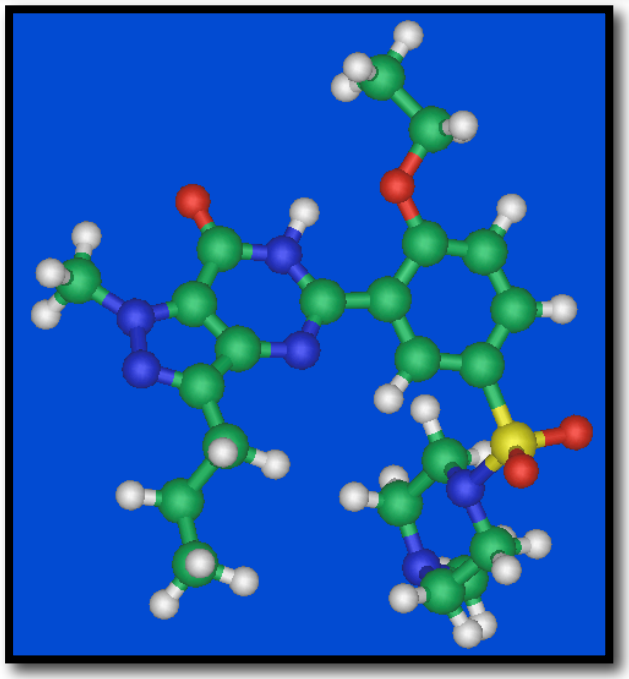
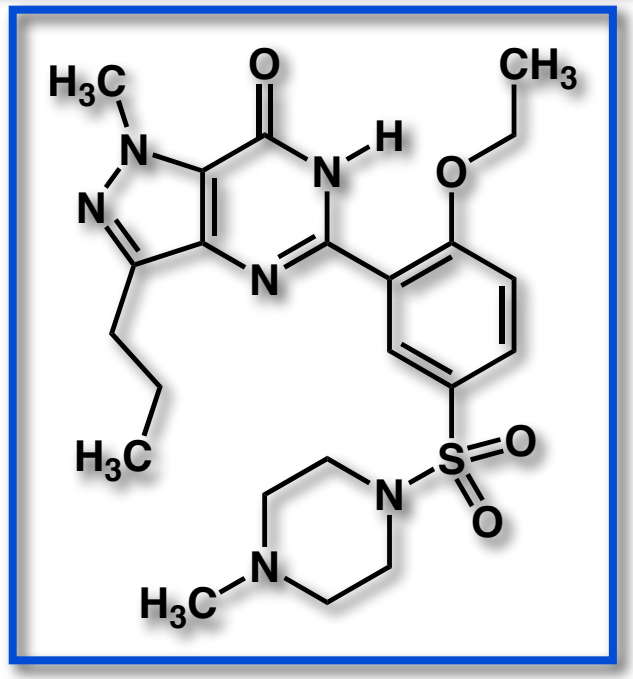
Unit One Part 2: naming and functional groups

- To write and interpret IUPAC names for small, simple molecules
- Identify some common functional groups found in organic molecules





viagra™ (trade name)
sildenafil (trivial name)
5-(2-ethoxy-5-(4-methylpiperazin-1-ylsulfonyl)phenyl)-1-methyl-3-propyl-1*H*-pyrazolo[4,3-*d*] pyrimidin-7(6*H*)-one

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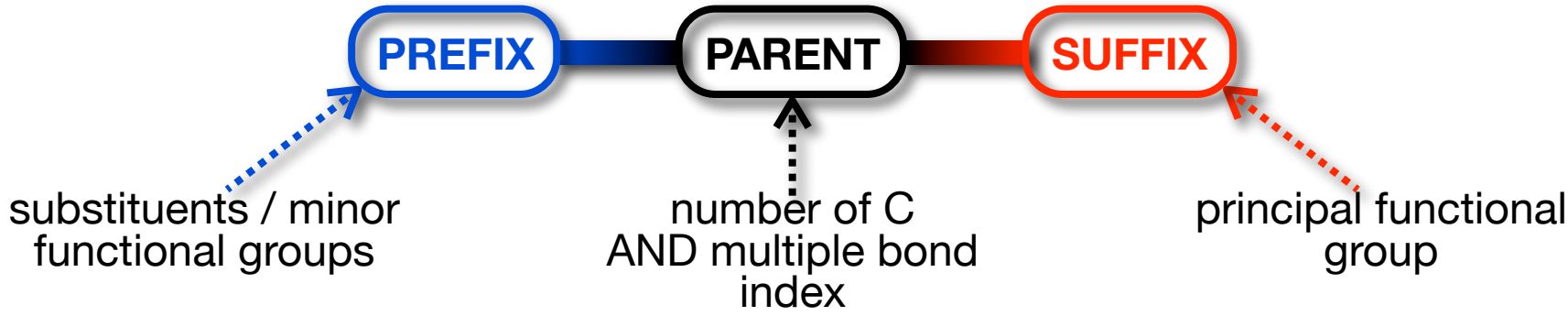
Systematic (IUPAC) naming

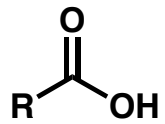
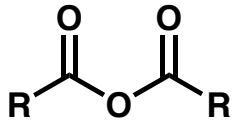
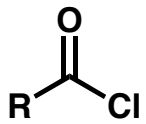
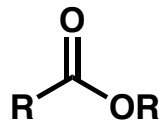
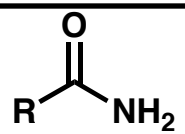
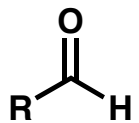
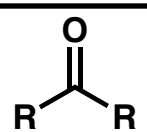


- Comprises of **three** main parts
- Note: **multiple bond index** is always incorporated in **parent** section

No. Carbons	Root	No. Carbons	Root
1	meth	6	hex
2	eth	7	hept
3	prop	8	oct
4	but	9	non
5	pent	10	dec

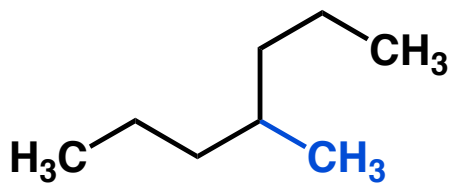
Bond	Multiple-bond index
C–C	an(e)
C=C	en(e)
C≡C	yn(e)

Systematic (IUPAC) naming: functional groups

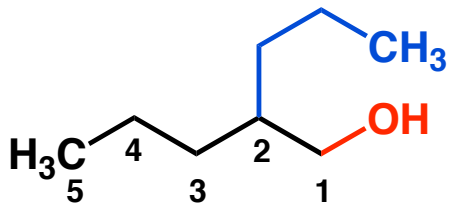
Functional group	Structure	Suffix	Prefix	General form
acid		–oic acid –carboxylic acid	carboxy	R-COOH
anhydride		–oic anhydride –carboxylic anhydride		R-C(O)OC(O)-R
acyl chloride		–oyl chloride -carbonyl chloride	chlorocarbonyl	R-COCl
ester		–oate –carboxylate	alkoxycarbonyl	R-COOR
amide		–amide –carboxamide	carbamoyl	R-CONH$_2$
nitrile		–nitrile	cyano	R-C≡N
aldehyde		–al –carbaldehyde	oxo	R-CHO
ketone		–one	oxo	R-CO-R
alcohol		–ol	hydroxy	R-OH
amine		–amine	amino	R-NH$_2$
ether		–ether	alkoxy	R-O-R
alkyl bromide (alkyl halide)			bromo (halo)	R-Br (R-X)

Nomenclature rules

1. **Parent** - root derived from number of carbon in longest unbranched chain containing functional group

