# Organic chemistry! Chapter 21

**Nov 4 – Nov 8** 

Video 25: Organic Molecules and Skeletal Structure

Video 26: Nomenclature

#### Next week: Nov 11 – Nov 14 (not in these notes)

Video 27: Conformation of alkanes

Video 28: Functional groups

Video 29: Stereochemistry and isomers

# Chapter 21

**Nov 4 – Nov 8** 

Video 25: Organic Molecules and Skeletal Structure

#### **Prof. Maureen McKeague**

**Department of Chemistry** 

@mmckeague



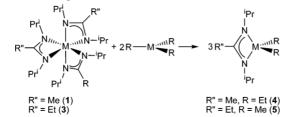
chem110-120.chemistry@mcgill.ca

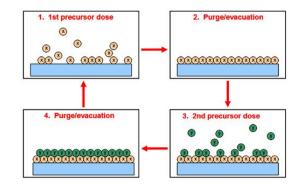
#### My diverse background in chemistry and biology

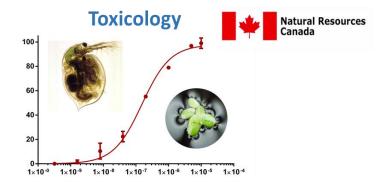
#### **Inorganic chemistry**

Carleton

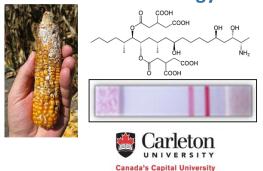
**Canada's Capital University** 







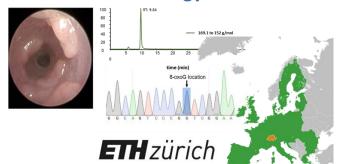
#### **DNA** nanotechnology



#### **Biotechnology**



#### **Chemical biology**



# Intro to Organic Structures

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# Birth of Synthetic Organic Chemistry

There was no concept of "synthesizing" compounds – compounds were separated and purified from natural sources



Synthesized urea from ammonium cyanate in 1828

-OCN

NH<sub>4</sub>+

**Cyanate ion** Ammonium ion

 $CO(NH_2)_2$ 

**Urea** 

Friedrich Wohler: 1800-1882

"In a manner of speaking, I can no longer hold my chemical water. I must tell you that I can make urea without the use of kidneys of any animal, be it man or dog."

Appearance: White solid

Density: 1.32 g/cm3

Melting point: 133 to 135 °C

# Organic Chemistry – A Brief History

#### 1892: International Congress of Chemistry developed "Geneva Nomenclature"

This remains the core (with continuous updates) of the IUPAC nomenclature that remains in use

(IUPAC = International Union of Pure and Applied Chemistry)



# Learning organic chemistry

It's hard work – it can be like learning a new language...

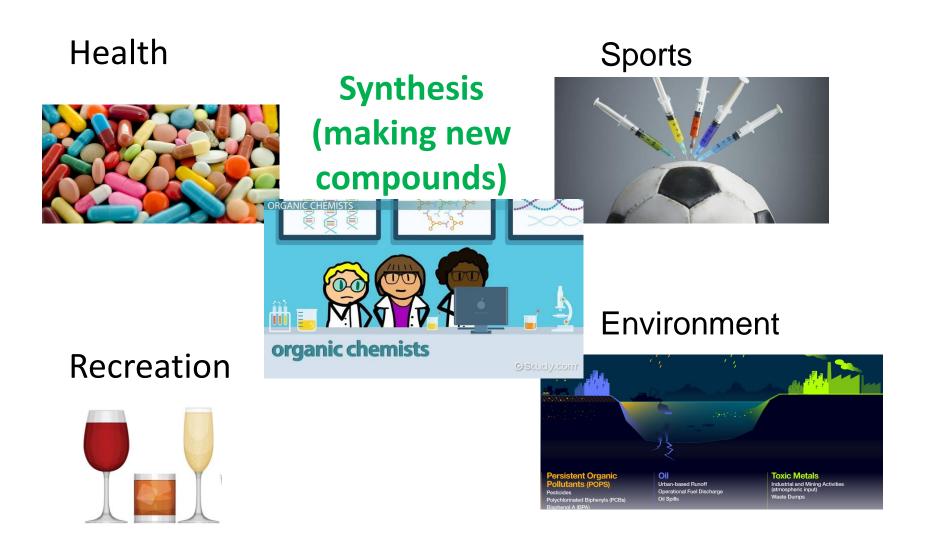
Imagine writing a poem or song

- -memorize ABC's
- -memorize sounds
- -learn words
- -write sentences
- -communicate your ideas in paragraphs, conversations

# Why do we care about organic chemistry?

What do you care about?

# Why do we care about organic chemistry?



#### Video demonstration

#### The Briggs-Rauscher Reaction

$$IO_3^- + 2H_2O_2 + CH_2(CO_2H)_2 + H^+ --> ICH(CO_2H)_2 + 2O_2 + 3H_2O$$
HO
OH

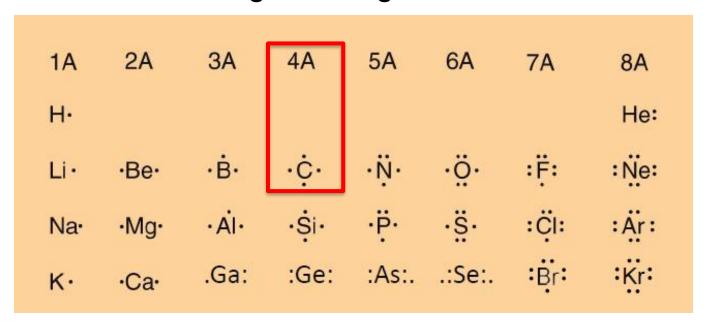
Colour comes from iodine (and iodine binding to starch – which isn't even participating in the overall reaction!)

