Chem 240
9.4.18

Chapter 3: Organic Compounds - Alkanes and Their Stereochemistry

Families of Organic Compounds

Organic compounds can be grouped into families by their common structural features

We shall survey the nature of the compounds in a tour of the families in this course

This chapter deals with *alkanes*, compounds that contain only carbons and hydrogens, all connected exclusively by single bonds

3.1 Functional Groups

Functional group - collection of atoms at a site within a molecule with a common bonding pattern

The group reacts in a typical way, generally independent of the rest of the molecule

*structural features of a molecule allow us to classify compounds into families called functional groups. The chemistry of every organic molecule, regardless of size & complexity, is determined by the functional groups

3.2 Alkanes and Alkane Isomers

Alkanes: Compounds with C-C single bonds and C-H bonds only (no functional groups)

Connecting carbons can lead to large or small molecules

The formula for an alkane with no rings in it must be C_nH_{2n+2} where the number of C's is "n"

Alkanes are **saturated** with hydrogen (no more can be added)
They are also called **aliphatic compounds**

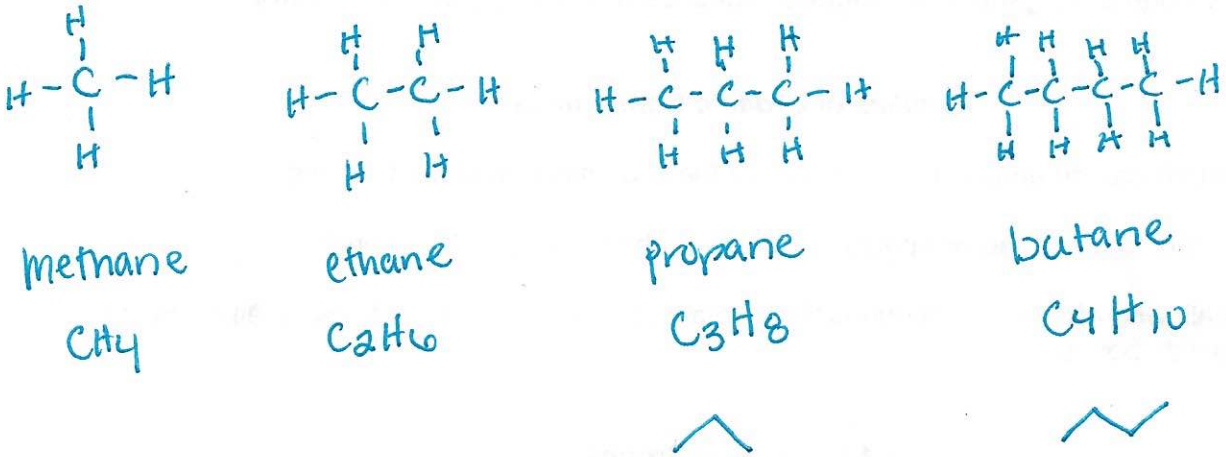
Names of Small Hydrocarbons

No. of Carbons	Formula Name	(C_nH_{2n+2})
1	Methane	CH_4
2	Ethane	C_2H_6
3	Propane	C_3H_8
4	Butane	C_4H_{10}
5	Pentane	C_5H_{12}

No. of Carbons	Formula Name	(C_nH_{2n+2})
6	Hexane	C_6H_{14}
7	Heptane	C_7H_{16}
8	Octante	C_8H_{18}
9	Nonane	C_9H_{20}
10	Decane	$C_{10}H_{22}$

↑ memorize →

Examples of Small Hydrocarbons



methane
CH_4

ethane
C_2H_6

propane
C_3H_8

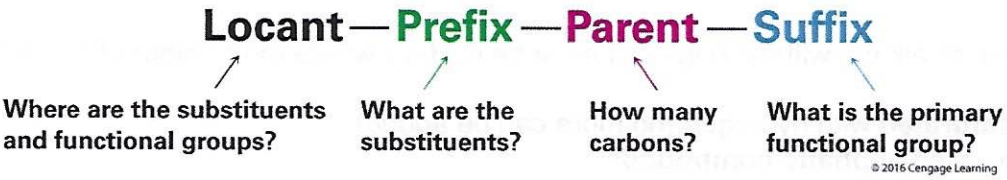
butane
C_4H_{10}

3.4 Naming Alkanes

IUPAC : International Union of Pure and Applied Chemistry

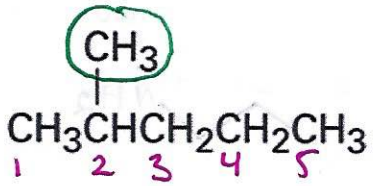
Compounds are given systematic names by a process that uses:

