CHEM 221 section 01

LECTURE #06 Thurs., Sept.22, 2005

ASSIGNED READINGS:

TODAY'S CLASS:

1.21	Lewis acids & bases
2.1-2.7	Naming organic compounds

NEXT CLASS: Ch.2: continue on…

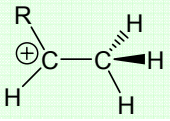
http://artsandscience.concordia.ca/facstaff/P-R/rogers

Common Lewis acids & Lewis bases

LEWIS ACIDS = e^- pair acceptors React with electron-rich species "electrophiles" *(Attracted to e^-s)* "E^+"	LEWIS BASES = e^- pair donors React with e^--deficient species "nucleophiles" *(Attracted to nuclei)* "Nu^-"
H^+ *(or δ^+ H)* } Empty s orbital *(or nearly empty)*	<u>Any</u> species with a lone pair
$\oplus CR_3$ } Empty p orbital	Can react in two ways: *Same mechanism, different outcome*
BR_3, AlR_3 } "trivalent elements" Empty p orbital	1. As a Brønsted base • React with δ^+ H atoms
Zn(II), Fe(III) } Metal cations: Empty orbitals…	2. As a nucleophile • React with δ^+ carbon or other non-H atoms

Example: Carbocations react with Lewis bases

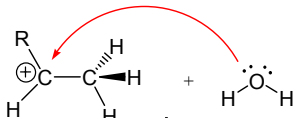
Highly electrophilic *(open shell carbon!)*



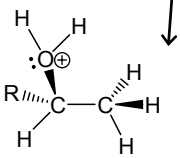
+

Lewis basic *(lone pair on O)*

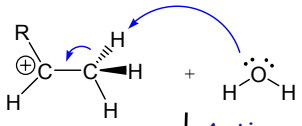
Depending on how the molecules collide, & other structural factors (*basicity, size, accessibility…see later…*), the rxn will occur in one of 2 ways:



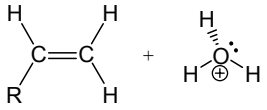
Acting as a Nu^-



Details in Ch.3, 4, 10, 11



Acting as a base



Details in Ch.11

Chapter 2: Introduction to Organic Compounds

Chapter Goals

To prepare ourselves for learning about chemical reactions

- Learn to draw & name common organic compounds - *nomenclature*
- Understand structure & physical properties - *molecular interactions*
- Understand the flexible nature of molecules - *conformations*

Chapter Outline:

2.1-2.7 Nomenclature of common organic compounds
alkanes, alkyl halides, ethers, alcohols, amines

2.8-2.9 Structures & physical properties of common compounds

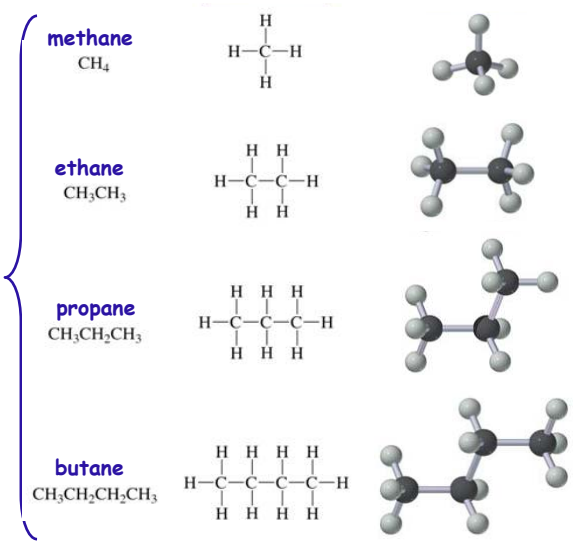
2.10-2.15 Conformations of alkanes & cycloalkanes

Alkanes: hydrocarbons containing only single bonds

- Hydrocarbons = compounds containing only C & H
- Alkane general formula: C_nH_{2n+2}

A "homologous series"

each member differs by one CH_2 "methylene" group



NAMING ALKANES

- Prefix based on: # C's
- Suffix based on: bonding all single C-C bonds
  ⇨ "_ane"