#### https://www.youtube.com/watch?v=Was YuiOk5xQ



## Why is carbon so special? Valence!

Review: Atoms lose/gain/share electrons to complete their octet – reach the noble gas configuration

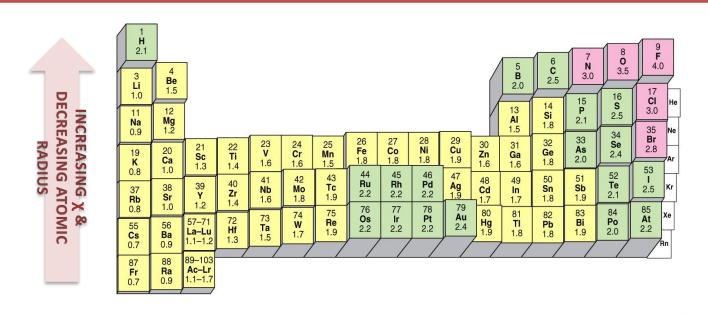


#### Carbon:

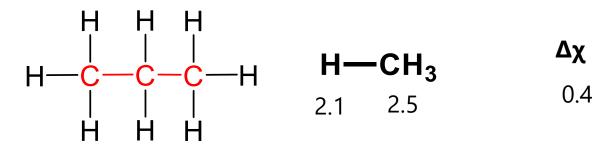
- Has 4 valence electrons
  - not realistic to be ionic (i.e. losing/gaining 4 is a lot)
  - Makes 4 bonds! (always!)

# Hydrocarbons and electronegativity

Review: Electronegativity— ability of an element to attract bonding electrons

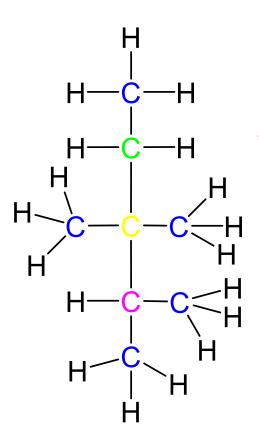


#### INCREASING $\chi$ & DECREASING ATOMIC RADIUS



# Organic chemistry is a whole subject because there is so much bonding diversity possible

One example of a molecule with just H and C (hence the name hydrocarbons)



Primary carbon = a carbon that forms only 1 bond with another carbon

Secondary carbon = is bonded with 2 other carbons

Tertiary carbon = is bonded with 3 other carbons

Quaternary carbon = is bonded with 4 other carbons

# More Bonding Diversity in Organic Molecules

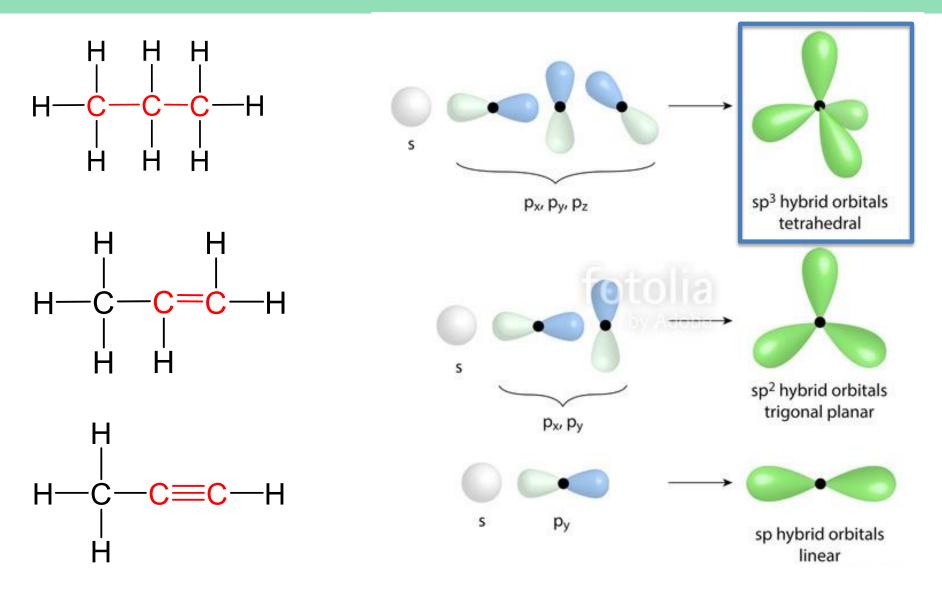
Single bond (also called **saturated**)
Saturated means "full" so a
saturated molecule is full of bonds
to as many other atoms as possible

Double bond (unsaturated)

Triple bond (unsaturated)

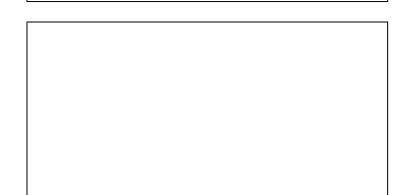
What exactly do you see for carbon hybridized orbitals?

## Bonding Diversity in Organic Molecules

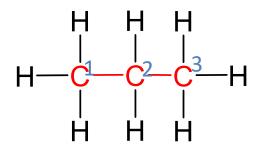


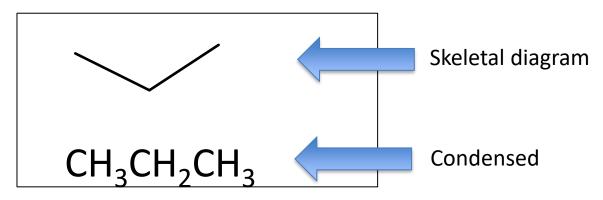
# Simplifying Organic Compounds (Drawing)

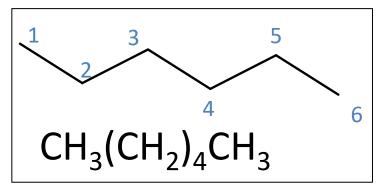
$$\begin{array}{c|ccccc} & & & & & & OH \\ & H_2 & H_2 & & | & & \\ C & C & C & C & CH_2 \\ H_3 & H_2 & H_2 & H_2 & \\ \end{array}$$

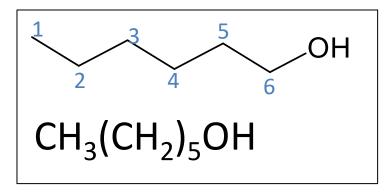


## Simplifying Organic Compounds (Drawing)





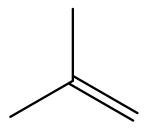




Have to write in all heteroatoms and anything attached to them at the end!

