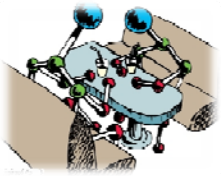


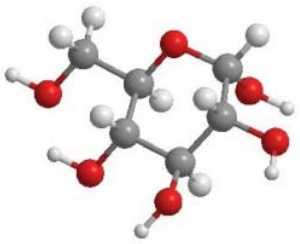
Chapter 10

ORGANIC CHEMISTRY

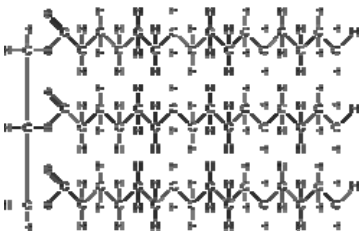
Part I

What Is Organic Chemistry?

- ***Organic chemistry*** is the field of science that studies the structure, properties, composition of hydrocarbons (compounds containing carbon and hydrogen). These compounds may contain some other elements, including oxygen, nitrogen and halogens.



Glucose molecule



Fat molecule

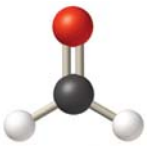
10.1

Why Carbon is Different

- *Electron configuration*: [He]$2s^2 2p^2$ shows that C atom effectively prohibits ion formation.
- In most of hydrocarbons, carbon atoms form *four bonds* with other atoms. These bonds are oriented in different directions.
- A C atom has a *small atomic radius* which gives rise to short, strong C–C bonds and, hence, stable compounds.
- *Hybridized* C atoms (*sp* and sp^2) can form strong π bonds with unhybridized *p* orbitals.

Methane
(4 σ bonds)

Carbon dioxide
(2 σ bonds & 2 π bonds)



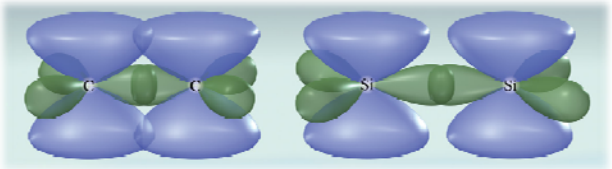
Formaldehyde
(3 σ bonds & 1 π bond)

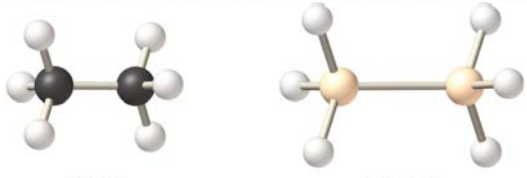
10.1

Chemistry of Carbon and Silicon

- Si atom is bigger than C atom. Thus, unhybridized *p orbitals do not overlap* effectively and, as a result, it is least likely to find π-bonding between Si atoms.

5	6	7
B	C	N
13	14	15
Al	Si	P
31	32	33
Ga	Ge	As
49	50	51
In	Sn	Sb
81	82	83
Tl	Pb	Bi





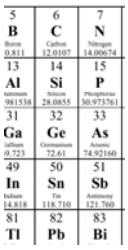
Ethane Disilane

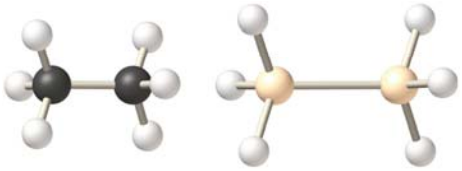
10.1

Chemistry of Carbon and Silicon

- Valence electrons in C atom have *n* = 2, while valence electrons in Si atom have *n* = 3 where *d* orbitals are there. *The empty d orbitals make Si-based compounds more reactive* and, hence, less stable compared to C-based compounds.

  Ethane is stable at normal condition, but disilane is not.



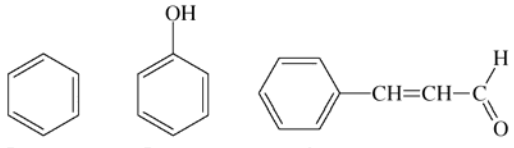


Ethane Disilane

10.1

Catenation

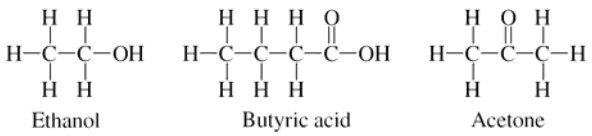
- ***Catenation*** is the process involving the carbon's formation of chains and rings containing single, double and triple bonds.