* helpful naming guide on pages 73-76 in textbook

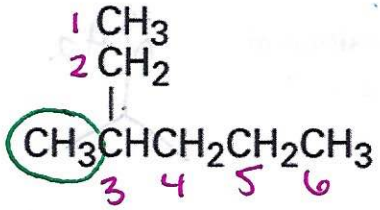


Follows specific rules:

1. Find the longest chain
2. Number the chain, Nearest branch with lowest number
3. Identify and # the substituents
4. Write as a single word
   - between prefixes
   , between words



2-methylpentane



3-methylhexane

Note: NOT 2-propylpentane
NOT 4-methylhexane

3.2 Alkane Isomers

CH_4 = methane, C_2H_6 = ethane, C_3H_8= propane ← NO ISOMERS

The molecular formula of an alkane with more than three carbons can give more than one structure
C_4 (butane) = butane and isobutane
C_5 (pentane) = pentane, 2-methylbutane, and 2,2-dimethylpropane

Alkanes with C's connected to no more than 2 other C's are **straight-chain** or **normal alkanes**

Alkanes with one or more C's connected to 3 or 4 C's are **branched-chain alkanes**

NO ISOMERS for methane, ethane & propane but more than 3 carbons can result in more than one structure

Constitutional Isomers

Isomers that differ in how their atoms are arranged in chains are called **constitutional isomers**

Compounds other than alkanes can be **constitutional isomers** of one another

They must have the same molecular formula to be isomers

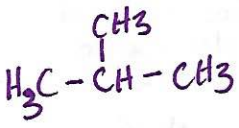
Isomer examples =

Different carbon skeletons
C_4H_{10}

$CH_3CH_2CH_2CH_3$

butane

and



2-methylpropane

Different functional groups
C_2H_6O

CH_3CH_2OH

ethanol

CH_3OCH_3

diethylether

*Remember how many bonds each atom needs to be "neutral"

Different position of functional groups C_3H_9N

isopropylamine

and

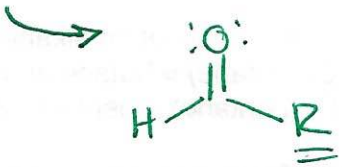
propylamine

3.3 Alkyl Groups

Alkyl group – remove one H from an alkane (a part of a structure)

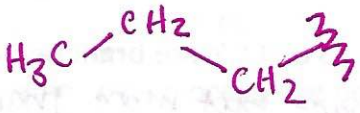
General abbreviation "R" (for Radical, an incomplete species or the "rest" of the molecule)

Name: replace *-ane* ending of alkane with *-yl* ending
$-CH_3$ is "methyl" (from methane)
$-CH_2CH_3$ is "ethyl" from ethane

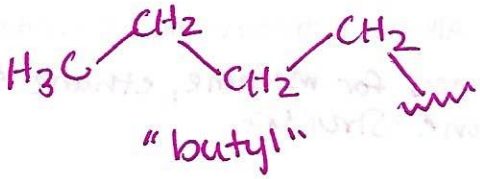


See Table 3.4 for a list

Basics:

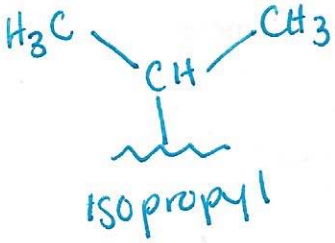


"Propyl"

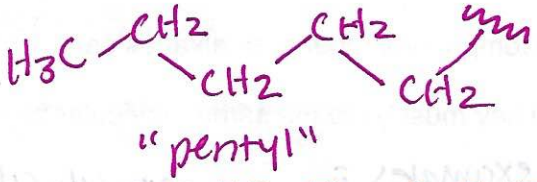


"butyl"

