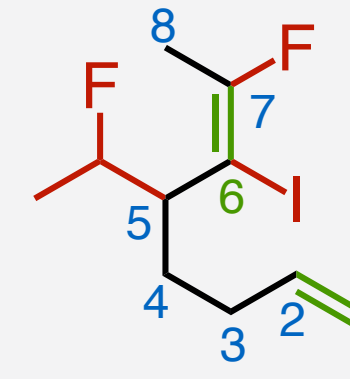
Advanced Examples of Branched Haloalkanes and Multifunctional Compounds



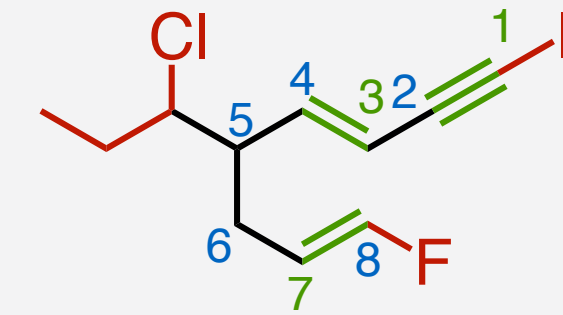
1,6-difluoro-3-(2-fluoroethyl)-2,5-dimethylhexane



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



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



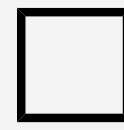
5-(1-chloropropyl)-8-fluoro-1-iodoocta-3,7-dien-1-yne

- **priority rules: alkane alkene, alkyne and halogens have no priority**
 - always search the **longest carbon chain**
 - the longer chain takes precedence, even even if halogens or alkenes are present
 - if a molecule contains an alkene or alkyne, they take precedence for finding longest chain
 - **halogen atoms never have priority**
 - they are always labeled with a prefix, the remaining nomenclature is as usual