Benzene Phenol Cinnamic aldehyde

Aromatic compounds

Aromatic compounds are organic compounds that contain one or more benzene rings.



Ethanol Butyric acid Acetone

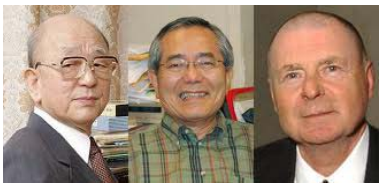
Aliphatic compounds

Aliphatic compounds are organic compounds that do not contain benzene rings.

10.2

Classes of Organic Compounds

- Carbon atoms can form endless number of different straight, branched and cyclic chains through catenation. So it is very common in organic chemistry to classify these molecules into specific classes.



Akira Suzuki Ei-ichi Negishi Richard Heck

These three scientists won the 2010 Nobel Prize for Chemistry for their discoveries that made it easier and cheaper to build long carbon chains in the lab, and use those chains to develop new drugs, build electronics, and more.

10.2

Alkanes

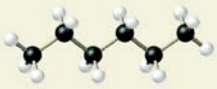
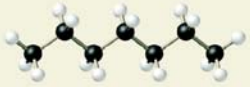
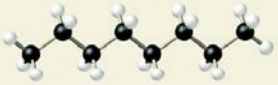
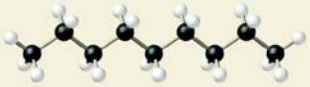
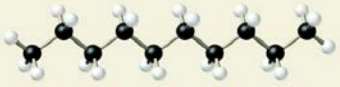
- ***Alkanes*** are simple organic compounds that consist of only carbon and hydrogen. They contain only single bonds.

Formula	Name	Model
CH_4	Methane	
C_2H_6	Ethane	
C_3H_8	Propane	
C_4H_{10}	Butane	
C_5H_{12}	Pentane	

General Formula
C_nH_{2n+2}

10.2

Alkanes

Formula	Name	Model
C_6H_{14}	Hexane	
C_7H_{16}	Heptane	
C_8H_{18}	Octane	
C_9H_{20}	Nonane	
$C_{10}H_{22}$	Decane	

General Formula
C_nH_{2n+2}

10.2

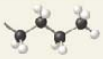
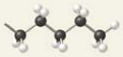
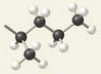
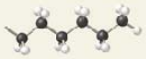
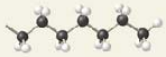
Alkyl Groups

- An ***alkyl group*** is a portion of a molecule that resembles an *alkane*. An alkyl group is formed by *removing one hydrogen* from the corresponding alkane.
- Alkyl groups are represented in organic compounds with ***R***.

Name	Formula	Model
Methyl	$-CH_3$	
Ethyl	$-CH_2CH_3$	
Propyl	$-CH_2CH_2CH_3$	
Isopropyl	$-CH(CH_3)_2$	

10.2

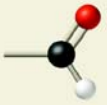
Alkyl Groups

Butyl	$-CH_2CH_2CH_2CH_3$	
tert-Butyl	$-C(CH_3)_3$	
Pentyl	$-CH_2CH_2CH_2CH_2CH_3$	
Isopentyl	$-CH(CH_3)CH_2CH_2CH_3$	
Hexyl	$-CH_2CH_2CH_2CH_2CH_2CH_3$	
Heptyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	
Octyl	$-CH_2CH_2CH_2CH_2CH_2CH_2CH_2CH_3$	

10.2

Functional Groups

- A ***functional group*** is a group of atoms that determines many of the molecule's properties, and that are responsible for chemical reactions.
- Some commonly important functional groups:
  - Alcohol.
  - Aldehydes.
  - Amines.
  - Amides.
  - Esters.

Name	Functional Group	Model
Alcohol	$-OH$	
Aldehyde	$-CHO$	
Carboxylic acid	$-COOH$	
Amine	$-NH_2$	

10.2

Functional Groups

Class	General Formula	Structure	Functional Group
Alcohol	ROH	—Ö—H	Hydroxy group
Carboxylic acid	RCOOH	—C(=O)—Ö—H	Carboxy group
Ester	RCOOR′	—C(=O)—Ö—R′	Ester group
Aldehyde	RCHO	—C(=O)—H	Carbonyl group
Ketone	RCOR′	—C(=O)—R′	Carbonyl group

R represents an alkyl group.