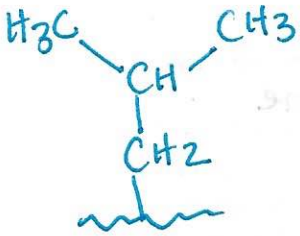
Common Names



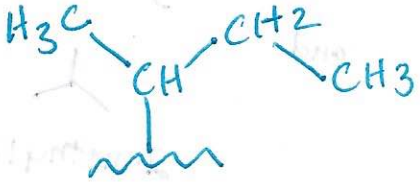
isopropyl



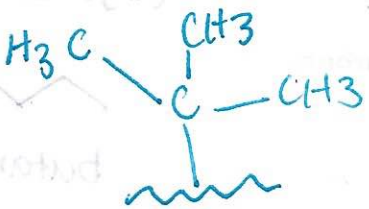
"pentyl"



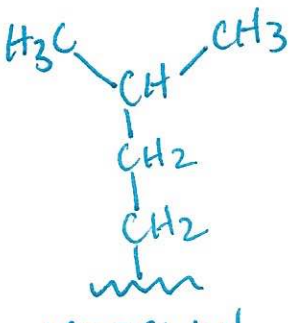
isobutyl

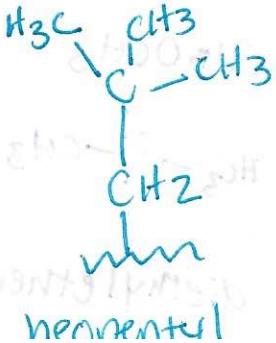


sec-butyl

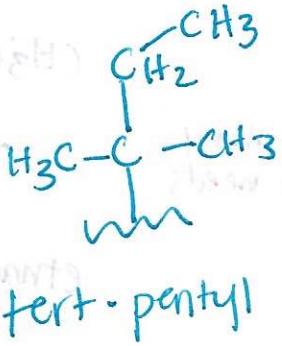


tert-butyl OR t-butyl





neopentyl



tert-pentyl

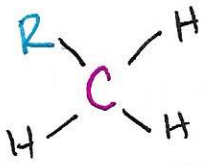
Types of Alkyl Groups

Classified by the connection site (See Figure 3.3)

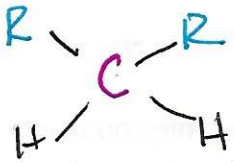
a carbon at the end of a chain (**primary alkyl group**)

a carbon in the middle of a chain (**secondary alkyl group**)

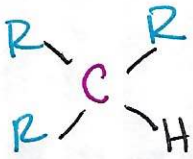
a carbon with three carbons attached to it (**tertiary alkyl group**)



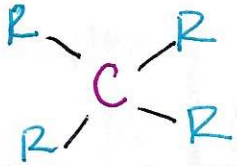
***Primary* carbon (1°) is bonded to one other carbon.**



***Secondary* carbon (2°) is bonded to two other carbons.**



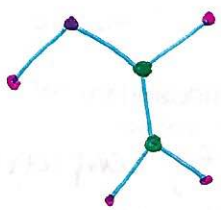
***Tertiary* carbon (3°) is bonded to three other carbons.**



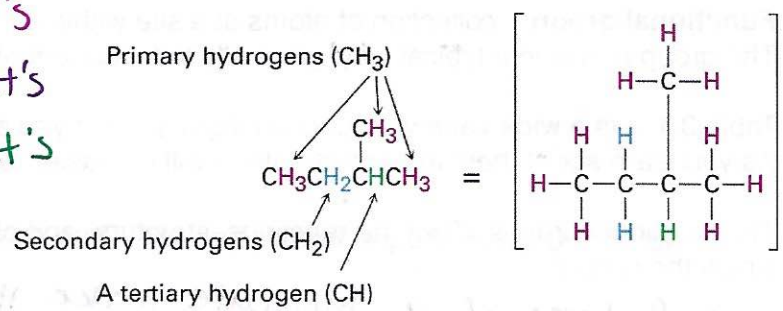
***Quaternary* carbon (4°) is bonded to four other carbons.**

Types of Hydrogen Atoms in Alkyl Groups

example!