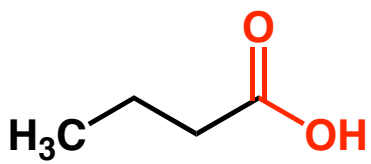


4-methylheptane

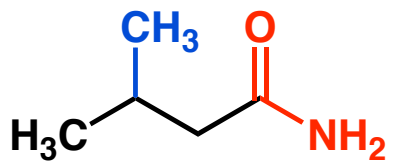


2-propyl-1-pentanol

2. **Suffix** - basic name derived by adding ending of major functional group (FG)

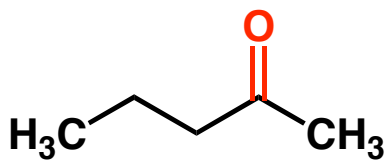


butanoic acid



3-methylbutanamide

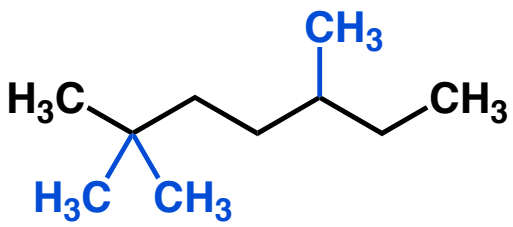
3. **Position** - position of FG denoted by Arabic numeral placed before whole name or just before ending. Numbering achieves lowest number for FG



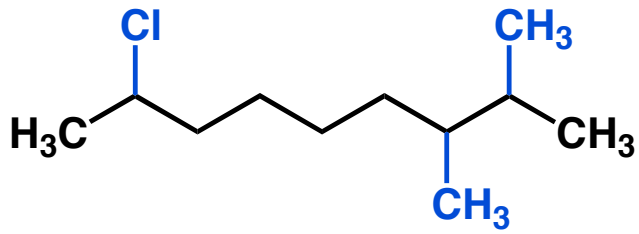
2-pentanone
pentan-2-one
NOT 4-pentanone

Nomenclature rules II

4. **Prefix** - substituents are designated by prefix & Arabic number indicating position (lowest possible numbering)

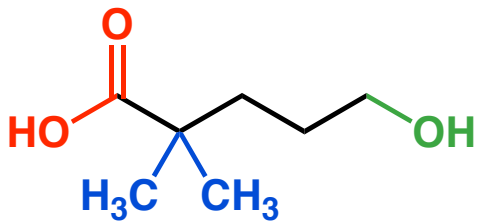


2,2,5-trimethylheptane
NOT 3,6,6-trimethylheptane

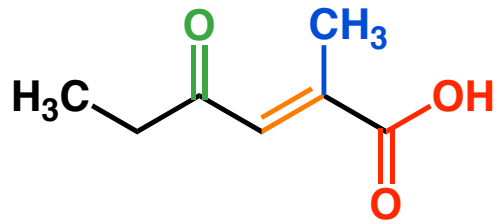


8-chloro-2,3-dimethylnonane
NOT 2-chloro-7,8-dimethylnonane

5. **FG** - if more than one FG name & number based on principle FG. List of priorities given in course notes. Multiple bonds are added to parent (end), all others are **prefixes**



5-hydroxy-2,2-dimethylpentanoic acid

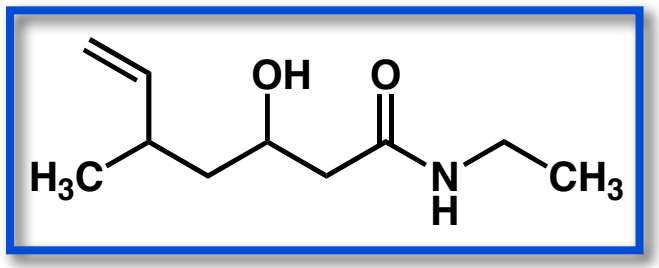


2-methyl-4-oxohex-2-enoic acid

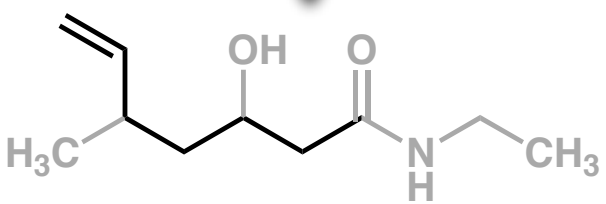
6. **Minor FG** - halo-, nitro- (-NO_2), nitroso- (-NO) & azo- (-N_2-) are considered substituents & not FG for nomenclature only

7. **Order** - substituents are written in alphabetical order

Examples: structure to name

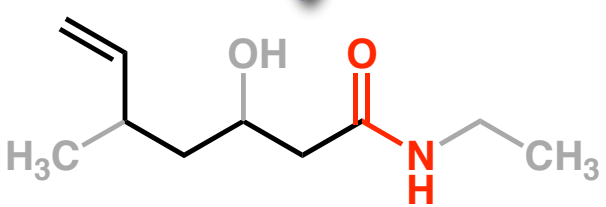


Step 1: root



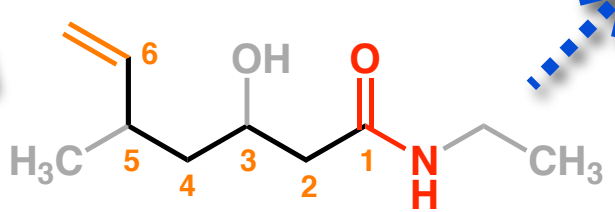
hept

Step 2: suffix



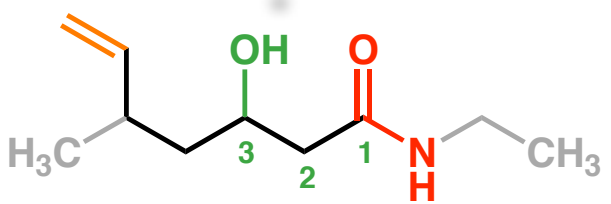
hept amide

Step 3: multiple-bond index



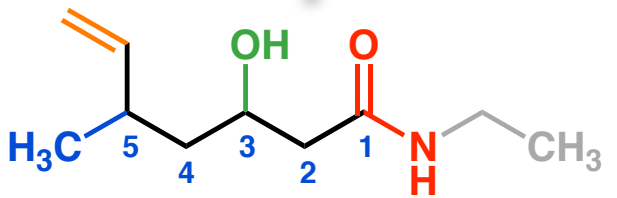
hept-6-enamide

Step 4: functional groups (prefix)



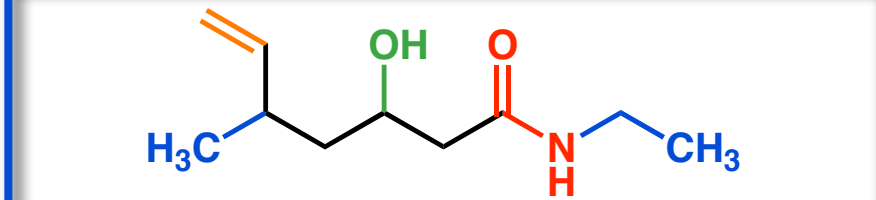
3-hydroxyhept-6-enamide

Step 5: substituents (prefix)



3-hydroxy-5-methylhept-6-enamide

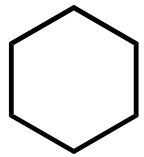
Step 7: complete



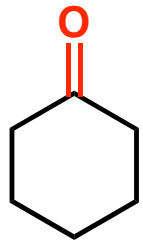
N-ethyl-3-hydroxy-5-methylhept-6-enamide