R′ represents a second alkyl group that may or may not be identical to the first alkyl group R.

10.2

Functional Groups

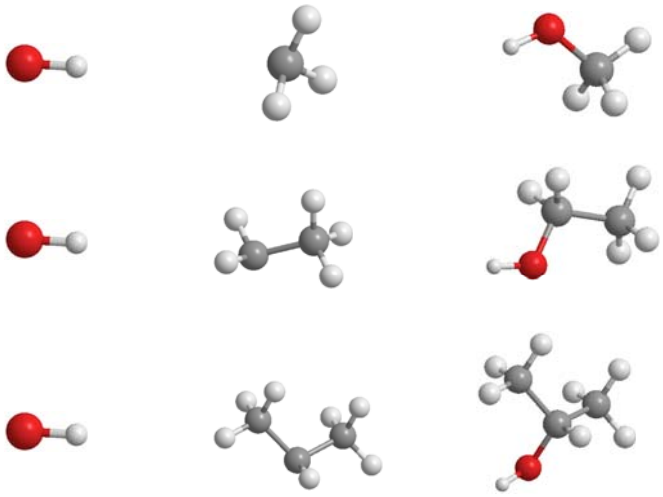
Amine	RNH_2	—N̈(H)—H	Amino group (primary, 1°)
Amine	RNR′H	—N̈(H)—R′	Amino group (secondary, 2°)
Amine	RNR′R″	—N̈(R″)—R′	Amino group (tertiary, 3°)
Amide	$RCONH_2$	—C(=O)—N̈(H)—H	Amide group (primary, 1°)
Amide	RCONR′H	—C(=O)—N̈(H)—R′	Amide group (secondary, 2°)
Amide	RCONR′R″	—C(=O)—N̈(R″)—R′	Amide group (tertiary, 3°)

1°, 2° and 3° indicate one, two, and three R groups bonded to the N atom, respectively