12 primary H's
2 secondary H's
2 tertiary H's



*bonus question... name that molecule!! ... 2,3-dimethylpentane

3.5 Properties of Alkanes

Called **paraffins** (low affinity compounds) because they do not react as most chemicals

They burn producing carbon dioxide, water, and heat

They react with Cl_2 in the presence of light to replace H's with Cl's (not controlled)

$$CH_4 + Cl_2 \xrightarrow{h\nu} CH_3Cl + HCl$$

$$CH_3Cl \xrightarrow{Cl_2} CH_2Cl_2 + HCl$$

$$CH_2Cl_2 \xrightarrow{Cl_2} CHCl_3 + HCl$$

$$CHCl_3 \xrightarrow{Cl_2} CCl_4 + HCl$$

Boiling points and melting points increase as the size of alkane increases

Forces between molecules (temporary dipoles, dispersion) are weak

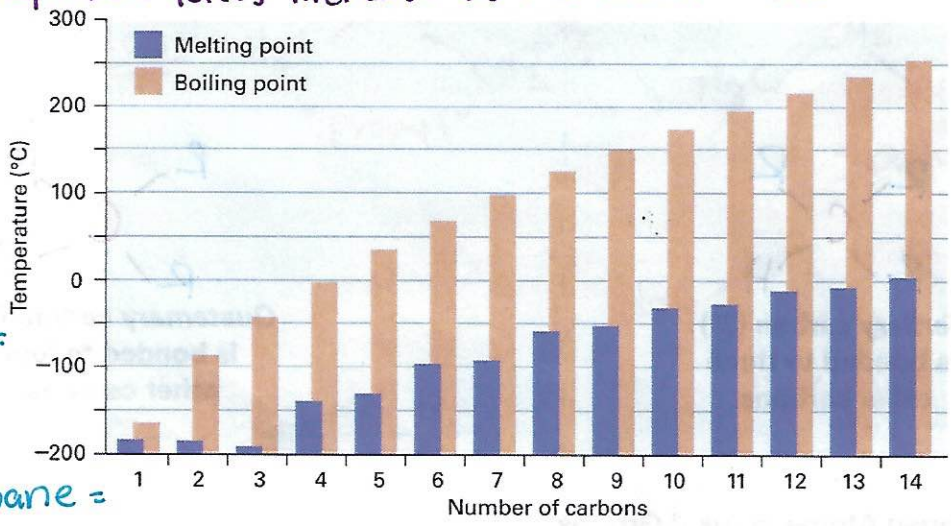
Branching? • BP & mp increase as the chain lengthens and molecular weight increa
• Dispersion forces increase as the molecule size increases

Branching lowers an alkane BP
for example:

Pentane = 36.1 deg

2 methylbutane = 27.9 deg

2,2-dimethylpropane = 9.5° deg



Functional Groups

Functional group - collection of atoms at a site within a molecule with a common bonding pattern
The group reacts in a typical way, generally independent of the rest of the molecule

Table 3.1 lists a wide variety of functional groups that you should recognize
As you learn about them in each chapter it will be easier to recognize them

The functional groups affect the reactions, structure, and physical properties of every compound in which they occur

Structural features of a molecule make it possible to classify compounds into families called functional groups. The chemistry of every organic molecule regardless of size and complexity is determined by the functional groups it contains

Reminder: Functional Groups can often be prefixes or suffixes
If there is more than one of the same functional group we use "di", "tri", etc.

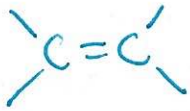
Types of Functional Groups: Multiple Carbon-Carbon Bonds

Alkenes have a C-C double bond – ene

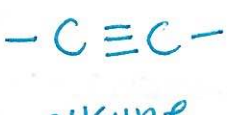
Alkynes have a C-C triple bond – yne

Arenes have special bonds represented as alternating single and double C-C bonds in a six-membered ring

Examples



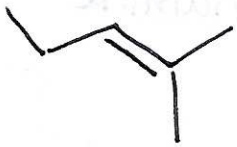
alkene



alkyne

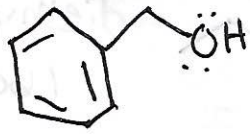
arene / aromatic ring

"benzene" OR "phenyl"



2-methyl-2-pentene
OR
2-methylpent-2-ene

1-butyne
OR
but-1-yne
OR
butyne



phenylmethanol
hydroxymethylbenzene

Functional Groups with a Single Carbon Bonded to an Electronegative Atom

Alkyl halide: C bonded to halogen (C-X)

Alcohol: C bonded O of a hydroxyl group (C-OH)

Ether: Two C's bonded to the same O (C-O-C)

Amine: C bonded to N (C-N)

Thiol: C bonded to SH group (C-SH)

Sulfide: Two C's bonded to same S (C-S-C)

Bonds are polar, with partial positive charge on C (δ+) and partial negative charge (δ-) on electronegative atom

* lower case delta "δ" means "partial"

Examples

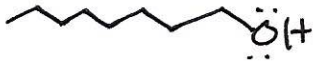
alkyl halides

Bromo-
Iodo-
Fluro-
chloro-

dichloromethane

Iodopropane

alcohols -ol



octanol

Ether

* note: name the sides alphabetically

diethyl ether
(bat!)