Nomenclature of Cyclic Alkanes



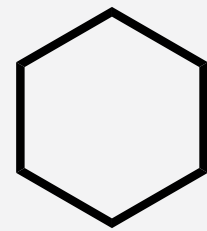
cyclopropane



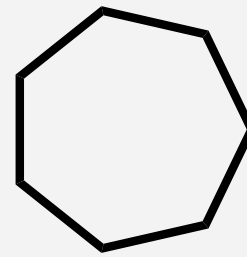
cyclobutane



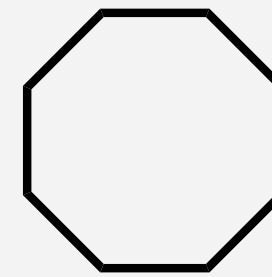
cyclopentane



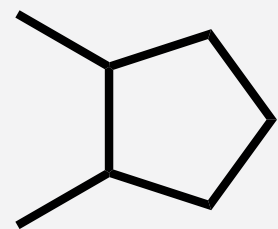
cyclohexane



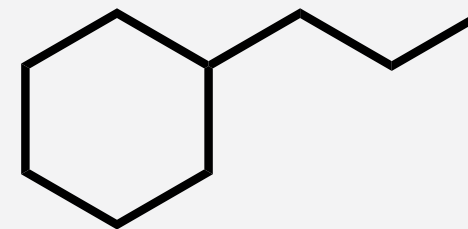
cycloheptane



cyclooctane



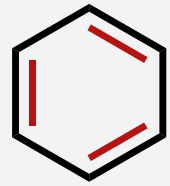
1,2-dimethylcyclopentane



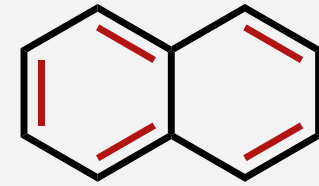
propylcyclohexane

Nomenclature of Aromatic Compounds

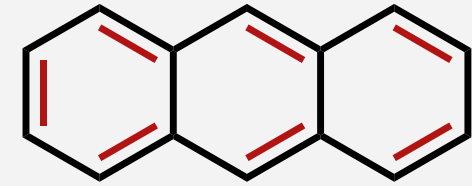
benzene



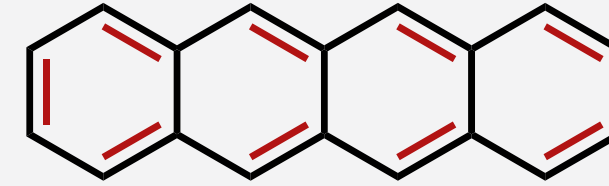
naphthalene



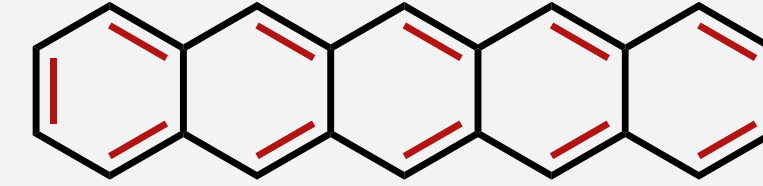
anthracene



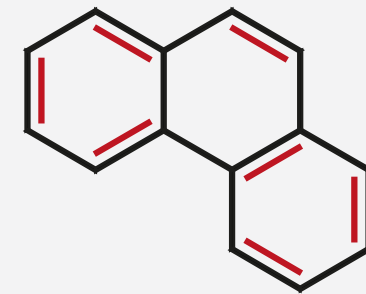
tetracene



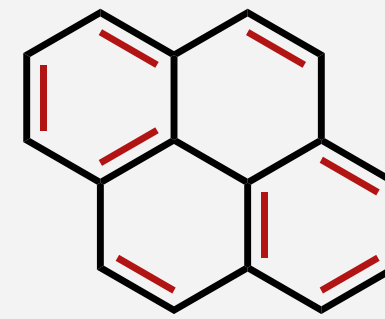
pentacene



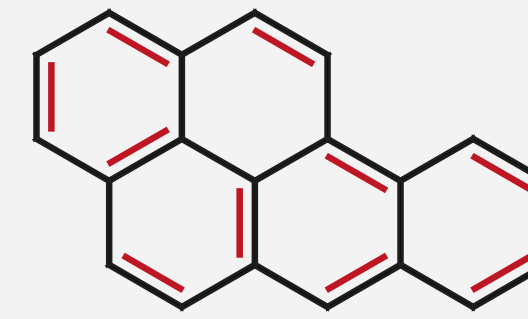
phenanthrene



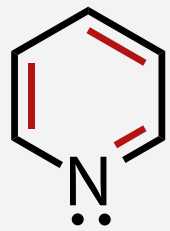
pyrene



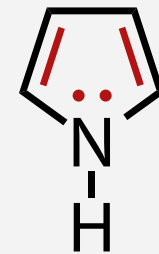
benzopyrene



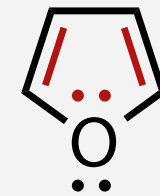
pyridine



pyrrol



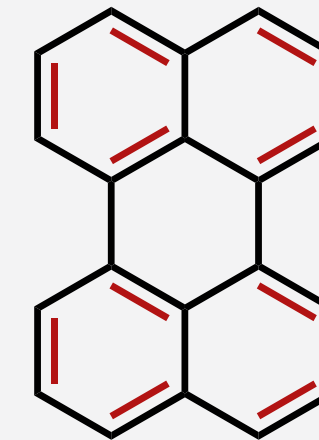
furan



thiophene

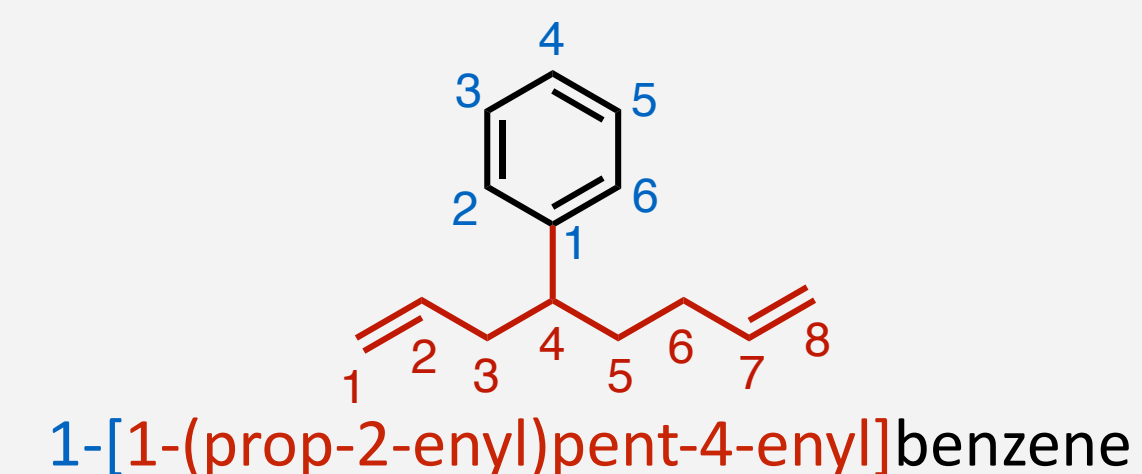
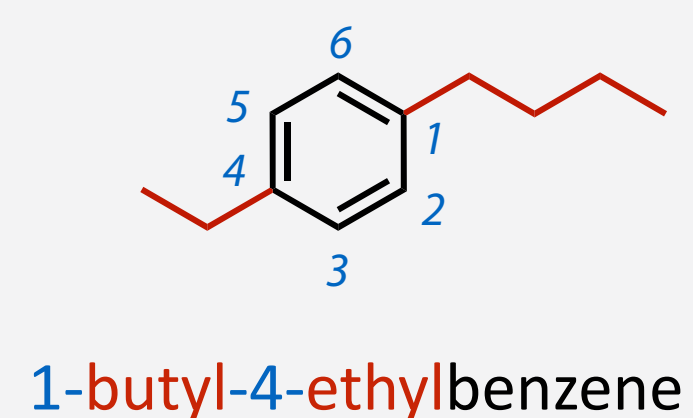
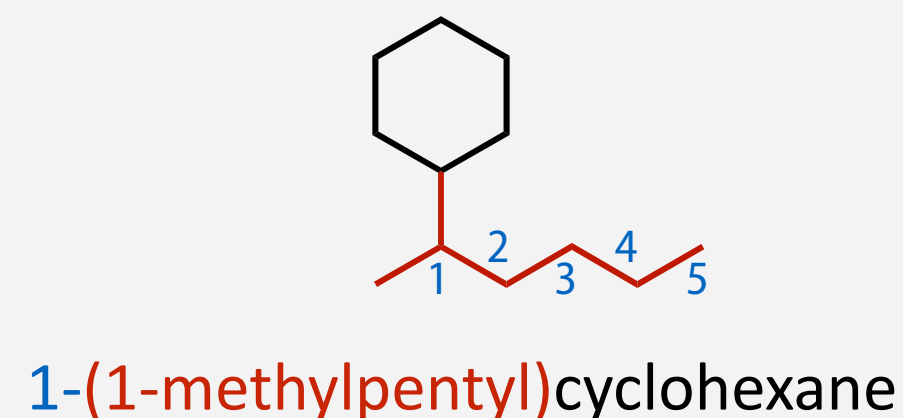


perylene



Naming of Cyclic and Aromatic Compounds

1. in compounds containing C, H, and halogens , the cycle is always considered as the parent chain and the alkyl residue(s) as the substituent(s)
2. name all residues attached to the cycle as “alkyl” residues
 - if side chains are branched, apply the same rules iteratively: find the longest carbon chain, etc.
3. 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 chain decide (iterative)
4. apply the same rules for substituents naming and ordering as described previously



Summary of the Priority Rules on Following Slides

		>		>		>		>		>	—OH	>	—NH_2
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-

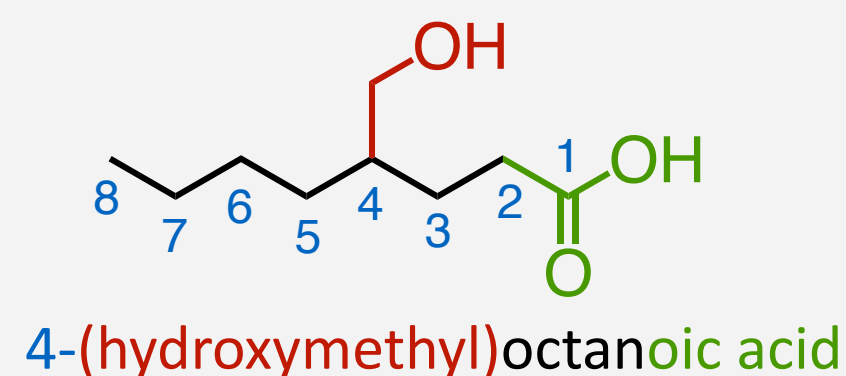
no priority

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

- alkanes, alkenes, alkynes and halogen do not possess any priority
- functional group with the higher priority defines 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 (except when in side groups)

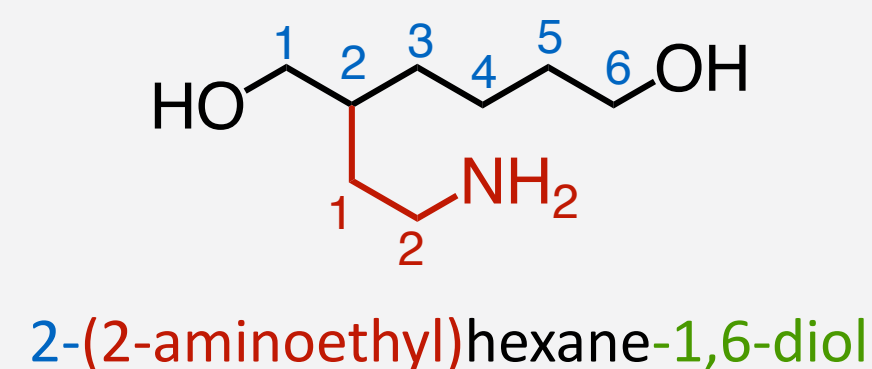
Priority Rules Summary To Determine Parent Chain

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



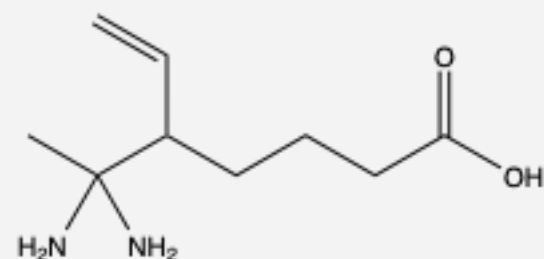
- if more than one type of functional group, the one with higher priority decides
- carboxylic acid is principal characteristic group because higher in priority than alcohol
- parent chain is longest carbon chain containing carboxylic acid