10.2

Examples of Alcohols

Hydoxy group + Alkyl group = Alcohol



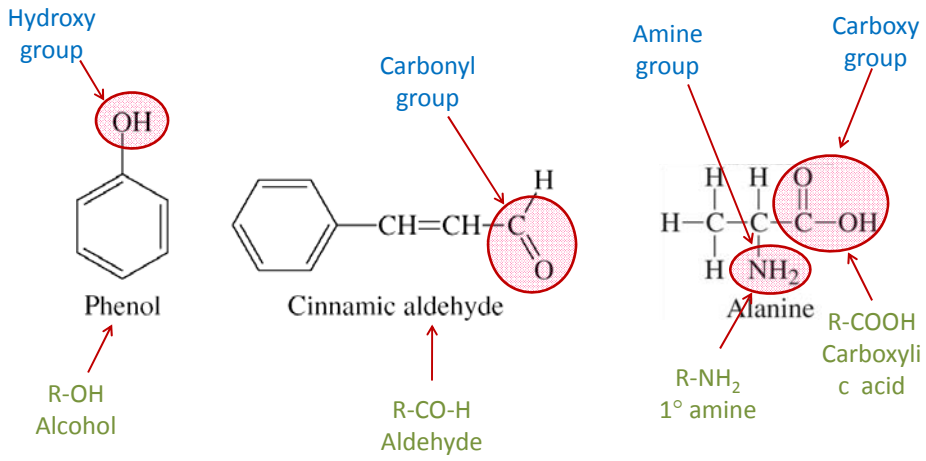
Methanol

Ethanol

Isopropanol *or* Isopropyl alcohol

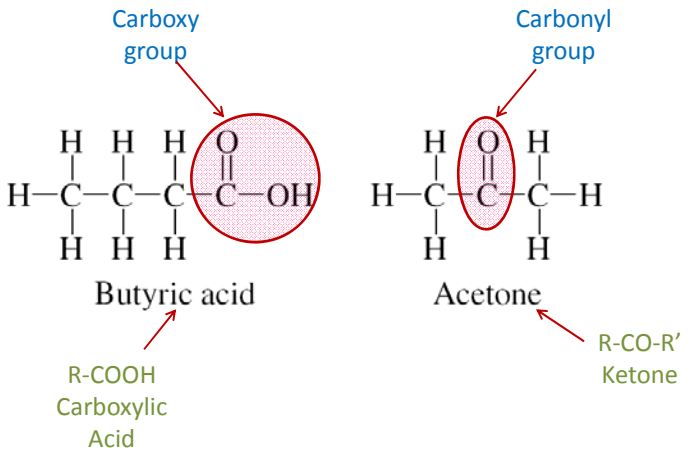
10.2

Identifying Functional Groups



10.2

Identifying Functional Groups



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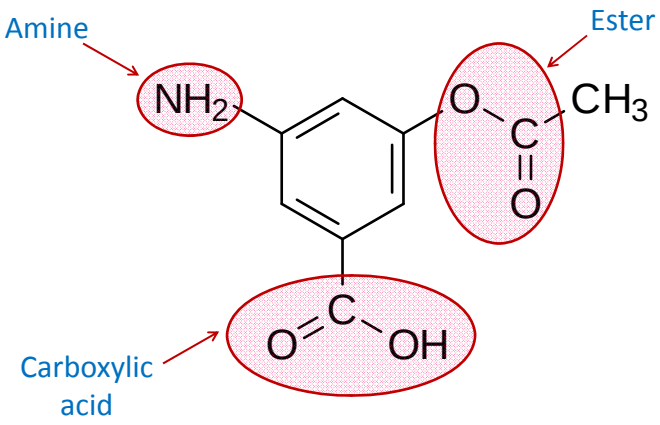
10.2

Identifying Functional Groups



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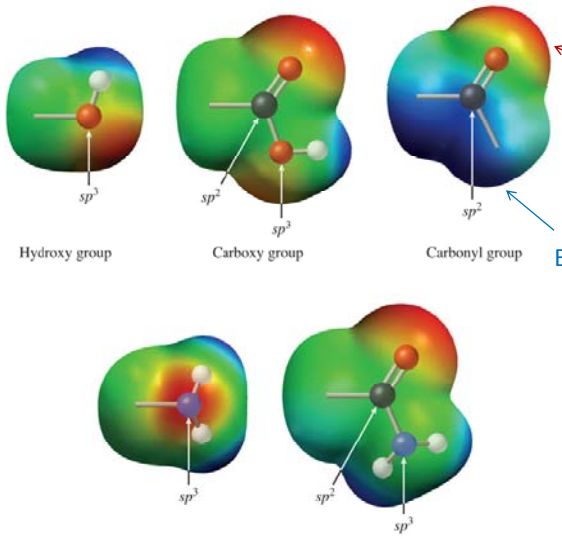
10.2

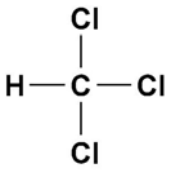
Electrostatic maps of selected functional groups

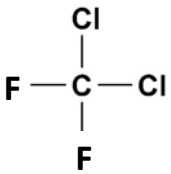


10.2

Names of Organic Compounds

- Organic compounds are named using IUPAC rules.
- There are:
  - ***Systematic names***: names that are based on IUPAC system.
  - ***Trivial names***: names that are commonly used but are not based on IUPAC system.





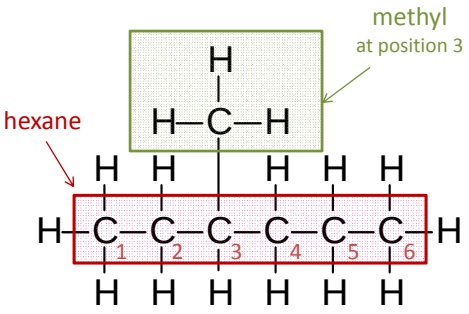
Systematic Name	Trichloromethane	Dichlorodifluoromethane
Trivial Name	Chloroform	Freon

10.2

Naming Organic Compounds (*Nomenclature*)

- ***How to name alkanes.***

1. Identify the longest continuous carbon chain to get the parent name.
2. Number the carbons in the continuous chain, beginning at the end closest to the *substituent*.
3. Identify the *substituent* and use a number and a prefix to specify location and identity, respectively.



3-Methylhexane

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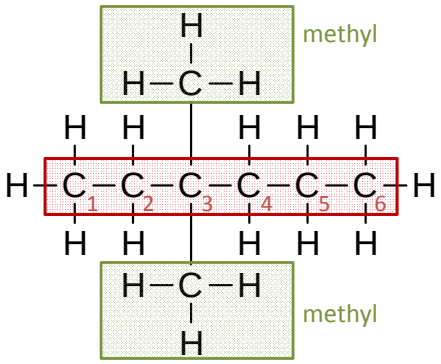
10.2

Naming Organic Compounds

- ***How to name alkanes.***

4. When two or more substituents are there:
   - o If they are identical, use prefixes (di, tri, tetra, …) to indicates the number of substituents.
   - o Also, use numbers as usual to indicate which C atom they are bonded to.



