CHEM110 – Chapter 2 The Language of Chemistry

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2.2 THREE-DIMENSIONAL STRUCTURES

In addition to representing structures

 also need to depict way chemical bonds break or form

Use MECHANISTIC ARROWS



2.2 THREE-DIMENSIONAL STRUCTURES

Bond breaking

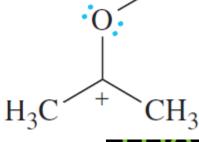
$$H \stackrel{\frown}{-} Cl \longrightarrow H^+ + Cl^-$$

Bond making

$$H_3$$
C CH_3 H_3 C CH_3

Charge neutralisation

$$H_3C$$
 CH_3
 H_3C





2.3 NOMENCLATURE

- Systematic naming of compounds
- International Union of Pure and Applied Chemistry (IUPAC)
- Common unsystematic names rather than systematic IUPAC name
 - The systematic name of water is oxidane
 - Only a small number of common compound names are accepted by IUPAC



1. The element closer to the left of the periodic table appears first

2. First element retains its elemental name.

3. The second element is named with the suffix -ide

4. A prefix specifying the number of atoms present is included when > 1 atom

TABLE 2.4 Common roots for naming compounds.

| Element | Full name | Root |
|---------|------------|---------|
| As | arsenic | arsen- |
| Br | bromine | brom- |
| C | carbon | carb- |
| Cl | chlorine | chlor- |
| F | fluorine | fluor- |
| Н | hydrogen | hydr- |
| Ĭ | iodine | iod- |
| N | nitrogen | nitr- |
| O | oxygen | ox- |
| Р | phosphorus | phosph- |
| S | sulfur | sulf- |



TABLE 2.5 Number prefixes for chemical names.

| Number | Prefix | Example | Name |
|--------|--------|-----------------------|--------------------------|
| 1 | mono- | CO | carbon monoxide(a) |
| 2 | di- | SiO_2 | silicon dioxide |
| 3 | tri- | \mathbf{NI}_3 | nitrogen triiodide |
| 4 | tetra- | SnCl ₄ | tin tetrachloride |
| 5 | penta- | PCl_5 | phosphorus pentachloride |
| 6 | hexa- | SF_6 | sulfur hexafluoride |
| 7 | hepta- | IF_7 | iodine heptafluoride |

⁽a) The final 'o' of the prefix is omitted in this case.



Worked Example 2.9 – page 49

Name the following binary compounds: SO_2 , CS_2 , BCI_3 , BrF_5 , N_2O_5



- Hydrogen requires special consideration
 - With elements from group 1 and 17
 - GROUP 1 Lithium hydride LiH
 - GROUP 17 Hydrogen fluoride HF
 - With elements from groups 2 and 16, except oxygen
 - GROUP 2 Calcium hydride CaH₂
 - GROUP 16 Hydrogen sulfide H₂S
 - Groups 13, 14 and 15
 - Unsystematic names e.g. B₂H₆ diborane



 Binary (containing 2) ionic compounds are written with the cation first and then the anion, which takes the suffix –ide, last

Potassium iodide
 KI

Calcium fluoride CaF₂

Ionic compounds may contain polyatomic ions

Ammonium NH₄⁺

• Nitrate NO₃-



2.3 NOMENCLATURE: OXOANIONS

- 1. The root name arises from the central atom
 - e.g. carbonate CO₃²-
- 2. When an element forms 2 different oxoanions, the one with fewer oxygen atoms ends in —ite, the one with more oxygens ends in —ate
 - Sulfite SO₃²⁻
 - Sulfate SO₄²⁻



2.3 NOMENCLATURE: OXOANIONS

- 3. Four oxoanions for chlorine, bromine and iodine.

