Alkanes

EQ

1. **How will I define Hydrocarbons?**
2. **Compare and contrast the 3 types of hydrocarbons (Alkanes, alkenes, alkynes).**

- Hydrocarbons: Compounds made of hydrogen and carbon only.
- Aliphatic (means "fat") - Open chain
- Aromatic - ring

Open chain Hydrocarbons:

Type of hydrocarbon	Alkane	Alkene	Alkyne
Suffix	-ane	-ene	-yne

Open chain Hydrocarbons:

Type of hydrocarbon	Alkane	Alkene	Alkyne
Suffix	-ane	-ene	-yne
Carbon Carbon Bond	single	double	triple

Open chain Hydrocarbons:

Type of hydrocarbon	Alkane	Alkene	Alkyne
Suffix	-ane	-ene	-yne
Carbon Carbon Bond	single	double	triple
General Formula	C_nH_{2n+2}	C_nH_{2n}	C_nH_{2n-2}

Prefixes (page 2)

# of C	Prefix	# of C	Prefix
1	Meth	9	Non
2	Eth	10	Dec
3	Prop	11	Undec
4	But	12	Dodec
5	Pent	13	Tridec
6	Hex	20	Icos
7	Hept	21	Henicos
8	Oct	30	Triacont

Chemical Structures

- 1. Molecular Model (Ball and stick)
- 2. Molecular Formula (Chemical formula)
- 3. Structural Formula
- 4. Condensed structure
- 5. Skeletal Structure

Functional Group

- **Definition: A group of atoms within a large molecule that has a characteristic behavior.**
- **Functional groups determine the chemistry of every organic compound.**

Functional Group

- **Functional groups described in this text can be divided into three categories;**
- **i. Functional groups with carbon-carbon multiple bonds.**
- **ii. Groups in which carbon forms a single bond to an electronegative atom.**
- **iii. Groups with a carbon-oxygen double bond.**

Functional Groups

- **1. Functional groups with Carbon Carbon bonds (C—C, C=C, C≡C , aromatic ring)**

- **Functional groups with Carbon Carbon bonds**

Family Name	Functional Group Structure	Simple Example	Name ending
Alkane	| | -C-C- | |	ethane	-ane
Alkene	| | C=C | |	ethene	-ene
Alkyne	-C≡C-	ethyne	-yne
Arene (Aromatic)	See text	benzene	none

Functional Groups

- **2. Functional groups with Carbon singly bonded to an *electronegative atom*:**
- **(Halide, alcohol, ether, amine, imine, nitrile, thiol, sulfide, disulfide)**

- **Functional groups with Carbon singly bonded to an electronegative atom**

Family Name	Functional Group Structure	Simple Example	Name ending
Halide	| -C-X |	Chloromethane	none
Alcohol	| . -C-OH | .	Methanol	-ol
Ether	| | -C-O-C- | |	Dimethyl ether	ether

- **Functional groups with Carbon singly bonded to an electronegative atom**

Family Name	Functional Group Structure	Simple Example	Name ending
Amine	| .. -C-N - | |	Methylamine	-amine
Imine	| .. C=N - |		none
Nitrile	.. -C≡N	Ethanenitrile	-nitrile
Nitro	| -C-NO_2 |	nitromethane	none

- **Functional groups with Carbon singly bonded to an electronegative atom**

Family Name	Functional Group Structure	Simple Example	Name ending
Thiol	| -C-SH |	Methanethiol	-thiol
Sulfide	| | -C-S-C- | |	Dimethyl sulfide	sulfide
Disulfide	| | -C-S-S-C- | |	Dimethyl disulfide	Disulfide

Functional Groups

- **3. Functional groups with a Carbon-Oxygen double bond: (Carbonyl groups) (Aldehyde, Ketone, Carboxylic acid, Ester, Amide, Acid chloride)**

- **3. Functional groups with a Carbon-Oxygen double bond:**

Family Name	Functional Group Structure	Simple Example	Name ending
Aldehyde	O | || | -C-C-H- | |	H	-al
Ketone	O | || | -C-C-C- | |		-one
Carboxylic acid	O | || | -C-C-OH | |		-oic acid

- **3. Functional groups with a Carbon-Oxygen double bond:**

Family Name	Functional Group Structure	Simple Example	Name ending
Ester	O . | || | -C-C-O-C- | |		-oate
Amide	O | || | -C-C-N- | |		-amide

- **3. Functional groups with a Carbon-Oxygen double bond:**

Family Name	Functional Group Structure	Simple Example	Name ending
Carboxylic acid anhydride	O O | || || | -C-C-O-C-C- | |		-oic anhydride
Carboxylic acid chloride	O | || . -C-C-Cl		-oyl chloride

EQ: How do I identify, define and draw alkanes and alkane isomers?