Examples: name to structure

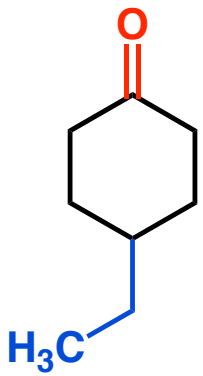
- Draw the structure for **4-ethyl-3-hydroxycyclohexanone** (please)



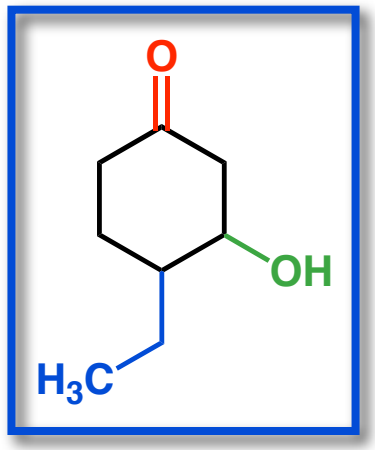
draw the root
4-ethyl-3-hydroxy**cyclohexanone**



add major functional group
4-ethyl-3-hydroxy**cyclohexanone**



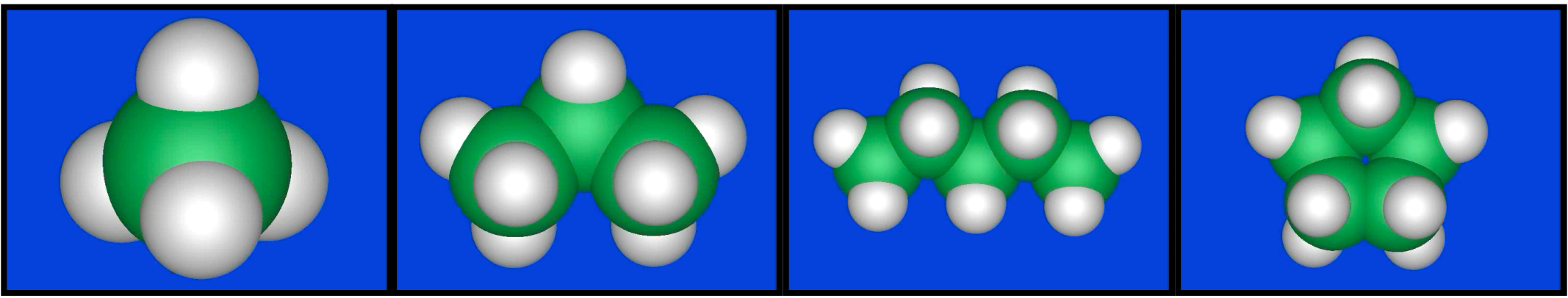
add substituent
4-ethyl-3-hydroxy**cyclohexanone**

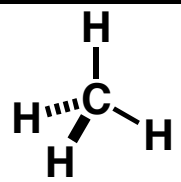


add minor functional group
4-ethyl-3-hydroxycyclohexanone

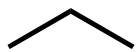
Functional groups: alkanes

- **Saturated hydrocarbons** - contain only C & H and no multiple bonds
- Non-cyclic alkanes have the formula $\mathbf{C_nH_{2n+2}}$



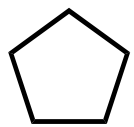


methane
CH_4

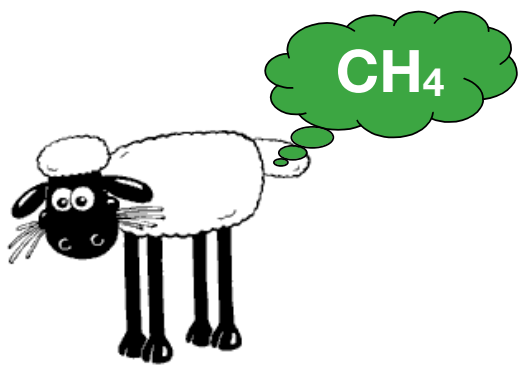


propane
C_3H_8

pentane
C_5H_{12}

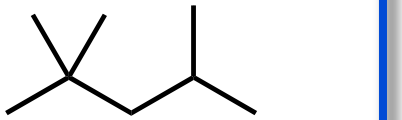


cyclopentane
C_5H_{10}

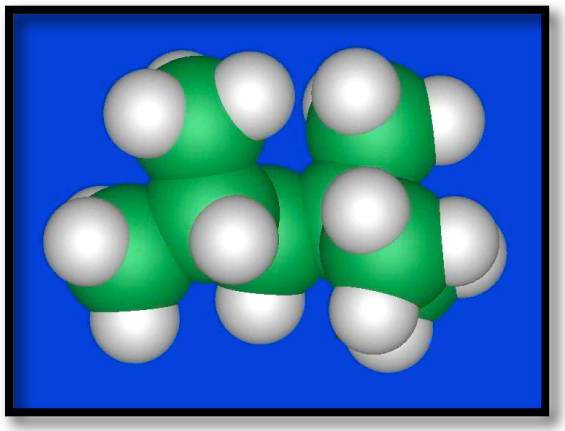


- Alkanes are a little dull - used as solvents or burnt as fuel
- Methane is a fuel, a chemical feedstock & a green house gas

Functional groups: alkanes II

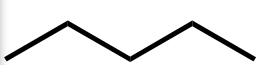


isooctane
2,2,4-trimethylpentane
C_8H_{18}

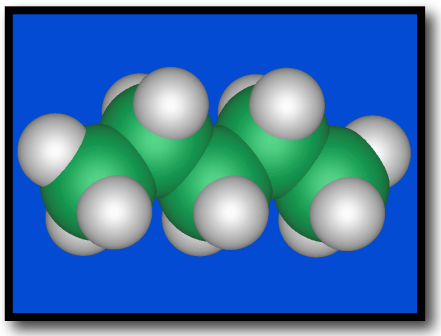


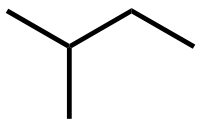
- Isooctane is used in petrol - branched structure means it burns smoothly
- Octane is a long change and burns explosively
- Octane number of petrol is based on isooctane = 100 & heptane = 1
  Unleaded 91 petrol = 91% isooctane & 9% heptane

- **Structural isomers** have same formula but different atoms joined differently
- Isomers can have very different properties



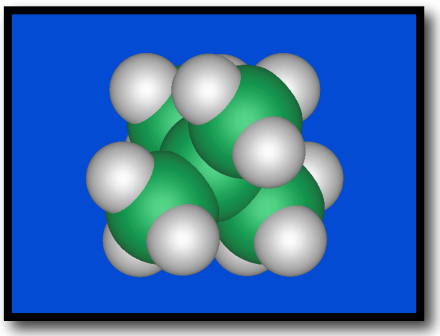
pentane
bp 36.2˚C



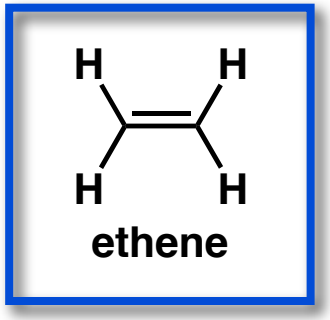


2-methylbutane
bp 28˚C

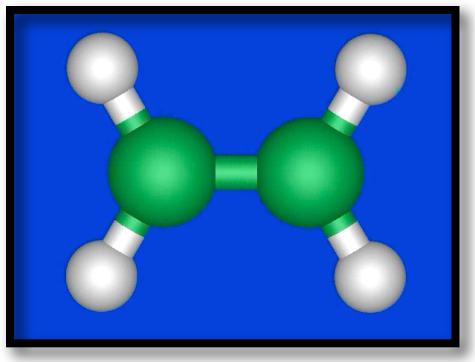
2,2-dimethylpropane
bp 9.6˚C



Functional groups: alkenes

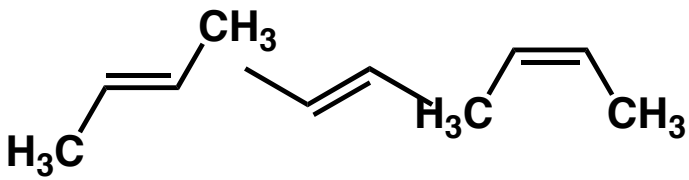


ethene

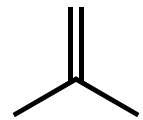


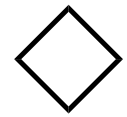
- **Ethene** - simplest alkene. Very important industrially
- Carbon is **trigonal planar** - flat and triangular!
- New form of isomerism - **configurational isomers**
- All atoms bonded in the same manner but different orientation in space

