CHEM 221 section 01 *based on original Lect07 but changed extensively…*

LECTURE #08 Thurs., Sept.29, 2005

ASSIGNED READINGS:

TODAY'S CLASS:

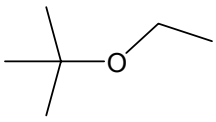
Finish nomenclature
Start structure-properties relationships

NEXT CLASS: continue with Ch.2

http://artsandscience.concordia.ca/facstaff/P-R/rogers

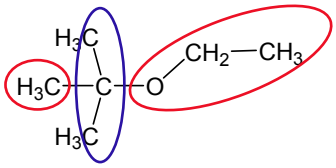
Continuing on with nomenclature…

Strategy: 1st assemble the name without the #s, then add position #s



An ether:
named as substituted alkane

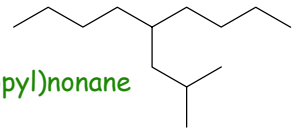
represents→



3-carbon parent chain: propane
substituents: methyl
ethoxy

START WITH: __-ethoxy-__-methylpropane

CORRECT NAME: 2-ethoxy-2-methylpropane

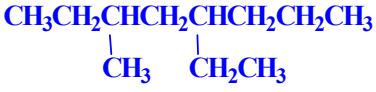
- **Numbers are used only in systematic names, not in common names**
  - A number & a word are separated by a hyphen:
    2-methylpropane 
  - A number & a number are separated by a comma:
    2,2-dimethylpropane 
  - A branched substituent is named systematically, in parentheses
    with point of attachment to parent chain
    labeled as C-1 of the substituent
    5-(2-methylpropyl)nonane 

- **Substituents are always listed in alphabetical order (by name)**
  - prefixes *di, tri, tetra…* indicate HOW MANY of that substituent
    ∴ are not used in alphabetization
  - prefixes *cyclo*, *iso*, *neo* ARE PART OF THE NAME of the substituent
    ∴ are used in alphabetization
    except: *sec* & *tert* *(don't know why!)*

Continuing with guidelines from last class…

1. Find longest continuous chain of carbons (= parent)
2. Number chain to give substituent(s) lowest possible #
3. Number the substituents to yield the lowest possible numbers in the name of the compound

i.e.,: Focus on minimizing the # given to the substituent that is closest to the end of the chain (either end!)



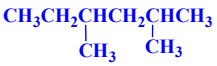
8-carbon parent chain: octane
with substituents: methyl
ethyl

START WITH: __-ethyl-__-methyloctane

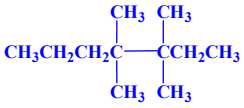
Because the CH_3 is closer to the end of the parent chain! → 5-ethyl-3-methyloctane

versus 4-ethyl-6-methyloctane

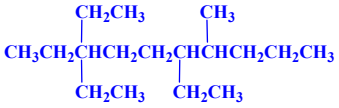
4. Number in direction that gives lowest possible numbers to <u>all</u> substituents (really the same thing as we just saw…)



2,4-dimethylhexane



3,3,4,4-tetramethylheptane



3,3,6-triethyl-7-methyldecane

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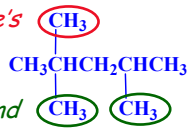
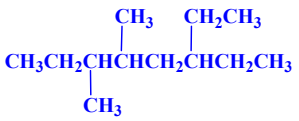
5. When the "1st" substituents are the same distance from each end of the chain: *# in direction that gives the lowest possible # to the substituent that is **next-closest** to the chain's end*

So: minimize this one's position #

Each is on a C 2nd from the end

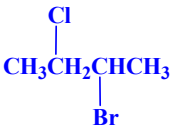


2,2,4-trimethylpentane
not
2,4,4-trimethylpentane
because 2<4

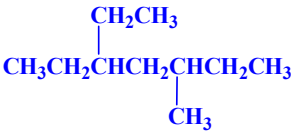


6-ethyl-3,4-dimethyloctane
not
3-ethyl-5,6-dimethyloctane
because 4<5

6. If the <u>same</u> numbers result from both numbering directions: *the 1st group in the NAME receives the lowest number* (alphabetically…)



2-bromo-3-chlorobutane
not
3-bromo-2-chlorobutane

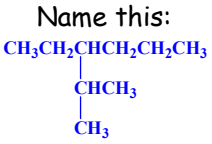


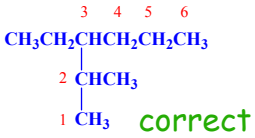
3-ethyl-5-methylheptane
not
5-ethyl-3-methylheptane

NOTE: numbering based on what comes 1st in the name is ONLY done when the substituents are ALL symmetrically attached like this (*i.e.,* all substituents are equal distances from the ends)

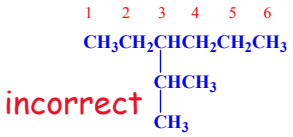
7. If two hydrocarbon chains in molecule have the same # of carbons: *parent = one with the most substituents*

Name this:





3-ethyl-2-methylhexane
(two substituents)



3-isopropylhexane
(one substituent)

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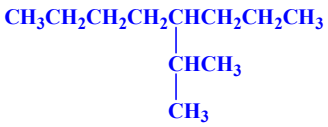
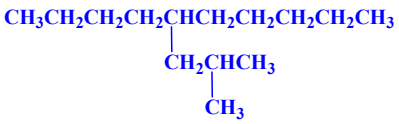
8. Certain common nomenclatures are ok in the IUPAC system
(But, it is still better to use fully systematic names.)



