CHEM 221 section 52

LECTURE #03

Thurs., Jan.17, 2008

ASSIGNED READINGS:

## TODAY'S CLASS:

- 2.1 Introduction to naming organic compounds
- 2.8-2.9 Dependence of physical properties on structure

NEXT CLASS: Ch.2: continue with 2.2-2.7, etc...

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## Chapter 2: Introduction to Organic Compounds

#### Chapter Goals

To prepare ourselves for learning about common organic reactions (have already seen acid-base reactions of organic molecules...)

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

<u>Chapter Outline</u>: (but not in this order in class)

- 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

We've been using these already on examples on the board...

## Rules for drawing skeletal / line structures (2.3)

Drawings that give idea of molecule's general shape:

- Bonds & angles shown: chains = zigzags, rings = polygons
- C & H atoms not shown: vertices = C atoms, missing bonds = Hs
- H-atoms bonded to heteroatoms always shown: NH, OH, etc
  - · Lone pairs on heteroatoms optional
  - but helpful on N (basic!) & O (polarity reminder)
- Formal charges are ALWAYS shown: if not zero...

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Its pure skeletal (line) structure:



#### A mixed-style structure



Two condensed representations: CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CHCHCH<sub>2</sub>CCH

$$CH_3CH_2CH_2CH=CHCH_2C=CH$$

Naming organic compounds: NOMENCLATURE How to "point" to different parts of a molecule: General descriptive terminology



Note: the *iso, sec, tert* names are commonly used

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but they do not appear in proper systematic names

Substituent (hydrocarbon-based group) (symbol, abbreviation & name)			Class a	f compounds	Comments		
(CH <sub>2</sub> ) <sub>n</sub> CH <sub>3</sub> or branched	-R	alkyl	C <sub>n</sub> H <sub>n+2</sub>	Alkanes	See Table 2.2 for structures & common names of alkyl groups		
—CH₃	—Me	methyl	)				
-CH <sub>2</sub> CH <sub>3</sub>	—Et	ethyl					
-(CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	—Pr	propyl	Must be	come very familiar			
-CH(CH <sub>3</sub> ) <sub>2</sub>	— <i>i-</i> Pr	isopropyl	groups				
-(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	—Bu	butyl					
— <i>C</i> ( <i>C</i> H <sub>3</sub> ) <sub>3</sub>	<i>—t-</i> Bu	tert-butyl	J				
-CH=CH <sub>2</sub>		vinyl	$R_2C = CR_2$	Alkenes	] Discussed later		
–C≡CH		acetylide	R <i>C</i> ≡CR	Alkynes	$\int$ in Chem221.		
	Ph	phenyl	C <sub>6</sub> H₅R	Aromatic hydrocarbons	Chemistry discussed in later courses.		

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## How to "point" to different parts of a molecule: General descriptive terminology



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

## 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  $\delta^*/\delta^-$  centres have nucleophilic / basic lone pairs

#### 2.) multiple bonds

 $\pi$ -electron density is exposed & polarizable very attractive to electrophiles (see Ch.3,4)

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Functional group (symbol & name)		Class of compounds (based on functional gp)		Descr	iptors	Examples	
_x	Halide	R—X	Alkyl halides	1° 2° 3°	RCH <sub>2</sub> -X R <sub>2</sub> CH-X R <sub>3</sub> C-X		
—он	Hydroxyl	R—OH	Alcohols	1º 2º 3º	RCH <sub>2</sub> -OH R <sub>2</sub> CH-OH R <sub>3</sub> C-OH		
—NH₂	Amino	R—NH <sub>2</sub>	Amines	1° 2° 3°	R-NH <sub>2</sub> R <sub>2</sub> NH R <sub>3</sub> N		
-0-	Оху	R—O—R	Ethers	Symmetric Asymmetric	R-O-R R-O-R'		
0    C	Carbonyl	O II R—C—R	Ketones; if ≥1 R=H: Aldehydes	0    Acyl halides <i>OR</i> R—C—X Acid halides		Chemistry of these types	
о ॥ _с_он	Carboxyl	O II R—C—OH	Carboxylic acids	O II R—C—OR Esters	O II R—C—NR <sub>2</sub> Amides	of compounds (including IUPAC names) discussed in	
—C≡N	Cyano	R—C≡N	Nitriles				
	Nitro	R—NO <sub>2</sub>	Alkyl nitrates				

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## Alkanes: hydrocarbons containing only single bonds

Hydrocarbons = compounds containing only C & H

Alkane general formula: C<sub>n</sub>H<sub>2n+2</sub>



Table 2.1	Nomenclature and				
Number of carbons	Molecular formula	Name	Condensed structure	Boiling point (°C)	Memorize: prefixes for 1.12 C's
1	CH <sub>4</sub>	methane	CH <sub>4</sub>	-167.7	101-12-03
2	$C_2H_6$	ethane	CH <sub>3</sub> CH <sub>3</sub>	-88.6	
3	C <sub>3</sub> H <sub>8</sub>	propane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	-42.1	Straight-chain
4	C <sub>4</sub> H <sub>10</sub>	butane	CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	-0.5	alkanag ana
5	C5H12	pentane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	36.1	urkunes ure
6	C <sub>6</sub> H <sub>14</sub>	hexane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>	68.7	commonly
7	C <sub>7</sub> H <sub>16</sub>	heptane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	98.4	called
8	C8H18	octane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>	127.7	<i>n</i> -alkanes
9	C9H20	nonane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>7</sub> CH <sub>3</sub>	150.8	( <i>n</i> for <i>normal</i> )
10	$C_{10}H_{22}$	decane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>8</sub> CH <sub>3</sub>	174.0	
11	C11H24	undecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>9</sub> CH <sub>3</sub>	195.8	
12	C12H26	dodecane	CH <sub>3</sub> (CH <sub>2</sub> ) <sub>10</sub> CH <sub>3</sub>	216.3	

