

(16) Today

Next Class (17)

Section 3.2: Alkanes and Isomers

Section 3.5 - 3.7: Properties and Conformations of Alkanes

Section 3.4: Nomenclature

Section 3.5 - 3.7: Properties and Conformations of Alkanes

Chap 4 Cycloalkanes
Section 4.1 Naming Cycloalkanes and Halogen Substituents

(18) Second Class from Today

Third Class from Today (19)

Sections 4.3 – 4.8 Stability of Cycloalkanes and Conformations of Cyclohexanes

Sections 5.1 – 5.5
Chirality and Determining the Configuration of Chiral Centers

Sections 5.1 – 5.5
Chirality and Determining the Configuration of Chiral Centers

Sections 5.6 – 5.12
Diastereomers, N,P, and S, and Prochirality

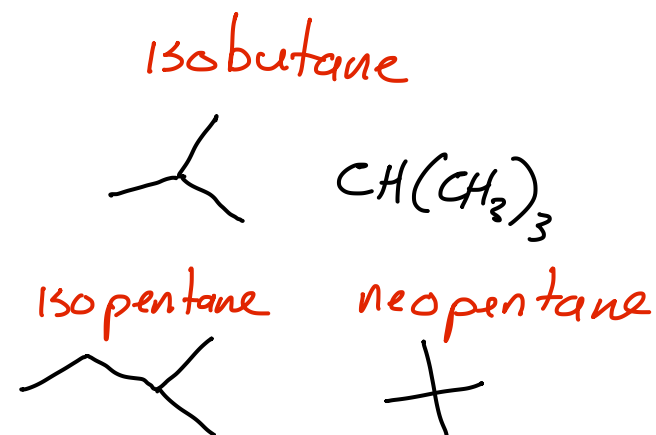
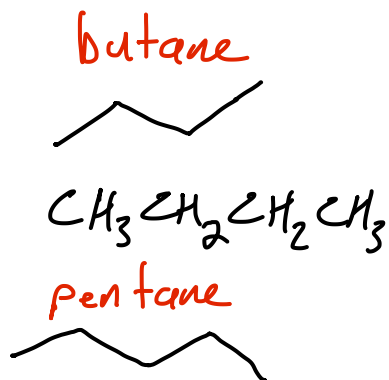
Office Hours moved from 12:20 to 1:20 to 3:00 to 4:00 for the foreseeable future

Rework Test 1 and hand in on Wednesday, October 15. Rework means that you should, on a separate piece of paper, write a more complete answer for any question that you did not received full credit for. I do NOT need the test back.

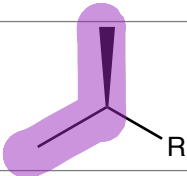
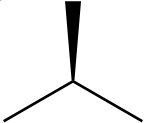
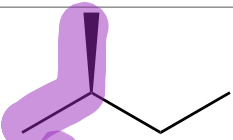
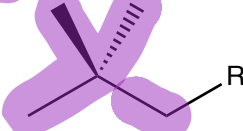
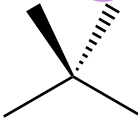
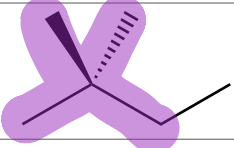
Nomenclature of Alkanes: Original Scheme based names on number of C atoms present but nonsystematic nomenclature becomes problematic quickly....

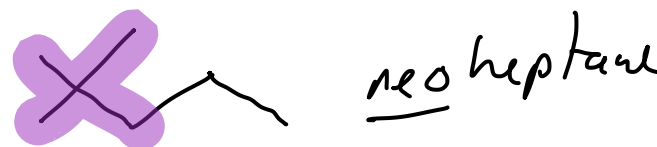
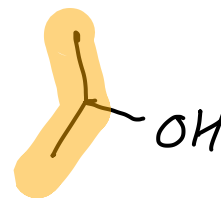
Sections 3.2 – 3.4

methane	CH ₄	1 isomer
ethane	C ₂ H ₆	1 isomer
propane	C ₃ H ₈	1 isomer
butane	C ₄ H ₁₀	2 isomers
pentane	C ₅ H ₁₂	3 isomers
hexane	C ₆ H ₁₄	5 isomers
heptane	C ₇ H ₁₆	...
octane	C ₈ H ₁₈	
nonane	C ₉ H ₂₀	
decane	C ₁₀ H ₂₂	
undecane	C ₁₁ H ₂₄	
dodecane	C ₁₂ H ₂₆	



