Chem 150, Spring 2015

Unit 5 - Hydrocarbons

Organic Chemistry and Hydrocarbons

- Organic chemistry is the chemistry of **carbon**
  - Carbon is unique among the elements in its ability to bond to itself and other elements in so many different ways.
  - It was originally thought that only living systems could make organic molecules.
  - Friedrich Wöhler demonstrated in 1828 that this was not the case.

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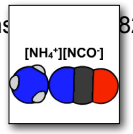

Chem 150, Unit 5: Hydrocarbons 2

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Chem 150, Unit 5: Hydrocarbons 2

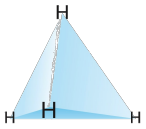
9.1 The Special Properties of Carbon

TABLE 9.2 Bonding Patterns for a Carbon Atom

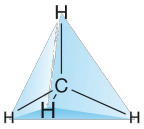
Bonds Formed	Lewis Structure	Example
Four single bonds		 **CH_4, methane**
One double bond Two single bonds		 **CH_2O, formaldehyde**
Two double bonds		**CO_2, carbon dioxide**
One triple bond One single bond		**HCN, hydrogen cyanide**

Tetrahedral Geometry

- When a carbon atom has four single bonds, the arrangement of atoms forms a tetrahedron.
- The VSEPR model (Valence-shell electron pair repulsion model) predicts this geometry.



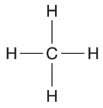
The four hydrogen atoms form the corners of a three-sided pyramid . . .



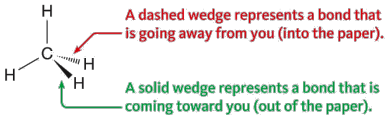
. . . with the carbon atom at the center of the pyramid.

Lewis and Wedge-Dash Structures

- Lewis structures are used even though they show bonds at right angles to one another.
- To show the 3-dimensional structure chemists show perspective with wedges and dashed lines.



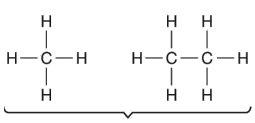
A Lewis structure: does not show the actual position of the atoms.



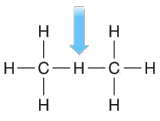
A wedge–dash structure: shows the actual positions of the atoms.

Hydrogen Atoms Form One Bond

- Because hydrogen only forms one bond, hydrogen is never found between two other atoms.



These are real compounds.
Each hydrogen atom forms one bond.



This is an impossible molecule.
The central hydrogen forms two bonds.

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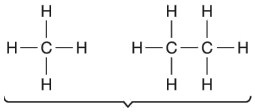

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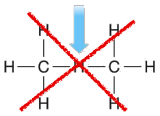

This is an impossible molecule.
The central hydrogen forms two bonds.

9.2 Linear Alkanes: The Foundation of Organic Chemistry

- Compounds that contain only carbon and hydrogen are called hydrocarbons.
- Hydrocarbons are classified by the types of carbon-carbon bonds they contain:
  - **Alkanes** (only single bonds)
  - **Alkenes** (at least one double bond)
  - **Alkynes** (at least one triple bond)
  - **Aromatic** (alternating pattern of single and double bonds in a ring)

Classes of Hydrocarbons

TABLE 9.3 Classes of Hydrocarbons

Class	Description	Example
Alkane	Alkanes do not contain double or triple bonds.	 Propane
Alkene	Alkenes contain at least one carbon–carbon double bond.	 Propene
Alkyne	Alkynes contain at least one carbon–carbon triple bond.	 Propyne
Aromatic compound (Arene)	Aromatic compounds contain a six-membered ring of carbon atoms, linked by alternating single and double bonds.	 Benzene

Constructing a Linear Alkane

1. Start with the skeletal structure which shows only the carbon atoms and carbon-carbon bonds.
2. Add bonds until each carbon atom is surrounded by four bonds.
3. Add hydrogen atoms to complete the structure.