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



- 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**

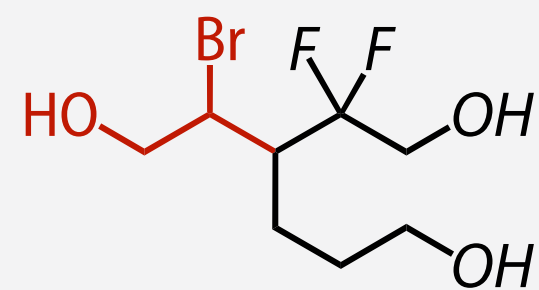


5-(1,1-diaminoethyl)hept-6enoic acid

- 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

Priority Rules Summary To Determine Parent Chain

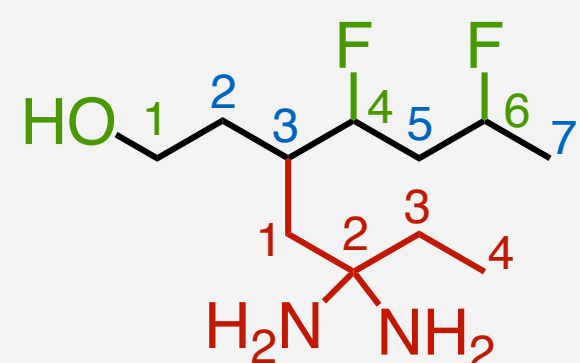
4. identify the chain that has the **maximum number of substituents**



2,2-difluoro-3-(1-bromoethyl)
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)

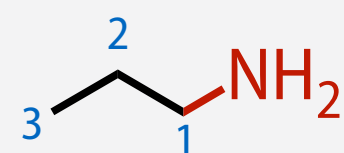
Nomenclature of Amines

1. identify the longest chain to which the amine is attached, name it, append suffix “amine”

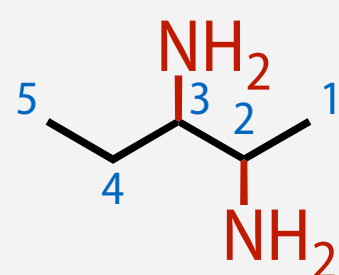
- parent chain is the one with maximum number of amine functions, even if molecule contains longer chains
- indicate their position with numbers (locants)

2. if multiple amines attached to same chain, use number prefix (di, tri, tetra, etc.)

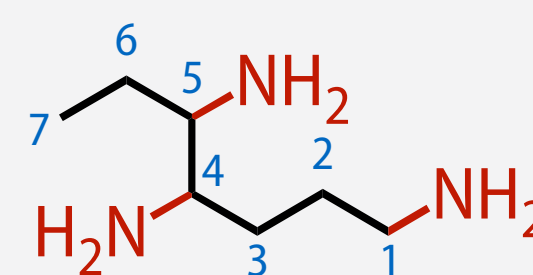
- combine their position numbers, separated by commas



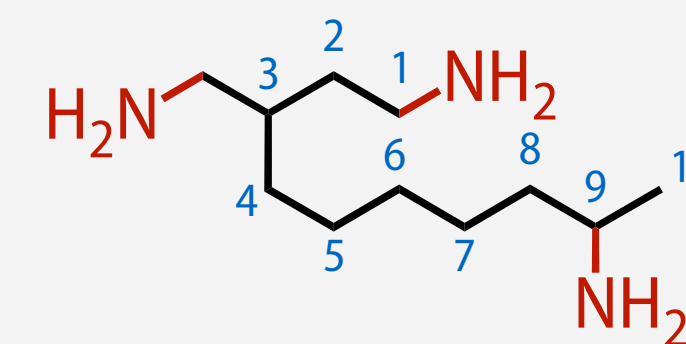
propan-1-amine



pentane-2,3-diamine



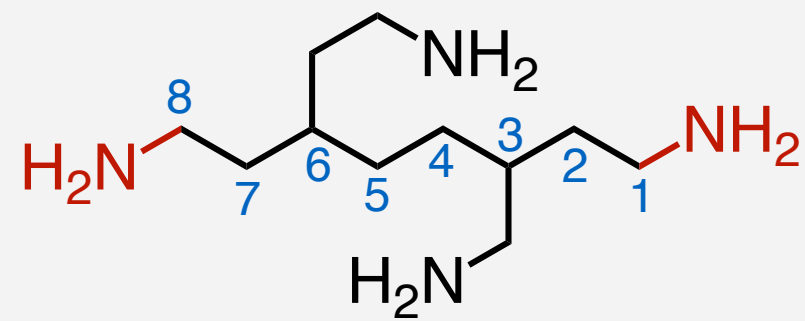
heptane-1,4,5-triamine



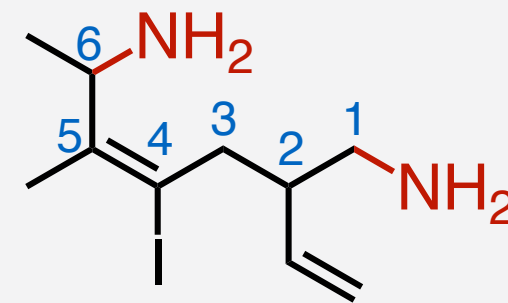
3-(aminomethyl)decane-1,9-diamine

- if amine is in a side branch (or if higher priority groups are present), use instead prefix “amino”

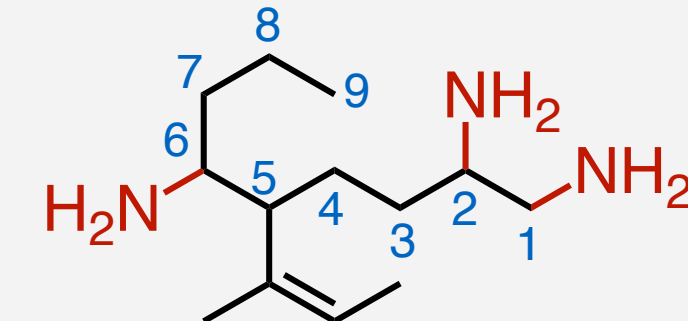
Advanced Examples of Branched Amines and Multifunctional Compounds



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



4-iodo-5-methyl-2-vinylhept-4-ene-1,6-diamine



5-(1-methyl-prop-1-enyl)nonane-1,2,6-triamine

- **priority rules: amine > (arene, alkene, alkyne, halogen)**
 - always search the **longest chain** that contains the **maximum number of amines**
 - this chain takes precedence, even even if longer alkyl chain or other groups 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”

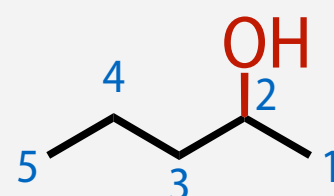
Nomenclature of Alcohols and Thiols

1. identify longest chain to which alcohol/thiol is attached, append suffix “ol”/“thiol”

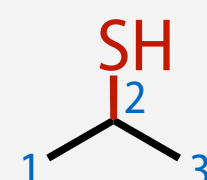
- parent chain is the one with maximum number of hydroxy or thiol functions, even if molecule contains longer chains
- indicate their position with numbers (locants)

2. if multiple alcohols/thiols attached to same chain, use number prefix (di, tri, tetra, etc.)