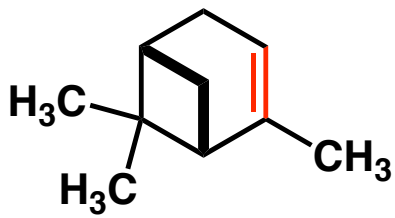

1-butene
C_4H_8

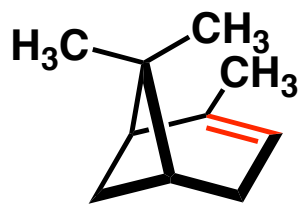


trans-2-butene *cis*-2-butene
C_4H_8


2-methylpropene
C_4H_8

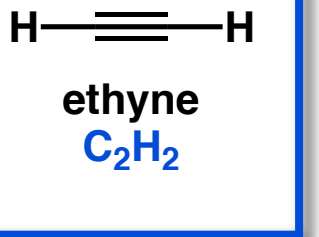

cyclobutane
C_4H_8



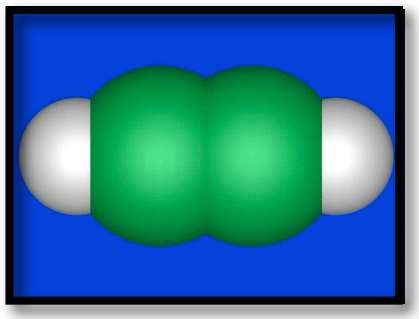


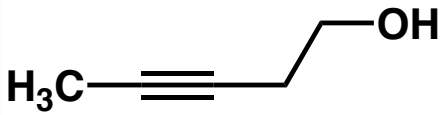
(1*R*,5*R*)-2,6,6-trimethylbicyclo[3.1.1]hept-2-ene
α-pinene

Functional groups: alkynes & cyclic structures

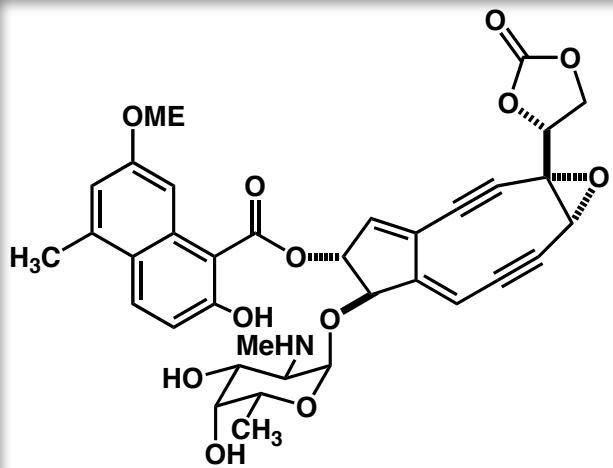


ethyne
C_2H_2





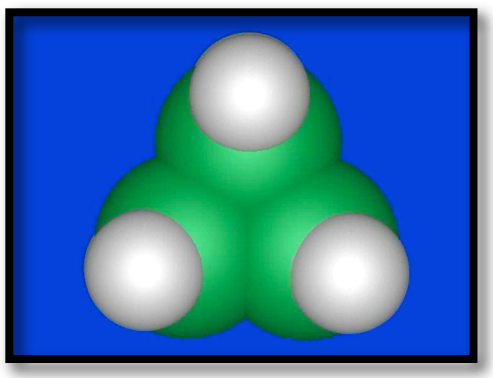
pent-3-yn-1-ol
NOT pent-2-yn-5-ol

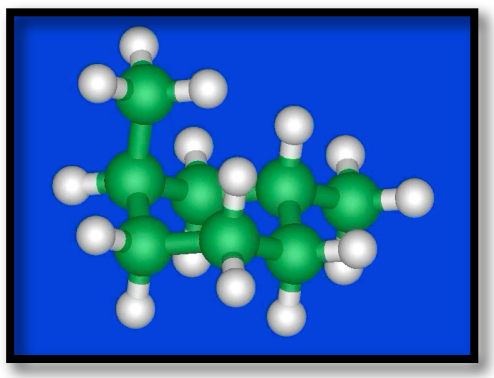


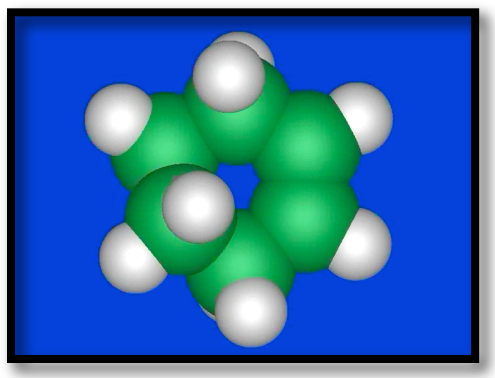
neocarzinostatin chromophore A

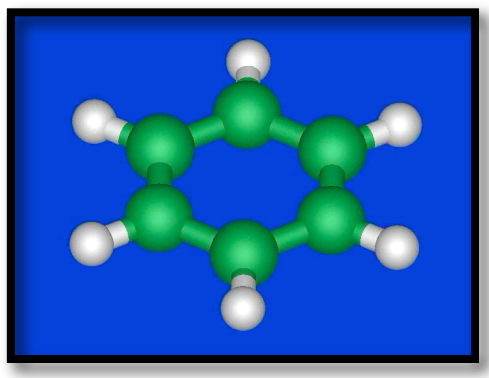
- Ethyne is an explosive gas
- Triple bond makes molecular **linear** (cylinder)
- Examples found in nature (example cleaves DNA)