 Distinguished by prefixes and suffixes -
 - Hypobromite BrO
 - Bromite BrO₂
 - Bromate BrO₃-
 - Perbromate BrO₄⁻
- 4. A polyatomic anion with a charge more negative than 1may add H⁺ to give another anion. Named from the parent anion by adding the word hydrogen
 - Hydrogen phosphate HPO₄²⁻
 - Dihydrogen phosphate H₂PO₄-



Composed primarily of carbon and hydrogen atoms

 Naming system based on number of carbons in the main part of the molecule

 parent molecule

Start with FUNCTIONAL GROUPS



FUNCTIONAL GROUPS

- A group of one or more atoms within a molecule,
 bonded together in a particular way
- Usually the point of reaction within a molecule
- Organic molecules are named according to functional groups (as well as the parent)
- Molecules containing same functional group tend to behave in chemically similar ways



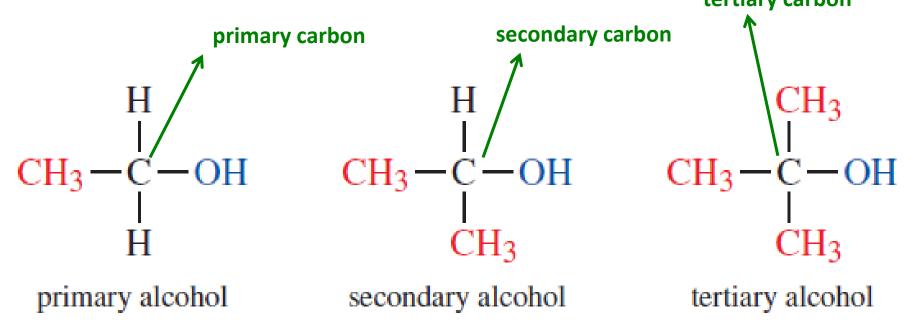
| Functional group | Name of group | Found in | R = |
|----------------------|---------------|------------------|--------|
| R—O | hydroxyl | alcohols | С |
| O C H | carbonyl | aldehydes | C or H |
| R C R | carbonyl | ketones | С |
| O C OH | carboxyl | carboxylic acids | C or H |

Table 2.7



2.3 NOMENCLATURE: ALCOHOLS

 Hydroxyl (-OH) functional group attached to other carbon atoms





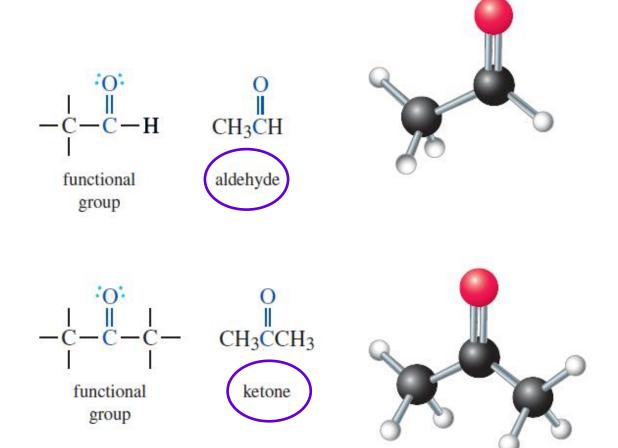
Worked Example 2.10 – page 51

Write condensed structural formulae for the two alcohols with the molecular formula C₃H₈O. Classify each as primary, secondary or tertiary.



2.3 NOMENCLATURE: CARBONYL GROUPS

Carbonyl (C=O) functional group





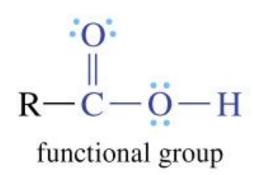
Worked Example 2.11 – page 52

Write condensed structural formulae for the two aldehydes with the chemical formula C_4H_8O .

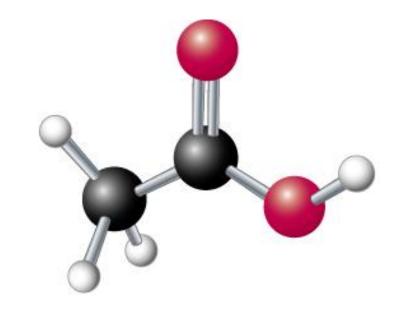


2.3 NOMENCLATURE: CARBOXYLIC ACIDS

Carboxyl group → –COOH









Worked Example 2.12 – page 53

Write condensed structural formulae for the carboxylic acid with the molecular formula $C_3H_6O_2$.