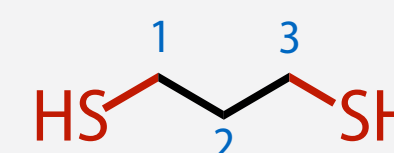
- combine their position numbers, separated by commas



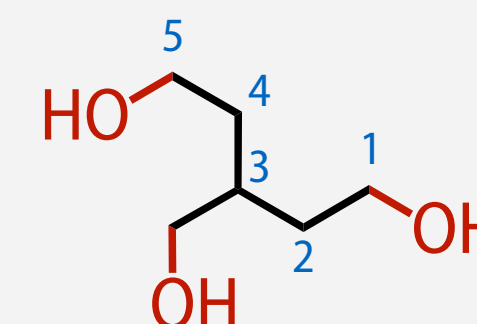
pentan-2-ol



propane-2-thiol



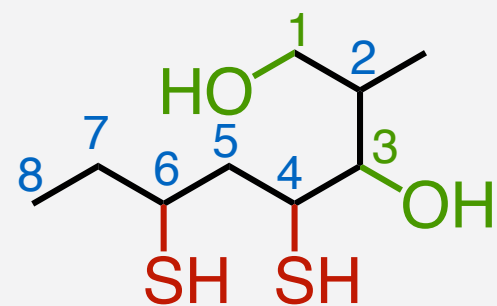
propane-1,3-dithiol



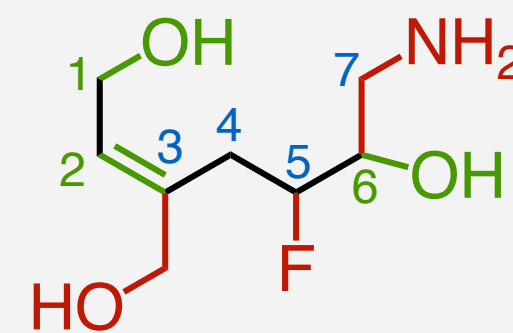
3-(hydroxymethyl)pentane-1,5-diol

- if alcohol is in a side branch (or if higher priority groups are present), use instead prefix “hydroxy”
- if thiol is in a side branch (or if higher priority groups are present), use instead prefix “sulfanyl”

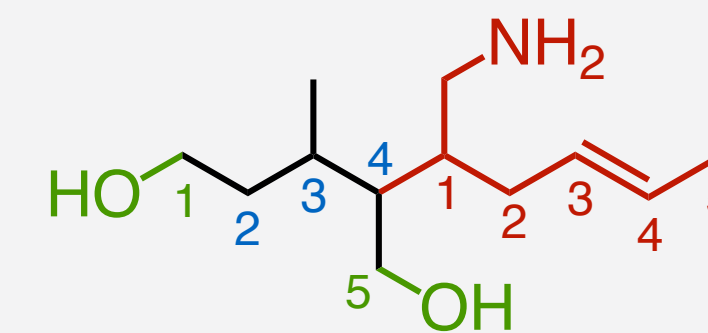
Advanced Examples of Branched Alcohols and Multifunctional Compounds



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



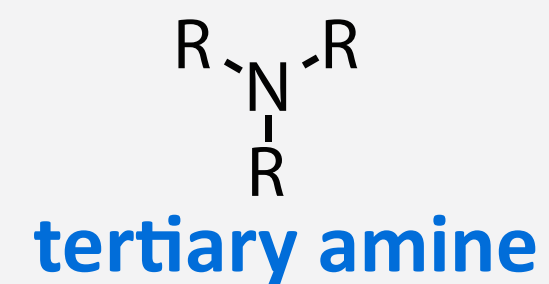
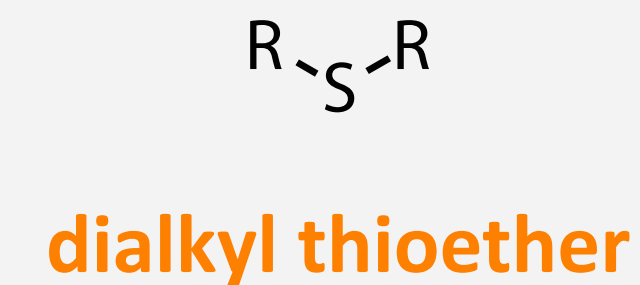
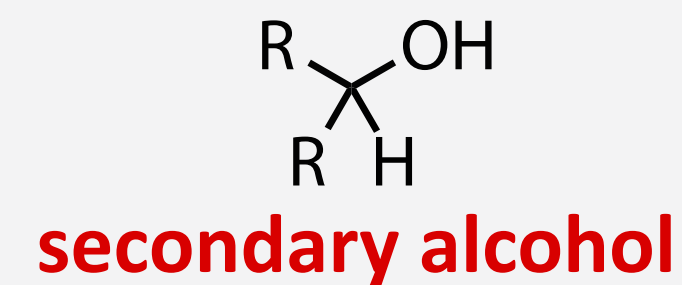
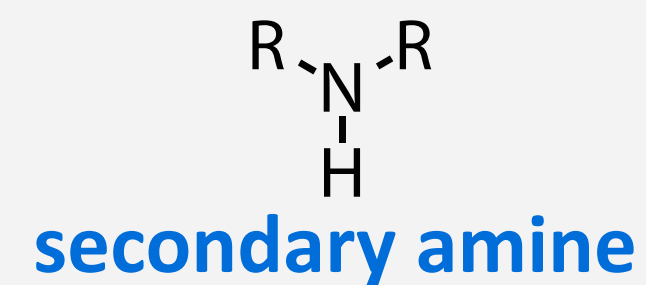
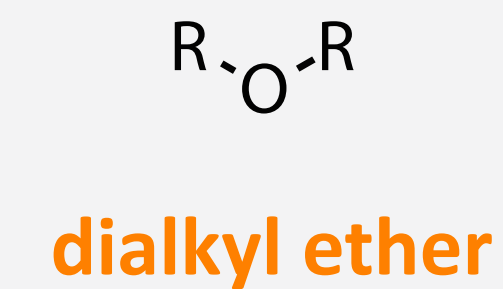
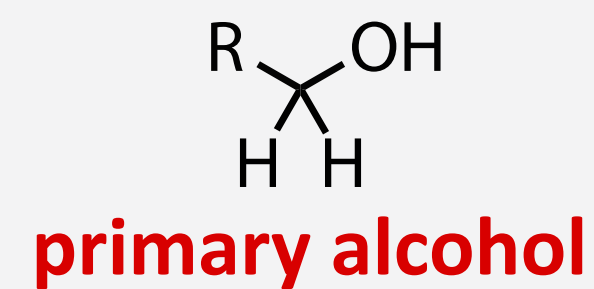
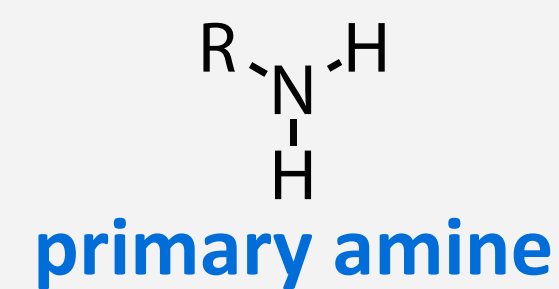
7-amino-5-fluoro-3-(hydroxymethyl)hept-2-ene-1,6-diol



