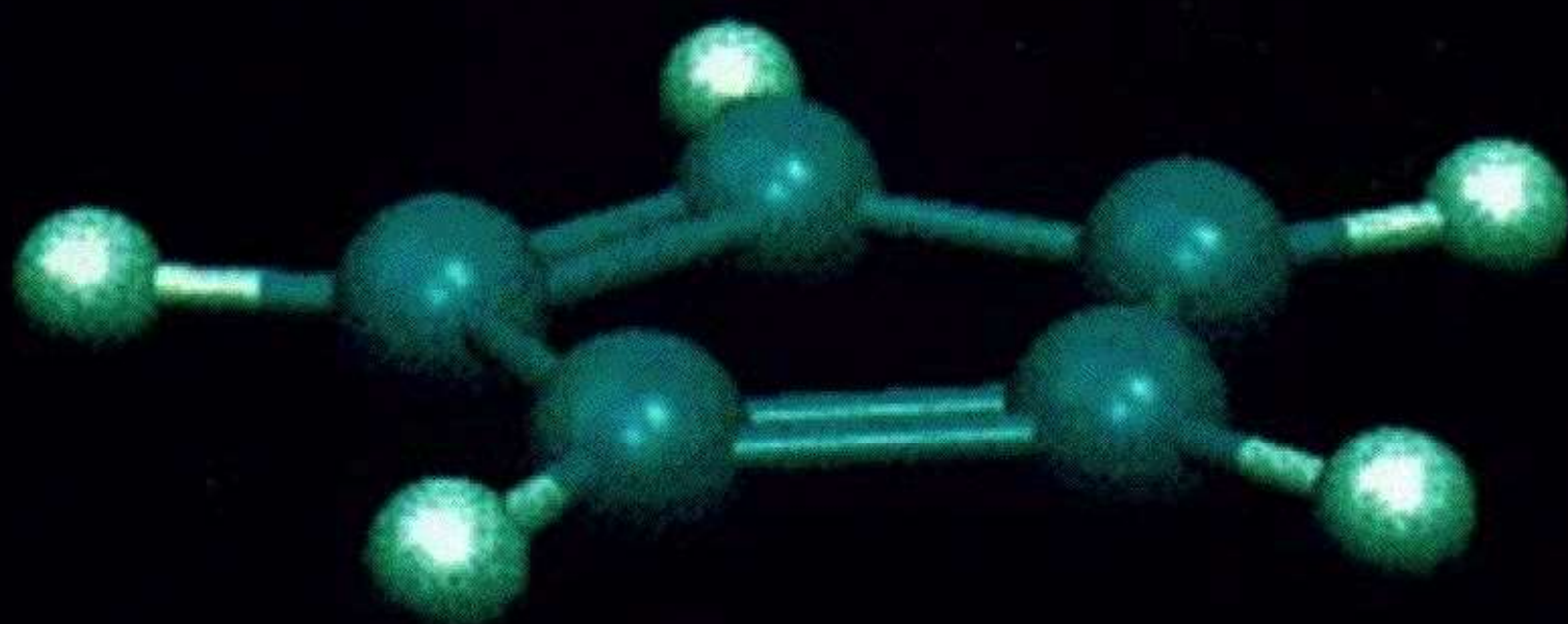
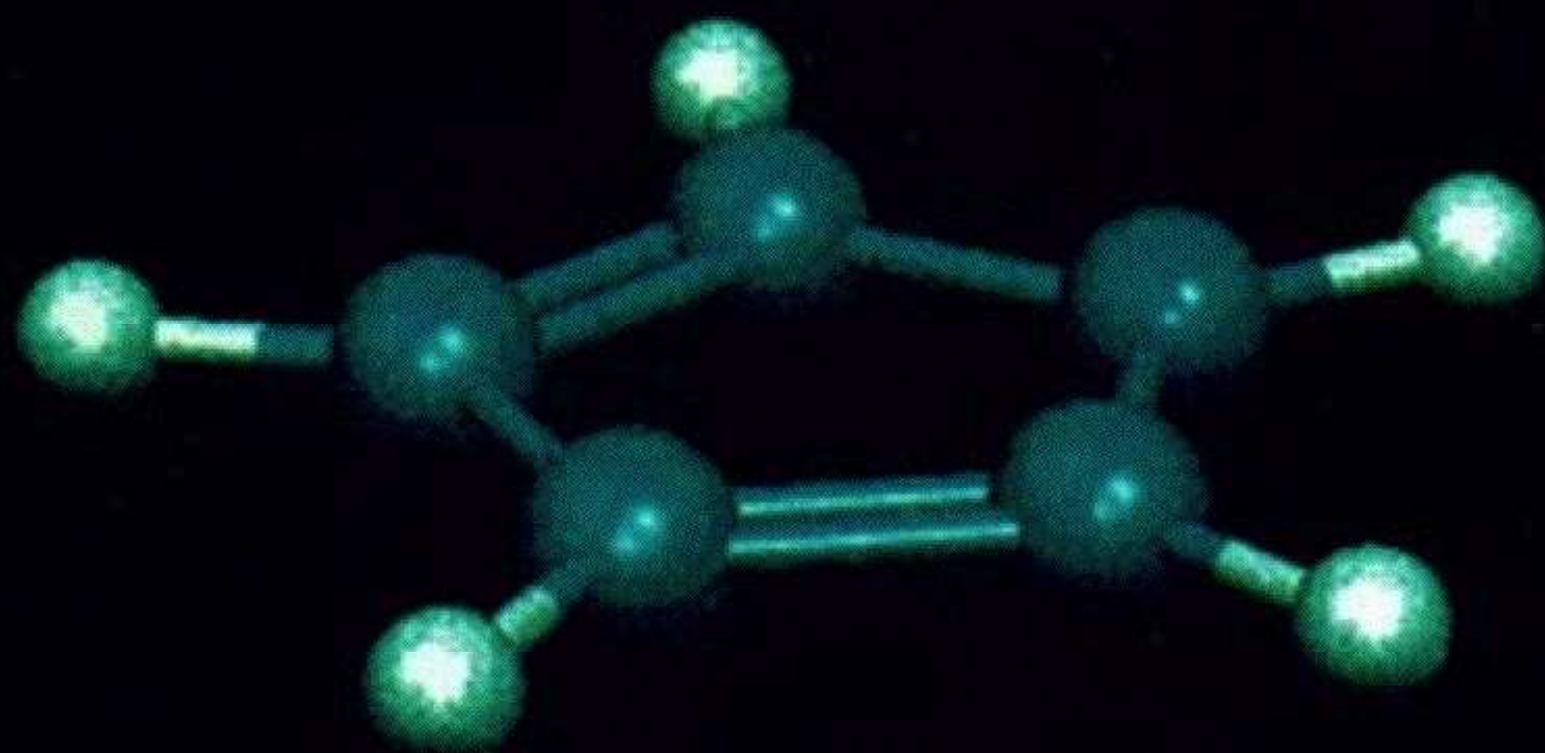