Cycloalkanes and cycloalkenes

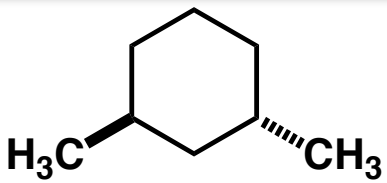




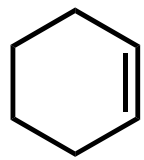




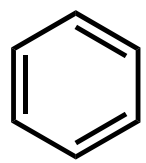
cyclopropane



1,3-dimethylcyclohexane



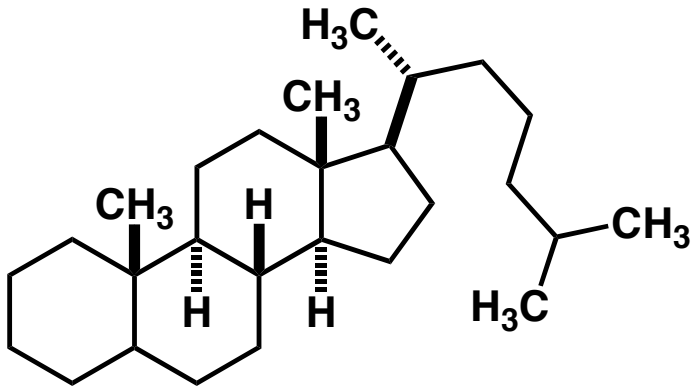
cyclohexene



benzene

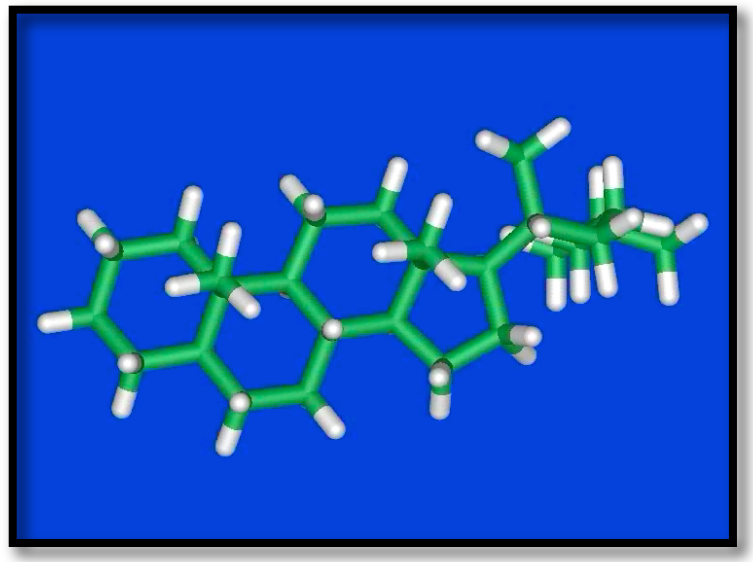
- Cyclic hydrocarbons are common - note that most are not flat

Cyclic structures in nature

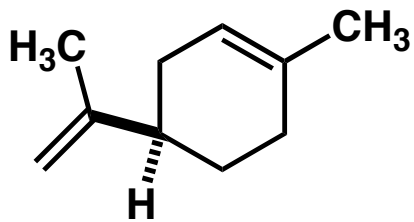


(8*R*,9*S*,10*S*,13*R*,14*S*,17*R*)-10,13-dimethyl-17-(6-methylheptan-2-yl)-hexadecahydro-1*H*-cyclopenta[*a*]phenanthrene

cholestane - steroid



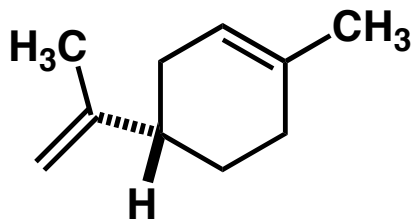
- Ring systems are common in natural products & pharmaceuticals
- Example below shows the importance of another form of **isomerism** - **stereoisomers**



(*R*)-1-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene

(*R*)-limonene

smells of oranges

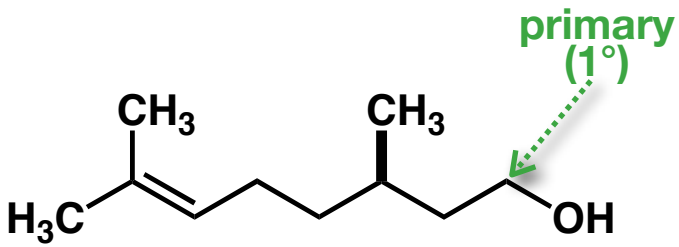


(*S*)-1-methyl-4-(prop-1-en-2-yl)cyclohex-1-ene

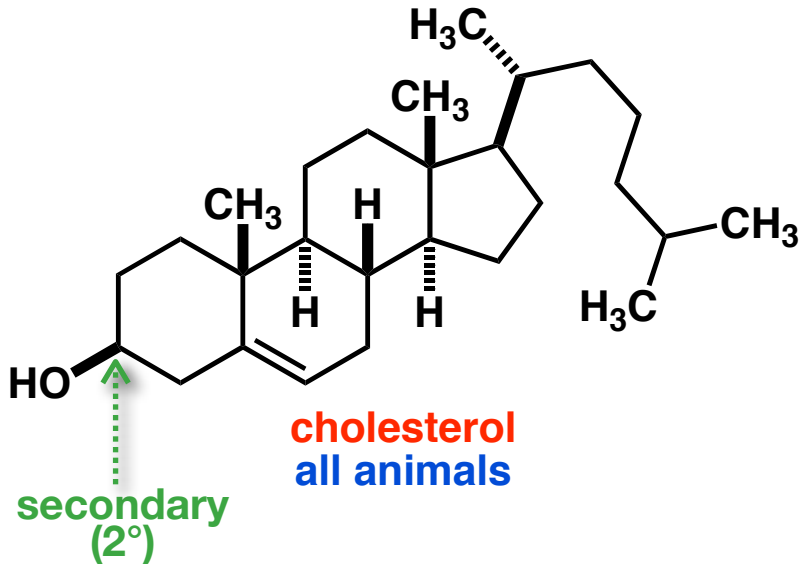
(*S*)-limonene

smells of lemons

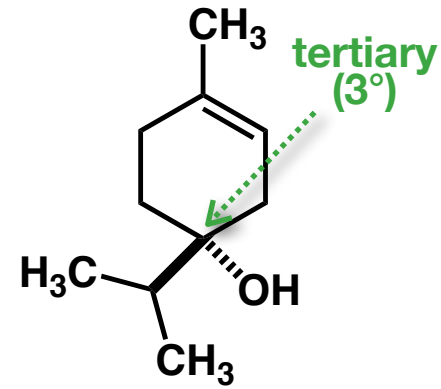
Functional groups: alcohols



(*R*)-3,7-dimethyloct-6-en-1-ol
citronellol
citronella oil

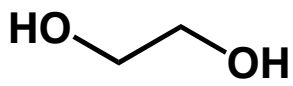


cholesterol
all animals

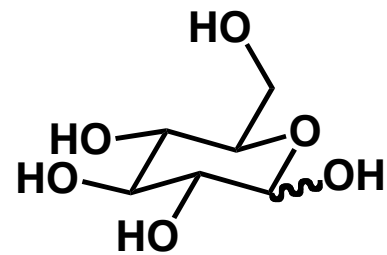


(*R*)-1-isopropyl-4-methylcyclohex-3-enol
terpinen-4-ol
tea tree oil

- Alcohols contain OH (hydroxy) group
- Found in many natural systems (especially on Friday night)
- Three classes depending on how many **C** attached to **C–OH**
- Compounds can have more than one OH (improves water solubility)



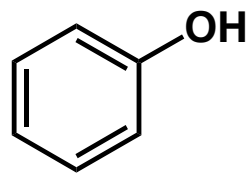
1,2-ethandiol
ethylene glycol
antifreeze



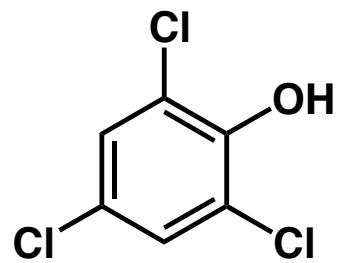
6-(hydroxymethyl)-tetrahydro-2*H*-pyran-2,3,4,5-tetraol
glucose
sugar I guess!