- Contain only CARBON and HYDROGEN and only SINGLE BONDS between the carbons
 - $-C_nH_{2n+2} \rightarrow$ Acyclic alkanes (carbons joined in chains)
 - C_nH_{2n} → Cycloalkanes (carbons joined in rings)
- Sometimes called SATURATED HYDROCARBONS
 - all the carbon-carbon bonds are single
- Two parts to the name
 - Prefix → # carbons in the chain
 - Ending → "-ane" indicating an alkane



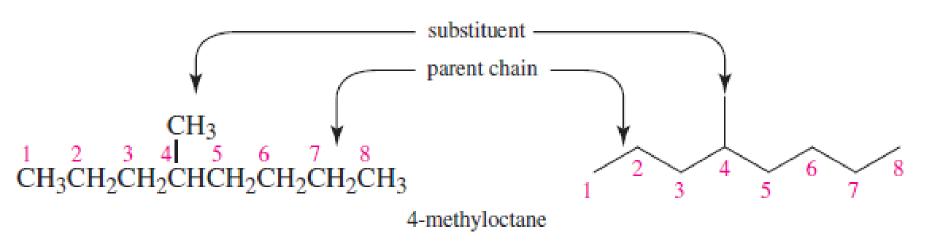
| meth- | |
|-------|----|
| | 1 |
| eth- | 2 |
| prop- | 3 |
| but- | 4 |
| pent- | 5 |
| hex- | 6 |
| hept- | 7 |
| oct- | 8 |
| non- | 9 |
| dec- | 10 |



- 1. Name for alkane with unbranched chain of carbon atoms consists of a prefix showing the number of carbon atoms in the chain, and the ending —ane
- 2. For branched-chain alkanes → the longest chain of carbon atoms is the parent chain and its name is the root name

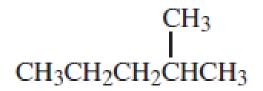


- Parent chain: the longest carbon chain
- Substituents: any branch off the parent chain

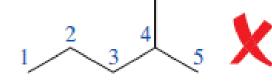




3. One substituent → number the parent chain so that the carbon atom bearing the substituent is given the lowest possible number

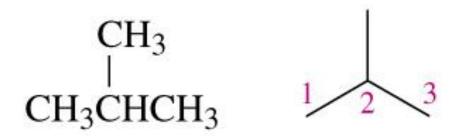








4. Give the substituent on the parent chain a name and a number. The number shows the carbon atom of the parent chain to which the substituent is bonded. Use a hyphen to connect the number to the name.



2-methylpropane

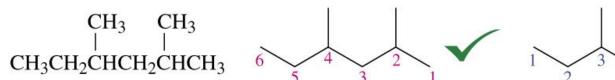


TABLE 2.9 Names, formulae and abbreviations of the most common alkyl groups.

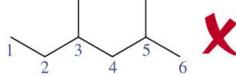
| Name | Condensed structural formula | Abbreviation |
|------------|--|--------------|
| methyl | $-CH_3$ | Me |
| ethyl | $-CH_2CH_3$ | Et |
| propyl | —CH ₂ CH ₂ CH ₃ | Pr |
| isopropyl | —СНСН ₃ | i-Pr |
| | $^{1}_{\mathrm{CH}_{3}}$ | |
| butyl | —CH ₂ CH ₂ CH ₂ CH ₃ | Bu |
| isobutyl | −CH ₂ CHCH ₃ | i-Bu |
| | $^{ m I}_{ m CH_3}$ | |
| sec-butyl | −CHCH2CH3 | s-Bu |
| | $^{ m I}_{ m CH_3}$ | |
| tert-butyl | CH ₃ | <i>t</i> -Bu |
| | -CCH ₃ | |
| | CH ₃ | |



5. If two or more identical substituents, number the parent chain from the end that gives the lowest numbers to the substituents. The number of times the substituent occurs is indicated by the prefixes *di-, tri-, tetra-, penta-, hexa-,* and so on.



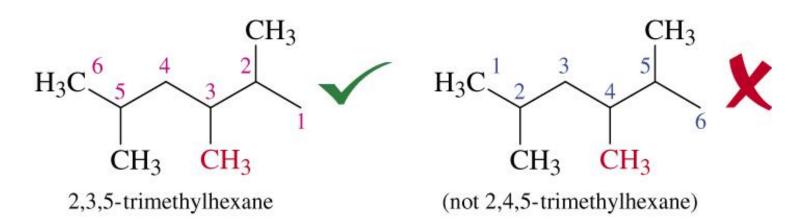
2,4-dimethylhexane



(not 3,5-dimethylhexane)



6. If step 5 leads to more than one possibility, number the parent chain such that the first point of difference has the lowest possible number.

