# Learning Guide for Chapter 4 - Alkanes

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#### I. Introduction to Alkanes

What is an alkane? hydrocarbon with only C-C single bonds

Why are we starting with them? simplest organic compounds framework for all the others

Straight-chain alkanes

Draw the line structure for the alkanes given below, and give their molecular formula.

methane	CH <sub>4</sub>		hexane	$C_6H_{14}$	$\sim$
ethane	C <sub>2</sub> H <sub>6</sub>	H <sub>3</sub> C-CH <sub>3</sub>	heptane	C <sub>7</sub> H <sub>16</sub>	$\sim \sim \sim$
propane	C <sub>3</sub> H <sub>8</sub>	$\sim$	octane	C <sub>8</sub> H <sub>18</sub>	$\sim$
butane	$C_4H_{10}$	$\sim$	nonane	C <sub>9</sub> H <sub>20</sub>	$\sim \sim \sim$
pentane	C <sub>5</sub> H <sub>12</sub>	$\sim$	decane	C <sub>10</sub> H <sub>22</sub>	$\sim$

What pattern do each of the formulas follow?  $C_n H_{2n+2}$ 

Why does this pattern occur? 2 H's for every C, 1 more on each end Branched alkanes

Draw all of the branched alkanes having 6 carbons. What are these compounds called?



What formula do all of these alkanes have?  $C_6H_{14}$  same as straight-chain We will learn how to name these compounds later in this chapter.

#### Cyclic alkanes

Draw the line structure for the cyclic alkanes given below, and give their molecular formula.



What pattern do these molecular formulas have, and why?

 $C_nH_{2n}$  2 H's for every C - no ends

Draw the line structures of all of the constitutional isomers of cyclopentane.



What happens to the molecular formula when more than one ring is present?

subtract 2 for every ring

# III. Physical properties, sources, and uses of alkanes

#### **Physical Properties of Alkanes**

What intermolecular force affects alkanes? van der Waals forces

What is the surface tention like, and how would you see this?

very low; small drops, doesn't bead up

Are alkanes soluble in water? Why or why not? no - can't break into H-bonding network

Are alkanes more or less dense than water? Why?

less dense; weak intermolecular forces farther apart, lots of H's

Match up the following alkanes with their boiling points.

first look for size (MW); if two are the same, branched



Which of the following molecules would you expect to have a higher melting point, and why?



What state of matter would you expect to find the following substances in at 25°C, 1 atm:

propane 3 C - gas	
hexane 6 C - liquid	1-4 C's - gases 5-17 C's - liquids 18 C's and up - solids
decane 10 C - liquid	
eicosane 20 C - solid	

Sources of alkanes

What are the two principle sources of alkanes? petroleum, natural gas

List some products of petroleum distillation. Which do you think is the most profitable? gasoline, kerosene, diesel, heating oil, petroleum jelly, paraffin wax, asphalt

What happens to the properties of the distillation products as the temperature goes up?

liquids get thicker, then turn to waxy solids

Uses of alkanes

What is the most common use of alkanes? burned for fuel

What is the problem with this? not renewable, generates CO<sub>2</sub>, may be causing global warming

What else can alkanes be used for? making plastics, pharmaceuticals, fertilizers

IR Spectroscopy

What bands do alkanes have?

C-H stretching 3000-2850 cm<sup>-1</sup> CH<sub>2</sub> bending 1460, 1380 cm<sup>-1</sup>



Why is it especially useful to remember these frequencies?

nearly all compounds have them - useful to orient yourself

How can you tell alkanes apart from other functional groups?

no other functional group bands

#### **III. Reactions of Alkanes**

How reactive are alkanes? not very - no functional groups

What are the three most common reactions of alkanes?

combustion, hydrocracking, and halogenation

Why aren't these reactions used in the laboratory?

they give mixtures of products two require high temps and pressures

Complete the following reactions and give what type they are:

halogenation

 $CH_4 + excess Cl_2 \xrightarrow{hv \text{ or}} CH_3Cl + CH_2Cl_2 + CHCl_3 + CCl_4$ heat

multiple products - have to separate

hydrocracking

$$\begin{array}{c} H_2, heat \\ \hline \\ catalyst \\ or \\ \end{array} \begin{array}{c} + \\ + \\ + \\ \end{array} \end{array}$$

combustion

used to make gasoline

 $+ 5 O_2 \longrightarrow 3 CO_2 + 4 H_2 O$ 

releases energy as heat or pressure

When can halogenation be useful?

when only one product is formed - we'll see how later

Why is hydrocracking useful?