Table 2.1 Nomenclature and Physical Properties of Straight-Chain Alkanes

Number of carbons	Molecular formula	Name	Condensed structure	Boiling point (°C)
1	CH_4	methane	CH_4	−167.7
2	C_2H_6	ethane	CH_3CH_3	−88.6
3	C_3H_8	propane	$CH_3CH_2CH_3$	−42.1
4	C_4H_{10}	butane	$CH_3CH_2CH_2CH_3$	−0.5
5	C_5H_{12}	pentane	$CH_3(CH_2)_3CH_3$	36.1
6	C_6H_{14}	hexane	$CH_3(CH_2)_4CH_3$	68.7
7	C_7H_{16}	heptane	$CH_3(CH_2)_5CH_3$	98.4
8	C_8H_{18}	octane	$CH_3(CH_2)_6CH_3$	127.7
9	C_9H_{20}	nonane	$CH_3(CH_2)_7CH_3$	150.8
10	$C_{10}H_{22}$	decane	$CH_3(CH_2)_8CH_3$	174.0
11	$C_{11}H_{24}$	undecane	$CH_3(CH_2)_9CH_3$	195.8
12	$C_{12}H_{26}$	dodecane	$CH_3(CH_2)_{10}CH_3$	216.3

Memorize: prefixes for 1-12 C's

Straight-chain alkanes are commonly called *n*-alkanes (*n* for *normal*)

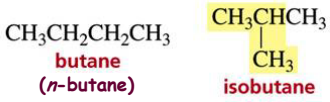
An "alkyl group" = an alkane-type chain bonded to something else

e.g., methyl (CH_3—),
pentyl ($CH_3CH_2CH_2CH_2CH_2$—)
etc...

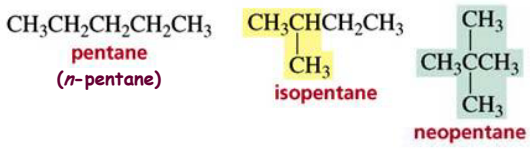
For chains of ≥ 4 carbons: branched isomers also possible

- Isomers = different molecules with same molecular formula
  - Constitutional isomers: same molecular formula, different connectivity (different atoms connected to each other)

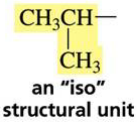
C_4H_{10}

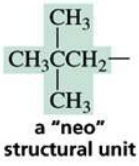


C_5H_{12}



Common motifs:





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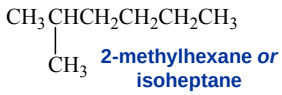
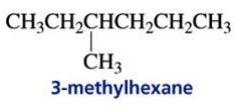
Drawing isomers: start with straight chain, then add braches

Try C_7H_{16}: *7C's straight*

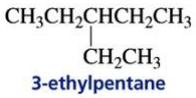
$CH_3CH_2CH_2CH_2CH_2CH_2CH_3$ Heptane (systematic IUPAC name) *or* *n*-heptane (common name)

6C's + 1 CH_3 substituent



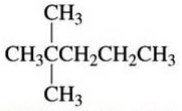


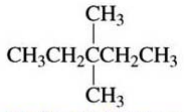
5C's + 1 CH_2CH_3 substituent

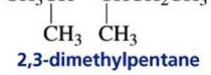


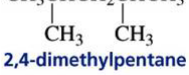
*Note: **no neoheptane**, since 3 isomers have a C bonded to 4C's…*

5C's + 2 CH_3 substituents

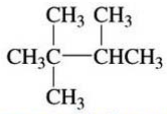








4C's + 3 CH_3 substituents



We'll learn to name these systematically soon…

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Important: A compound can have more than one name, but a name must specify only one compound

Two systems of nomenclature:

1. Common names

- Historical
- Not necessarily based on structure
- Too many to memorize for all known compounds…but…
- Still in use for common compounds
  - on chemical bottles…
  - need to know motifs: *normal, iso, neo*