3,3-Dimethylhexane

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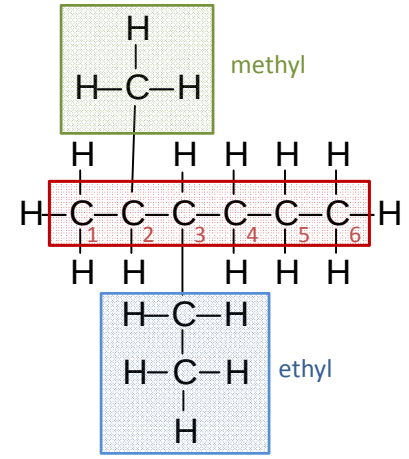
10.2

Naming Organic Compounds

- ***How to name alkanes.***

4. When two or more substituents are there:
   - o If they are <u>not</u> identical, follow the same procedure for identical substituents. However, the substituent names must be put in an *alphabetical order*. (prefixes are not used to determine the alphabetization)



3-Ethyl-2-methylhexane

Notice that incorrect numbering would lead to the name <u>3-isopropylhexane</u>.
To name alkanes, you need to choose the longest chain with the *higher number of substituents*.

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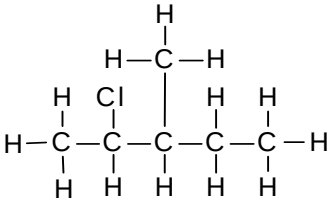
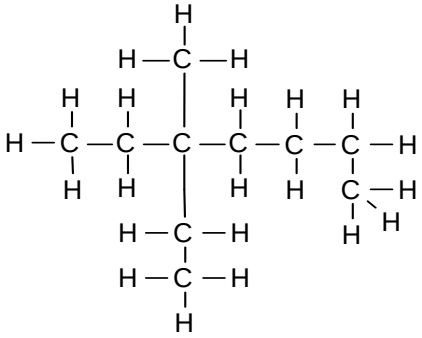
10.2

Naming Organic Compounds

- <u>Exercise:</u>
  Name the following organic compounds:



2-Chloro-3-methylpentane



3-Ethyl-3-methylheptane

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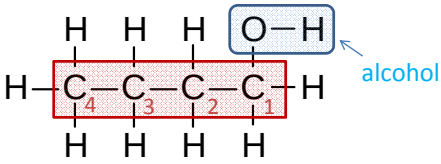
10.2

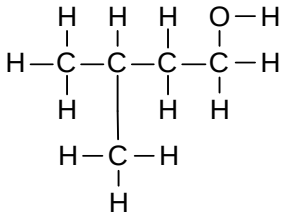
Naming Organic Compounds Containing Functional Groups

- ***How to name alcohols.***

1. Identify the longest chain that includes the –OH group.
2. Change the –*e* ending to -*ol*.
3. Do numbering such that the –OH group is given the lowest number.
4. If the chain also contains an alkyl substituent, give the –OH the lowest number.



1-Butanol



3-Methyl-1-butanol

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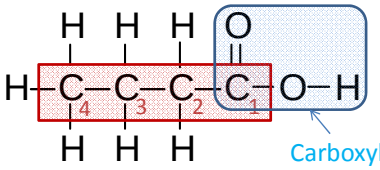
10.2

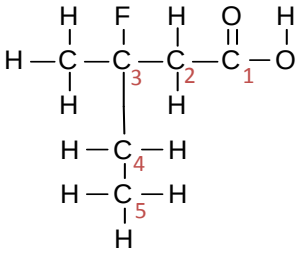
Naming Organic Compounds Containing Functional Groups

- ***How to name carboxylic acids.***

1. Identify the longest chain that includes the carboxyl group.
2. Change the – *e* ending to – *oic acid*.
3. Do numbering starting with the carbonyl (C=O) carbon.
4. Use numbers and prefixes to indicate the position and identity of any substituents.