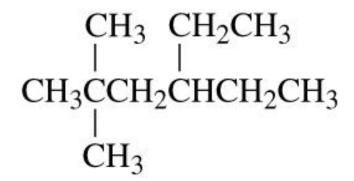


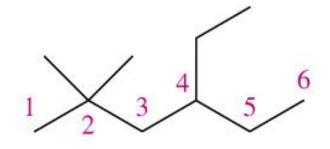


7. If there are two or more substituents list them in alphabetical order. If there are different substituents in equivalent positions on opposite ends of the parent chain, the substituent of lower alphabetical order is given the lower number.



8. The prefixes *di-, tri-,* and hyphenated prefixes such as *sec-* and *tert-* are disregarded for the purposes of alphabetical ordering.



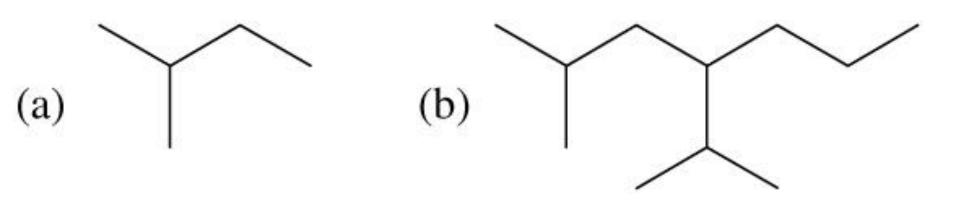


4-ethyl-2,2-dimethylhexane (not 2,2-dimethyl-4-ethylhexane)



Worked Example 2.13 – page 56

Write IUPAC names for the following alkanes:

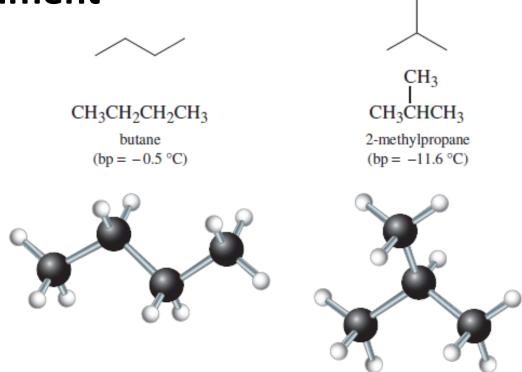




2.3 ISOMERISATION: ALKANES

Constitutional isomers

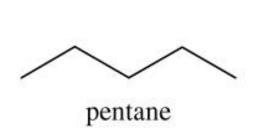
 compounds with the same chemical formula but different order of attachment

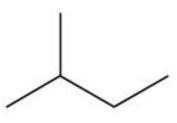


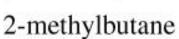


2.3 ISOMERISATION: ALKANES

 C_5H_{12}









2,2-dimethylpropane



Worked Example 2.14 – page 58

Do the structural formulae in each of the following pairs of molecules represent the same compound or constitutional isomers?

(a)
$$CH_3CH_2CH_2CH_2CH_3$$
 and $CH_3CH_2CH_2$ | (each is C_6H_{14}) $CH_2CH_2CH_3$

CH₃ CH₃ CH₃ CH₃ (b) CH₃CHCH₂CH and CH₃CHCHCH₃ (each is
$$C_7H_{16}$$
)
$$\begin{array}{c|cccc} CH_3 & CH_3$$



Worked Example 2.15 – page 59

Draw the structural formulae for the five constitutional isomers with the molecular formula C_6H_{14} .



GENERAL ORGANIC NOMENCLATURE

Page 59-60

Please go over yourselves

Practice Exercise 2.19 and Review Exercise
2.8



LEARNING OBJECTIVES

- Understand measurement and units relevant to studies in chemistry
- Learn different representations for molecules
- Be able to name chemical species using conventional chemical nomenclature



Ch 2 – Wrap up

- Summary pg 61
- Key Concepts and Equations pg 62
- Key Terms pg 63
- Review Questions pg 63
- Review Problems pg 64
- Additional Problems pg 68