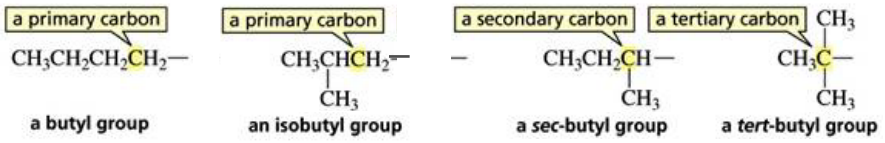
2. Systematic names (IUPAC)

- Unambiguous names
- Based on structure
  - Length of carbon chain
  - Bonding in chain
  - Positions of substituents
  - *etc.*
- Once you learn the rules, you can figure out names as required (less memorizing)
- *First: learn alkyl groups & functional groups*

First: different types of C's & H's

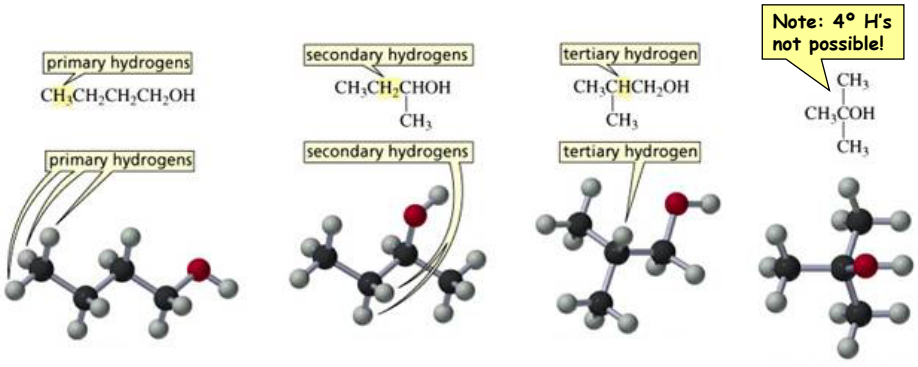
DESCRIBE CARBON ATOMS: Based on # of C's the C is bonded to

1 ⇨ primary 1°
2 ⇨ secondary 2°
3 ⇨ tertiary 3°
4 ⇨ quaternary 4°



First: different types of C's & H's

DESCRIBE HYDROGEN ATOMS: Based on type of C the H is bonded to



We will see: this is related to common names of some types of compounds

2.1 Nomenclature of Alkyl Substituents

Table 2.2 Names of Some Alkyl Groups

methyl	CH_3-
ethyl	CH_3CH_2-
propyl	$CH_3CH_2CH_2-$
isopropyl	$CH_3CH(CH_3)-$
butyl	$CH_3CH_2CH_2CH_2-$
isobutyl	$CH_3CH(CH_3)CH_2-$
sec-butyl	$CH_3CH_2CH(CH_3)-$
tert-butyl	$(CH_3)_3C-$
pentyl	$CH_3CH_2CH_2CH_2CH_2-$
isopentyl	$CH_3CH(CH_3)CH_2CH_2-$

Note: the *iso, sec, tert* names are commonly used
but they do not appear in proper systematic names

Substituent (hydrocarbon-based group) (symbol, abbreviation & name)			Class of compounds		Comments
$-(CH_2)_nCH_3$ or branched…	—R	**alkyl**	C_nH_{n+2}	**Alkanes**	See Table 2.2 for structures & common names of alkyl groups
$-CH_3$	—Me	methyl	Must become very familiar with these common alkyl groups		
$-CH_2CH_3$	—Et	ethyl			
$-(CH_2)_2CH_3$	—Pr	propyl			
$-CH(CH_3)_2$	—*i*-Pr	isopropyl			
$-(CH_2)_3CH_3$	—Bu	butyl			
$-C(CH_3)_3$	—*t*-Bu	*tert*-butyl			
$-CH{=}CH_2$		vinyl	$R_2C{=}CR_2$	**Alkenes**	Discussed later in Chem221.
$-C{\equiv}CH$		acetylide	$RC{\equiv}CR$	**Alkynes**	
$-C_6H_5$	**—Ph** 	**phenyl**  A benzene ring as a substituent…	C_6H_5R	**Aromatic hydrocarbons**	Chemistry discussed in later courses.