Functional groups: phenols and ethers

Phenols



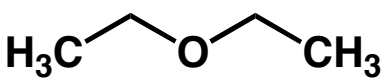
phenol
carbolic acid



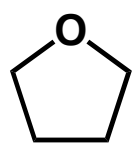
2,4,6-trichlorophenol
TCP
antiseptic

- Phenols are distinct from alcohols as attached to phenyl ring - acidic O–H

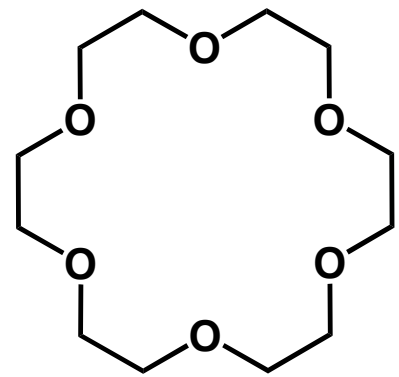
Ethers



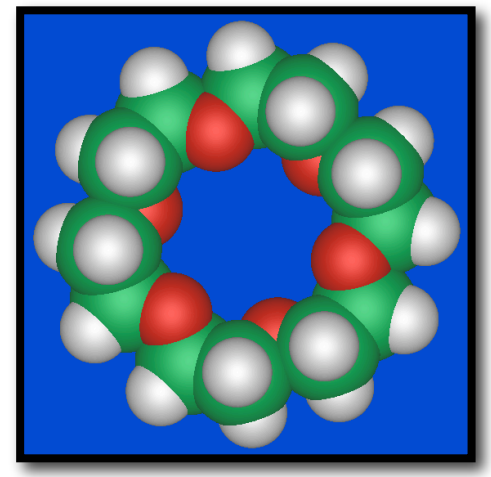
ethoxyethane
diethyl ether
ether



tetrahydrofuran
THF

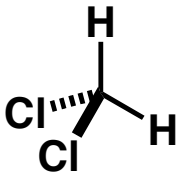


18-crown-6

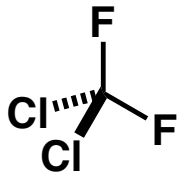


- Most commonly used as solvents
- 18-Crown-6 enables metal cations (M^+) to dissolve in organic solvents

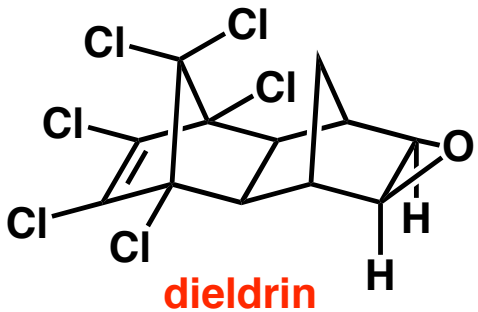
Functional groups: alkyl halides and thiols



dichloromethane
DCM



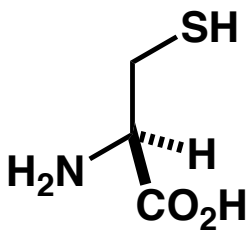
dichlorodifluoromethane
Freon (refrigerant)
a CFC



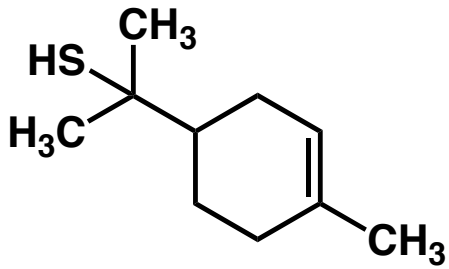
dieldrin

- Alkyl halides are incredibly useful compounds - used extensively
- Down side is they appear to be bad for us and the environment

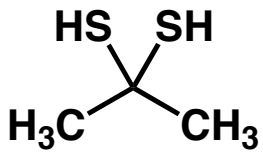
Thiols



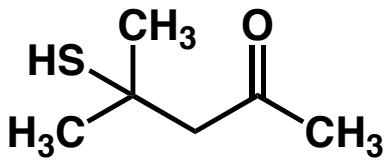
(*R*)-2-amino-3-sulfanylpropanoic acid
cysteine



2-(4-methylcyclohex-3-enyl)propane-2-thiol
taste of grapefruit



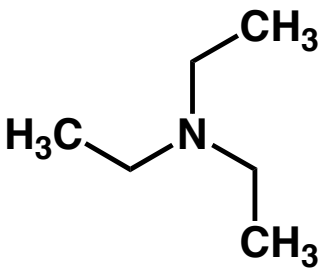
propane-2,2-dithiol



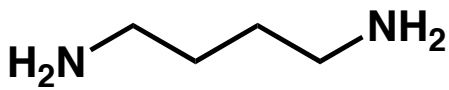
4-methyl-4-sulfanylpentan-2-one

- Thiols are the sulfur analogue of alcohols - and they smell, bad...
- Humans can detect 2×10^{-5} ppb of the second compound (1 drop in a lake)
- One of the last two compounds is the smelliest known - but no one is prepared to make them again to find out which!

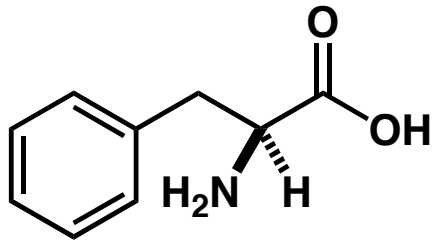
Functional groups: amines



triethylamine
smells of fish

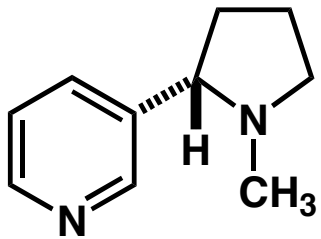


butane-1,4-diamine
putrescine
smells of decay

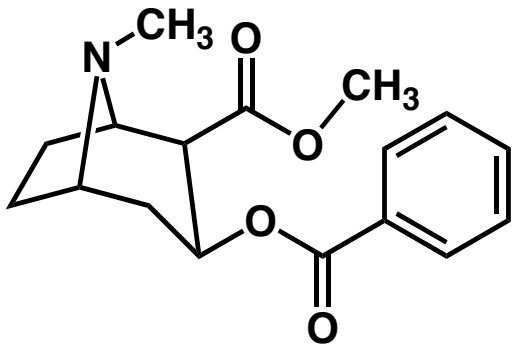


(*S*)-2-amino-3-phenylpropanoic acid
phenylalanine
amino acid

- Vital in biological systems
- Many smell (bad but not as bad as thiols)
- Found in many compounds that are physiologically active...