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



5-isobutyldecane
or
5-(2-methylpropyl)decane

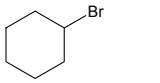
2.3 Naming cyclic alkanes: "cycloalkanes"

1. If ring = parent: add "cyclo" just before parent chain's name

cyclopropane

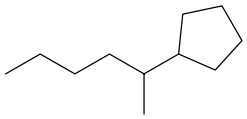
cyclobutane

cyclopentane



bromocyclohexane

2. If ring = substituent: *i.e.,* if longest chain is NOT the ring
"cycloalkyl-" as substituent name

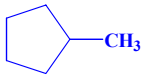


2-cyclopentylhexane

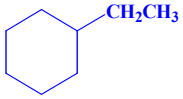
3. When ring has substituents:
   - 1 substituent: attachment C = C-1 (but omit "1-" in name)
   - 2 substituents: list in alphabetical order
     lowest in alphabet (1st listed…) labeled as on C-1
     (different than for acyclic compounds!)
   - > 2 substit.'s: choose C-1 so rest of position #s are minimized

Nomenclature of Cycloalkanes

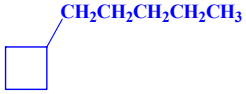
1. No number is needed for a single substituent on a ring
   (but it is not technically wrong to include the 1)



methylcyclopentane

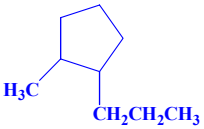


ethylcyclohexane

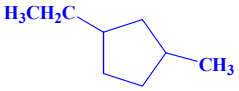


1-cyclobutylpentane

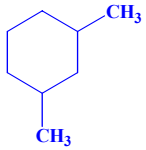
2. If two: Name substituents in alphabetical order
   Lowest # given to group listed 1st in alphabet



1-methyl-2-propylcyclopentane



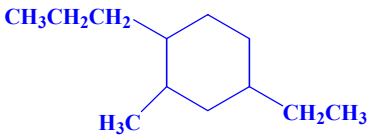
1-ethyl-3-methylcyclopentane



1,3-dimethylcyclohexane

3. If there are more than two substituents:
   choose C-1 such that the other substituent #s are the smallest possible
   i.e., C-1 is the C with the other substituents closest to it !

Strategy: choose a C-1, & start #ing towards the closest substituent, then try all other possible C-1's & see which yields lowest #s



__-ethyl-__-methyl-__-propylcyclohexane

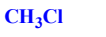
4-ethyl-2-methyl-1-propylcyclohexane

not
1-ethyl-3-methyl-4-propylcyclohexane
because2<3

not
5-ethyl-1-methyl-2-propylcyclohexane
because 4<5

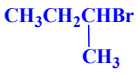
If number as	we'll have groups on
Propyl on C-1:	1…2…4… ← Lowest #s
Methyl on C-1:	1…2…5…
Ethyl on C-1:	1…3…4…

2.4 Nomenclature of Alkyl Halides

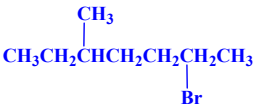

chloromethane

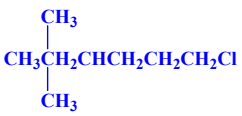

fluoroethane

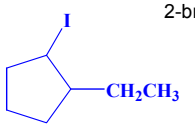

2-iodopropane

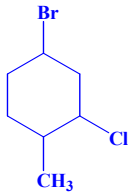

2-bromobutane

In the IUPAC system:
alkyl halides are named as substituted alkanes


2-bromo-5-methylheptane


1-chloro-5,5-dimethylhexane


1-ethyl-2-iodocyclopentane

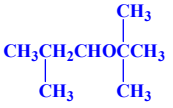

4-bromo-2-chloro-1-methylcyclohexane

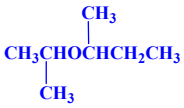
2.5 Nomenclature of Ethers

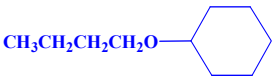
Common names:
Name the two alkyl groups + add "ether"


ethyl methyl ether


diethyl ether


tert-butyl isobutyl ether

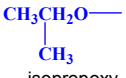

sec-butyl isopropyl ether

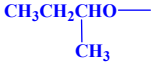

cyclohexyl isopentyl ether

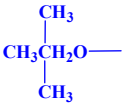
IUPAC systematic name: -OR group named as a substituent:


methoxy


ethoxy


isopropoxy

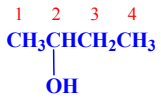

sec-butoxy


tert-butoxy

2.6 Nomenclature of Alcohols

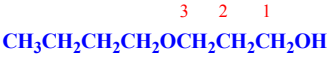
IUPAC naming: the OH functional group is "important enough" to name the compound after it…
→ use suffix "-ol"