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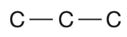

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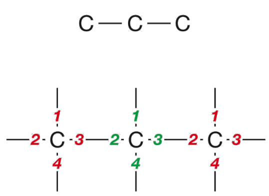

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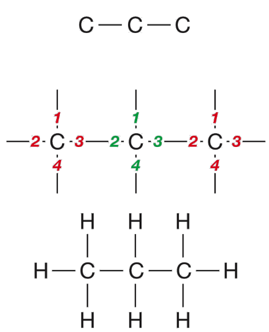

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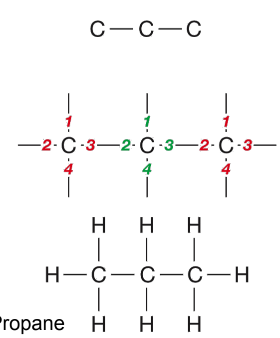
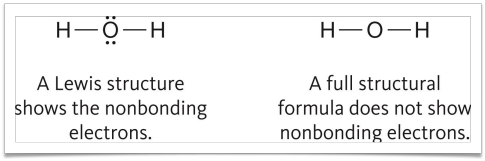


Propane

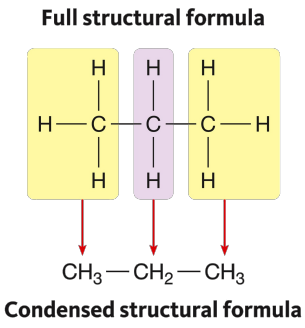
Types of Structures

- There are ways to simplify the way we draw structural formulas.
  - For example, often the non-bonding electrons are omitted from structures with the assumption they are there.



Types of Structures

- Full structural formulas show every atom and bond in a molecule, but do not show nonbonding electrons.
- Condensed structural formulas list all the carbons individually and the hydrogen atoms that are bonded to a carbon are written immediately after the carbon atom.



Try It!

Question:
Draw the full and condensed structural formulas for pentane. The skeletal structure is

C–C–C–C–C

Naming Linear Alkanes

- There is a systematic way of naming organic molecules that conveys structural informations.
- For examples
  - The names for all **alkanes** end with **-ane**.
  - The prefix tells you the number of carbons in an alkane chain.

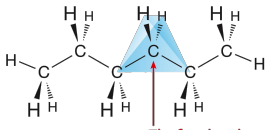
Naming Linear Alkanes

TABLE 9.4 The Names and Structures of the First Ten Linear Alkanes

Name and Molecular Formula	Condensed Structural Formula
Methane (CH_4)	CH_4
Ethane (C_2H_6)	$CH_3—CH_3$
Propane (C_3H_8)	$CH_3—CH_2—CH_3$
Butane (C_4H_{10})	$CH_3—CH_2—CH_2—CH_3$
Pentane (C_5H_{12})	$CH_3—CH_2—CH_2—CH_2—CH_3$
Hexane (C_6H_{14})	$CH_3—CH_2—CH_2—CH_2—CH_2—CH_3$
Heptane (C_7H_{16})	$CH_3—CH_2—CH_2—CH_2—CH_2—CH_2—CH_3$
Octane (C_8H_{18})	$CH_3—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_3$
Nonane (C_9H_{20})	$CH_3—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_3$
Decane ($C_{10}H_{22}$)	$CH_3—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_2—CH_3$

Each Carbon Atom in an Alkane Forms a Tetrahedral Arrangement

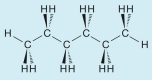
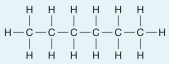
- Each of the carbon atoms is at the center of a tetrahedral arrangement.
- In larger alkanes, this arrangement forces the carbon chain into a zigzag shape.
- The term *linear* is misleading because carbon atoms in an alkane cannot really from a straight line.



The four bonds around this carbon atom form a tetrahedral arrangement.

Common Ways to Represent Organic Molecules

TABLE 9.5 Common Ways to Represent Hexane, an Organic Molecule

Structure	Type of Structure and Uses of This Type
	**Wedge–dash structure** Shows the actual positions of atoms and bonds in the molecule.
	**Full structural formula** Shows all of the bonds and atoms in the molecule.
$CH_3—CH_2—CH_2—CH_2—CH_2—CH_3$ or $CH_3(CH_2)_4CH_3$	**Condensed structural formula** Shows all of the atoms in a compact format.
	Line structure Shows the carbon framework in a simple, easy-to-draw format.
C_6H_{14}	**Molecular formula** Useful for writing balanced equations.

Try It!

Try It!