But before getting into the systematic nomenclature of Substituted Alkanes: non-IUPAC names based on total number of C atoms present

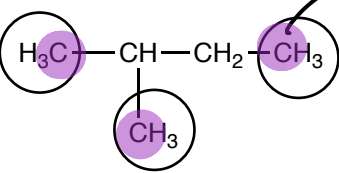
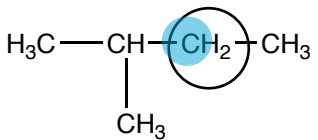
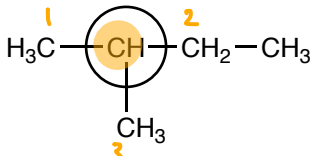
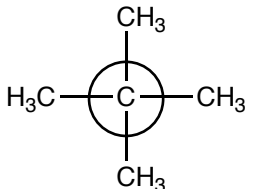
the "iso" group		
isobutane	$R = \text{CH}_3$ (4 C's)	
isopentane	$R = \text{CH}_2\text{CH}_3$ (5 C's)	
isohexane	$R = \text{CH}_2\text{CH}_2\text{CH}_3$ (6 C's)	
the "neo" group		
neopentane	$R = \text{H}$ (5 C's)	
neohexane	$R = \text{CH}_3$ (6 C's)	



Each of these molecules could be used as an adjective to describe a group; for example, the top one where the R is not defined we could say that the defined parts are an isopropyl group. It's three carbons (propane) in the shape of the iso group.

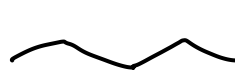
But before getting into the systematic nomenclature of Substituted Alkanes: non-IUPAC names based on total number of C atoms present and position of functional group

Degree of Substitution

1° primary (<i>n</i>-) 
2° secondary (<i>sec</i>-, <i>s</i>-) 
3° tertiary (<i>tert</i>-, <i>t</i>-) 
4° quaternary 

this carbon is "primary" (1°) because it is directly bonded to 1 C atom

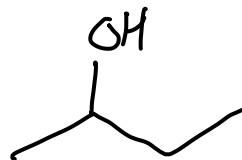
n-pentane



n-pentanol



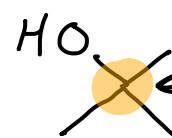
1°



sec-butanol because OH on 2° C

t-butanol

tertiary alcohol with 4 C atoms

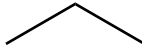
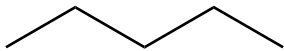
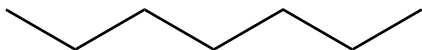
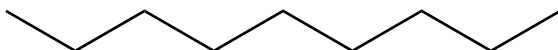
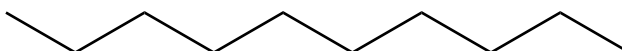
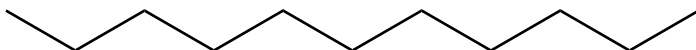
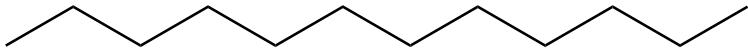


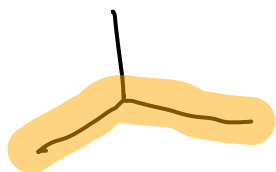
this C

is a tertiary C atom 'cu2

3 C atoms are bonded to it

Nomenclature of Alkanes: IUPAC Names based on the number of C's in the longest continuous chain of C atoms

