Copyrighted Material

In this chapter, we are faced with a large amount of factual material to digest. It is not very challenging intellectually, but it takes time to absorb. It is important to study the material a little at a time, and to solve at least half of the exercises. <u>You should use the interactive menu on the</u> <u>CD when you start problem solving</u>. Working problems is by far the best way to learn this topic. Once you have mastered nomenclature problem solving, you will gain two distinct skills. First you have learned essential vocabulary. Secondly, you will have taken a great step forward in learning to 'read' a chemical structure accurately, which is a crucial factor in mastering organic synthesis, the most challenging and aesthetically pleasing part of Organic Chemistry.

We shall start by discussing the basic rules of nomenclature, and work examples for alkanes, alkenes and alkynes. Then we shall study the nomenclature of common functional groups. Work hard and good luck.

I. INTRODUCTION TO IUPAC NOMENCLATURE

We are aware that there are millions of known organic compounds. Thus, there is a need to develop a systematic method for naming compounds so that scientists across the world would be able to recognize, or rapidly work out, structures without having to memorize huge numbers of names. The method that was adopted was devised by the International Union of Pure and Applied Chemistry (IUPAC). The basic format for all IUPAC names is summarized in the text box below.

Basic Format of IUPAC Names MATERIAL J.M.E. QUIRKE 9/1/1999

- **1**. Substituents are placed in alphabetical order at the beginning of the name.
- 2. The position of each substituent is listed at the beginning of the name, also.
- **3**. The final 'word' in the name defines:

i.

- a. The length of the longest carbon chain
- **b.** The number and the sites of carbon-carbon π bonds in the longest chain
- c. The nature and the position of the parent (dominant) functional group in the molecule
- **3**. The final 'word' is divided into three syllables:
 - **a**. The first syllable defines the chain length
 - **b**. The second syllable defines the number and the site of carbon-carbon π bonds in the longest chain as follows:
 - 'an' indicates zero carbon-carbon π bonds
 - ii. 'en' indicates a carbon-carbon double bond(s), C=C
 - iii. 'yn' indicates a carbon-carbon triple bond(s), C≡C
 - c. The third syllable indicates the parent functional group and is the 'family ending' of the name. If the molecule is an aliphatic hydrocarbon, *i.e.*, an alkane, alkene or alkyne, this syllable is omitted.

The IUPAC system seems complicated, but it is easy to use once you master a few simple concepts. To illustrate how IUPAC nomenclature works, we shall look at a IUPAC name and deduce the structure of the molecule. Clearly, you do not know the terminology yet, but you will soon be able to work out such structures on your own.



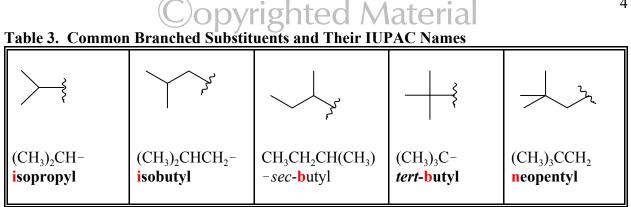
Chain Length*	Prefix	Chain Length*	Prefix	Chain Length*	Prefix
1 carbon	Meth	6 carbons	Hex	11 carbons	Undec
2 carbons	Eth	7 carbons	Hept	12 carbons	Dodec
3 carbons	Prop	8 carbons	Oct	20 carbons	Eicos
4 carbons	But	9 carbons	Non	30 carbons	Tricos
5 carbons	Pent	10 carbons	Dec	40 carbons	Tetracont

Copyrighted MaterialTable 1.Syllables That Define the Carbon Chain Length

II.C NAMING AND NUMBERING STRAIGHT CHAIN ALKYL SUBSTITUENTS: MULTIPLE SUBSTITUENTS

Guidelines for Naming Straight Chain Alkyl Substituents

- 1. **Redraw the structure**.
- 2. Identify the longest carbon chain bearing the parent functional group.
- 3. Number the longest chain (left-to-right or right-to-left) so that the parent group, if any, is assigned the lowest number possible.
- Identify the branches on the longest chain. These are the sites of the substituents.
 Number the position of each branch point, keeping the numbers as low as possible.
- The numbering format MUST assign the lowest number possible to the parent group.
 Name the substituent by counting the number of carbons on the branch and
- adding 'yl' to the appropriate prefix from Table 1. For example, if the alkyl substituent contains two carbons, it will be an ethyl group.
- 7. **List the substituents, and their positions, in alphabetical order at the beginning of the name**. If a molecule has an ethyl group at position 3, it is a 3-ethyl-compound. If there is more than one substituent of the same type, see Section II.C.1.
- Note Every substituent MUST be accompanied by a number



Note: The red letter in bold face is the one used in the alphabetizing process.

These branched substituents are not a challenge in nomenclature. Once the branched substituent is identified, numbered and named, it is treated like any other substituent. The only awkward issue is to know which letter in the substituent is used in the alphabetizing process, see Table 3.

The alternative approach to naming branched substituents is to number the site of the substituent on the longest chain and name the entire substituent is placed in parenthesis, immediately after the numbered site. When identifying the branching site on the substituent, start the numbering from the longest chain of the molecule and place these numbers within the parenthesis. The carbon attached to the longest chain will be C-1.

© COPYRIGHTED MATERIAL J.M.E. QUIRKE 9/1/1999

II.C.1 Working With More Than One Substituents of the Same Type

When a compound bears several substituents of the same type, list all of them together, numbering the positions of each substituent, and adding a prefix that designates the total number of these substituents present. The prefixes are listed in Table 2. For example, a molecule bearing three methyl substituents, two of which are attached to C-3 and one to C-4 would be named a 3.3.4trimethyl system. Notice, we used the term '3,3,4' to indicates the locations of the substituents. The term 'tri' confirms the fact that three identical groups are present. Note

If there is more than one parent functional group, we would also use the prefixes in Table 2 below. You can download this table from the CD.

# Substituents	Prefix	# Substituents	Prefix
2	Di	6	Hexa
3	Tri	7	Hepta
4	Tetra	8	Octa
5	Penta	9	Nona

Prefixes Defining The Number of Identical Substituents Present Table 2.