# **BASIC TRAINING IN CHEMISTRY**

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**STEVEN HOENIG**



# **Basic Training in Chemistry**

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# **Basic Training in Chemistry**

**Steven L. Hoenig**

*Ridgewood, New York*

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**To Lena and Alan**

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## Preface

This book was written as a quick reference to the many different concepts and ideas encountered in chemistry. Most books these days go into a detailed explanation of one subject and go no further. This is simply an attempt to present briefly some of the various subjects that make up the whole of chemistry. The different subjects covered include general chemistry, inorganic chemistry, organic chemistry, and spectral analysis. The material is brief, but hopefully detailed enough to be of use. Keep in mind that the material is written for a reader who is familiar with the subject of chemistry. It has been the author's intention to present in one ready source several disciplines that are used and referred to often.

This book was written not to be a chemistry text unto itself, but rather as a supplement that can be used repeatedly throughout a course of study and thereafter. This does not preclude it from being used by others that would find it useful as a reference source as well.

Having kept this in mind during its preparation, the material is presented in a manner in which the reader should have some knowledge of the material. Only the basics are stated because a detailed explanation was not the goal but rather to present a number of chemical concepts in one source.

The first chapter deals with material that is commonly covered in almost every first year general chemistry course. The concepts are presented in, I hope, a clear and concise manner. No detailed explanation of the origin of the material or problems are presented. Only that which is needed to understand the concept is stated. If more detailed explanation is needed any general chemistry text would suffice. And if examples are of use, any review book could be used.