Alkanes

- **A. Alkanes are formed by overlap of carbon sp^3 orbitals.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **B. Alkanes are described as saturated hydrocarbons...**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **B. Alkanes are described as saturated hydrocarbons...**
- **1. They are <u>hydrocarbons</u> because they contain only carbon and hydrogen.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **B. Alkanes are described as saturated hydrocarbons ...**
- **2. They are <u>saturated</u> because there are maximum possible number of hydrogens per carbon (all the bonds are single bonds).**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **3. The general formula for alkanes is C_nH_{2n+2}**
- **4. Aliphatic (means fatty) compounds .**

EQ: How do I identify, define and draw alkanes and alkane isomers?

Alkanes Lab

- Complete the worksheet as you build models of the different alkanes.

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **C. For alkanes with four or more carbons, the carbons can be connected in more than one way.**
- **1. If the carbons are in a row, the alkane is a straight-chain alkane (*n*-alkane). (n stands for normal)**
- **2. If the carbon chain has a branch, the alkane is a branched-chain alkane.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **Straight-chain alkanes are named according to the number of carbons in their chain.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

What are ISOMERS?

- **Alkanes with the same molecular formula but different structural formula are <u>isomers</u>.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- **1. Isomers whose atoms are connected differently are <u>constitutional</u> isomers. Constitutional isomers are always different compounds with different properties but with the same molecular formula.**
- **2. A given alkane can be drawn in different ways.**

EQ: How do I identify, define and draw alkanes and alkane isomers?

- Lets try to draw some isomers on Page 11 of the packet…

EQ: What are alkyl groups?

Alkyl Group

EQ: What are alkyl groups?

- **An alkyl group is the <u>partial structure</u> that results from the removal of a hydrogen atom from an alkane.**
- **An alkyl group is always attached to a parent chain (it is a branch), it does not exist on it's own.**

EQ: What are alkyl groups?

- **1. Alkyl groups are named by replacing the –ane of an alkane by –yl.**
- **Meth*ane* CH_4 Meth*yl* $-CH_3$**
- **Eth*ane* C_2H_6**
- **Eth*yl* $-C_2H_5$ *or* $-CH_2CH_3$**

EQ: What are alkyl groups?

- *2.* ***n*-Alkyl groups are formed by removal of a hydrogen from an end carbon of a straight-chain alkane.**
- **propyl is -$CH_2CH_2CH_3$**
- ***The terminal C is attached to the parent chain***

EQ: What are alkyl groups?

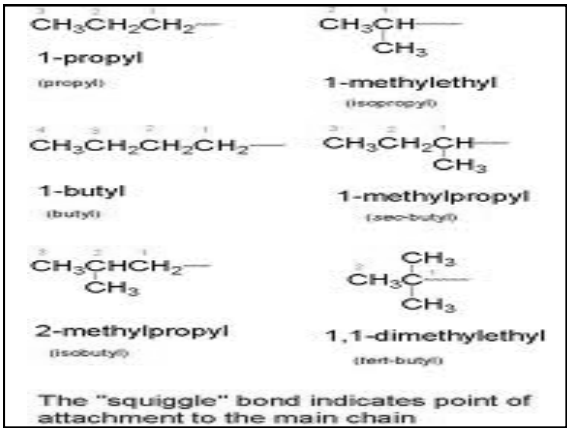
- **3. Branched-chain alkyl groups are formed by removal of a hydrogen atom from an internal carbon.**
- **isopropyl is** ~CH-CH_3
- |
- CH_3
- ***The central C is attached to the parent chain***

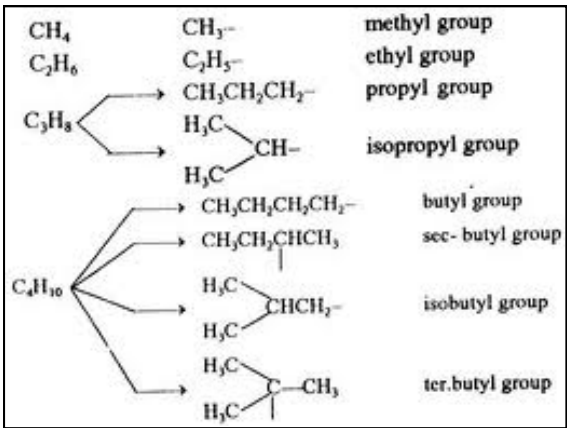
EQ: What are alkyl groups?