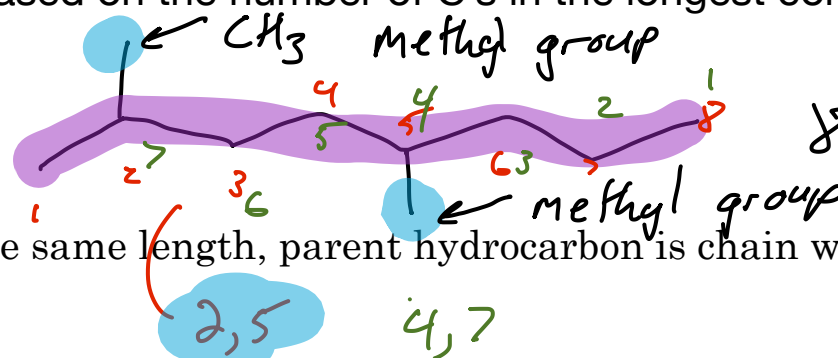
methane	CH_4	
ethane	CH_3CH_3	
propane	$\text{CH}_3\text{CH}_2\text{CH}_3$	
butane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_3$	
pentane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
hexane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
heptane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
octane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
nonane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
decane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
undecane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	
dodecane	$\text{CH}_3\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_2\text{CH}_3$	



Nomenclature of Alkanes: IUPAC Names based on the number of C's in the longest continuous chain of C atoms

Determine longest continuous chain.

- This is the **parent hydrocarbon**
- If compound has two or more chains of the same length, parent hydrocarbon is chain with greatest number of substituents



List the name of **substituent(s)** before the name of the parent hydrocarbon along with the number of the carbon to which it is attached--Substituents are listed in alphabetical order – neglecting prefixes such as di- tri- tert- etc.

- Find and list all of the substituents
- Names of alkyl substituents are based on the length of the substituent.
- Names for branched substituent such as *sec*-butyl and *tert*-butyl are acceptable, but systematic substituent names are preferable.
 - The numbering system for a branched substituent begins with the carbon attached to the parent hydrocarbon
 - This number together with the substituent name is placed inside parentheses
- Number the substituents
 - in the direction that gives the **lower number** for the **lowest-numbered** substituent. (Lowest possible number for all substituents on the parent chain)
 - When both directions yield the same lower number for the lowest numbered substituent, select the direction that yields the lower number for the next lowest numbered substituent
 - If same substituent numbers are obtained in either direction, number in the direction giving lowest number to the first (alphabetically) named substituent

Form of name: #-followed by substituent name followed by parent hydrocarbon name

position#-**stuff hanging off longest chain****longest chain of C atoms****functional group ending**

2,5 - dimethyl octane

Nomenclature of Alkanes: IUPAC Names based on the number of C's in the longest continuous chain of C atoms

Determine longest continuous chain.

- This is the **parent hydrocarbon**
- If compound has two or more chains of the same length, parent hydrocarbon is chain with greatest number of substituents

List the name of substituent(s) before the name of the parent hydrocarbon along with the number of the carbon to which it is attached--Substituents are listed in alphabetical order – neglecting prefixes such as di- tri- tert- etc.