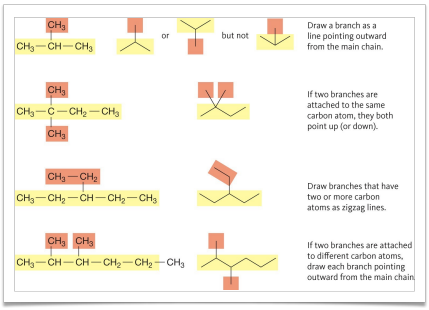
Question:

Draw the line structure for pentane. The skeletal structure is

C–C–C–C–C

9.3 Branched Alkanes, Cycloalkanes, and Isomers

- Alkanes in which the carbon atoms do not form a single continuous chain are branched alkanes.



Isomers

- Compounds that have the same molecular formula but different structures are called isomers.
- There are several types of isomers in organic chemistry.
- Constitutional isomers have their atoms connected to one another in a different order (for example: branched versus linear).
- Constitutional isomers have different shapes, which in turn give them different physical and chemical properties.

Properties of Two Constitutional Isomers

TABLE 9.6 The Properties of Two Constitutional Isomers

	Butane	Isobutane
Molecular formula	C_4H_{10}	C_4H_{10}
Condensed structural formula	$CH_3-CH_2-CH_2-CH_3$	$CH_3-CH(CH_3)-CH_3$
Line structure		
Appearance at room temp.	colorless, odorless gas	colorless, odorless gas
Boiling point	−0.5°C	−11.7°C
Freezing point	−138.3°C	−159.4°C
Density of liquid at −20°C	0.620 g/mL	0.605 g/mL
Amount of energy obtained from burning one gram of this compound	10.92 kcal	10.89 kcal

Properties of Two Constitutional Isomers

TABLE 9.7 Pentane and Its Isomers

	Pentane	Isopentane	Neopentane
Skeleton structure	C—C—C—C—C	C | C—C—C—C	C | C—C—C | C
Condensed structural formula	$CH_3—CH_2—CH_2—CH_2—CH_3$	$CH_3—CH(CH_3)—CH_2—CH_3$	$CH_3—C(CH_3)_2—CH_3$
Line structure			
Physical properties	melts at −129.8°C boils at 36.1°C density: 0.56 g/mL	melts at −159.9°C boils at 29.9°C density: 0.62 g/mL	melts at −16.8°C boils at 9.4°C density: 0.59 g/mL

Recognizing Constitutional Isomers

- Constitutional isomers of an alkane have a different bonding pattern.
  - It is important to distinguish this from different configurations of the same molecule.

These are different molecules with the chemical formula C_5H_{12}.

Pentane	Isopentane	Neopentane
C—C—C—C—C	C | C—C—C—C	C | C—C—C | C

Recognizing Constitutional Isomers

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These are different representations of the same molecule.

$CH_3—CH_2—CH_2—CH_2—CH_3$ $\quad$ $CH_3—CH_2—CH_2—CH(CH_3)$ $\quad$ $CH_3—CH_2—CH(CH_3)_2$

Cycloalkanes

- A cycloalkane is an alkane in which the carbon atoms are arranged in a ring.
  - We name cycloalkanes by adding the prefix *cyclo-* to the names of the corresponding linear alkanes.
  - Cycloalkanes and alkanes are closely related, but they are not isomers because the ring has two fewer hydrogen atoms.
- Alkanes and cycloalkanes are called saturated hydrocarbons because they contain no double or triple bonds (“saturated” with hydrogen).

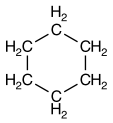
The Structures and Names of Some Cycloalkanes

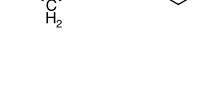
TABLE 9.8 The Structures and Names of Some Cycloalkanes

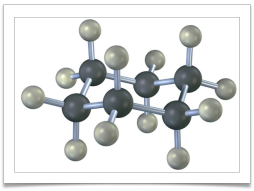
Name	Condensed Structural Formula	Line Structure
cyclopropane	CH_2 / CH_2-CH_2	△
cyclobutane	CH_2-CH_2 / CH_2-CH_2	□
cyclopentane	CH_2, CH_2, CH_2, CH_2-CH_2	⬠
cyclohexane	CH_2, CH_2, CH_2, CH_2, CH_2, CH_2	⬡

The Structures and Names of Some Cycloalkanes

Cyclohexane

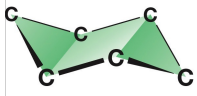




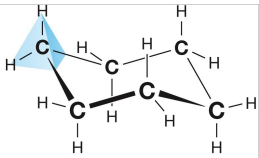


The Structures and Names of Some Cycloalkanes

Cyclohexane



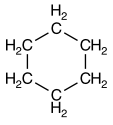
The chair conformation of the carbon ring in cyclohexane.

