## Introduction to Organic Functional Groups

Constitutional isomers: Klein 4.3
Alkane nomenclature: Klein 4.1-4.2
Functional groups: Klein 2.3
Alkyl halide nomenclature: Klein 7.2

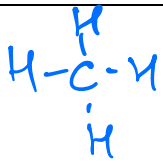
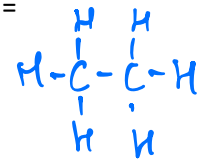
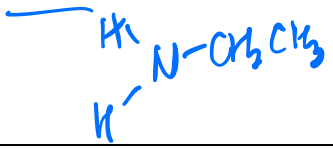
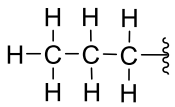
### A. Alkanes and Alkyl Groups

Boring!

=a.k.a. Saturated hydrocarbons or aliphatics

-General formula for alkanes=

*1. Naming alkanes*

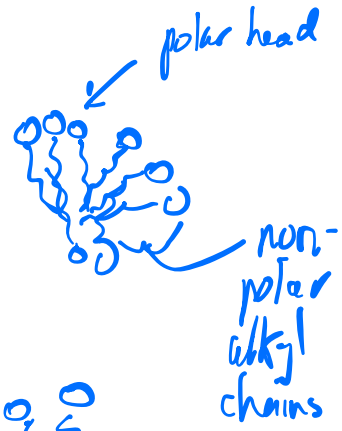
| alkane structure | name | alkyl piece structure | name | no. of C's |
|---|---|---|---|---|
| $CH_4$ =  | methane | $H_3C$- | methyl | 1 |
| $CH_3$-$CH_3$ =  | ethane | $H_3CCH_2$-  | ethyl | 2 |
| $CH_3CH_2CH_3$ | propane | $H_3CCH_2CH_2$- =  | propyl | 3 |
| $CH_3CH_2CH_2CH_3$ | butane | $CH_3CH_2CH_2CH_2$- | butyl | 4 |
| $CH_3CH_2CH_2CH_2CH_3$ | pentane | $CH_3CH_2CH_2CH_2CH_2$- | pentyl | 5 |
| $CH_3CH_2CH_2CH_2CH_2CH_3$ | hexane | $CH_3CH_2CH_2CH_2CH_2CH_2$- | hexyl | 6 |
| $CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ | heptane | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2$- | heptyl | 7 |
| $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | octane | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2$- | octyl | 8 |
| $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | X nonane | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2$- | nonyl X | 9 |
| $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$ | X | $CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_2$- | X | 10 |
| | | | | |

Comments: —

*mostly Greek prefixes used ✓

*Other notable alkyl chains*

| systematic or official name | common name | no. of C's (Note: including $CO_2H$ carbon) |
|---|---|---|
| dodecyl | lauryl | 12 |
| tetradecyl | myristyl | 14 |
| **hexadecyl** | palmityl | **16** |
| **octadecyl** | stearyl | **18** |
| eicosyl | arachidyl | 20 |




**KNOW… 1-8, 16 & 18

*2. Alkane properties=*

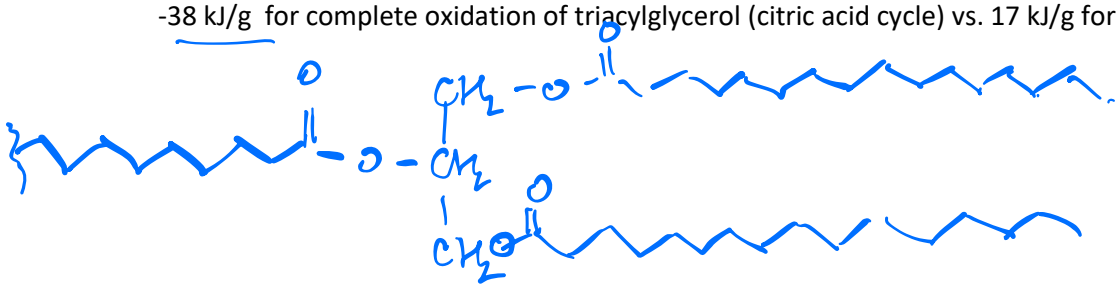
-they are hydrophobic (water fearing) or lipophilic in nature; they glob together like droplets or grease balls oil

-longer chains have higher boiling points

-fatty acids=long alkyl chains with carboxylic acid groups on end

-fatty acids form micelles in aqueous solutions; fatty acids (triacylglycerols specifically) are an important constituent of lipids and cell membranes and a great source of energy in cells.