Butanoic acid



3-Fluoro-3-methyl-pentanoic acid

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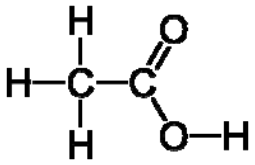
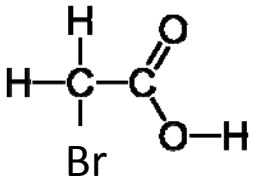
10.2

Naming Organic Compounds Containing Functional Groups

What is the name of the carboxylic acids shown below?





Ethanoic acid

Acetic acid ⟵ *Trivial name* ⟶ Bromoacetic acid

Bromoethanoic acid

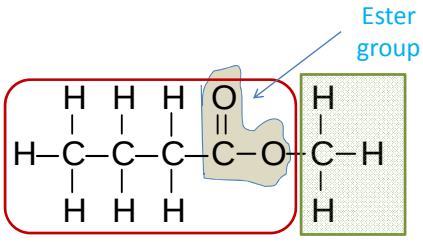
10.2

Naming Organic Compounds Containing Functional Groups

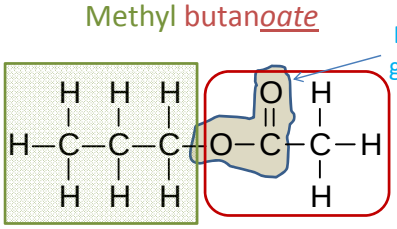
- ***How to name esters.***

  Esters are named as derivatives of carboxylic acids by:

  - locating the ester group.
  - locating the main carbon chain and replacing the *–ic acid* ending with *–oate*.
  - locating the substituent.

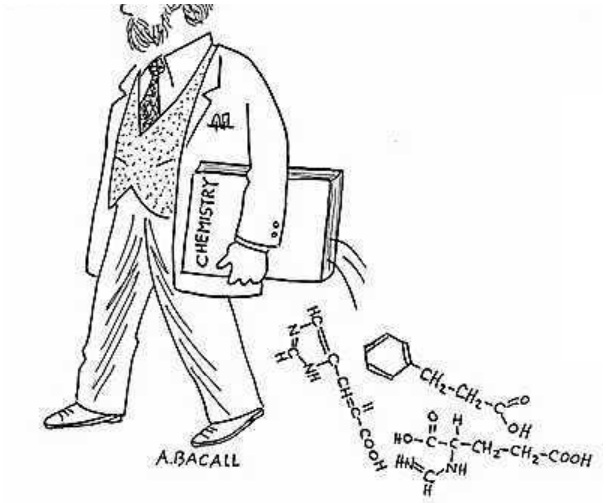


Methyl butan*oate*



Propyl ethan*oate*

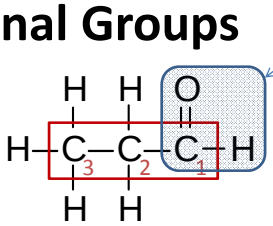
Propyl acetate



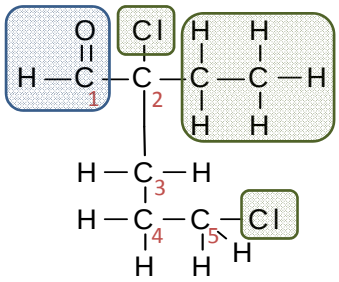
Naming Organic Compounds Containing Functional Groups

- ***How to name aldehydes.***

1. Identify the longest chain that includes the carbonyl group.
2. Change the *–e* ending to - *al*.
3. Number starting with the carbonyl (C=O) carbon.
4. Use numbers and prefixes to indicate the position and identity of any substituents.



Propan*al*



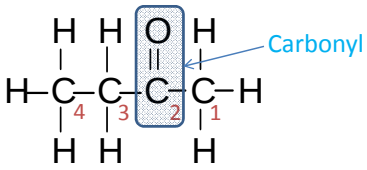
2,5-Dichloro-2-ethylpentan*al*

10.2

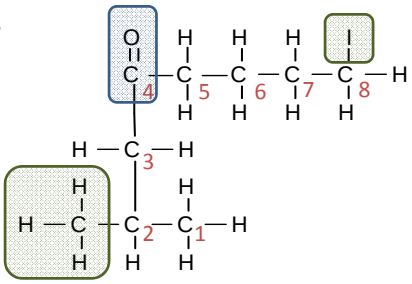
Naming Organic Compounds Containing Functional Groups

- ***How to name ketones.***

1. Identify the longest chain that includes the carbonyl group.
2. Change the *–e* ending to - *one*.
3. Number to give the carbonyl group (C=O) the *lowest possible number*.
4. Use numbers and prefixes to indicate the position and identity of any substituents.