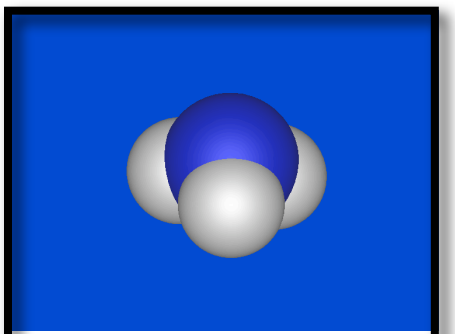


(*S*)-3-(1-methylpyrrolidin-2-yl) pyridine
nicotine

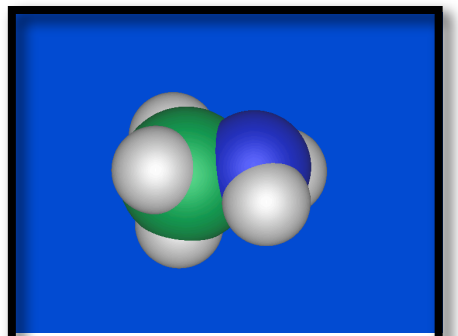


methyl 3-(benzoyloxy)-8-methyl-8-aza-bicyclo[3.2.1]octane-2-carboxylate
cocaine

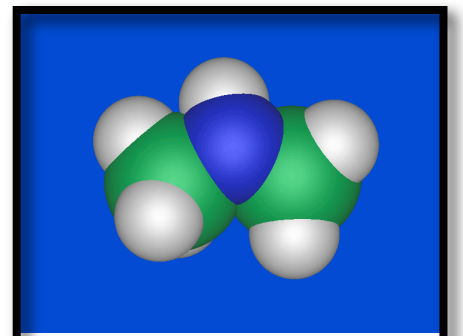
Functional groups: amines II



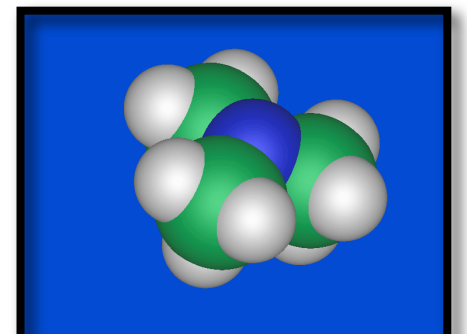
ammonia



methylamine
1° amine

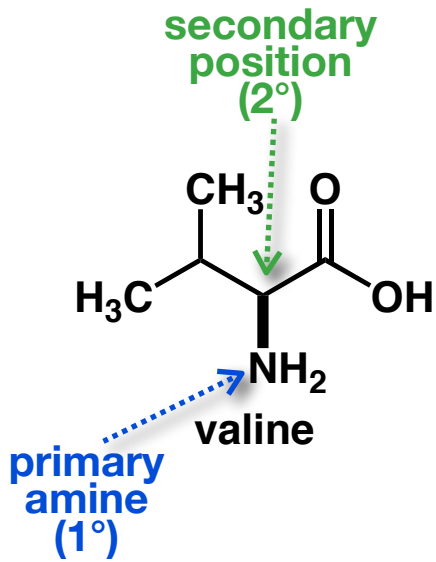


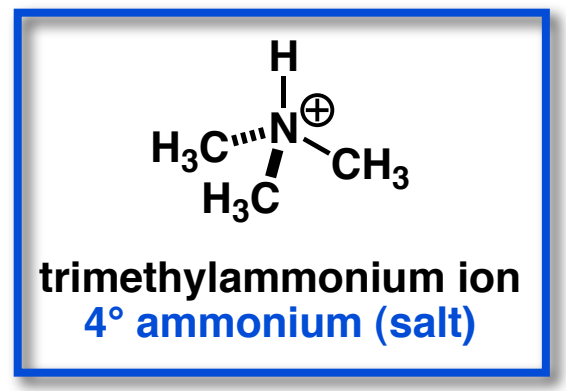
dimethylamine
2° amine



trimethylamine
3° amine

- Just to confuse, **amines** are labeled by the number of **C** attached
- This is different to **alcohols** (labeled by **C** attached to **C**–OH)





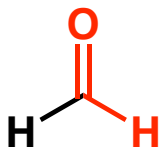
trimethylammonium ion
4° ammonium (salt)

If add four groups everything changes!

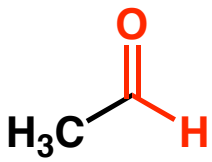
Functional groups: the carbonyl group

- **Carbonyl** group **C=O** – analogous to alkene
- Two groups, **aldehydes RCHO** and **ketones $R_2C=O$**

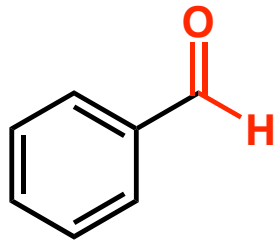
Aldehyde



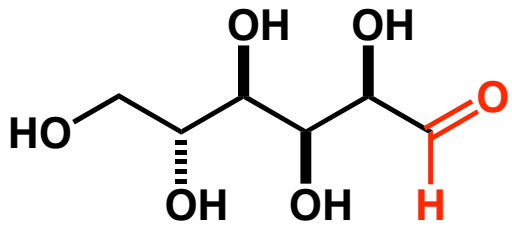
methanal
formaldehyde



ethanal
acetaldehyde

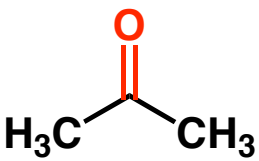


benzaldehyde

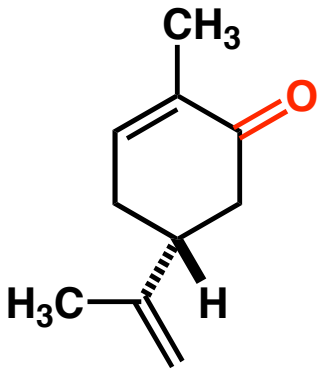


(2*R*,3*S*,4*R*,5*R*)-2,3,4,5,6-pentahydroxyhexanal
glucose

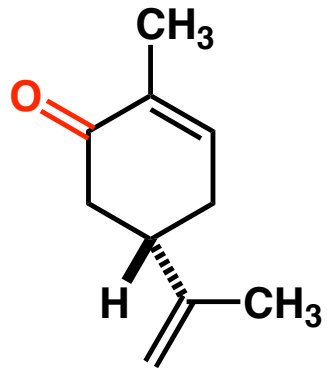
Ketones



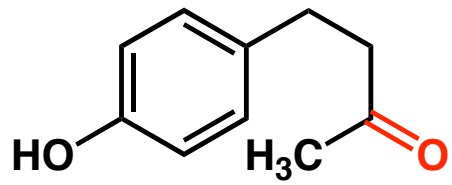
propanone
acetone



(*R*)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-enone
(*R*)-carvone
spearmint

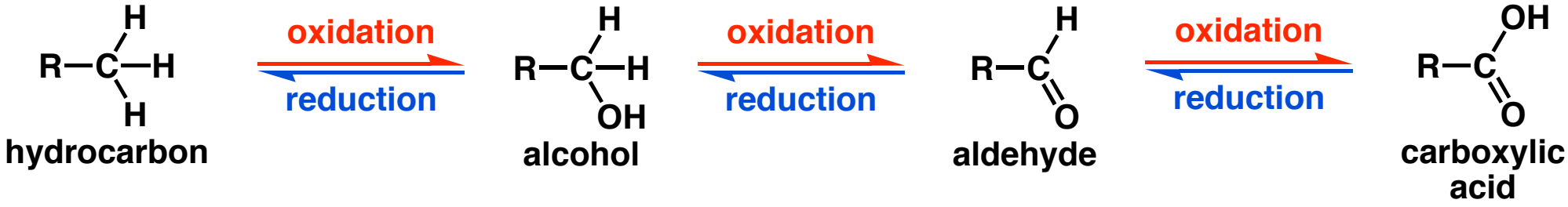


(*S*)-2-methyl-5-(prop-1-en-2-yl)cyclohex-2-enone
(*S*)-carvone
caraway



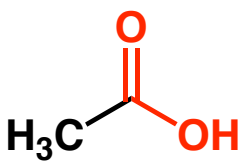
4-(4-hydroxyphenyl)butan-2-one
raspberry ketone

Functional groups: carboxylic acids & derivatives

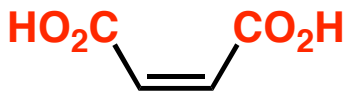


hydrocarbon — alcohol — aldehyde — carboxylic acid

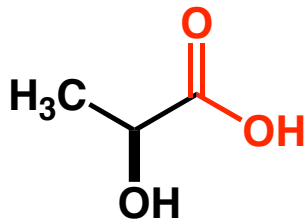
- Many of the functional groups are 'linked'
- If we replace one **C–H** at a time by a **C–O** we see how these groups relate