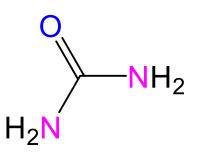
# Bonding Diversity and Skeletal Structures

Triple bond is straight!



Cyclic Compound





#### **Heteroatoms**

- Oxygen
- Nitrogen
- Phosphorus
- Sulfur
- Halides

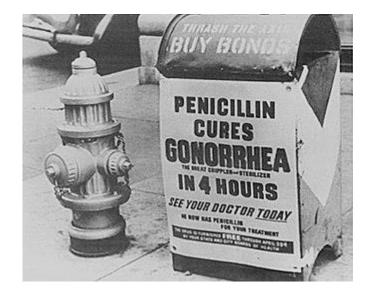
# Chapter 21

**Nov 4 – Nov 8** 

Video 26: Nomenclature

# Importance of Organic Chemistry: Penicillin





Alexander Fleming discovered (its properties) in 1928

1) 1% yield by extracting from mold

# Importance of Organic Chemistry: Penicillin

HCI-H<sub>2</sub>NCH—CH C(CH<sub>3</sub>)<sub>2</sub> (1) C<sub>6</sub>H<sub>5</sub>OCH<sub>2</sub>COCl
CO NH—CHCO<sub>2</sub>H (3) C<sub>5</sub>H<sub>5</sub>N

OC(CH<sub>3</sub>)<sub>3</sub>
II, D-
$$\alpha$$

S

C<sub>6</sub>H<sub>5</sub>OCH<sub>2</sub>CONHCH—CH C(CH<sub>3</sub>)<sub>2</sub>

CO NH—CHCO<sub>2</sub>H

OH

(1) KOH (one equiv.)

(2) C<sub>6</sub>H<sub>11</sub>N=C=NC<sub>6</sub>H<sub>11</sub>

IV

S

C<sub>6</sub>H<sub>5</sub>OCH<sub>2</sub>CONHCH—CH C(CH<sub>3</sub>)<sub>2</sub>

CO—N—CHCO<sub>2</sub>K

penicillin V potassium
(potassium phenoxymethylpenicillinate)

John C Sheehan and Kenneth R. Henery-Logan, **THE TOTAL SYNTHESIS OF PENICILLIN V.** *J. Am. Chem. Soc.* **1957**, *79*, 1262-1263.

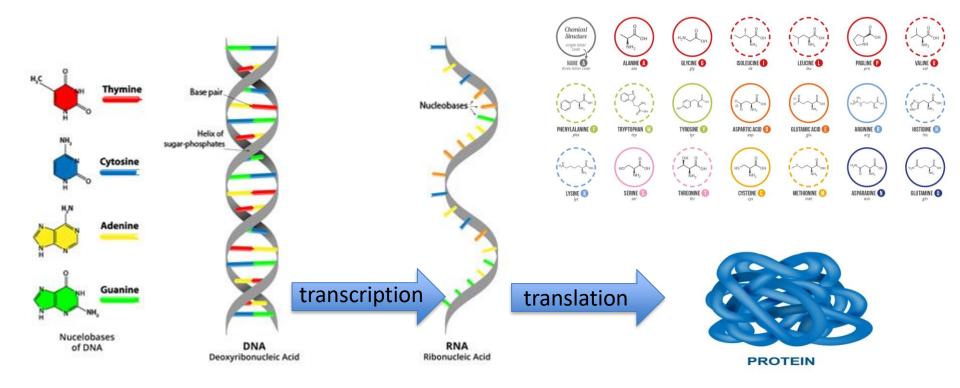
- 2) "Total" chemical synthesis of penicillin
  - 4 or more synthetic steps
  - 0.6% yield

# Importance of Organic Chemistry: Penicillin

- 3) Production through fermentation (bioengineering/biotechnology)
- 10% yield!