4-(1-(aminomethyl)pent-3-enyl)3-methylpentane-1,5-diol

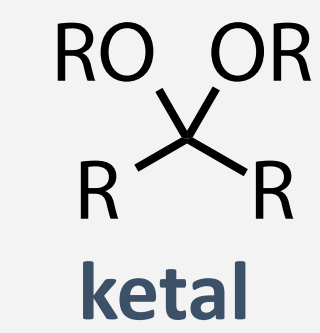
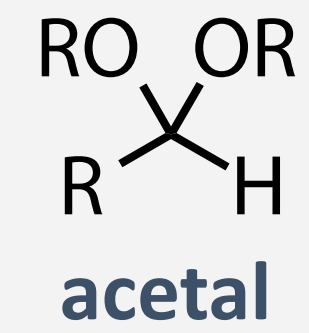
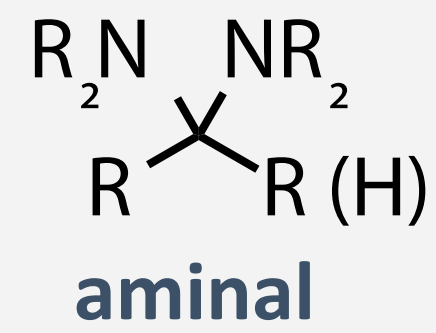
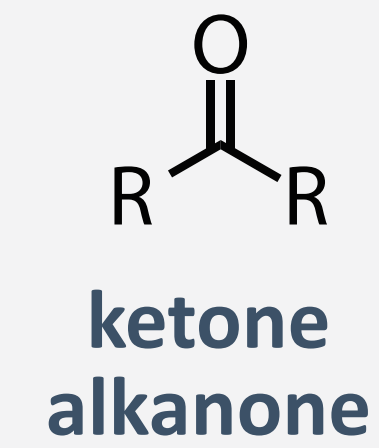
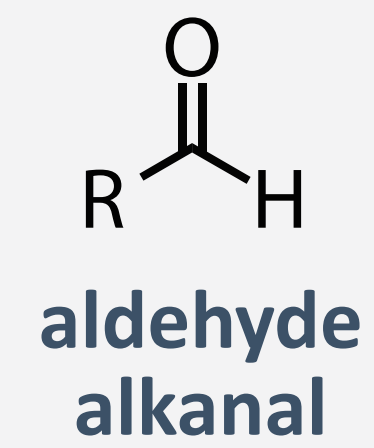
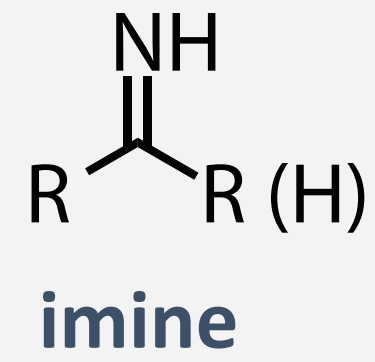
- **priority rules: alcohol > amine > (arene, alkene, alkyne, halogen)**
 - always search the **longest chain** that contains the **maximum number of alcohols**
 - this chain takes precedence, even even if longer alkyl chains or other groups present
 - suffixes of alkenes/alkynes and alcohols can be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

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



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

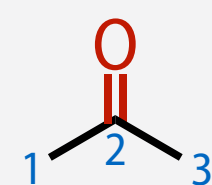
Nomenclature of Ketones and Aldehydes

1. identify the longest chain to which ketone/aldehyde is attached, append suffix “one”/“al”

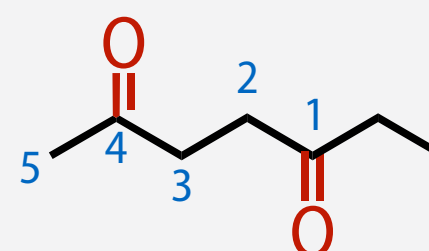
- parent chain is the one with maximum number of ketone/aldehyde functions, even if molecule contains longer chains
- indicate their position with numbers (locants)

2. indicate the position of the ketone on the chain with number

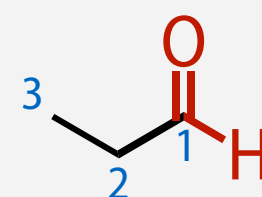
- aldehyde must always be terminal, no number, and its position is assumed to be 1



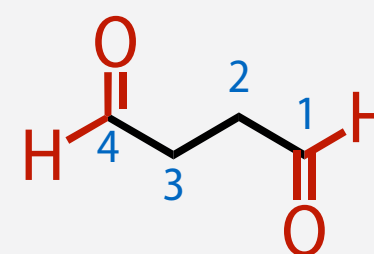
propan-2-one



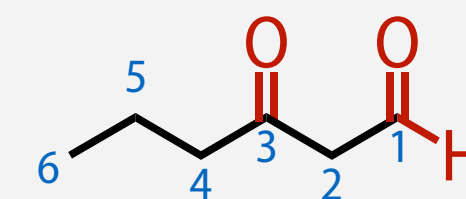
heptane-2,5-dione



propanal



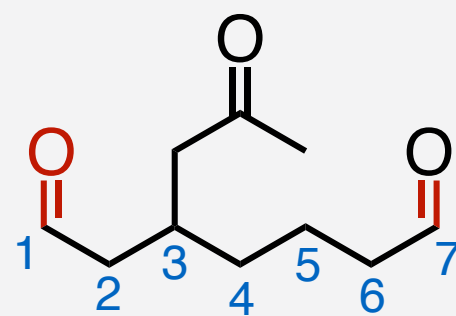
1,4-butanedial



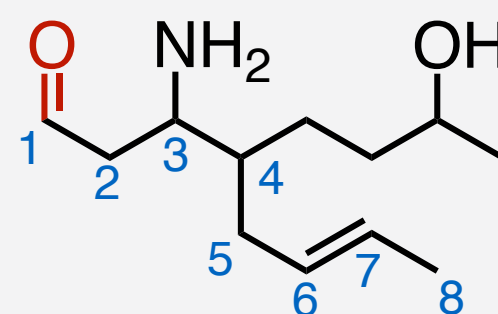
3-oxohexanal

- if aldehyde/ketone is in a side branch (or if higher priority groups are present), use instead prefix “oxo”

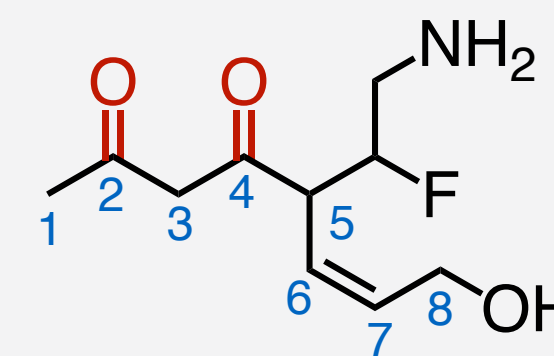
Advanced Examples of Branched and Multifunctional Compounds