- **The prefixes *sec*- and *tert*- refer to the degree of substitution at the branching carbon atom.**

EQ: What are alkyl groups?

- **There are four possible degrees of alkyl substitution for carbon.**
- **1. A primary carbon is bonded to one other carbon.**
- **2. A secondary carbon is bonded to two other carbons.**
- **3. A tertiary carbon is bonded to three other carbons.**
- **4. A quaternary carbon is bonded to four other carbons.**
- ***** The symbol R refers to the rest of the molecule.**





EQ: How do I name and draw structures of alkanes?

- **The system of nomenclature used is the IUPAC system. *(International Union of Pure and Applied Chemistry)***

- **In this system, a chemical name has a *prefix*, a *parent, Locant* and a *suffix*.**

-The *prefix* shows Where and what substituents

- The *parent* shows the number of carbons in the principal chain.

- Locant - Location of functional group

- The *suffix* identifies the functional group family.

EQ: How do I name and draw structures of alkanes?

Naming Branched-Chain Alkanes

1. Find the parent hydrocarbon.

a. Find the longest continuous chain of carbons, and use its name as the parent name.

b. If two chains have the same number of carbons, choose the one with more branch points.

EQ: How do I name and draw structures of alkanes?

2. Number the atoms in the parent chain.

a. Start numbering at the end nearer the first branch point.

b. If branching occurs at equal distance from both ends, begin numbering at the end nearer the second branch.

EQ: How do I name and draw structures of alkanes?

3. Identify and number the substituents.

a. Give each substituent a number that corresponds to its position on the parent chain.

b. Two substituents on the same carbon receive the same number.

```
      CH3
       |
CH3-CH-CH2-CH-CH2-CH3
       |
      CH3
```

EQ: How do I name and draw structures of alkanes?

4. Write the name as a single word.

a. Use hyphens to separate prefixes and commas to separate numbers.

b. Use the prefixes, *di-, tri-, tetra-* if necessary, but don't consider them for alphabetizing.

```
      CH3
       |
CH3-CH-CH2-CH-CH2-CH3
       |
      CH3
```

Properties of Alkanes

- **i. Alkanes are chemically inert to most laboratory reagents.**

Properties of Alkanes

- **- Alkanes undergo a Substitution reaction.**
- **Why? Because the only have H bonded to C**

Properties of Alkanes

- **ii. Alkanes react with O_2**
- **(Reaction with O_2 is called a combustion reaction.**
- **example: $C_3H_8 + O_2 \rightarrow CO_2 + H_2O$**

Properties of Alkanes

- **ii. Alkanes react with Cl_2**
- **Reaction with Cl_2 :**

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

Properties of Alkanes

- iii. The boiling points and melting points of alkanes increase with increasing molecular weight.
- iv. Increased branching lowers an alkane's boiling point.

Conformation Of Ethane

1) Rotation is possible around carbon-carbon single bonds.

--The different arrangements of atoms that result from rotation are conformer.

EQ: What do I understand by the term conformation?

Conformation Of Ethane

2) Conformations can be represented in two ways.

a) Sawhorse representations of alkanes view the C-C bond from an oblique angle.

b) Newman projections represent the two carbon atoms by a circle.

EQ: What do I understand by the term conformation?

Conformation Of Ethane

a) In a staggered conformation, hydrogens are as far apart as possible.

b) In an eclipsed conformation, hydrogens are as close together as possible.

c) For most compounds, a staggered conformation is more stable than an eclipsed conformation.

Cycloalkanes

- 1.State the characteristics of cycloalkanes.
- 2.How do I name and draw the molecular structural and skeletal structure for cycloalkanes?
- 3.What are cis-trans isomers? How do I name and draw the molecular structural using cis-trans isomerism?
- 4.How do I differentiate between constitutional isomers and stereoisomers?

EQ: How do I name and write structures for cycloalkanes?