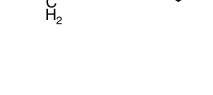


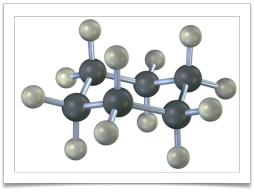
The full structure of cyclohexane (The tetrahedral arrangement around the leftmost carbon is shown by shading.)

The Structures and Names of Some Cycloalkanes

Cyclohexane







9.4 Naming Branched Alkanes: The IUPAC System

- Organic chemists have devised a systematic method for naming organic molecules
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(Structural Formula) → 2-methylbutane (IUPAC name)

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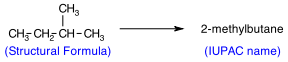


(Structural Formula) → 2-methylbutane (IUPAC name)

- That person can then give that name to another person, who could then convert it back into a structure.

2-methylbutane (IUPAC name) → 

(Structural Formula)

9.4 Naming Branched Alkanes: The IUPAC System

- The IUPAC names can help us distinguish the different options from the last set of clicker questions

A. different molecules that are **not isomers**.
- (These will have different chemical formulas and different IUPAC names)

B. different molecules that are **isomers**.
- (These will have the same chemical formula, but different IUPAC names)

C. different representations of the **same molecule**.
- (These will have the same chemical formula, and the same IUPAC name)

9.4 Naming Branched Alkanes: The IUPAC System

- The longest continuous carbon chain in a molecule is the *principal carbon chain*.
  - It will be used to create the root name.
- The *branches* are any other carbons attached to the principal chain that are not included in the chain
  - The are called alkyl groups.
  - We name alkyl branches by replacing the *–ane* ending of the corresponding alkane with the *–yl* ending.

The Structures of Common Alkyl Groups

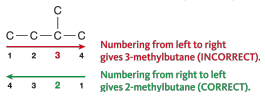
TABLE 9.9 The Structures of Common Alkyl Groups

Number of Carbon Atoms	Structure	Name
1	CH_3	methyl
2	CH_2-CH_3	ethyl
3	$CH_2-CH_2-CH_3$	propyl
3	$CH_3-CH(CH_3)$	isopropyl
4	$CH_2-CH_2-CH_2-CH_3$	butyl

Naming Branched Alkanes Continued

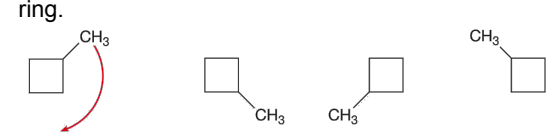
- Steps in creating an IUPAC name for an alkane:

1. Identify and name the **principal carbon chain**.
2. Identify and name **alkyl substitutent groups** that are not part of the principle carbon chain.
3. Number the carbon atoms in the principal chain starting from the end that is closest to an alkyl group, and use these numbers to locate where the alkyl groups are attached to the principal chain.
2. Assemble the complete name by writing the name of the branch in front of the name of the principal chain.



Naming Cycloalkanes

- When naming cycloalkanes, you do not write a number to show the location of the alkyl group because there is only one possible molecule that we can make by connecting a single alkyl group to a ring.



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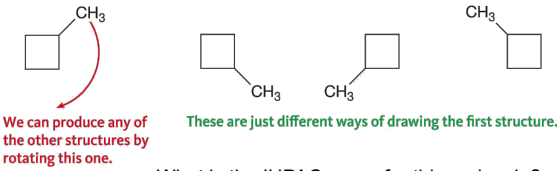
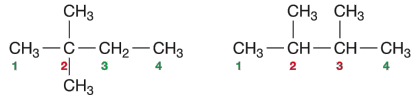


What is the IUPAC name for this molecule?

Alkane With Two or More Identical Branches

- When an alkane has two or more identical branches, we use the prefixes *di-, tri-, tetra-* to show the number of identical alkyl groups.
- Each group gets a number separated by commas.
- Regardless of the number of branches, we number the principal chain from the side that is closest to a branch.

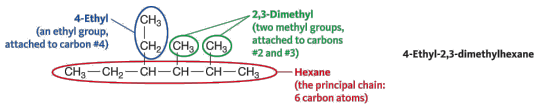


2,2-Dimethylbutane
(Both methyl groups are attached to carbon #2 in the principal chain.)