-38 kJ/g for complete oxidation of triacylglycerol (citric acid cycle) vs. 17 kJ/g for carbohydrates and proteins



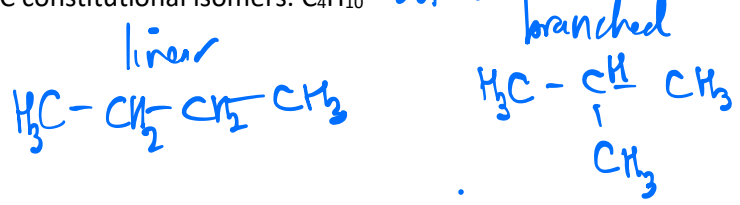
triacylglycerol (triglycerides)

*3. Constitutional isomers*

= same number and type of atoms, but different bonding arrangement

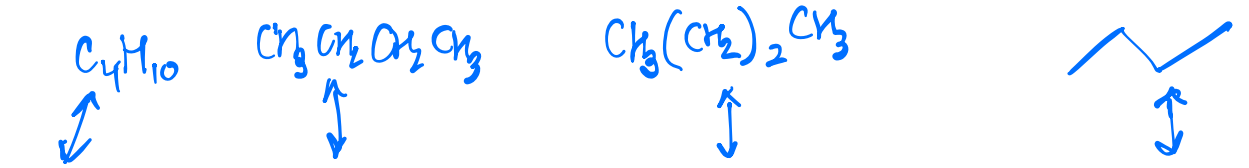
*Key*-→ not all alkyl groups are linear; branching can occur

-e.g. 4 C constitutional isomers: $C_4H_{10}$ butane



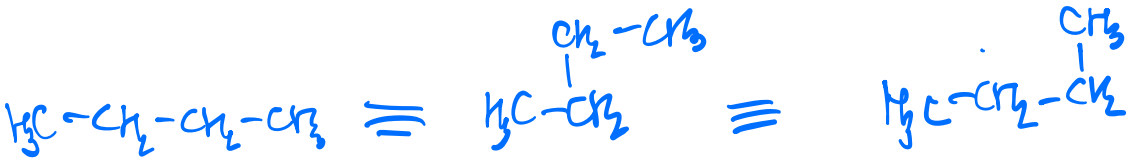

two constitutional isomers

Side bar: *Depicting organic chemical structures*



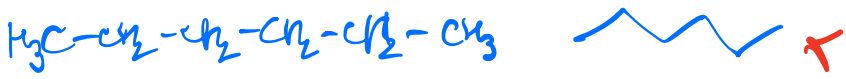
formula condensed highly condensed skeletal

**C-C SIGMA BONDS CAN FREELY ROTATE !

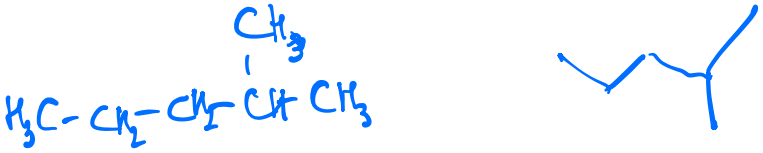


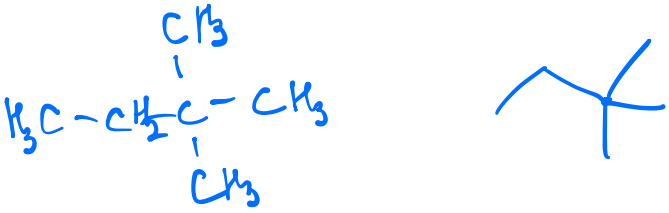
EXAMPLE with hexane ($C_6H_{14}$): 5 constitutional isomers