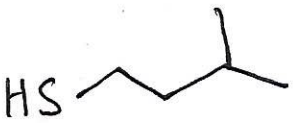
ethyl methyl ether

Amines -amine

$-\ddot{N}H_2$ methanamine
OR
$H_3C-\ddot{N}H_2$

Thiols

* note: The carbon bound to the thiol group takes priority when counting -thiol



3-methylbutane-1-thiol

Groups with a Carbon-Oxygen Double Bond (Carbonyl Groups)

Aldehyde: one hydrogen bonded to C=O

Ketone: two C's bonded to the C=O

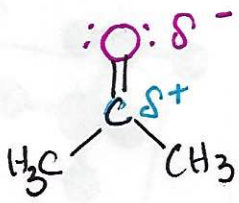
Carboxylic acid: OH bonded to the C=O

Ester: C-O bonded to the C=O

Amide: C-N bonded to the C=O

Acid chloride: Cl bonded to the C=O

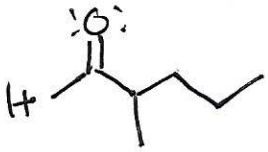
Carbonyl C has partial positive charge (δ+)
Carbonyl O has partial negative charge (δ-).



acetone - a typical carbonyl compound
Carbonyl C has a partial positive charge
Carbonyl O has a partial negative cha

Examples

Aldehydes 



"-al"

2-methylpentanal

Ketones 

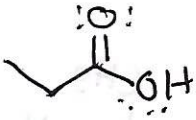
"-one"

aka-acetone

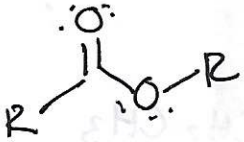
propanone

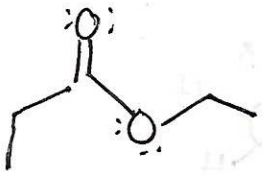
carboxylic acids

"-oic acid"