2,3-Dimethylbutane
(One methyl group is attached to carbon #2 and one is attached to carbon #3.)

Alkane With Two or More Different Branches

- In molecules that have alkyl groups that are different sizes, we list the alkyl groups **alphabetically**.
- If we have two or more identical branches, we ignore the prefix (*di-, tri-, tetra-*) when we alphabetize the names.
- If both ends of the principal chain are the same distance from a branch, proceed to the next branch to determine numbering.

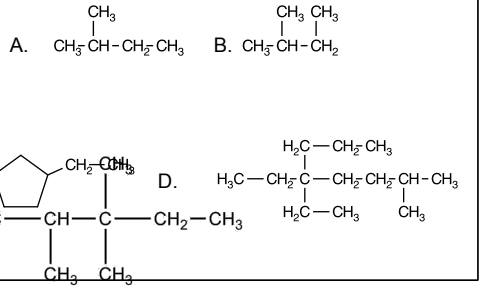


4-Ethyl-2,3-dimethylhexane

Try It!

Questions:

Name the following molecules



Try It!

Questions:
Draw structures for the following named molecules

A. 4-propylheptane
B. 4-isopropyl-2-methylheptane
C. ethylcylcohexane
D. 5-butyl-2,3,4-trimethyldecane

9.5 Functional Groups

- A functional group is a group of atoms that have distinct chemical and physical properties.
  - They can be added as substituents onto an alkane.
- Organic chemists use functional groups to group organic molecules into families.
  - Alkanes represent the family that has no functional groups.

9.5 Functional Groups

- A funct ave distinct
  - They an alka
- Organi roup organic
  - Alka func

TABLE 9.10 Some Representative Functional Groups in Organic Chemistry

Functional Group	Name	An Example of a Compound That Contains This Group:
	alkene	$CH_3-CH=CH_2$ propene
	alkyne	$CH_3-C\equiv CH$ propyne
	chloroalkane	$CH_3-CH_2-CH_2-Cl$ 1-chloropropane
	alcohol	$CH_3-CH_2-CH_2-OH$ 1-propanol
	amine	$CH_3-CH_2-CH_2-NH_2$ propylamine
	aldehyde	$CH_3-CH_2-C(=O)-H$ propanal
	carboxylic acid	$CH_3-CH_2-C(=O)-OH$ propanoic acid

9.5 Functional Groups

- A functional group is a group of atoms that have distinct chemical and physical properties.
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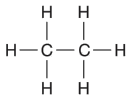
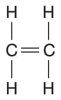
Chem 150, Unit 5: Hydrocarbons 36

9.6 Alkenes and Alkynes

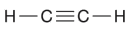
- While most of the functional groups contain carbons other than carbons and hydrogen, alkenes and alkynes contain functional groups that are hydrocarbons.
- Any hydrocarbon that contains at least one double or triple bond is called an unsaturated hydrocarbon.



Ethane (C_2H_6)
An alkane



Ethylene (C_2H_4)
An alkene



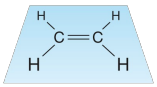
Acetylene (C_2H_2)
An alkyne

Alkenes Contain a Trigonal Planar Arrangement of Atoms

- The two carbon atoms that form the double bond adopt a trigonal planar arrangement.

Trigonal planar arrangement of bonds around a carbon atom

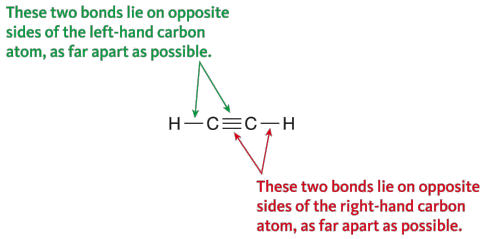
The actual structure of ethylene: each carbon atom forms a trigonal planar arrangement.



Side view of ethylene (all six atoms can be placed on a flat surface)

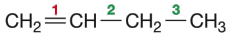
Alkynes are Linear

- The triple bond in an alkyne and the two adjacent single bonds form a straight line.

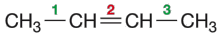


Naming Alkenes and Alkynes

1. Find the long chain of carbons that contains the double or triple bond; this will be the principle carbon chain.
2. Change the ***–ane*** ending of the alkane to ***–ene*** for an alkene or ***–yne*** for an alkyne.
3. Number the carbon-carbon bonds starting from the end closest to the functional group, and use these numbers to identify the position of the multiple bond.
4. Assemble the name by writing the number followed by the name (a hyphen separates numbers from words).