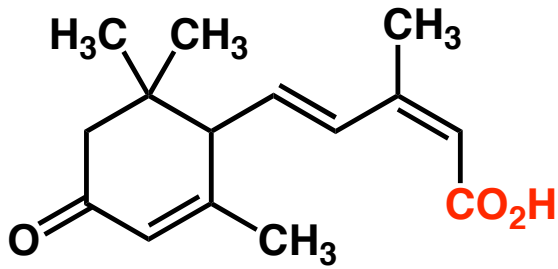
ethanoic acid
acetic acid
vinegar



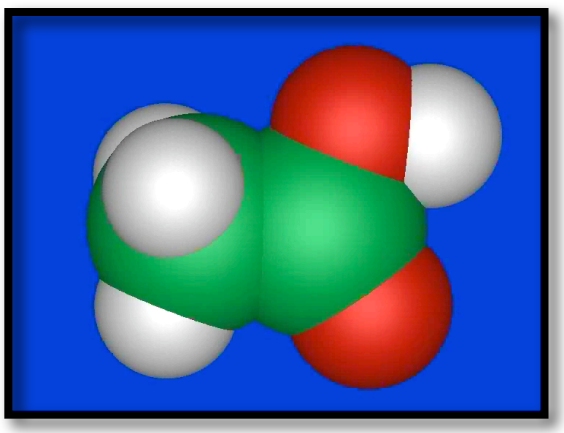
maleic acid



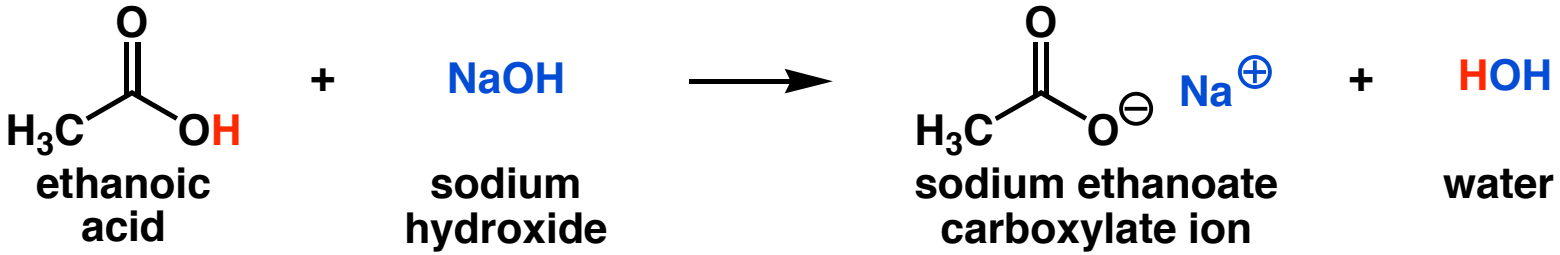
(*S*)-2-hydroxypropanoic acid
L-(+)-lactic acid



(2*Z*,4*E*)-3-methyl-5-(2,6,6-trimethyl-4-oxocyclohex-2-enyl)penta-2,4-dienoic acid
abscisic acid
leaf fall

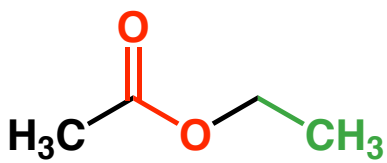


Functional groups: derivatives

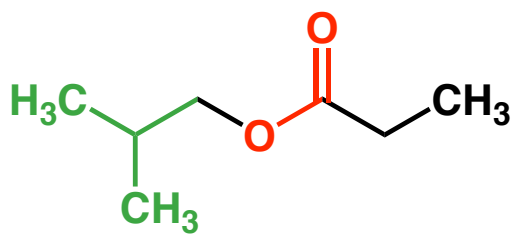


- Reaction of a **carboxylic acid** with a **base** (*eg.* NaOH) gives **carboxylate ion**

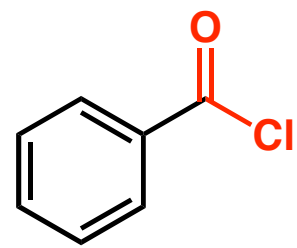
Derivatives



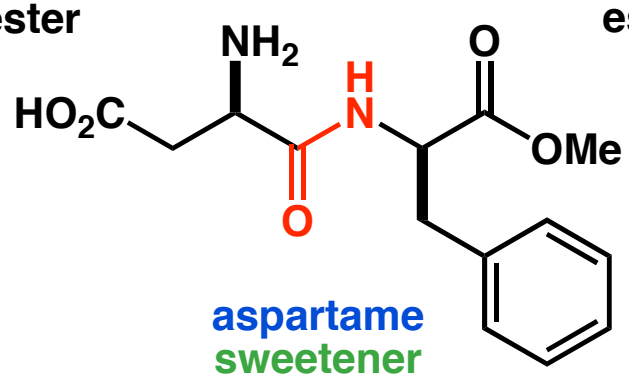
ethyl ethanoate
ethyl acetate
solvent
ester



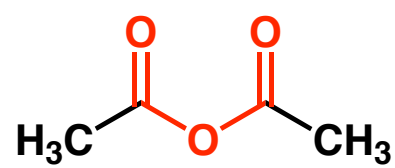
2-methylpropyl propanoate
isobutyl propionate
smell of rum
ester



benzoyl chloride
acid chloride



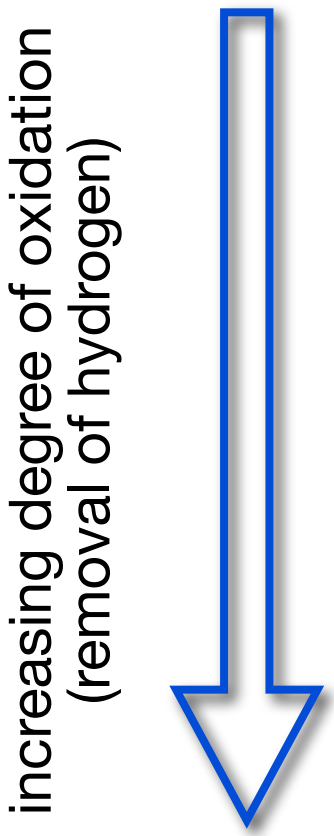
aspartame
sweetener
amide



ethanoic anhydride
acetic anhydride
acid anhydride

Classification of functional groups

- Functional groups can be classed by the degree of **oxidation** (removal of **H**)

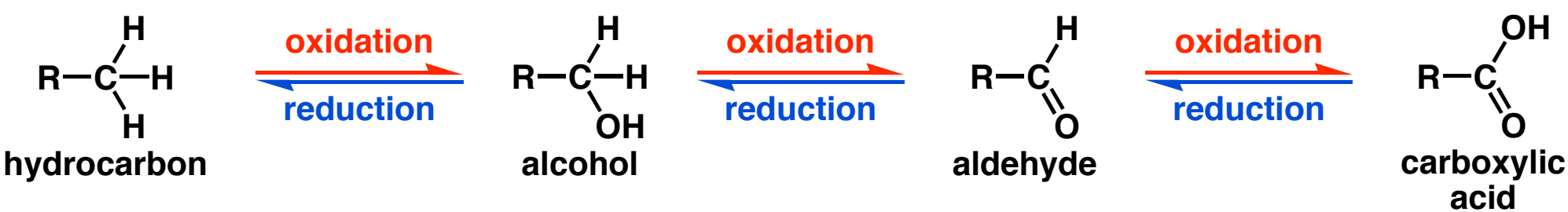


alkanes

alcohols ethers amines alkyl halides thiols

aldehydes ketones

carboxylic acids esters amides acyl chlorides acid anhydrides nitriles



Overview

What have we learnt?

- How to name simple organic molecules
- To recognise common functional groups
- Common examples of these functional groups

What's next?

- To looking at the bonding in molecules in detail
- To understand how bonding effects the shape of molecules