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



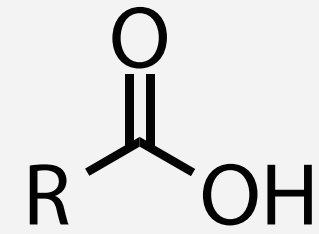
3-amino-4-(3-hydroxybutyl)oct-6-enal



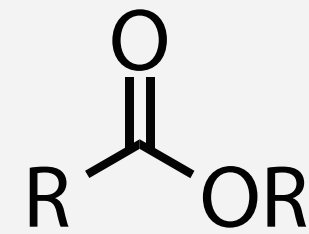
5-(2-amino-1-fluoroethyl)-8-hydroxyoct-6-ene-2,4-dione

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

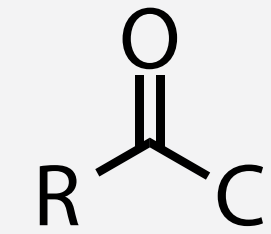
Trivalent Functional Groups



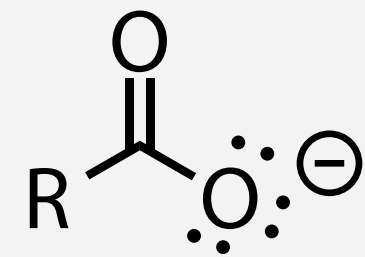
carboxylic acid



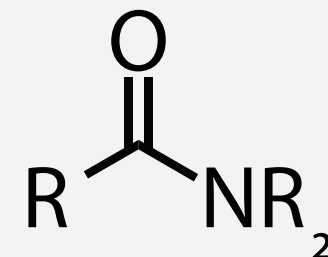
carboxylic acid ester



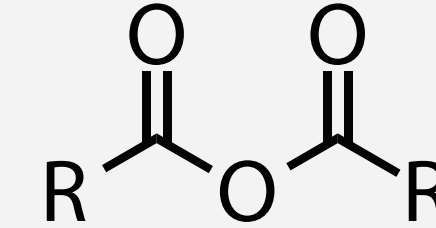
carboxylic acid chloride



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”

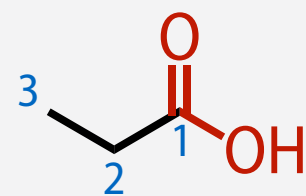
Nomenclature of Carboxylic Acids

1. identify the longest chain which contains the acid, append suffix “oic acid”

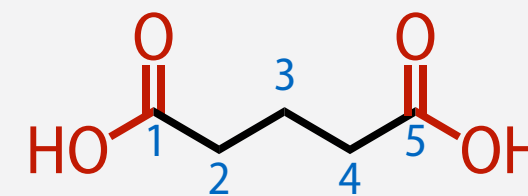
- parent chain is the one with maximum number of carboxylic acid functions, even if molecule contains longer chains
- carboxylic acid(s) are always terminal, no number needed

2. if multiple acids within the same chain, use number prefix (di)

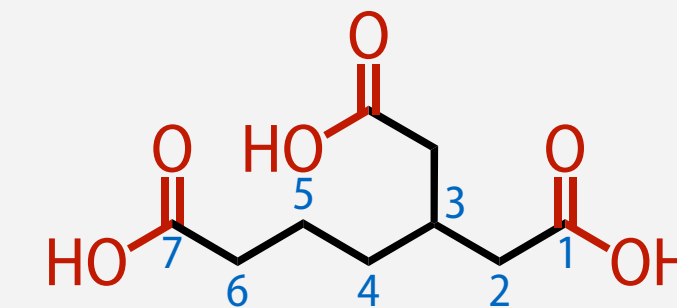
- there cannot be more than two acids on the main chain



propanoic acid



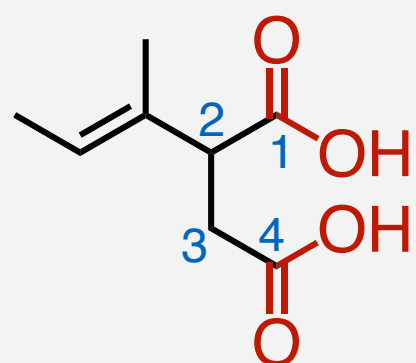
pentanedioic acid



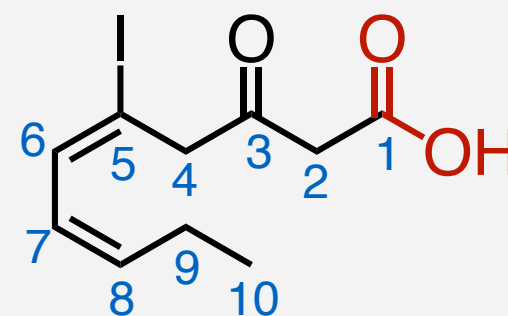
3-(carboxymethyl)
heptanedioic acid

- if carboxylic acid is in a side branch (or if higher priority groups are present), use instead prefix “carboxy”

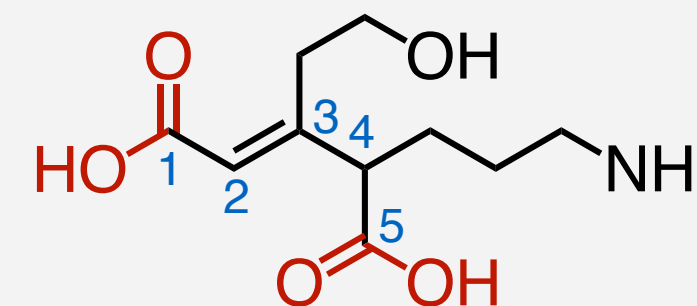
Advanced Examples of Branched and Multifunctional Compounds



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



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

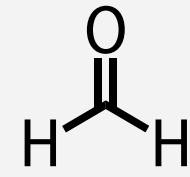


4-(3-aminopropyl)-3-(2-hydroxyethyl)pent-2-enedioic acid

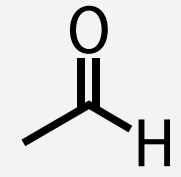
- **priority rules: acid > ester > amide > aldehyde > ketone > alcohol > amine > ...**
- always search **longest chain** that contains the **maximum number of acids**
- this chain takes precedence, even if longer alkyl chains or other groups present
- suffixes of alkenes/alkynes and aldehydes can be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