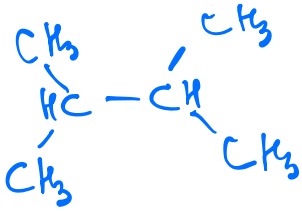
1. C-C-C-C-C-C

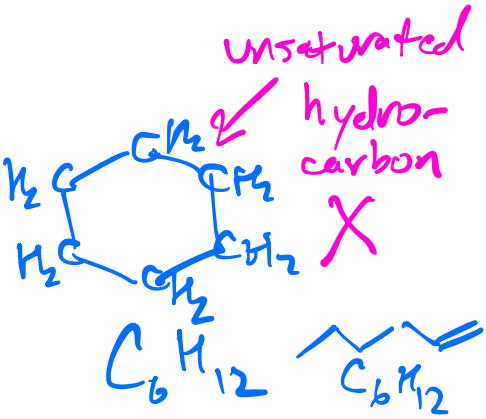
linear 

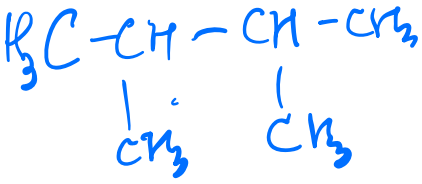
2.

3. 

4. 

5. 

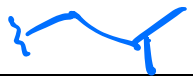
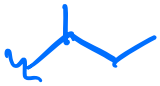


Lots of other examples; see book and assigned questions for more details (not worth more discussion)
-e.g.

| # of C's | # of constitutional isomers |
|---|---|
| $C_7H_{16}$ | 9 |
| $C_8H_{18}$ | 18 |
| $C_{10}H_{22}$ | 75 |
| $C_{15}H_{32}$ | 4,347 |
| $C_{20}H_{42}$ | 366,319 |

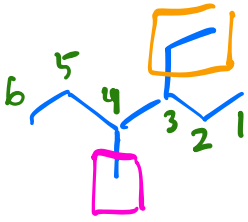
*4. Common names for some common constitutional isomer groups*

| group | name | skeletal representation |
|---|---|---|
| $CH_3$-$CH(CH_3)$- | isopropyl | Y-shape |
| $CH_3$-$CH(CH_3)$-$CH_2$- | isobutyl |  |
| $CH_3CH_2CH(CH_3)$- | sec-butyl |  |
| $(CH_3)_3C$- | tert-butyl | |

*add these to the list of groups that you need to know

*5. Nomenclature of Alkanes*
How to name alkanes....

1st example: $CH_3CH_2CH(CH_3)CH(CH_2CH_3)CH_2CH_3$ (1 2 3 4 5 6)



*all alkanes have ___-ane___ as the suffix

**a) Find longest chain and name**

*in our example..... 6 C's = hex-

**b) Name and number substituents**
*-number from end that gives lowest number or numbers*

methyl ethyl

3-methyl, 4-ethyl or 3-ethyl, 4-methyl

-If multiple substituents of the same type, then use the prefixes di , tri , tetra etc. as necessary.

**c) Alphabet wins naming if there is a choice**

*-lowest number goes to substituent with first name alphabetically*

* 3-ethyl, 4-methyl

-hyphenated prefixes like *sec* and *tert* and di-, tri-, tetra-, penta- etc. are *not* used when alphabetizing

Final name of example: 3-ethyl, 4-methylhexane

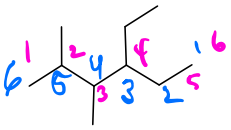
-most organic chemists refer to molecules by their key/critical functional groups, i.e. alkane, alcohols, alkyl halides carboxylic acids, etc.

This is because the functional groups are the most important part when discussing molecular properties and reactions.

*Additional rules…*

**d) Correct name will use the lowest number for substituents**

example




-analysis: 4-ethyl-2,3-dimethylhexane

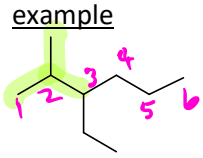
NOT… 2,3 dimethyl-4-ethylhexane → NOT alphabetically listed

NOT… 4,5-dimethyl-3-ethylhexane → higher numbers (12 total vs. 9 total for correct answer)

* "di" ignored in alphabetizing

**e) Simplest substituent names preferred over complex**

example

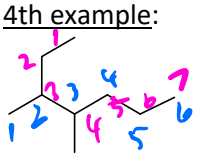



-analysis: 3-ethyl, 2-methylhexane

NOT… 4-ethyl, 5-methylhexane (higher numbers)

NOT… 3-isopropyl-hexane (more complex substituent: isopropyl vs. ethyl and methyl)

4th example:



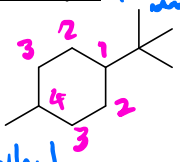
-analysis: 3,4-dimethylheptane NOT 4,5-dimethylheptane

End 9/2/26

6. Nomenclature of Cycloalkanes

**a) count the number of C's in cyclic structure/ring and name using prefix for linear (acyclic) alkanes**
**b) use** cyclo- **prefix**
**c) name each substituent on ring**
**d) if two or more substituents AND same priority (alkyl, halo), lowest numbering first,**
**e) if numbering same, then number alphabetically**

example 1-tert-butyl

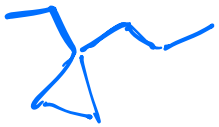


1-tert-butyl-4-methyl cyclohexane

4-methyl

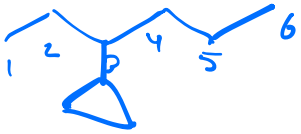
example—naming cycloalkyl substituents: draw 3-cyclopropylhexane

cyclopropyl



1-ethyl-1-propyl cyclopropane

See receptor worksheet for halide nomenclature



*7. Other functional groups*

*You must recognize all these, but you don't need to know the nomenclature right now.

a) Simple functional groups

(1) alkyl halides: -X, where X= F, Cl, Br or I

e.g.

common name: propyl iodide

1-iodo propane

"official IUPAC nomenclature"

(2) ethers: -OR, where R= alkyl

e.g. $CH_3CH_2CH_2\underset{\displaystyle CH_3}{\underset{|}{CH}}-OCH_3$ $-\overset{|}{\underset{|}{C}}-O-\overset{|}{\underset{|}{C}}-$

(3) alcohols: -OH

e.g.

isopropyl alcohol

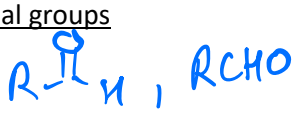
(4) amines: $-NH_2$

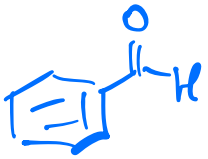
e.g.

$H_2N-\underset{\displaystyle CH_3}{\underset{|}{CH_2}}$ ethyl amine

Carbonyl

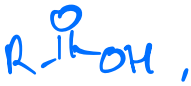
b) C=O functional groups

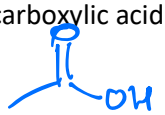
(1) aldehyde =  , RCHO

e.g.  benzaldehyde

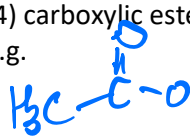
(2) ketone =

e.g. acetone

(3) carboxylic acid =  , RCOOH, $RCO_2H$

e.g.  acetic acid

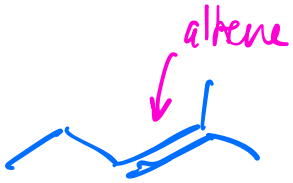
(4) carboxylic ester = , where R and R' are alkyl groups

e.g.  ethyl acetate

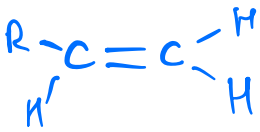
(5) carboxylic amide =

c) Unsaturated hydrocarbon functional groups

-contain pi bonds

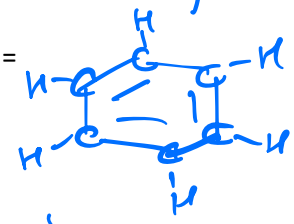



(1) alkene =

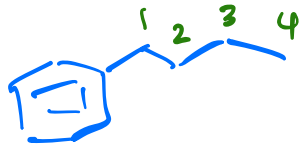
e.g. 

(2) alkyne =

e.g.