makes gasoline out of higher boiling petroleum fractions

Why is combustion useful?

releases lots of energy - powers cars, trucks, planes, trains, boats; can be used to create steam, turn turbines to generate electricity

Why is it hazardous? alkanes are easily ignited, can get out of control

What can happen when combustion takes place without enough heat or oxygen?

can get carbon monoxide - poisonous (car exhaust)

unburned carbon (soot) - particulates  $2 C_4 H_{10} + O_2 \longrightarrow 8 C + 10 H_2 O$ 

hydrocarbon fragments - smog

# IV. Nomenclature of Alkanes, Cycloalkanes, and Bicyclic Alkanes

Who created the current rules for naming organic compounds? **IUPAC** What is the purpose behind these rules?

- 1) only one name per compound
- 2) name shows structure of the compound

Step 1: Finding the principle chain (or ring).







Step 3: Name and order the substituents, add them to the root name.





What if the substituents are branched?



Will you ever have an "ane" inside the name of a compound? no! always yl-yl-yl-ane

Common names for branched substituents:



these are becoming less commonly used but you still need to be able to recognize them!

Name the following compounds.





nonane 3-ethyl 5-(2-methylpropyl)

3-ethyl-5-(2-methylpropyl)nonane

less common: 3-ethyl-5-isobutylnonane

## **IV. Conformations of Straight and Branched Alkanes**

When we imagine an organic molecule, say methanol, we picture the atoms as holding still. Give some examples of why this isn't accurate.

molecules are zipping through space (air molecules: 1000 mph)

molecules are tumbling through space

bonds are vibrating

As a molecule rotates around a single bond, what are the different positions called?

conformations

**Ethane** 

Make a model of ethane. Turn it so that you are looking down the C-C bond. Then draw a Newmann projection, and label one of the dihedral angles.



eclipsed - higher energy electron clouds repel each other

Now turn the top atom so that the H's in front fall in between the H's in back. Label the two conformations. Which is higher in energy? Why?



staggered - lower energy electron clouds have more room

Plot the energy of the molecule as it rotates all the way around:



## Propane

Make a model of propane. What would its two conformations look like?



What would a graph of their energy look like?

# same pattern, slightly wider apart (13.8 KJ/mol)

Make a model of butane. How many different conformation does it have? Which are the highest and lowest energies? Draw them in a circle as you rotate around the bond, starting at a 0° angle for the two methyl groups.



Graph the energy of these bonds.



#### **BRING MODELS**

V. Stability of cycloalkanes

Below are the heats of formation of the first 6 cyclic alkanes. Which is the most stable? Which have more energy than their constituent elements?

cyclopropane	+17.8 kJ/mol
cyclobutane	+6.9 kJ/mol
cyclopentane	-15.3 kJ/mol
cyclohexane	-20.7 kJ/mol) most stable
cycloheptane	-17.0 kJ/mol
cyclooctane	-15.7 kJ/mol

What makes the least stable rings so high in energy?



Why don't cyclopentane and cyclooctane have these problems?



we draw it flat, but it isn't

envelope conformation relieves angle strain, torsional strain

angles are bent, substituents staggered

Why does cyclohexane have the lowest energy of all the rings?



all angles 109.5° - no angle strain all substituents staggered - no torsional strain

show model

## VI. Conformations of Cyclohexane

Why do we study the conformations of cyclohexane in more detail than other rings?

they are the most stable, commonly found in nature

Below is a representation of a cyclohexane as seen from the top. Draw in the H's, showing their orientation.



Below is a representation of a cyclohexane as seen from the side. What is it called, and why?



Here is a representation including the H's. Label them as going up or down.

3



2

1

since this view is from the side, the H's goin up are on top, going down are on the bottom

Draw them in on your own, and label the axial and equatorial H's.



axial - straight up or straight down, alternating

equatorial - slanted up or down, alternating parallel to next line over, make a W

What pattern do you see?

ax/up, eq/down ax/down, eq/up

no lines are straight across!

Flip the structures below into the other chair conformation.





same energy

1 ax, 1 cq

1 ax, 1 v

same number of axial and equatorial - same energy





2 ax, 1 eq higher energy

1 ax, 2 eq

lower energy

if there are more axial than equatorial substituents, that conformation will be higher in energy

LG Ch 4 p 15







2 ax, 2 eq larger subst axial 2 ax, 2 eq larger subst eq

higher energy

lower energy

if there are the same number of axial and equatorial substituents, but one substituent is larger, then it will prefer the equatorial position



a quaternary carbon is too large to fit in the axial position; only one conformation will exist