Cycloalkanes

- **Cycloalkanes are also called alicyclic compounds.**
- **General formula of cycloalkanes: CnH2n or (CH2)n**

EQ: How do I name and write structures for cycloalkanes?

Cycloalkanes

- **1) A 3 carbon cycloalkane is called cyclopropane.**
- **It's skeletal structure:**

- **2) A 4 carbon cycloalkane is called cyclobutane.**
- **It's skeletal structure:**

EQ: How do I name and write structures for cycloalkanes?

Cycloalkanes

- **3) A 5 carbon cycloalkane is called _____**
- **It's skeletal structure:**

- **4) A 6 carbon cycloalkane is called _____**
- **It's skeletal structure:**

EQ: How do I name and write structures for cycloalkanes?

Naming Substituted Cycloalkanes

- **i. Count the number of carbon atoms in the ring, and add the prefix *cyclo-* to the name of the corresponding alkane.**

- **ii. For two or more substituents, begin numbering at the group with alphabetical priority, and give the other substituents the lowest possible number.**

	Acyclic alkanes (open chain alkanes)	Cyclic alkanes (ring compounds)
Rotation around C-C bond	**Free Rotation**	**More constrained (rigid planar molecule)**
Isomerism	**Constitutional isomers**	**Stereoisomers**
Examples	**1,2-dichloropropane**	**1,2-dichlorocyclopropane**

	Stereoisomers (cis-trans isomers)	**Constitutional Isomers**
Definition	**Compounds that have their atoms connected in the same way but differ in 3 dimensional orientation.**	**Compounds which have the same molecular formula but different structural formula.**
Examples		

Cis-trans isomerism in cycloalkanes

- **1. Unlike open-chain alkanes, cycloalkanes have much less rotational freedom.**
- **a. Very small rings are rigid.**
- **b. Large rings have more rotational freedom.**

Cis-trans isomerism in cycloalkanes

- 2. Cycloalkanes have a "top" side and a "bottom" side.
- a. If two substituents are on the same side of a ring, the ring is cis-disubstituted.
- b.If two substituents are on opposite sides of a ring, the ring is trans-disubstituted.

Cis-trans isomerism in cycloalkanes

- 3. Substituents in the two types of disubstituted cycloalkanes are connected in the same order but differ in the spatial orientation.
- a. These cycloalkanes are stereoisomers that are known as cis-trans isomers.
- b. Cis-trans isomers are stable compounds that can't be interconverted.

Conformation Of Cycloalkanes

- **Cyclopropane:**
- **Molecular Formula: C3H6**
- **Structure:**
- **Bond angle: 60º (C prefers to have a bond angle of 109.5º)**
- **Angle strain: The strain introduced into a molecule when a bond angle is deformed from its ideal value.**
- **Reactivity: Due to angle strain, it makes it more reactive than unstrained alkanes**
- **C-H bonds: All 6 C-H bonds have eclipsed arrangement.**

Conformation Of Cycloalkanes

- **Cyclobutane and cyclopentane:**
- **Molecular Formula: C4H8; C5H10**
- **Structure:**
- **Bond angle: 90º and 108º (C prefers to have a bond angle of 109.5º)**
- **They are slightly puckered rather than flat. The puckering makes the C-C-C bond angle bit smaller and increases angle strain but relieves the eclipsing interactions of adjacent C-H bonds.**

Cyclohexanes

- **Chair conformation: cyclohexane.**
- **a. The chair conformation of a cyclohexane is strain-free.**
- **b. In a standard drawing of cyclohexane the lower bond is in front.**

Axial and equatorial bonds in cyclohexane

- **1. There are two kinds of positions on a cyclohexane ring.**
- **a. Six axial hydrogens are perpendicular to the plane of the ring.**
- **b. Six equatorial hydrogens are roughly in the plane of the ring.**

Axial and equatorial bonds in cyclohexane

- **1. Each carbon has one axial hydrogen and one equatorial hydrogen.**
- **2. Each side of the ring has alternating axial and equatorial hydrogens.**
- **3. All hydrogens on the same side of the ring are cis.**

Conformational mobility of cyclohexanes

- **Different chair conformations of cyclohexanes interconvert by a ring-flip.**
- **After a ring-flip, an axial bond becomes an equatorial bond and vice versa.**
- **Both conformations aren't equally stable at room temperature.**
- **In methylcyclohexane, 95% of molecules have the methyl group in the equatorial position.**
- **Steric strain:**