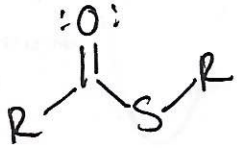


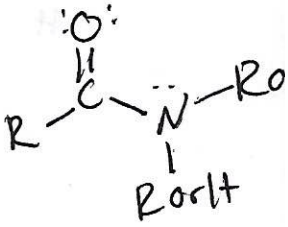
propanoic acid

Esters 

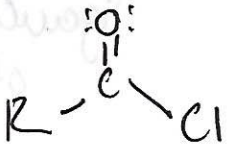


ethyl propanoate

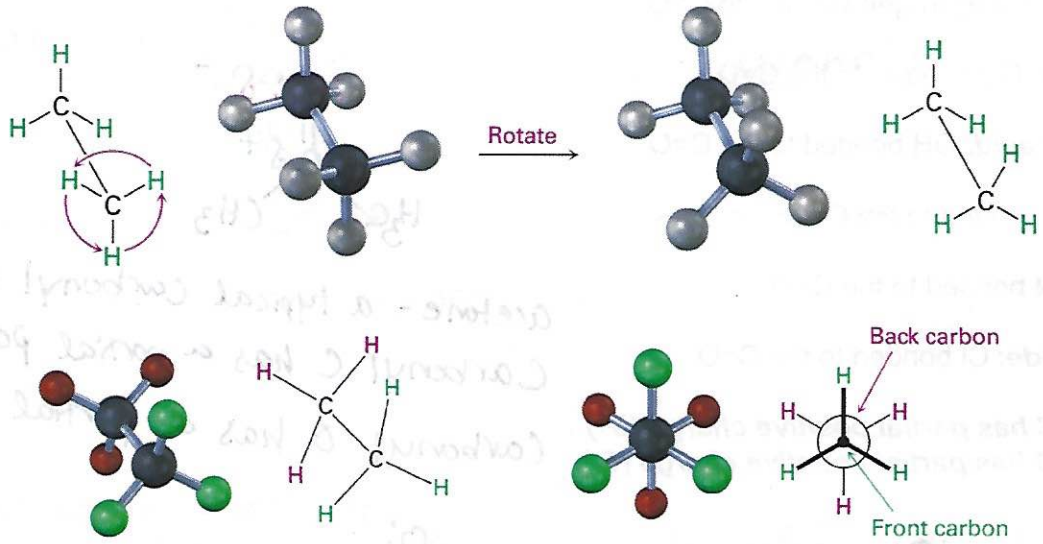
Thioester 

Amide 

ethanamide

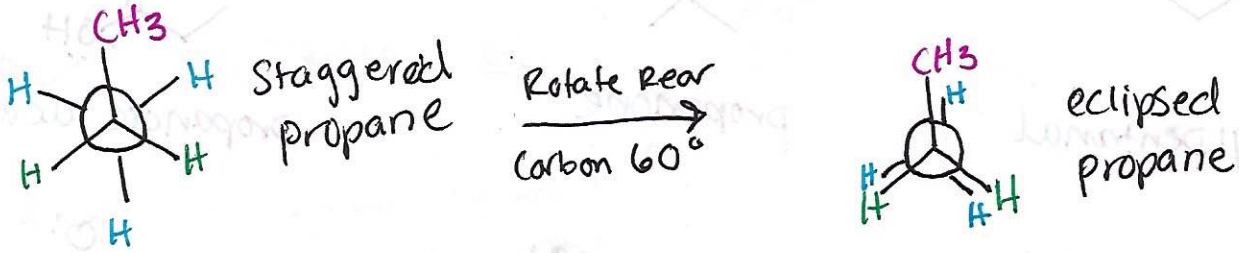
Acid chloride 

3.6 Conformations of Ethane



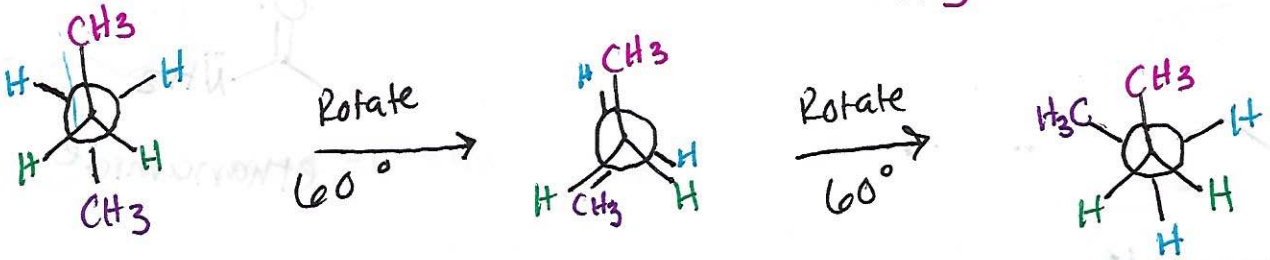
*viewed down the C2-C3 bond

Conformations of Propane $CH_3CH_2CH_3$



*viewed down the C2-C3 bond

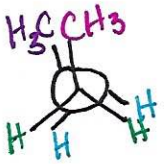
Conformations of Butane $CH_3CH_2CH_2CH_3$



