Advanced Chemistry: Chapter 12 Notes. Organic Chemistry & Alkanes

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I. Defining Organic Molecules.

Organic Chemistry- The study of carbon-containing molecules

Organic molecules are characterized by:

1. Containing tetravalent carbon atoms: always forming 4 bonds Due to sp^3 hybridization

2. All bonds between atoms are covalent bonds
   -some intermolecular attractions occur but are less common due to nonpolar bonding between C-H

3. Polar bonds occur when carbon is bonded to (N, O, F, & Cl)
   -other polar bonds are found with (H-O & H-N)

4. Carbon can form multiple bonds by sharing more than 1 pair of electrons with other atoms
   -based on the hybridization of carbon: double bond = sp^2 and triple bond = sp

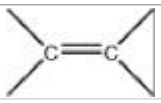
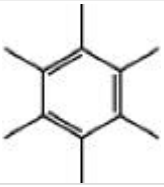
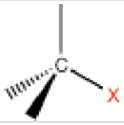
5. Organic molecules have specific three dimensional shapes
   -due to # of electron dense regions- (bonded & lone pairs of electrons about central carbons)

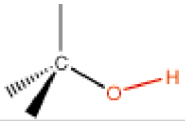
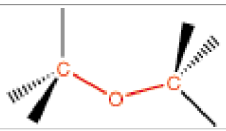
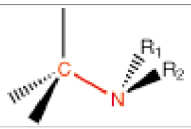
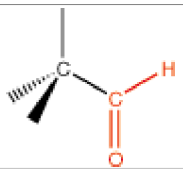
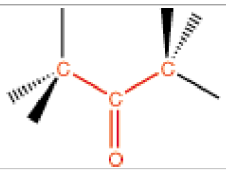
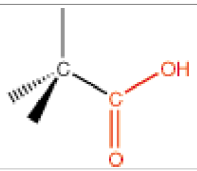
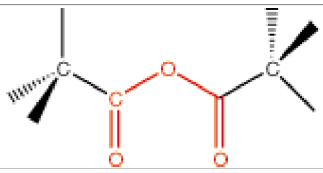
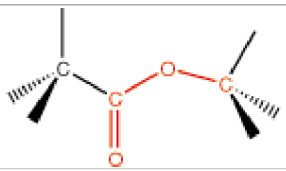
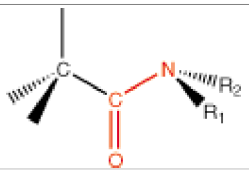
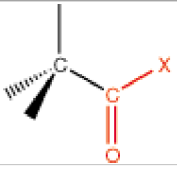
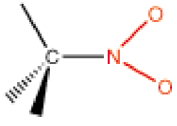
6. Organic molecules commonly contain H, N, & O (also Cl, P, & S)

II. Families of Organic Molecules

Hydrocarbon- compound containing carbon & hydrogen
Most organic molecules have hydrocarbons that function as the skeletal framework of the molecule
Molecules differ by:

a. structure of the parental hydrocarbon chain (skeletal framework)
b. addition of functional groups: R represents any alkyl group (alkane group attached to another)

Hydrocarbon Functional Groups			
Family	Functional Group	Functional Group Structure	Prefix/Infix/Suffix
1. Alkane	none	none	-ane
2. Alkene	carbon/carbon double bond		-ene
3. Alkyne	carbon/carbon triple bond		-yne
4. Arene	resonant hexacyclic triene		none
5. Alkyl Halide	carbon-halogen		-none

6. Alcohol	hydroxyl		-ol
7. Ether	ether linkage		-oxy-
8. Amine	amine		-amine 1º, 2º & 3º
9. Aldehyde	terminal carbonyl		-al
10. Ketone	axial carbonyl		-one
11. Carboxylic Acid	carboxyl		-oic acid
12. Acid Anhydride	dicarboxyl linkage		anhydride
13. Ester	ester linkage		-ate
14. Amide	amide linkage		-amide 1º, 2º & 3º
15. Nitrile	nitrile		-nitrile
16. Acyl Halide	carbonyl w/ halide		-ate
17. Nitro compounds	carbon-nitro		nitro-

18. Thiols	sulfhydryl	-SH	-thiol

III. Alkanes

Alkane- Hydrocarbon with the maximum number of hydrogen atoms per carbon (considered "saturated with hydrogen atoms")

General formula → C_nH_{2n+2}

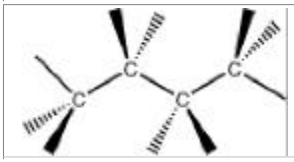
1. All bonds between carbons are single covalent bonds; sp3 hybridization
2. The chain of carbons must be in open form (non-cyclic structures)

-a.k.a. – saturated hydrocarbon or aliphatic hydrocarbon

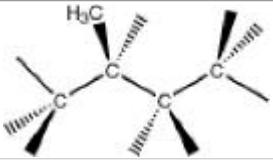
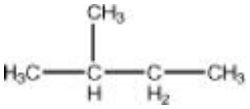
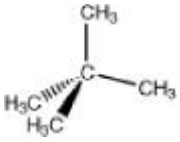
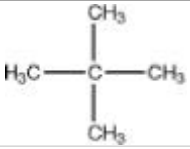
A. Isomerization

Isomers- Compounds with the same formula but having different molecular structures

1. constitutional isomers- isomers that differ by the order of attachment of their atoms
   a. straight-chained- alkanes where each carbon is bonded to a maximum of 2 other carbons.