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

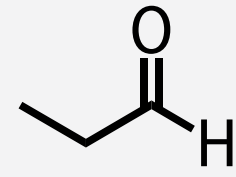
aldehydes



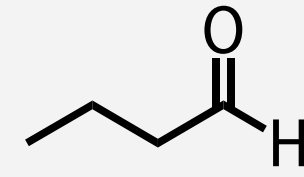
formaldehyde
methanal



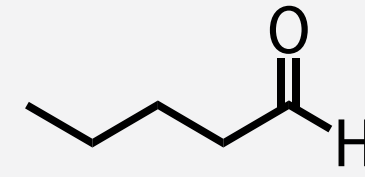
acetaldehyde
ethanal



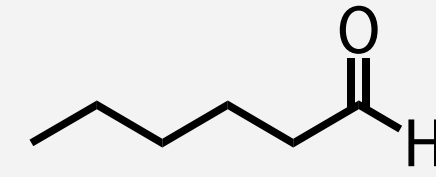
propionaldehyde
propanal



butyraldehyde
butanal

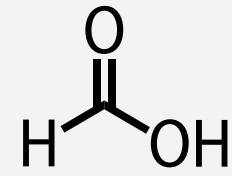


valeraldehyde
pentanal

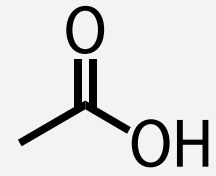


capronaldehyde
hexanal

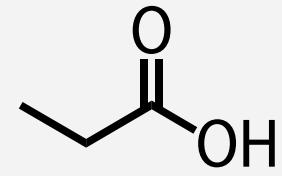
carboxylic acids



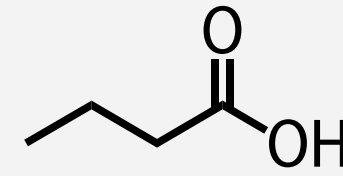
formic acid
methanoic acid



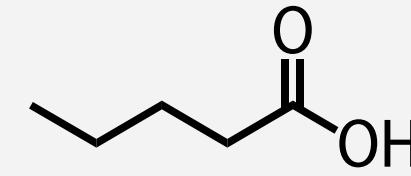
acetic acid
ethanoic acid



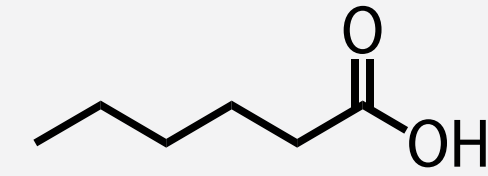
propionic acid
propanoic acid



butyric acid
butanoic acid

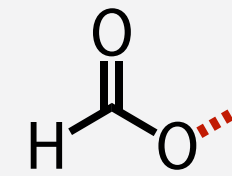


valeric acid
pentanoic acid

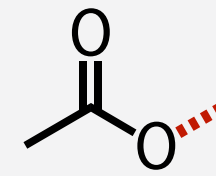


caproic acid
hexanoic acid

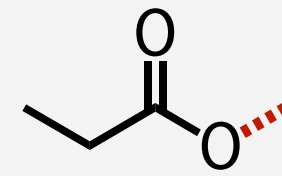
esters



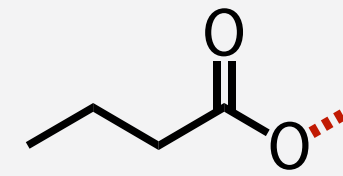
formate
methanoate



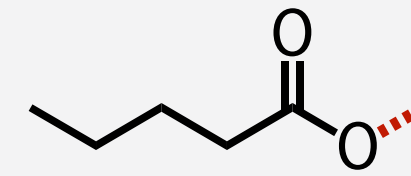
acetate
ethanoate



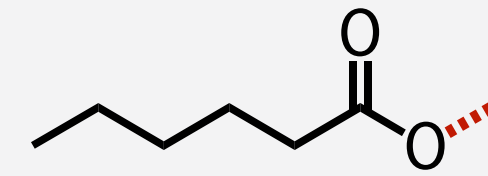
propionate
propanoate



butyrate
butanoate

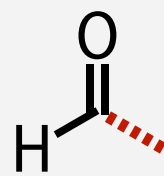


valerate
pentanoate

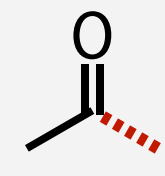


caproate
hexanoate

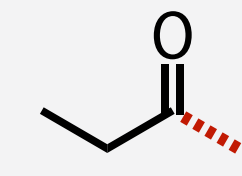
acyl residues



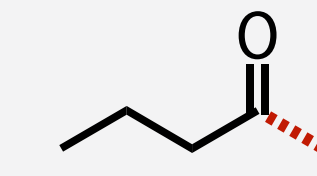
formyl
methanoyl



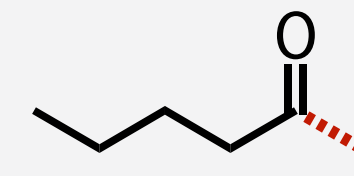
acetyl
ethanoyl



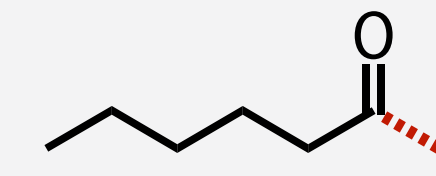
propionyl
propanoyl



butyryl
butanoyl



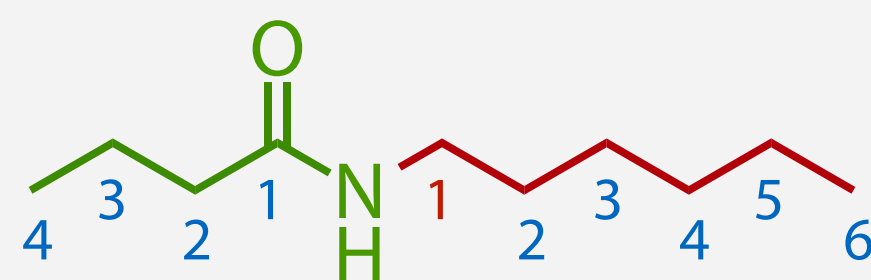
valeryl
pentanoyl



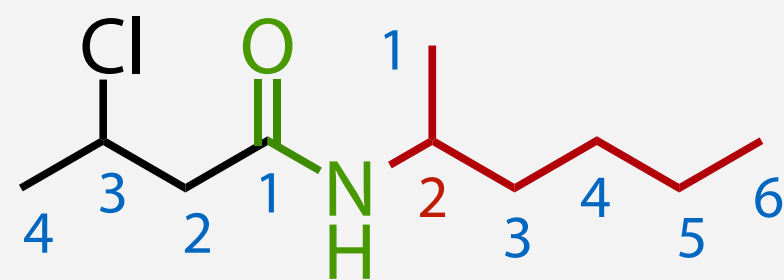
caproyl
hexanoyl

Nomenclature of Carboxylic Acid Amides

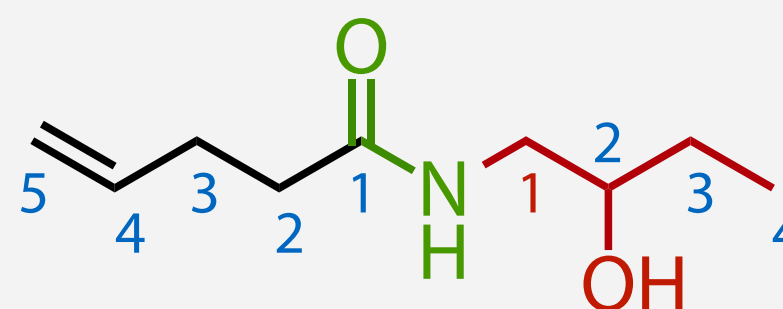
1. identify the longest chain to which the amide C=O is attached, name it, append suffix “amide”
2. prepend the name with the remaining residue, ended by “yl” (use number prefix if necessary)
3. carboxylic acid amide(s) always terminal, no number needed
4. if two carboxylic acid amides attached to same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