1-Butene



2-Butene

Cycloalkenes

- A cycloalkene is a ring of carbon atoms with a double bond.

TABLE 9.11 The Structures and Names of Some Cycloalkenes

Name	Condensed Structural Formula	Line Structure
cyclopropene	CH_2 / $CH{=}CH$	
cyclobutene	$CH_2{-}CH_2$ / $CH{=}CH$	
cyclopentene	CH_2, CH_2, CH_2 / $CH{=}CH$	

Other Notes on Naming

- The principal chain is always the longest chain that *includes* the functional group.
- The principal chain is numbered from the side closest to the functional group, regardless of the positions of the branches.
- There are commonly used names, called trivial names, that were given to compounds before the IUPAC system was developed. They are sometimes used almost exclusively.

9.7 *Cis* and *Trans* Isomers of Alkenes

- In an alkane the single bond permits free rotation of the two carbon atoms that it joins.
- Carbon-carbon double bonds do not permit free rotation.
- We can often produce two forms of a compound with an otherwise identical name (stereoisomers).
  - Unlike constitutional isomers, stereoisomers produce the same IUPAC name, but they are different molecules.
  - The prefixes *cis* and *trans* are used to distinguish the two isomers.
    - *Cis*—groups are on the "same side"
    - *Trans*—groups are on the "opposite sides"

9.7 *Cis* and *Trans* Isomers of Alkenes

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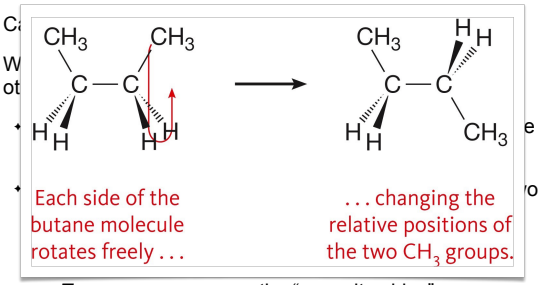
- C
- W ot



  - *Trans*—groups are on the "opposite sides"

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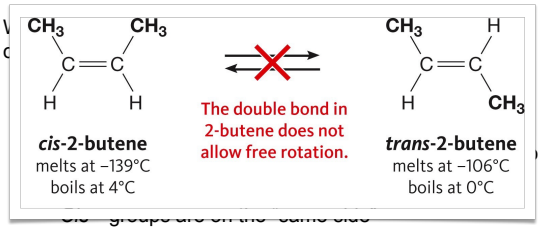

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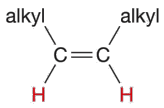
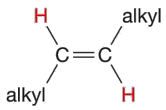
Chem 150, Unit 5: Hydrocarbons 43

Example of *Cis* and *Trans*

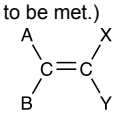


***Cis* isomer:** The two hydrogen atoms are on the same side of the double bond.



***Trans* isomer:** The two hydrogen atoms are on opposite sides of the double bond.

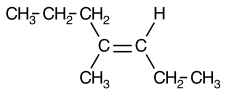
Cis and *Trans* isomers occur whenever A ≠ B AND X ≠ Y (Both conditions have to be met.)



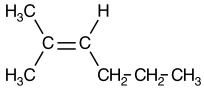
Try It!

Questions:
Give the IUPAC name for the following compound.

A.



B.



Try It!

Questions:

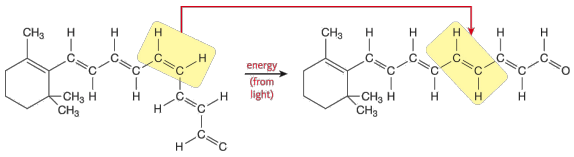
Draw the structures of the following named molecules.

A. *cis*-3-heptene

B. *trans*-3-methyl-3-hexene

Cis-Trans Isomerism and Vision

- The key chemical step in seeing is the conversion of cis-retinal to trans-retinal which requires energy that is supplied by the light that enters the eye.
- When it returns, it releases the energy which is passed to the optic nerve and on to the visual center of the brain.

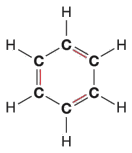


***Cis*-retinal** ***Trans*-retinal**

9.8 Benzene and Aromatic Compounds

- Benzene has six carbon atoms arranged in a ring with one hydrogen atom bonded to each carbon.