Compounds are classified based on reactivity

FUNCTIONAL GROUPS = centres of reactivity in compounds

- basis for classifying compounds
- functional groups contain:

1.) heteroatoms
atoms that are not carbon or hydrogen
more electronegative: result in δ^+/δ^- centres
have nucleophilic / basic lone pairs

2.) multiple bonds
π-electron density is exposed & polarizable
very attractive to electrophiles (see Ch.3,4)

Functional group (symbol & name)		Class of compounds (based on functional gp)		Descriptors		Examples
—X	Halide	R—X	Alkyl halides	1° 2° 3°	RCH_2-X R_2CH-X R_3C-X	
—OH	Hydroxyl	R—OH	Alcohols	1° 2° 3°	RCH_2-OH R_2CH-OH R_3C-OH	
—NH_2	Amino	R—NH_2	Amines	1° 2° 3°	R-NH_2 R_2NH R_3N	
—O—	Oxy	R—O—R	Ethers	Symmetric Asymmetric	R-O-R R-O-R'	
O ‖ —C—	Carbonyl	O ‖ R—C—R	Ketones; if ≥1 R=H: Aldehydes	O ‖ R—C—X Acyl halides *OR* Acid halides		Chemistry of these types of compounds (including IUPAC names) discussed in later courses.
O ‖ —C—OH	Carboxyl	O ‖ R—C—OH	Carboxylic acids	O ‖ R—C—OR Esters	O ‖ R—C—NR_2 Amides	
—C≡N	Cyano	R—C≡N	Nitriles			
—NO_2	Nitro	R—NO_2	Alkyl nitrates			

(15)

Naming common compounds

"Common names" of compounds: alkyl group + compound type

CH_3OH methyl alcohol	$CH_3CH_2NH_2$ ethylamine	$CH_3CH_2CH_2Br$ propyl bromide	$CH_3CH_2CH_2CH_2Cl$ butyl chloride
CH_3I methyl iodide	CH_3CH_2OH ethyl alcohol	$CH_3CH_2CH_2NH_2$ propylamine	$CH_3CH_2CH_2CH_2OH$ butyl alcohol

(16)

Systematic names: one long word, made up of 3 main parts:

PREFIX — INFIX — SUFFIX

PREFIX

Based on length of longest continuous C chain ("parent") PLUS: parent chain descriptor preceded by positions & names of substituents

Substituents:
alkyl
halo
hydroxy
amino (alkylamino, di/trialkylamino)
alkoxy

Parent:
meth–
eth–
prop–
but–
pent–
hex–
hept–
oct–
non–
dec–

INFIX

Based on C-C bond type in backbone

Infix:
single only –an–
≥ 1 double –en–
≥ 1 triple –yn–

SUFFIX

Based on most important functional group

Conventions:
- treat halides simply as substituents on chain
- ethers named as alkoxy substituents on chain

Suffix:
Alkanes: –e
Alcohols: –ol
Amines: –amine
Carboxylic acids: –oic acid

See Bruice Table 2.3

Compound class	Systematic IUPAC name	Common name
Alkyl halide	Substituted alkane $CH_3CH_2FCH_2CH_2CH_3$ 2-fluoropentane	*Alkyl* group to which halogen is attached, plus *halide* ←*sec*-pentyl fluoride *(Bad --- name is non-unique!)*
Ether	Substituted alkane $CH_3CH_2OCH_2CH_3$ ethoxyethane	*Alkyl* group attached to oxygen, plus *ether* ← diethyl ether
Alcohol	Functional group suffix is *-ol* $(CH_3)_3COH$ 2-methyl-2-propanol	*Alkyl* group to which OH is attached, plus *alcohol* ← t-butanol
Amine	Functional group suffix is *-amine* $CH_3CH_2NHCH_3$ N-methylethanamine	*Alkyl* groups attached to N, plus *amine* ← ethylmethylamine

But: what about when the chains are more complicated?