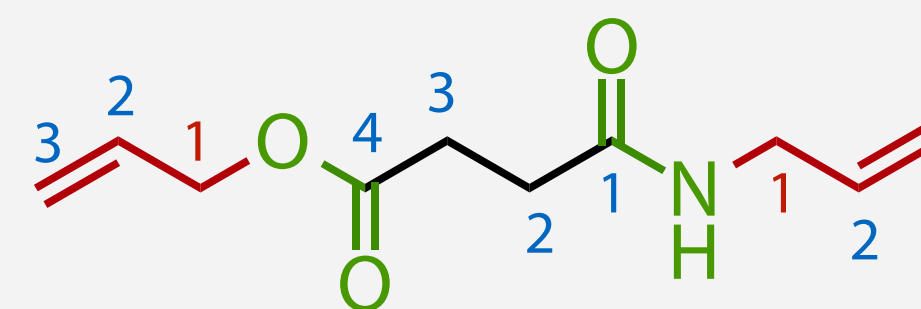
hexyl butanamide
old: butanoic acid
hexyl amide



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 butandioate
old: butandioic acid
di(2-propenyl) amide

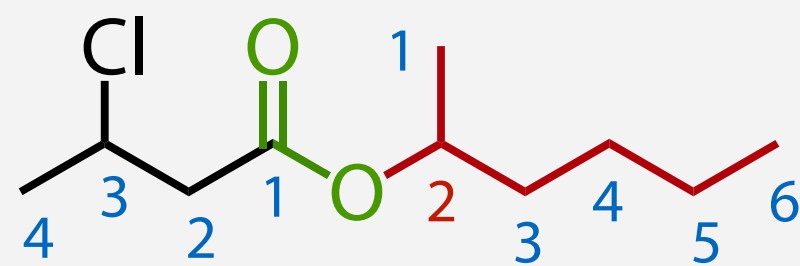
- alternatively, name like a carboxylic acid, append residue ended by “yl”, append “amide”
- naming of compounds with >2 amides (i.e., in side chains) complex but rarely needed

Nomenclature of Carboxylic Acid Esters

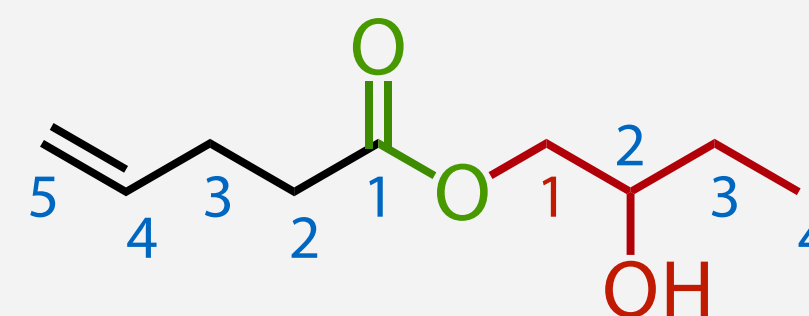
1. identify the longest chain to which the ester C=O is attached, name it, append suffix “oate”
2. prepend the name with the remaining residue, ended by “yl” (use number prefix if necessary)
3. carboxylic acid ester(s) always terminal, no number needed
4. if two carboxylic acid esters attached to same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



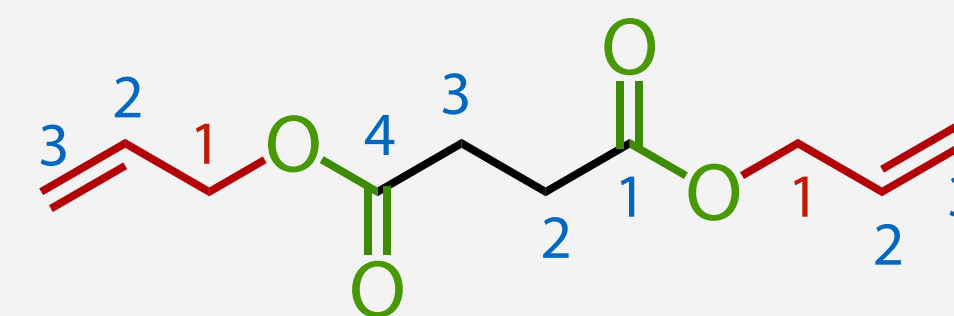
hexyl butanoate
old: butanoic acid
hexyl ester



1-methylpentyl 3-chlorobutanoate
old: 3-chlorobutanoic acid
2-hexyl ester



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



di(2-propenyl) butanedioate
or diallyl butanedioate
old: butanedioic 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

		>		>		>		>		>	—OH	>	—NH_2
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-

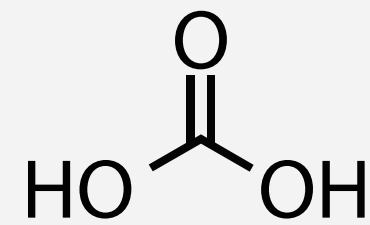
no priority

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

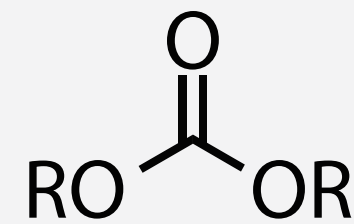
- alkanes, alkenes, alkynes and halogen do not possess any priority
- functional group with the higher priority defines the naming of the parent chain (using the suffix)
- functional group with a lower priority treated as a substituent (using prefix nomenclature)
- alkene/alkyne are concatenated with other suffixes (except when in side groups)

Naming of Simple Compounds with Tetravalent Functional Groups

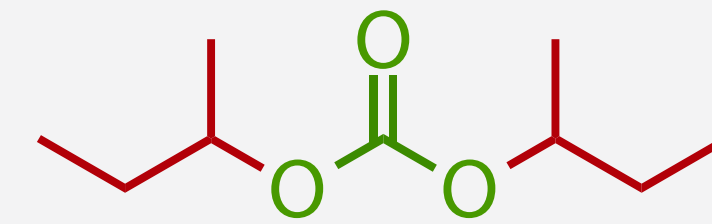
- in tetravalent functional groups, carbon has four bonds connected to heteroatom(s)



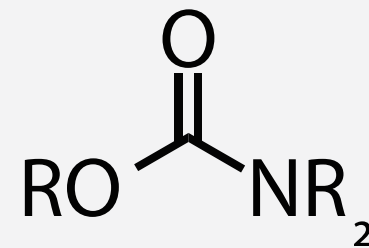
carbonic acid



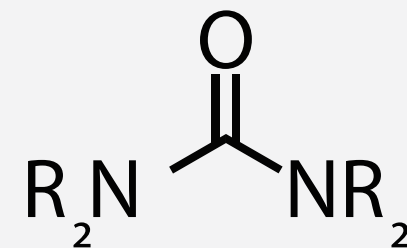
carbonate



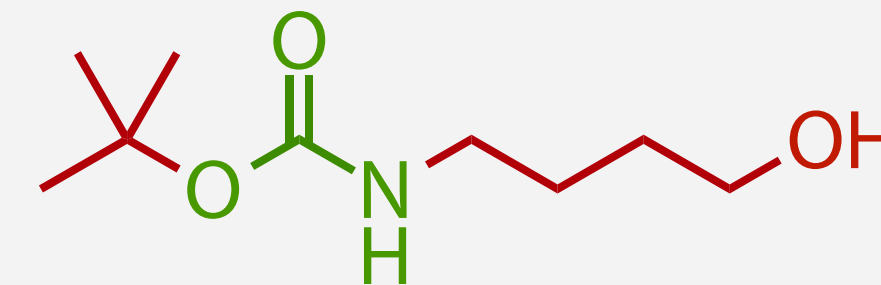
di(1-methylpropyl) carbonate



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