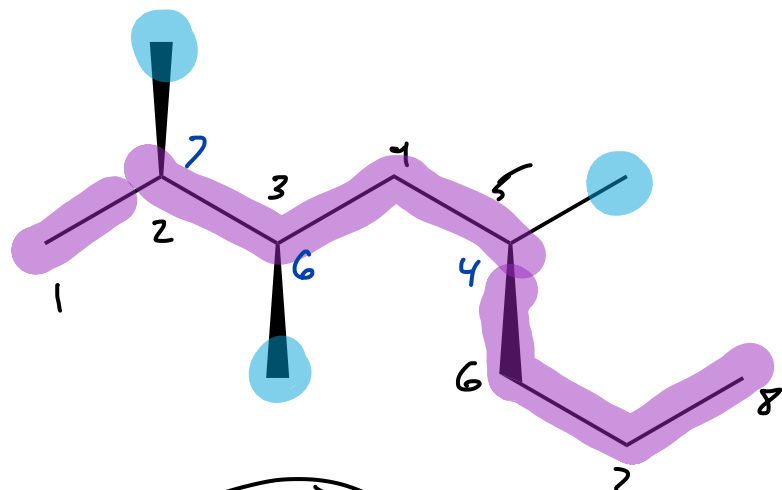
- Find and list all of the substituents
- Names of alkyl substituents are based on the length of the substituent.
- Names for branched substituent such as *sec*-butyl and *tert*-butyl are acceptable, but systematic substituent names are preferable.
 - The numbering system for a branched substituent begins with the carbon attached to the parent hydrocarbon
 - This number together with the substituent name is placed inside parentheses
- Number the substituents
 - in the direction that gives the lower number for the lowest-numbered substituent. (Lowest possible number for all substituents on the parent chain)
 - When both directions yield the same lower number for the lowest numbered substituent, select the direction that yields the lower number for the next lowest numbered substituent
 - If same substituent numbers are obtained in either direction, number in the direction giving lowest number to the first (alphabetically) named substituent

Form of name: #-followed by substituent name followed by parent hydrocarbon name

position#-**stuff hanging off longest chain**longest chain of C atoms**functional group ending**

Nomenclature of Alkanes

position#-**stuff hanging off longest chain**longest chain of C atoms**functional group ending**



2,3,5-trimethyloctane

2,3,5
4,6,7

Nomenclature of Alkanes

position#-**stuff hanging off longest chain**longest chain of C atoms**functional group ending**

longest chain:

7

parent alkane name:

heptane

functional group (?) and position:

none ✓

substituent names:

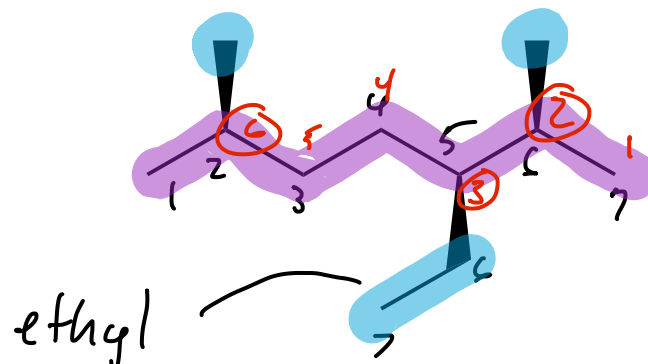
two methyl groups

ethyl

substituent positions:

2, 5, 6

2, 3, 6



tie for longest chain

3-ethyl-2,6-dimethylheptane

longest chain: 6

parent alkane name:

hexane

functional group (?) and position:

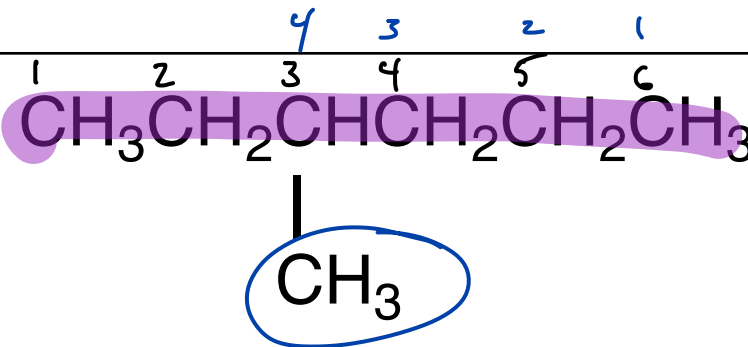
no

substituent names:

methyl

substituent positions:

3
or
4



name:

3-methylhexane

longest chain: 7

parent alkane name:

heptane

functional group (?) and position:

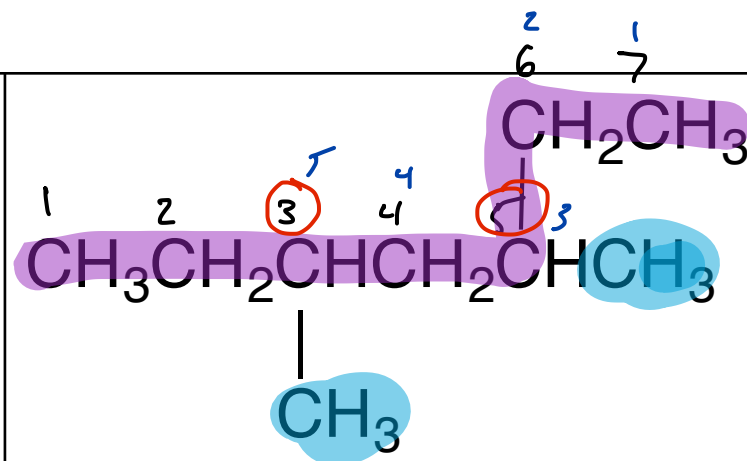
no

substituent names:

two methyl groups

substituent positions:

3,5 or 3,5



name:

3,5-dimethylheptane

longest chain: 8

parent alkane name:

octane

functional group (?) and position:

no halogens are
substituents

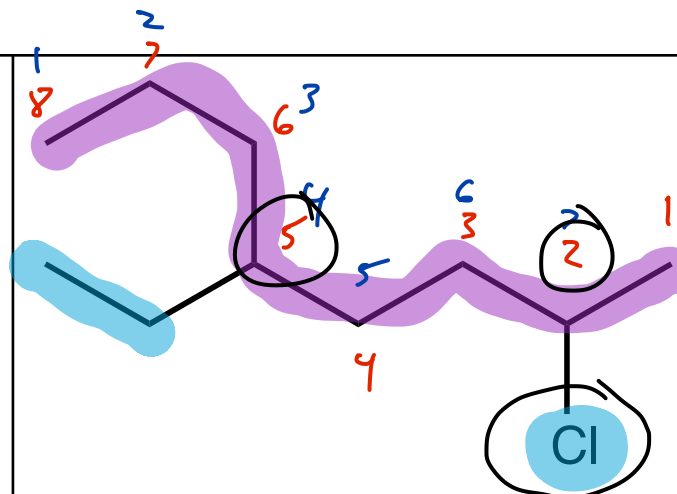
substituent names:

- ethan-yl

chlor-yl

substituent positions:

2, 5 or 4, 7



halogen lop off "ine" ending
name: replace with "o"

2-chloro-5-ethyl octane

longest chain: 7

parent alkane name:

heptane

functional group (?) and position:

not by nomenclature rule

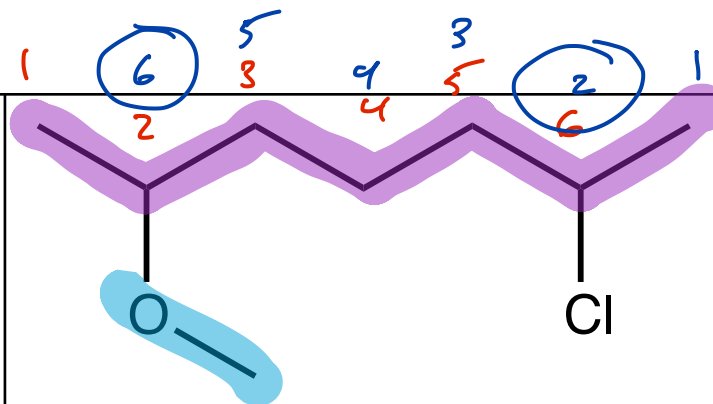
substituent names:

chlorine $\rightarrow$ chloro

methane $\rightarrow$ methoxy
oxy

substituent positions:

2,6 or 2,6
| |
methoxy chloro



name:

2-chloro-6-methoxyheptane

tie breaker is which
substituent come first
in the alphabet