Butan*one*



8-Iodo-2-methyl-4-octan*one*

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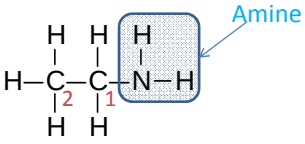
10.2

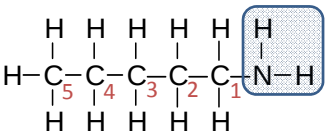
Naming Organic Compounds Containing Functional Groups

- ***How to name primary amines.***

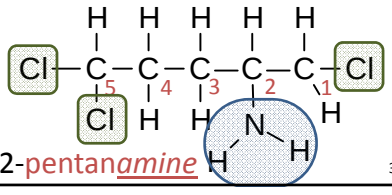
1. Identify the longest chain that includes the $–NH_2$ group.
2. Change the *–e* ending to - *amine*.
3. Number C atoms so that the C atom to which the $–NH_2$ group is bonded is given the *lowest possible number*.
4. Use numbers and prefixes to indicate the position and identity of any substituents.



Ethan*amine*



1-Pentan*amine*



1,5,5-Trichloro-2-pentan*amine*

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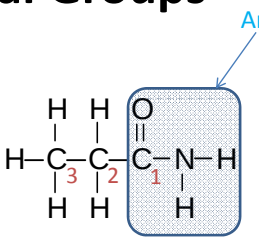
10.2

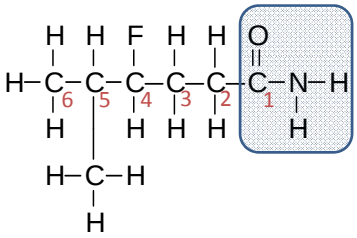
Naming Organic Compounds Containing Functional Groups

- ***How to name primary amides.***

  Primary amides can be named as derivatives of carboxylic acids by replacing the *–ic acid* ending with – *amide*.



Propan*amide*



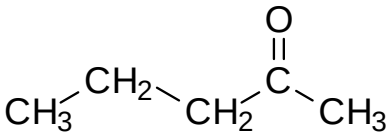
4-Fluoro-5-methylhexan*amide*

10.2

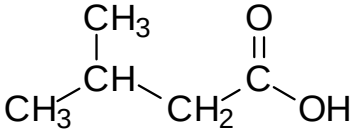
Naming Organic Compounds

- Exercise:

  Name the following compounds.



2-pentanone

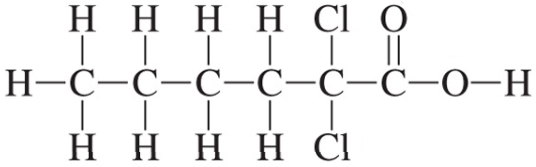


3-methylbutanoic acid

10.3

Representing Organic Molecules

- ***Kekulé structure***: It is similar to Lewis structure but without showing the lone pairs. It is very commonly used in organic chemistry.



Kekulé structure

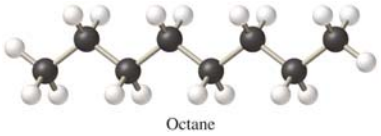
- *What is the name of this compound?*

  2,2-Dichlorohexanoic acid.

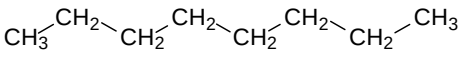
10.3

Representing Organic Molecules

- ***Condensed structural formula***: (or ***Condensed Structure***): It shows the same information as a structural formula but in a condensed form.



Octane



$CH_3CH_2CH_2CH_2CH_2CH_2CH_2CH_3$

$CH_3(CH_2)_6CH_3$

C_8H_{18}

Ball-and-stick structure

Structural formula

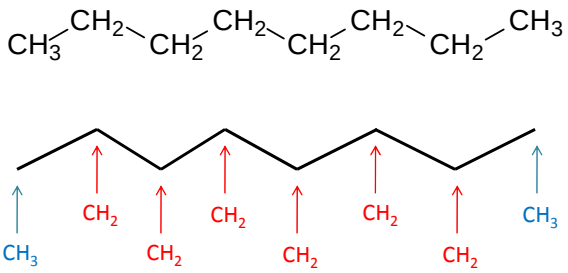
Condensed structure

Molecular formula

10.3

Representing Organic Molecules

- ***Skeletal Structure***: It consists of straight lines that represent C-C bonds. H atoms bonded to C atoms are not shown. Atoms other than carbon or hydrogen (*Heteroatoms*) are shown explicitly.