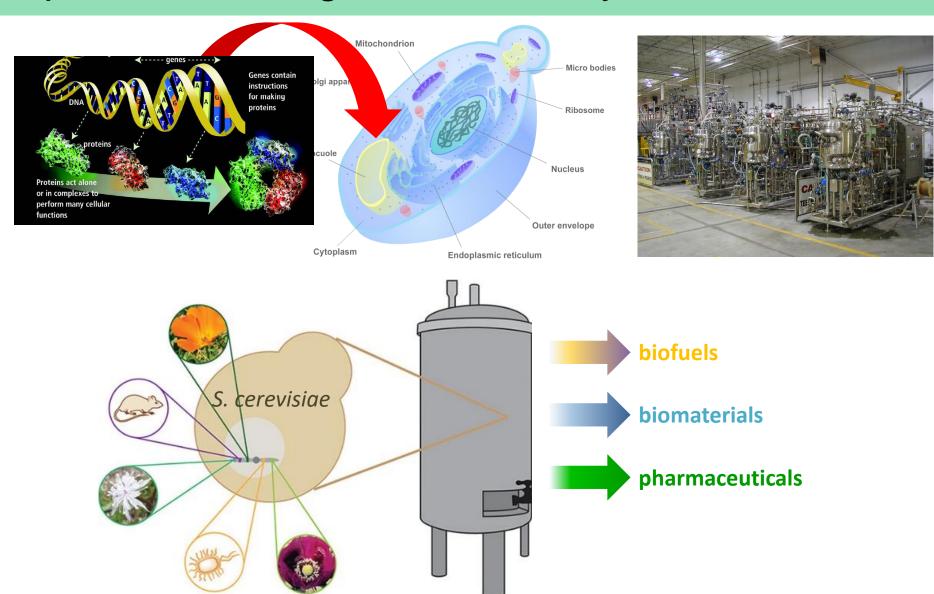


# Importance of Organic Chemistry



#### Enzymes (proteins) do the chemical synthesis!

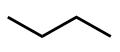
# Importance of Organic Chemistry



## Nomenclature, physical properties, and chemical properties: Group similar organic compounds together

#### **HYDROCARBONS**

#### CYCLIC HYDROCARBONS

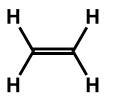


Saturated Alkane

Suffix: -ane



Cycloalkane



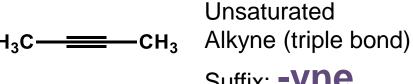
Unsaturated Alkene (double bond)

Suffix: -ene

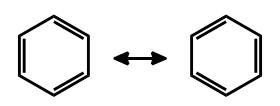


Cycloalkene

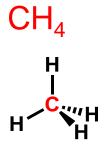
## **AROMATICS** (BENZENE RINGS)



Suffix: **-yne** 

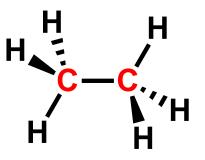


Simplest Alkane: CH<sub>4</sub>



**METHANE** 

CH<sub>4</sub> CH<sub>3</sub>CH<sub>3</sub> METHANE CH<sub>4</sub>
ETHANE C<sub>2</sub>H<sub>6</sub>



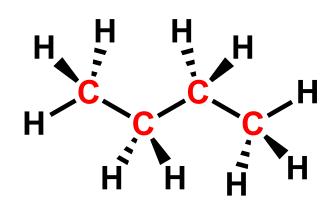
CH <sub>4</sub>	METHANE	$CH_4$	n=1
CH <sub>3</sub> CH <sub>3</sub>	ETHANE	$C_2H_6$	n=2
CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	<b>PROPANE</b>	$C_3H_8$	n=3

A trend in alkane molecular formula

 $C_nH_{2n+2}$ : Saturated hydrocarbon

CH <sub>4</sub>
CH <sub>3</sub> CH <sub>3</sub>
CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>

METHANE 
$$C_{4}$$
ETHANE  $C_{2}H_{6}$ 
PROPANE  $C_{3}H_{8}$ 
BUTANE  $C_{4}H_{10}$ 





CH<sub>4</sub> METHANE CH<sub>4</sub>

CH<sub>3</sub>CH<sub>3</sub> ETHANE C<sub>2</sub>H<sub>6</sub>

CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub> PROPANE C<sub>3</sub>H<sub>8</sub>

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub> BUTANE C<sub>4</sub>H<sub>10</sub>

**NOTICE a pattern:** 

 $C_nH_{2n+2}$ 

H H H H H H H C C H C H C C H

Same molecular formula : C<sub>4</sub>H<sub>10</sub> – but different structures/bonding – **Skeletal ISOMERS** 

CH<sub>4</sub>
CH<sub>3</sub>CH<sub>3</sub>
CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>
CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>
CH<sub>3</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>

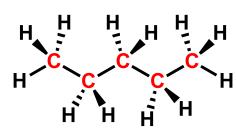
METHANE CH<sub>4</sub>

ETHANE  $C_2H_6$ 

PROPANE C<sub>3</sub>H<sub>8</sub>

BUTANE  $C_4H_{10}$ 

PENTANE C<sub>5</sub>H<sub>12</sub>



CH<sub>4</sub>
CH<sub>3</sub>CH<sub>3</sub>
CH<sub>3</sub>CH<sub>2</sub>CH<sub>3</sub>
CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>3</sub>
CH<sub>3</sub>(CH<sub>2</sub>)<sub>3</sub>CH<sub>3</sub>

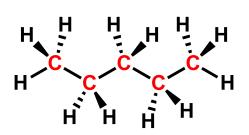


ETHANE  $C_2H_6$ 

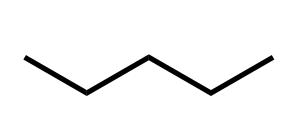
PROPANE C<sub>3</sub>H<sub>8</sub>

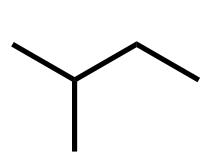
BUTANE  $C_4H_{10}$ 

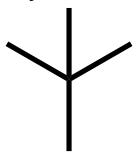
PENTANE C<sub>5</sub>H<sub>12</sub>



Same molecular formula :  $C_5H_{12}$  – but different structures/bonding – STRUCTURAL ISOMERS (later you will see these are specifically skeletal isomers)







# Nomenclature Saturated hydrocarbons Alkane Base Names You need to memorize the prefix!

CH <sub>4</sub>	METHANE	$CH_4$
CH <sub>3</sub> CH <sub>3</sub>	ETHANE	$C_2H_6$
CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	PROPANE	$C_3H_8$
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	BUTANE	$C_4H_{10}$
$CH_3(CH_2)_3CH_3$	PENTANE	$C_5H_{12}$
CH <sub>3</sub> (CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>	HEXANE	$C_6H_{14}$
$CH_3(CH_2)_5CH_3$	HEPTANE	$C_7H_{16}$
$CH_3(CH_2)_6CH_3$	OCTANE	$C_8H_{18}$
$CH_3(CH_2)_7CH_3$	NONANE	$C_9H_{20}$
$CH_3(CH_2)_8CH_3$	DECANE	$C_{10}H_{22}$