Formulas		
Formula Type	**Demonstrates**	**Example: BUTANE**
Molecular formula	shows ratio of atoms	C_4H_{10}
Structural formula	shows bonds and atoms	
Condensed formula	shows functionality of each carbon	CH_3-CH_2-CH_2-CH_3

   b. branched-chained-alkanes where an atom is bonded to 3 other carbons.

Examples of Branched Hydrocarbons		
Name	Structural Formula	Condensed Formula
2-Methylbutane		
2,2-Dimethylpropane		

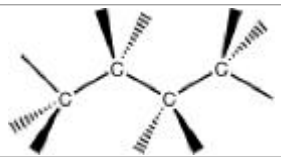
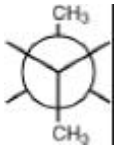
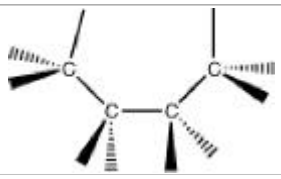
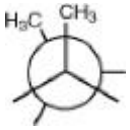
IV. Shapes of Organic Molecules

Conformation- 3-dimensional arrangement of atoms that result from free rotation about a single bond (sigma bond)

1. Staggered conformation- rotation occurs between 2 carbon atoms until atoms on adjacent carbons maximize their distances

   Newman projection- a molecular perspective that looks down the axis of a C -- C bond.

2. Eclipsed conformation- rotation that produces adjacent atoms to minimize their distances.

Conformations		
Conformation	Structural Formula	Newman Projection Model
Staggered		
Eclipsed		

V. Naming Alkanes- Nomenclature

IUPAC- International Union of Pure and Applied Chemistry
- Set up the rules by which organic compounds are named, but some common names still exist.

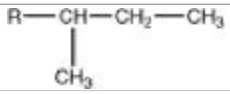
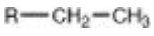
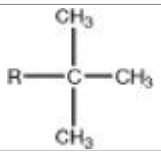
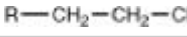
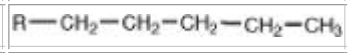
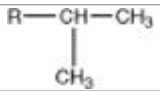
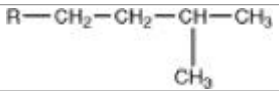
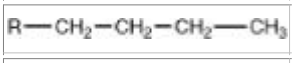
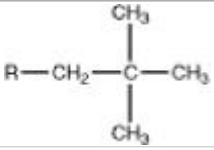
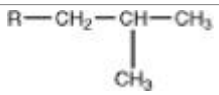
3 parts of any compound name
1. Prefix- describes the location of substituent(s) or functional group(s)
2. Root- describes how many carbons in the longest chain (parent chain)
3. Suffix- describes the family
   For alkanes the suffix is –ane

Root nomenclature- most are named for Greek numerals except for 1,2,3 &4 carbon molecules

IUPAC Prefixes of Unbranced Alkanes					
# of Carbons	**Prefix**	**# of Carbons**	**Prefix**	**# of Carbons**	**Prefix**
1	meth-	11	undec-	21	henicos
2	eth-	12	dodec-	22	docos-
3	prop-	13	tridec-	23	tricos-
4	but-	14	tetradec-	24	tetracos-
5	pent-	15	pentadec-	30	triacont-
6	hex-	16	hexadec-	31	hentriacont-

7	hept-	17	heptadec-	32	dotriacont-
8	oct-	18	octadec-	40	tetracont-
9	non-	19	nonadec-	50	pentacont-
10	dec-	20	eicos- (icos-)	100	hect-

Alkyl Groups- alkanes attached to a parent chain- change name ending from –ane to –yl

Names of Common Alkyl Group			
Name	Condensed Formula	Name	Condensed Formula
methyl		sec-butyl	
ethyl		tert-butyl	
propyl		pentyl	
isopropyl		isopentyl	
butyl		neopentyl	
isobutyl			

IUPAC Rules for Naming Alkanes

1. The general name of an open-ended saturated hydrocarbon is an alkane
2. For branched-chain hydrocarbons, the alkane corresponding to the longest chain of carbon atoms is taken as the parent chain and its name is the root name
3. Groups attached to the parent chain are called substituents and each is given a name and number. The number identifies which carbon it is attached to.
4. If there is one substituent, number the parent chain which gives the lowest number to the substituent carbon.
5. If a substituent occurs more than once, the number of each carbon is given and the numeric prefix for the number groups (di-, tri-, etc.).
   Number the chain that yields the lowest number for the first substituent.
6. If there are two or more different substituents, list them in alphabetic order and number the parent chain to give the lowest number for the first substituent. If two substituents have the same position on the chain, number the chain so that the alphabetic first has the lower number
7. The prefixes di-, tri-, etc. are not used in alphabetizing, only the substituent names.
8. Hyphenated prefixes, such as sec- and tert- are not considered when alphabetizing.
9. If the hydrocarbon forms a cyclic structure, the prefix cyclo- preceeds the prefix for the number of carbons in the cyclic structure.

Order of Precedence of Functional Groups for Identifying Family Name

Functional Group	Suffix if Higher	Prefix if Lower
Carboxyl	-oic acid	
Terminal Carbonyl	-al	oxo-
Axial Carbonyl	-one	oxo-
Hydroxyl	-ol	hydroxy-
Amine	-amine	amino-
Thiol	-thiol	mercapto-