An "alkyl group" = an alkane-type chain bonded to something else *e.g.*, methyl (CH<sub>3</sub>—), pentyl (CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>—) *etc...* 

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## For chains of $\geq$ 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)



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D	rawing isom	<b>ers:</b> start with st	raight chain, t	hen add brand	ches	
Т	<b>ry C<sub>7</sub>H</b> <sub>16</sub> :	<i>7C's straight</i> CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CI	Heptane (sy H <sub>2</sub> CH <sub>3</sub> or <i>n</i> -hept	stematic IUPAC nar tane (common name	ne) ∋)	
	6C's + 1 CH <sub>3</sub> substituent	CH <sub>3</sub> CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH CH <sub>3</sub> 2-methylhexa isoheptar	l <sub>3</sub> CH <sub>3</sub> CH nne or ne 3-n	or CH <sub>3</sub> CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> CH <sub>3</sub> 3-methylhexane		
$5C's + 1 CH_2CH_3$ substituent		√ <sub>3</sub> CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> ↓ CH <sub>2</sub> CH <sub>3</sub> 3-ethylpentane	CH <sub>2</sub> CHCH <sub>2</sub> CH <sub>3</sub>   Note: no n CH <sub>2</sub> CH <sub>3</sub> isomers have		e <u>3</u> 4C's	
	5C's + 2 CH <sub>3</sub> substituents	$\begin{array}{c} CH_3 \\   \\ CH_3CCH_2CH_2CH_3 \\ CH_3 \\ \textbf{2,2-dimethylpentane} \\ CH_3CH-CHCH_2CH_3 \\   \\ CH_3CH_3 \\ CH_3 \\ \textbf{2,3-dimethylpentane} \end{array}$	CH <sub>3</sub> CH <sub>3</sub> CH <sub>2</sub> CCH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub> CH <sub>3</sub> ,3-dimethylpentane CH <sub>3</sub> CHCH <sub>2</sub> CHCH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> CH <sub>3</sub> 2,4-dimethylpentane	$\begin{array}{c} 4C's + 3 CH_3\\ substituents\\ CH_3 CH_3\\ CH_3CH_3\\ CH_3CH_3\\ CH_3\\ CH_3\\ 2,2,3-trimethylbu\end{array}$	'H <sub>3</sub> tane	

We'll learn to name these systematically soon...

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# 2.8–2.9 Understanding relationships between chemical structure & properties...

#### Physical properties include:

- boiling point
- melting point
- solubility

#### Chemical properties:

- types of rxns that occur
- we're getting to those soon!

#### What determines the physical properties of a compound ?

 $\rightarrow$  Strength of interaction between the molecules

- what type(s) of interaction are occurring?
- how strong are those individual interactions?
- · how large are the regions over which these interactions operate?
  - how many points of contact with that interaction?
  - how many individual interactions of each type possible?

### → To predict: consider shape, polarity & size of the molecules

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## Longer alkyl chain ⇒ higher mp & bp

Boiling points: alka	nes	VS	alkyl	halides	22-	Table 2.6
Y =	Н		F	Cl	Br	Ι
CH <sub>3</sub> —Y	-161.7 °C	-	-78.4	-24.2	3.6	42.4
CH <sub>3</sub> CH <sub>2</sub> -Y	-88.6		-37.7	12.3	38.4	72.3
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> -Y	-42.1		-2.5	46.6	71.0	102.5
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -Y	-0.5		32.5	78.4	101.6	130.5
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>2</sub> -Y	36.1		62.8	107.8	129.6	157.0

Why?

Longer alkyl chain ⇒ lower solubility in polar solvents Alkanes: NONPOLAR ⇒ generally not water-soluble Alkyl halides: NEARLY NONPOLAR ⇒ soluble if R < 2 CH<sub>2</sub> long...

**Ethers:** AMPHIPHILIC  $\Rightarrow$  soluble if R < 3 CH<sub>2</sub> long...

**Alcohols:** AMPHIPHILIC  $\Rightarrow$  soluble if R < 4 CH<sub>2</sub> long

**Amines:** AMPHIPHILIC ⇒ similar to ROH, plus sol'y 1° > 2° > 3°

(17) Branching  $\uparrow$  solubility: less surface for H<sub>2</sub>O to solvate

#### For these compounds:

- 1) Classify by compound type
- 2) Draw, add polarities, identify polar vs. nonpolar regions
- 3) Identify relative strengths of intermolecular forces
- 4) Comment on expected relative boiling points
- 5) Comment on expected solubility in water...

 $(CH_3)_3CH$   $CH_3NH_2$   $CH_3(CH_2)_5OH$ 

## ASSIGNED READINGS & EXERCISES

# ESSENTIAL BEFORE NEXT LECTURE:

**Read:** Ch.2 sections 2.1, 2.8, 2.9

Memorize: names, structures & shorthands for... alkyl groups & functional groups

**Practice:** drawing isomers: linear, branched, etc predicting phys. properties from structures (19)