# Saturated hydrocarbons: Alkanes (–ane) ( $C_nH_{2n+2}$ )

CH <sub>4</sub>	METHANE	CH <sub>4</sub>
CH <sub>3</sub> CH <sub>3</sub>	ETHANE	C <sub>2</sub> H <sub>6</sub> -GASES
CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>	PROPANE	$C_3H_8$
CH <sub>3</sub> CH <sub>2</sub> CH <sub>2</sub> CH <sub>3</sub>	BUTANE	$C_4H_{10}$
$CH_3(CH_2)_3CH_3$	PENTANE	$C_5H_{12}$
$CH_3(CH_2)_4CH_3$	HEXANE	C <sub>6</sub> H <sub>14</sub>
$CH_3(CH_2)_5CH_3$	HEPTANE	C <sub>7</sub> H <sub>16</sub> LIQUIDS
$CH_3(CH_2)_6CH_3$	OCTANE	C <sub>8</sub> H <sub>18</sub>
$CH_3(CH_2)_7CH_3$	NONANE	C <sub>9</sub> H <sub>20</sub>
$CH_3(CH_2)_8CH_3$	DECANE	$C_{10}H_{22}$

### Comparing Physical Properties of Alkanes

Hydrocarbons are regarded as **non-polar** (the difference in electronegativity between C and H is very small).

The only intermolecular force present in hydrocarbons is **London Dispersion Force** 

Alkanes: become less volatile with increasing molar mass.

# Nomenclature: Cyclic hydrocarbons: cycloalkanes (C<sub>n</sub>H<sub>2n</sub>)

HEXANE 
$$C_6H_{14}$$

CYCLOHEXANE  $C_6H_{12}$ 

Just put "cyclo" in front of the alkane name

## Cycloalkanes (cycloxxxane)

METHANE  $CH_{4}$  = can't make a circle ETHANE  $C_2H_6$  = can't make a circle  $C_3H_8 = \Delta$  cyclopropane =  $C_3H_6$ **PROPANE**  $C_4H_{10} = \square$  cyclobutane =  $C_4H_8$ BUTANE  $C_5H_{12} =$  cyclopentane =  $C_5H_{10}$ PENTANE  $C_6H_{14}$  = etc, fill in the blanks! HEXANE **NOTICE** a pattern: HEPTANE  $C_7H_{16}$ OCTANE C<sub>n</sub>H<sub>2n</sub>  $C_9H_{20}$ NONANE  $C_{10}H_{22}$ DECANE

Chem 110

# Nomenclature: Alkenes ( $C_nH_{2n}$ ) – Base names

Same prefix (eth, prop, but...) different suffix!
-Change to "ene" instead of "ane"

#### **NOTICE a pattern:**

ETHENE	$C_2H_4$	$C_nH_{2n}$
PROPENE	$C_3H_6$	n 2n
BUTENE	$C_4H_8$	
PENTENE	$C_5H_{10}$	
HEXENE	$C_6H_{12}$	
HEPTENE	$C_7H_{14}$	
OCTENE	$C_8H_{16}$	Many structural isomers possible

# Physical Properties of Alkenes

ETHENE	$C_2H_4$
PROPENE	$C_3H_6$
BUTENE	$C_4H_8$
PENTENE	$C_5H_{10}$
HEXENE	$C_6H_{12}$
HEPTENE	$C_7H_{14}$
OCTENE	$C_8H_{16}$

**Boiling Point Increases** 

# Nomenclature: Alkynes ( $C_nH_{2n-2}$ )

Same prefix (eth, prop, but...) different suffix!
-Change to "yne" instead of "ane"

CH≡CH	ETHYNE	$C_2H_2$
CH≡CCH <sub>3</sub>	PROPYNE	$C_3H_4$
CH≡CCH <sub>2</sub> CH <sub>3</sub>	BUTYNE	$C_4H_6$
CH≡C(CH <sub>2</sub> ) <sub>2</sub> CH <sub>3</sub>	PENTYNE	$C_5H_8$
CH≡C(CH <sub>2</sub> ) <sub>3</sub> CH <sub>3</sub>	HEXYNE	$C_6H_{10}$
CH≡C(CH <sub>2</sub> ) <sub>4</sub> CH <sub>3</sub>	HEPTYNE	$C_7H_{12}$
CH≡C(CH <sub>2</sub> ) <sub>5</sub> CH <sub>3</sub>	OCTYNE	$C_8H_{14}$
CH≡C(CH <sub>2</sub> ) <sub>6</sub> CH <sub>3</sub>	NONYNE	$C_9H_{16}$
CH≡C(CH <sub>2</sub> ) <sub>7</sub> CH <sub>3</sub>	DECYNE	$C_{10}H_{18}$

#### **NOTICE a pattern:**

 $C_nH_{2n-2}$ 

## Degrees or units of unsaturation

How to calculate for any unsaturated molecule:

- 1) Calculate difference in # of hydrogens for the saturated version of the molecule vs the molecule at hand.
- 2) Divide the difference by 2

Example 1: How many degrees of unsaturation in octyne?