Full structural formulas for benzene:



The six electrons shown in red . . .

Line structures for benzene:

Aromatic Compounds

- Benzene was once thought to contain alternating double and single bonds, but it does not behave like an alkene.
- The three extra electron pairs move freely around the ring so a circle is often drawn to show these electrons.
- Compounds that contain the benzene ring are called aromatic compounds, reflecting their often pleasant fruity aromas.
- They are toxic and many are carcinogens, so the odors have no practical use.

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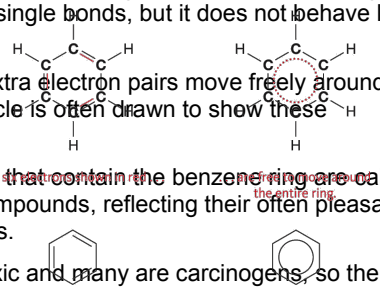

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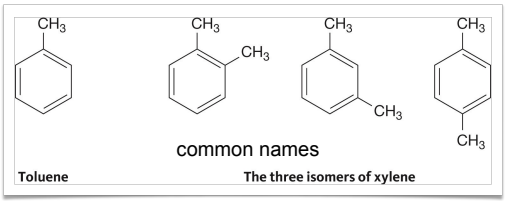
Chem 150, Unit 5: Hydrocarbons 49

Aromatic Compounds

- Common names are often used for aromatic compounds.
  - For benzene derivative can use the root name benzene and name them like cycloalkanes



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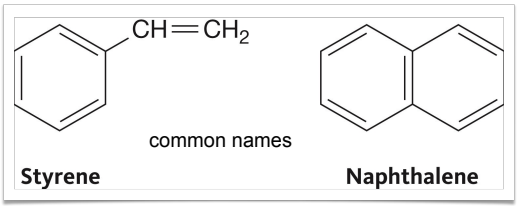

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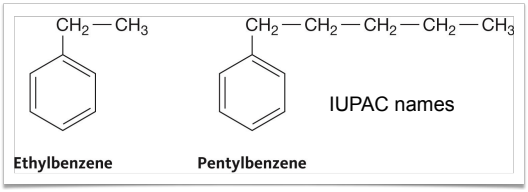

9.9 Properties of Hydrocarbons

TABLE 9.12 The Physical Properties of Hydrocarbons

Typical appearance	Liquids and gases are clear and colorless. Most solids are white or transparent (compounds with many double bonds can be brightly colored).
Typical density (liquids and solids)	0.6 to 0.9 g/mL (Most hydrocarbons float on top of water.)
State at room temperature	1 to 4 carbon atoms: gas More than 5 carbon atoms: liquid or solid (Compounds with more than 15 carbon atoms are usually solids, but the cutoff is quite variable; the shape of the molecule plays an important role in determining the melting point.)
Solubility in water	Very low: hydrocarbons are considered to be insoluble in water.

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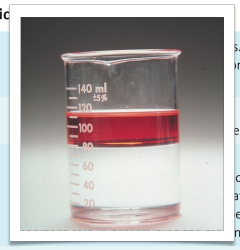

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The Effect of Size On the Physical Properties of Alkanes

TABLE 9.13 The Effect of Size on the Physical Properties of Alkanes

Compound	Attraction Between Molecules	Melting Point	Boiling Point	State at Room Temperature
Ethane (C_2H_6)	weakest	−183°C	−89°C	Gas
Butane (C_4H_{10})		−138°C	−1°C	Gas
Hexane (C_6H_{14})		−95°C	69°C	Liquid
Octane (C_8H_{18})	strongest	−57°C	126°C	Liquid

Combustion of Hydrocarbons

- The most important role of hydrocarbons in human society is as fuels.
  - Natural gas, gasoline, kerosene, diesel fuel, aviation gasoline, heating oil, and even candle wax are mixtures of hydrocarbons.
  - All hydrocarbons react with oxygen when they are heated producing carbon dioxide, water, and a great deal of energy.
  - Coal, petroleum, and natural gas are the *fossil fuels*, the remnants of living organisms from hundreds of millions of years ago.

Next Up

- Unit 6 - Hydration, Dehydration and Alcohols
  - Chapter 10 in Armstrong
  - Unit 6 assignments due 5. March, with deadline on 12. March