Systematic naming: a summary of the strategy

1.) Find longest continuous chain of carbons: PARENT CHAIN
- if 2 or more of same length:
  one with more substituents = parent chain

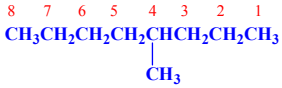
2.) Number C's in the chain
in direction that puts substituents on C's with lowest #'s possible

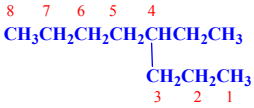
3.) Write substituents in alphabetical order (with position # 1st for each) followed by parent chain name
- if ≥ 1 identical substituent: use di, tri, tetra… to indicate quantity
  e.g., #,#,#-tri__
- but note: prefixes are not included in alphabetization
  except: *iso, neo* (non-systematic!) & cyclo ARE included

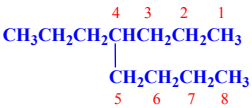
4.) MORE DETAILS: regarding direction of numbering
- if multiple substituents: # so the position #'s are as low as possible
  (the #s themselves, not their sum)
- if same in both directions: substit. 1st in alpha. listing gets lower #

2.2 Nomenclature of Alkanes

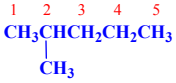
1. Determine the number of carbons in parent hydrocarbon



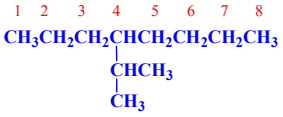




2. Number the chain so that the substituent gets the lowest possible number

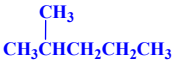


2-methylpentane



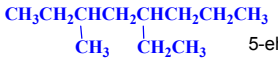
4-isopropyloctane

Better if you also systematically name the *i*-Pr substituent: 4-(1-methylethyl)octane



common name: isohexane
systematic name: 2-methylpentane

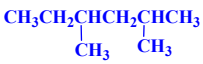
3. Number the substituents to yield the lowest possible numbers in the name of the compound



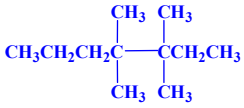
5-ehtyl-3-methyloctane
not
4-ethyl-6-methyloctane
because 3<4

(substituents are listed in alphabetical order)

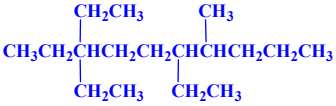
4. Assign the lowest possible numbers to all substituents



2,4-dimethylhexane



3,3,4,4-tetramethylheptane



3,3,6-triethyl-7-methyldecane

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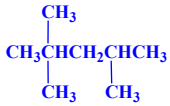
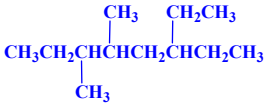
5. When both directions lead to the same lowest number for one of the substituents, the direction is chosen that gives the lowest possible number to one of the remaining substituents

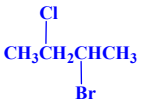


2,2,4-trimethylpentane
not
2,4,4-trimethylpentane
because 2<4

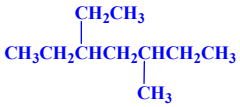


6-ethyl-3,4-dimethyloctane
not
3-ethyl-5,6-dimethyloctane
because 4<5

6. If the same number is obtained in both directions, the first group receives the lowest number



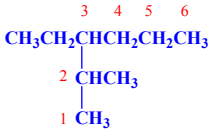
2-bromo-3-chlorobutane
not
3-bromo-2-chlorobutane



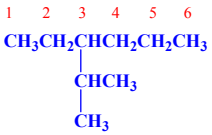
3-ethyl-5-methylheptane
not
5-ethyl-3-methylheptane

(22)

7. In the case of two hydrocarbon chains with the same number of carbons, choose the one with the most substituents

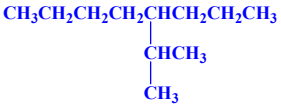


3-ethyl-2-methylhexane
(two substituents)

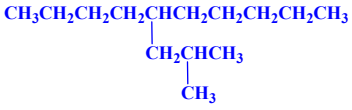


3-isopropylhexane
(one substituent)

8. Certain common nomenclatures are ok in the IUPAC system



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



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

But, it is still better to go 'fully systematic'

ASSIGNED READINGS

BEFORE NEXT LECTURE:

Read: Ch.2 up to 2.8

Practice: naming organic compounds