OCTYNE  $C_8H_{14} = 14$  hydrogens in molecule of interest What is the formula for a fully saturated version of a C8 "oct" molecule?  $C_8H_{18} = \text{so } 18$  hydrogens if the molecule was saturated

- 1) So, 18-14 = 4
- 2) 4/2 = 2

Therefore this molecule has 2 units of unsaturation

Chem 110

## How many units of unsaturation in cyclohexane?

HEXANE 
$$C_6H_{14}$$

CYCLOHEXANE  $C_6H_{12}$ 

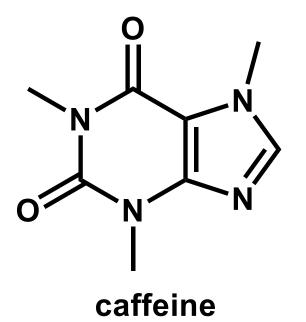
CHAINED alkanes (not cycloalkanes) have the maximum hydrogen per C (saturated)

- 1) So, 14-12 = 2
- 2) 2/2 = 1

Therefore this molecule has 1 unit of unsaturation

Chem 110

# How to calculate units of unsaturation for more complex molecules.



#### MEMORIZE THE FOLLOWING

- Double bond 1 unit of unsaturation
- 2. Triple bond 2 units of unsaturation
- B. Each ring 1 unit of unsaturation

4 double bonds; 2 rings Units of unsaturation = 4+2 =6

# IUPAC Nomenclature: For complicated organic compounds need to memorize these rules (or practice practice practice!)

#### For <u>alkanes</u> and their derivatives

- 1. <u>Find</u> the longest carbon chain. Use that number as the prefix + "ane" as the base name.
- 2. <u>Number the carbons</u> in the chain from the end nearest the first branch/substituent. (If there is a tie, give the lowest number to the lowest in alphabetical order i.e. ethyl lower than methyl)
- 3. <u>Identify substituents</u> (e.g. methyl, ethyl, bromo, chloro). If more than one substituent of the same kind is present, use the prefixes "di" for two, "tri" for three, "tetra" for four....
- 4. Locate the numbered carbon to which the substituents are attached.
- 5. Put substituents in <u>alphabetical order</u> (multiplier prefixes like "di", "tri" do not count).
- 6. Separate numbers from letters by a dash and write the <u>whole name</u> as one word with the basic name at the end.

#### For alkanes and their derivatives

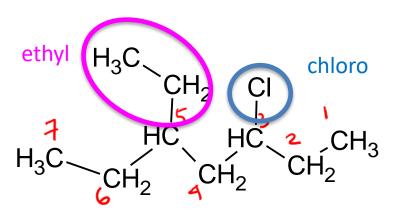
- Find the longest carbon chain. Use that number as the prefix + "ane" as the base name.
- 2. <u>Number the carbons</u> in the chain from the end nearest the first branch/substituent. (If there is a tie, give the lowest number to the lowest in alphabetical order i.e. ethyl lower than methyl)

$$H_3C$$
 $CH_2$ 
 $CH_2$ 
 $CH_3$ 
 $H_3C$ 
 $CH_2$ 
 $CH_2$ 
 $CH_3$ 
 $CH_2$ 
 $CH_3$ 

heptane

#### For alkanes and their derivatives

3. Identify substituents (e.g. methyl, ethyl, bromo, chloro). If more than one substituent of the same kind is present, use the prefixes "di" for two, "tri" for three, "tetra" for four....



# Naming Alkyl Substituents: most common

CH<sub>3</sub>—H Methane CH<sub>3</sub>— Methyl <u>Halides</u>

**CI** = chloro

Br = bromo

I = iodo

 $\mathbf{F} = fluoro$ 

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>—H

Propane

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>—

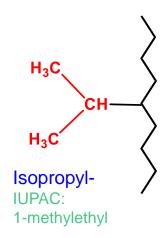
Propyl

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>—H
Butane

CH<sub>3</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>—

Butyl

# Naming Alkyl Substituents: common names FYI!



How most chemists name them (this is not the current IUPAC system)

CH<sub>3</sub>
CH
CH
CH
H<sub>3</sub>C

Isobutyl-

IUPAC: 2-methylpropyl

H<sub>3</sub>C CH<sub>2</sub>

sec-butylor s-butyl

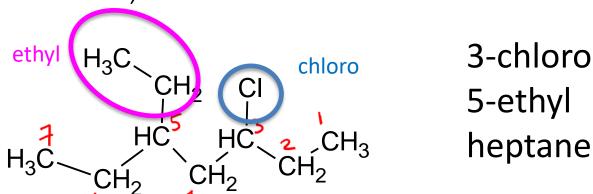
IUPAC: butan-2-yl

**IUPAC**: tert-butyl

# IUPAC Nomenclature: For complicated organic compounds need to memorize these rules (or practice practice practice!)

#### For alkanes and their derivatives

- 4. Locate the numbered carbon to which the substituents are attached.
- 5. Put substituents in <u>alphabetical order</u> (multiplier prefixes like "di", "tri" do not count).



#### note: it is NOT

3-ethyl

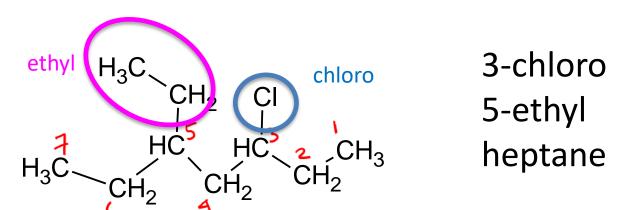
5-chloro

heptane (if the order of how you number the chain is tied on both side; you want the lowest number on the earliest letter in the alphabet)