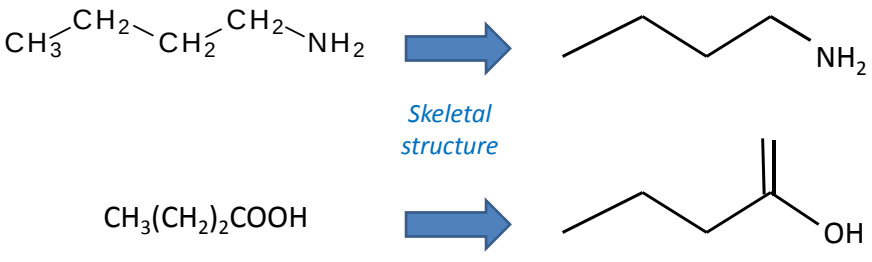


Skeletal structure

10.3

Representing Organic Molecules

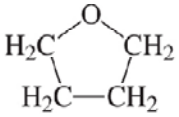
- ***Skeletal Structure***: It consists of straight lines that represent C-C bonds. H atoms bonded to C atoms are not shown. Atoms other than carbon or hydrogen (*Heteroatoms*) are shown explicitly.



10.3

Representing Organic Molecules

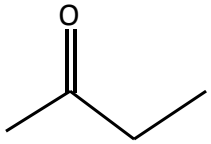
- Exercise:
  Give the skeletal structures of the following compounds.

Name	Structural Formula	Skeletal Structure
Propanone (acetone)	CH_3CCH_3 (O double-bonded to C)	
Ethylamine	$CH_3CH_2NH_2$	
Tetrahydrofuran		

10.3

Representing Organic Molecules

- Exercise:
  Write the molecular formula and a structural formula for the following molecule.



$CH_3COCH_2CH_3$ *Structural formula*

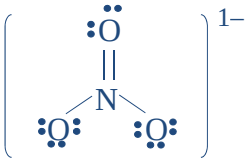
C_4H_8O *Molecular formula*

10.3

Resonance

- ***Resonance*** is repositioning of electrons to produce other equivalent structures of the molecule.
  - *You will need to review how to draw Lewis structures for simple organic compounds.*
- Example: Draw the Lewis structure of nitrate ion (NO_3^-) and show resonance structure.

# of valence electrons:
$(5+3\times6+1)e^- - 6e^- = 18e^-$

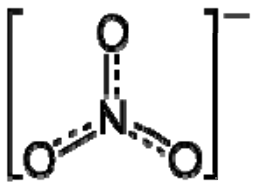


10.3

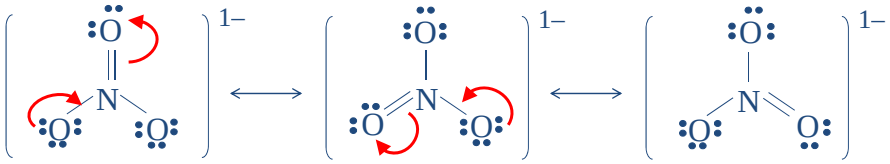
Resonance

☞ The nitrate ion structure is the average of all the three ***equivalent*** structures, not one of them.

☞ The three NO bonds are found from experiments to be identical.



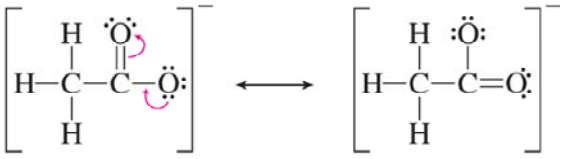
Resonance structures:



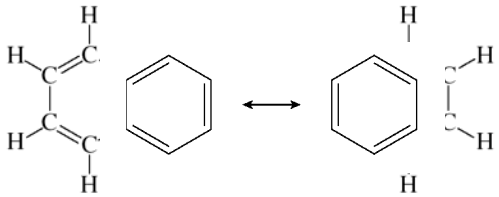
10.3

More Examples on Resonance Structures

- The anion produced from ethanoic acid.



- Benzene molecule (C_6H_6)



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