"anti" conformation of butane

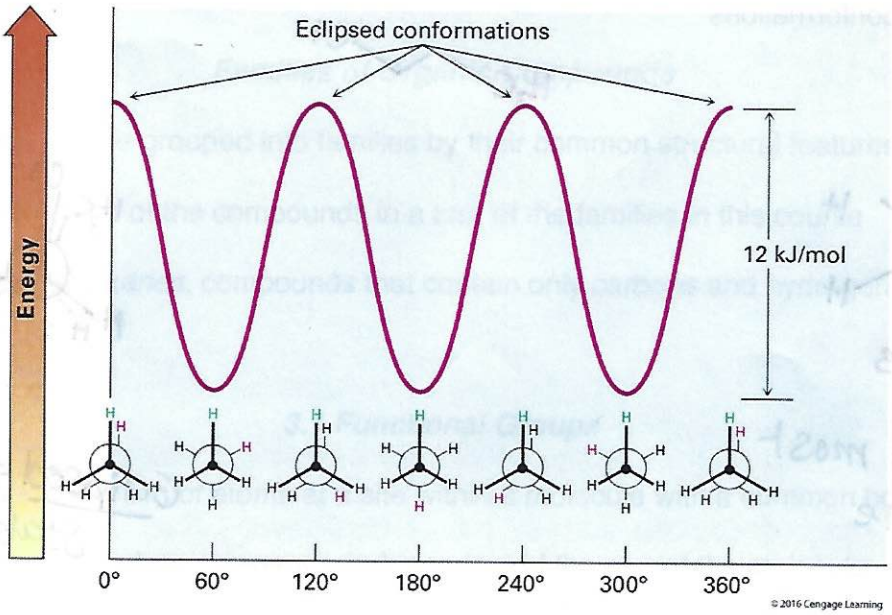
"eclipsed" conformation of butane

"gauche" conformation of butane

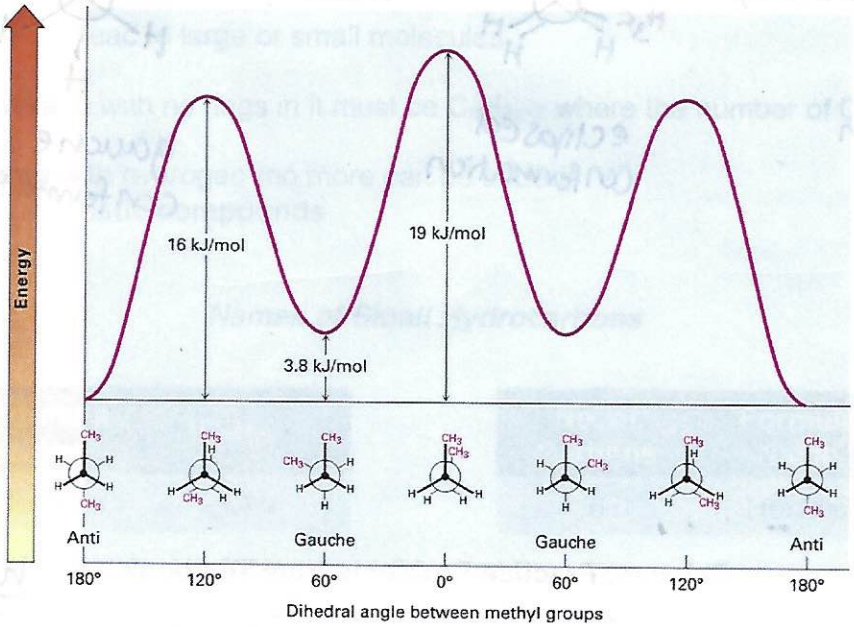


Rotate 60°

Conformations of Ethane

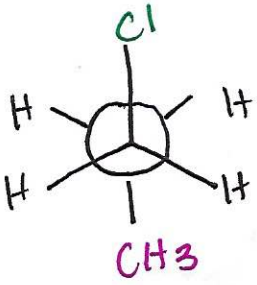


Conformations of Butane

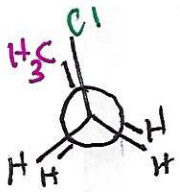


Newman Projection Practice

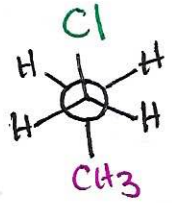
Sight along the C1 - C2 bond of 1-chloropropane and draw Newman projections of the most stable and least stable conformations



Staggard = most Stable

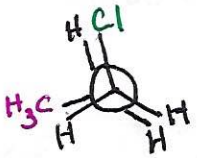


Eclipsed = least Stable



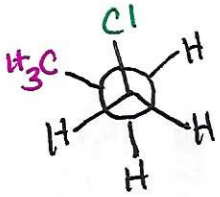
"anti" conformation
Lowest energy

Rotate 60°



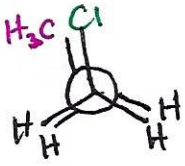
eclipsed conformation

Rotate 60°



gauche conformation

Rotate 60°



eclipsed
highest energy

Relevant Practice Problems from Textbook

Chapter 3: 2, 4-6, 8-12, 15-17 19, 21-25, 27-40, 42, 48, 49, 53 (9th ed)