(3) benzene/aromatic = 

-a.k.a. phenyl (Ph) ring

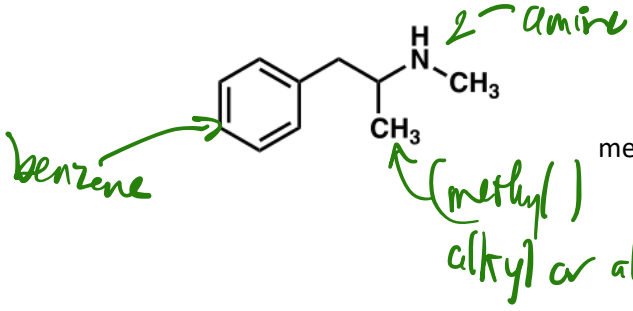



1-phenylbutane

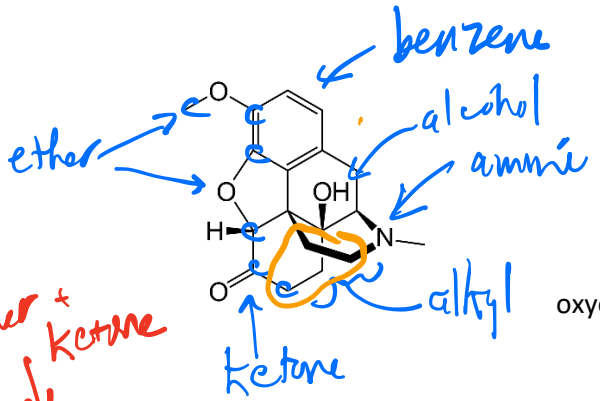
1-butylbenzene

Practice examples:

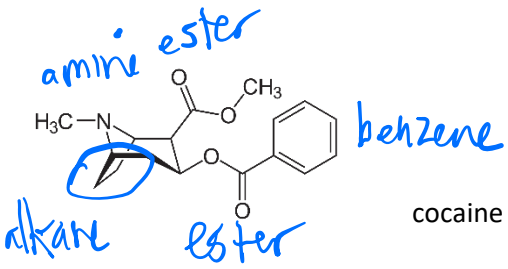
Show a complex structure with many of these functional groups, such as:



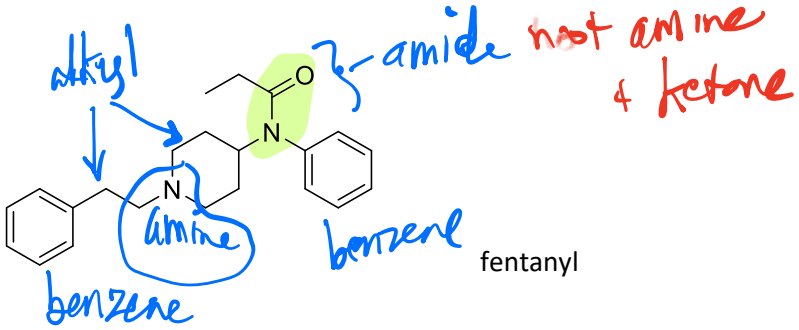

methamphetamine




oxycodone (oxycontin)




cocaine




fentanyl

*8. *Special topic: degree of unsaturation*

One pi bond or one ring structure = __1__ degree of unsaturation

Two pi bonds; two rings; or one ring + one pi bond = __2__ degrees of unsaturation

-e.g. $C_{10}H_{20}$ → "normal" saturated alkane would be.... $C_nH_{2n+2}$ 10 C's → H? 2(10)+2 = 22

→ $C_{10}H_{20}$ has __1__ degree of unsaturation, so you would expect it to have __one__ ring or __one__ pi bond

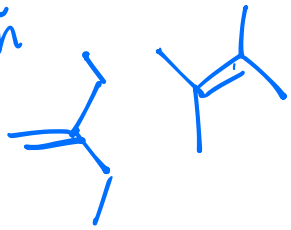
Possibilities...

examples to illustrate:

-2-hexene ($C_6H_{12}$) vs. hexane ($C_6H_{14}$); loss of two H's = 1 degree of unsaturation

Possible structures....

(constitutional isomers)



-benzene has __4__ degrees of unsaturation: $C_6H_6$; normal alkane would be $C_6H_{14}$

$C_nH_{2n+2}$

*9. Special designations for types of carbons:*

-defined by # of C's attached to C of interest

(1) 1 C attached = primary = $-CH_3$ = methyl

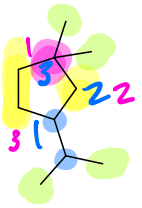
(2) 2 C's attached = secondary = $-CH_2-$ = methylene

(3) 3 C's attached = tertiary = –C–H = methine

(4) 4 C's attached = quaternary = –C– = quaternary carbon

Example will illustrate best:

dimethyl (1,1)-dimethyl vs. (3,3)-dimethyl



3-isopropyl-1,1-dimethylcyclopentane

isopropyl (3)-isopropyl vs. (1)-isopropyl

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