# IUPAC Nomenclature: For complicated organic compounds need to memorize these rules (or practice practice practice!)

#### For alkanes and their derivatives

6. Separate numbers from letters by a dash and write the <u>whole name</u> as one word with the base name at the end.



FINAL ANSWER: 3-chloro-5-ethylheptane

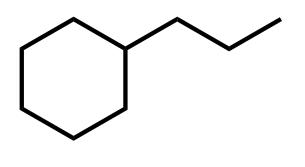
INGREDIENTS: WATER (75%), SUGARS (12%) (GLUCOSE (48%), FRUCTOSE (40%), SUCROSE (2%), MALTOSE (<1%)), STARCH (5%), FIBRE E460 (3%), AMINO ACIDS (<1%) (GLUTAMIC ACID (19%), ASPARTIC ACID (16%), HISTIDINE (11%), LEUCINE (7%), LYSINE (5%), PHENYLALANINE (4%), ARGININE (4%), VALINE (4%), ALANINE (4%), SERINE (4%), GLYCINE (3%), THREONINE (3%), ISOLEUCINE (3%), PROLINE (3%), TRYPTOPHAN (1%), CYSTINE (1%), TYROSINE (1%), METHIONINE (1%)), FATTY ACIDS (1%) (PALMITIC ACID (30%), OMEGA-6 FATTY ACID: LINOLEIC ACID (14%), OMEGA-3 FATTY ACID: LINOLENIC ACID (8%), OLEIC ACID (7%), PALMITOLEIC ACID (3%), STEARIC ACID (2%), LAURIC ACID (1%), MYRISTIC ACID (1%), CAPRIC ACID (<1%)), ASH (<1%), PHYTOSTEROLS, E515, OXALIC ACID, E300, E306 (TOCOPHEROL), PHYLLOQUINONE, THIAMIN, COLOURS (YELLOW-ORANGE E101 (RIBOFLAVIN), YELLOW-BROWN E160a), FLAVOURS (3-METHYLBUT-1-YL ETHANOATE, 2-METHYLBUTYL ETHANOATE, 2-METHYLPROPAN-1-OL, 3-METHYLBUTYL-1-OL, 2-HYDROXY-3-METHYLETHYL BUTANOATE, 3-METHYLBUTANAL, ETHYL HEXANOATE, ETHYL BUTANOATE, PENTYL ACETATE), 1510, NATURAL RIPENING AGENT (ETHENE GAS).

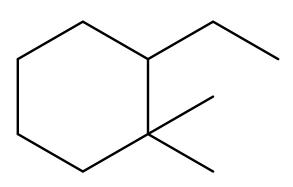
methyl (1R,2R,3S,5S)-3-benzoyloxy-8-methyl-8-azabicyclo[3.2.1]octane-2-carboxylate

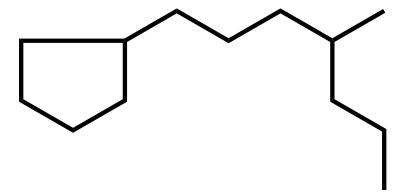
# cocaine

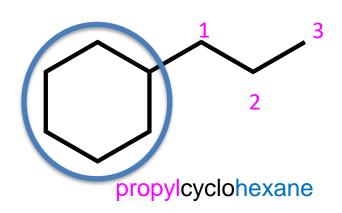
#### For cycloalkanes and their derivatives

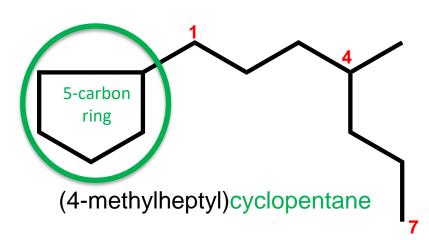
- 1. Determine the number of carbon atoms in the ring.
- 2. Add the prefix cyclo- to the name of the corresponding alkane.
- 3. If only one substituent: not necessary to designate number.
- 4. If two substituents: assign C1 to substituent first in the alphabet and number in the direction that gives next substituent the lowest number.
- 5. If three substituents or more: begin at the substituent that leads to the lowest overall (total) numbering of the other substituents.
- 6. When the ring is attached to an alkyl chain, the ring almost always gets priority/based name. (Note this is different than in the past). Even if the alkyl side chain is longer than the ring, even if the chain has bromo groups, double bonds, triple bonds; the ring gets the base name. This changes if the side chain is an alcohol, amine (etc) but we will NOT cover that.



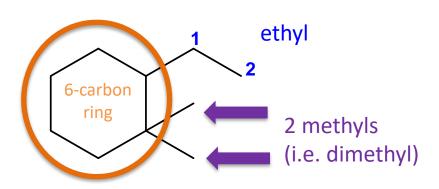








Even through the heptane chain is longer than the cycloalkane chain, the cyclo still gets the base name.



2-ethyl-1,1-dimethylcyclohexane 2 + 1 + 1 = 4

This compound will not be called 1-ethyl,2-2,dimethylcyclohexane 1 + 2 + 2 = 5

If three substituents or more: begin at the substituent that leads to the lowest overall (total) numbering of the other substituents.

### IUPAC Nomenclature: Alkenes/Cycloalkenes

# For alkenes, cycloalkenes and their derivatives CYCLOALKENES:

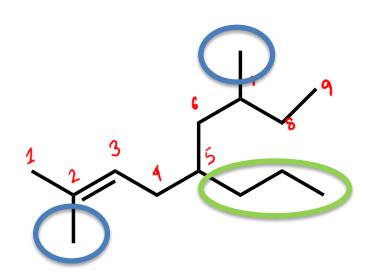
Number the carbons of the double bond as C1 and C2.

#### **ALKENES:**

- 1. Select the longest continuous chain of carbon atoms that contains both carbons of the double bond for the basic name (end with —ene).
- Number the carbons in the chain from the end nearest the first carbon of the double bond. The first carbon of the double bond is also the numbering of the double bond
- 3. Substituent numbering and identification same as alkanes.

NOTE: the double bond takes priority (compared to other substituents) regardless of "lowest total numbers"

#### **IUPAC Nomenclature**



- 1) 9 carbon chain with a double bond = Nonene
- 2) Where is the double bond starting? 2 Non-2-ene

3)

- -Two methyl groups (i.e. dimethyl)
- -one propyl group

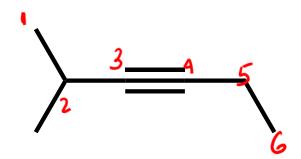
2,7-dimethyl-5-propylnon-2-ene

## **IUPAC Nomenclature: Alkynes**

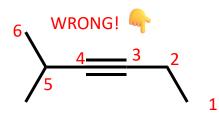
#### For alkynes and their derivatives

- Select the longest continuous chain of carbon atoms that contains both carbons of the triple bond for the basic name. (Name ends with – yne)
- 2. Number the carbons in the chain from the end nearest the first carbon of the triple bond. The first carbon of the triple bond is also the numbering of the triple bond
- 3. Substituent numbering and identification same as alkanes.