1. Determine the parent hydrocarbon that <u>contains the highest-priority functional group</u> *(here: the hydroxyl)*



2-butanol
or
butan-2-ol

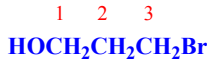
2-ethyl-1-pentanol
or
2-ethylpentan-1-ol



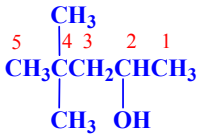
3-butoxy-1-propanol
or
3-butoxypropan-1-ol

Note: the position # for the –OH group can appear in 1 of 2 places:
(i) immediately before the "-ol" suffix
or (ii) before the parent chain's name

2. The highest-priority functional group suffix gets the lowest position number possible

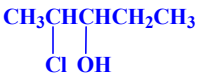


3-bromo-1-propanol

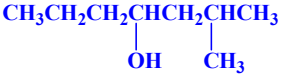


4,4-dimethyl-2-pentanol

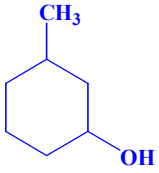
3. And…then give the lowest possible #s to the other substituents



2-chloro-3-pentanol
not
4-chloro-3-pentanol

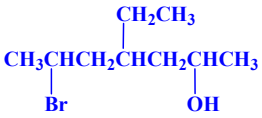


2-methyl-4-heptanol
not
6-methyl-4-heptanol

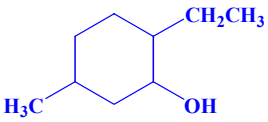


3-methylcyclohexanol
not
5-methylcyclohexanol

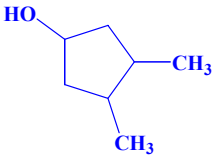
4. If there is more than one substituent, the substituents are cited in alphabetical order *(as always!)*
& the rest of the rules are followed too



6-bromo-4-ethyl-2-heptanol



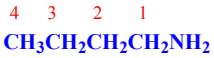
2-ethyl-5-methylcyclohexanol



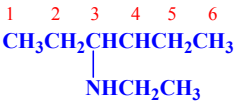
3,4-dimethylcyclopentanol

2.7 Nomenclature of Amines

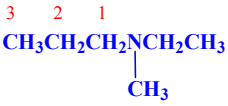
IUPAC naming: based on functional group, suffix "-amine"



1-butanamine
or
butan-1-amine

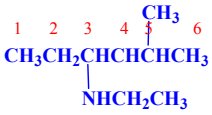


N-ethyl-3-hexanamine
or
N-ethylhexan-3-amine

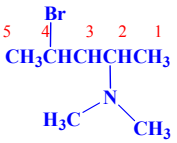


N-ethyl-N-methyl-1-propanamine
or
N-ethyl-N-methylpropan-1-amine

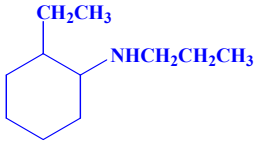
- The substituents are listed in alphabetical order and a number or an "*N*" is assigned to each one



N-ethyl-5-methyl-3-hexanamine



4-bromo-N,N-dimethyl-2-pentanamine



2-ethyl-N-propylcyclohexanamine

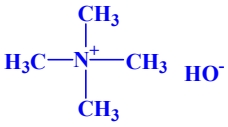
Naming Quaternary Ammonium Salts

Ionic compounds: name cation first, then name anion

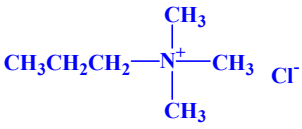
Common names:

1. Name all substituents on the nitrogen
2. Use suffix "-ammonium"
3. Name the counterion

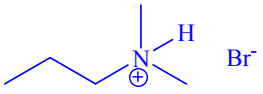
Don't worry about their IUPAC names



tetramethylammonium hydroxide



ethyltrimethylammonium chloride



dimethylpropylammonium bromide

We'll see how alkylammonium salts can form later…
but we DO know that amines can be protonated (act as base!)

A few more slides to come about structure & properties…

ASSIGNED READINGS

BEFORE NEXT LECTURE:

Read: Ch.2 up to 2.9

Practice: nomenclature & structural drawings