## **IUPAC Nomenclature: Alkynes**



2-methylhex-3-yne

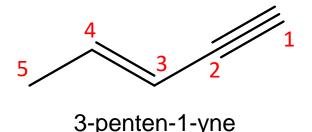


Could label chain either way to give **3-yne (the priority)**; so in this case SINCE the triple bond is a tie either way, you must go with the direction that gives the lowest total numbers! IUPAC left NOTHING up to choice/ambiguity!!!

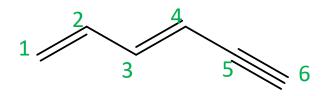
i.e. 2-methylhex-3-yne

BUT NOT: 5-methylhex-3-yne

## IUPAC Nomenclature: Alkynes + alkenes: important rule!



When both double and triple bonds are present, number the chain so that you get the lowest possible numbers even though this may at times give "-yne" a lower number than "-ene" like it is here.



1,3-hexadien-5-yne

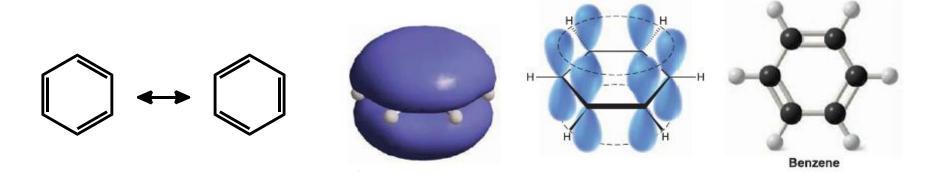
HOWEVER, when there is a choice in numbering (because it's a tie in total numbers either way), then double bonds (ene) are given the lowest numbers. This is because we always break a numbering tie with alphabetical order. In this case, — ene before -yne

# Summary for nomenclature of complex chains

- 1) Alkene/alkynes should be in the main chain and thus takes the "lowest number" priority (i.e. closer to #1 on the chain)
- 2) Then, after that, try to keep the numbers as low as possible for the rest of the substituents
- 3) If there is a "tie" in the substituents, then go with alphabetical order

Note: rule #1 has been slightly updated by IUPAC but is not reflected in the textbook yet. So we will keep this rule as is for simplicity in this course!

## AROMATICS (BENZENE RINGS):



Planar (all ring carbon atoms sp<sup>2</sup>)

Organic compounds that are not aromatic are classified as aliphatic compounds—they might be cyclic, but only **aromatic** rings have special stability (low reactivity).

## Aromatic Compounds – in nature (because they are stable!)

#### All the nucleotides!!!

#### Several amino acids

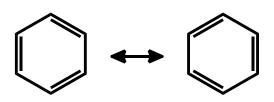
#### **Chlorophyll**

#### Heme

$$O$$
OHO $O$ OH $O$ OH $O$ OH

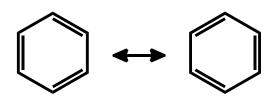
Chem 110 64

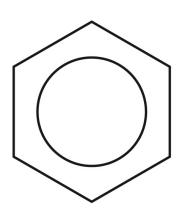
# AROMATICS (BENZENE RINGS):





# AROMATICS (BENZENE RINGS):



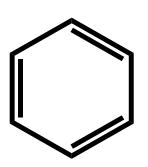




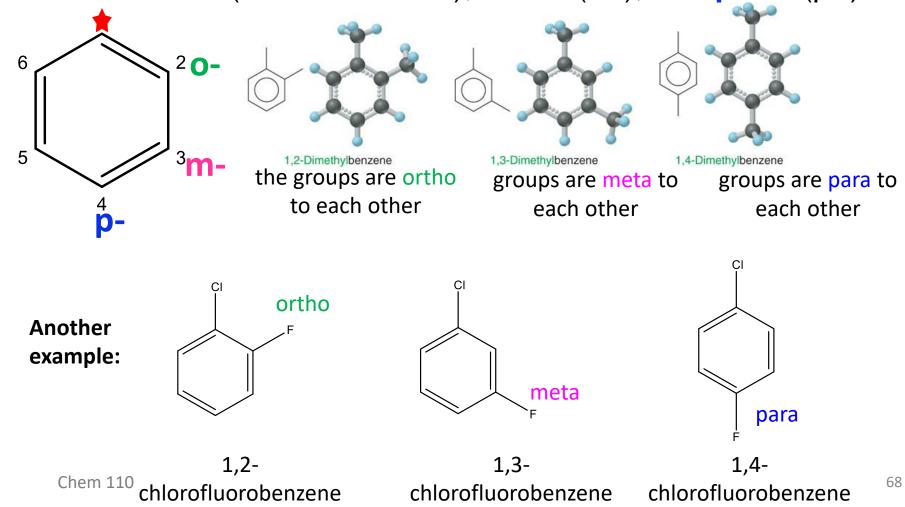


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# AROMATICS (BENZENE RINGS):



Older, yet <u>widely</u> used nomenclature, starts with substituent in location 1 of a benzene ring, and locations 2, 3, and 4 are denoted <u>ortho</u> (abbreviated o-), <u>meta-</u> (m-), and <u>para-</u> (p-).



# Congrats on surviving nomenclature!!!!

Funny "common" names

http://www.chm.bris.ac.uk/sillymolecules/sillymols.htm