The second chapter covers inorganic chemistry. Those most commonly encountered concepts are presented, such as, coordination numbers, crystal systems, and ionic crystals. More detailed explanation of the coordination encountered in bonding of inorganic compounds requires a deeper explanation than this book was intended for.

Chapter three consists mostly of organic reactions listed according to their preparation and reactions. The mechanisms of the various reactions are not discussed since there are numerous texts which are devoted to the subject. A section is devoted to the concept of isomers since any treatment of organic chemistry must include an understanding it. A section on polymer structures is also presented since it is impossible these days not to come across some discussion of it.

The fourth chapter covers instrumental analysis. No attempt is made to explain the inner workings of the different instruments or the mechanisms by which various spectra is produced. The material listed is for the use by those that are familiar with the different type of spectra encountered in the instrumental analysis of chemical compounds. The tables and charts would be useful for the interpretation of various spectra generated in the course of analyzing a chemical substance. Listed are tables that would be useful as for the interpretation of ultra-violet (uv), infra-red (ir), nuclear magnetic resonance (nmr) and mass spectroscopy (ms) spectra.

Chapter five consists of physical constants and unit measurements that are commonly encountered throughout the application of chemistry.

Chapter six contains certain mathematical concepts that are useful to have when reviewing or working with certain concepts encountered in chemistry.

*Steven L. Hoenig*

## **Acknowledgements**

I wish to express my deepest gratitude to Richard Leff, without whose faith and belief in me this book would not have been possible. And I wish to express my thanks to the following Richard Kolodkin, Robert Glatt, Cindy and Harriet Cuccias, and Anthony Woll, who know what the meaning of friendship is.

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## Chapter 1

### General Chemistry

1.1 Atomic Structure and the Periodic Table

1.2 Chemical Bonding

1.3 Gases

1.4 Solutions

1.5 Acids and Bases

1.6 Thermodynamics

1.7 Equilibria

1.8 Kinetics

### 1.1 Atomic Structure and the Periodic Table

#### 1.1.1 Constituents of the Atom

The atom of any element consists of three basic types of particles ... the electron (a negatively charged particle), the proton (a positively charged particle), and the neutron (a neutrally charged particle). The protons and neutrons occupy the nucleus while the electrons are outside of the nucleus. The protons and neutrons contribute very little to the total volume but account for the majority of the atom's mass. However, the atom's volume is determined by the electrons, which contribute very little to the mass. Table 1.1 summarizes the properties of these three particles.

Table 1.1. Properties of the Proton, Electron, and Neutron

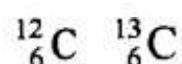
| Particle | Mass                      | Electric Charge                  | Unit Charge |
|----------|---------------------------|----------------------------------|-------------|
| Proton   | $1.672 \times 10^{-24}$ g | $+1.602 \times 10^{-19}$ coulomb | +1          |
| Electron | $9.108 \times 10^{-28}$ g | $-1.602 \times 10^{-19}$ coulomb | -1          |
| Neutron  | $1.675 \times 10^{-24}$ g | 0                                | 0           |

The **atomic number** (Z) of an element is the number of protons within the nucleus of an atom of that element. In a neutral atom, the number of protons and electrons are equal and the atomic number also indicates the number of electrons.

The **mass number** (A) is the sum of the protons and neutrons present in the atom. The number of neutrons can be determined by (A - Z). The symbol for denoting the atomic number and mass number for an element X is as follows:



Atoms that have the same atomic number (equal number of protons) but different atomic masses (unequal number of neutrons) are referred to as isotopes. For example, carbon consists of two isotopes, carbon-12 and carbon-13:



The **atomic mass unit** (amu) is defined as 1/12 the mass of a carbon-12 isotope. The relative **atomic mass** of an element is the weighted average of the isotopes relative to 1/12 of the carbon-12 isotope. For example, the atomic mass of neon is 20.17 amu and is calculated from the following data: neon-19 (amu of 19.99245, natural abundance of 90.92%), neon-20 (amu of 20.99396, natural abundance of 0.260%) and neon-21 (amu of 21.99139, natural abundance of 8.82%):

$$\begin{aligned} \text{a.m.} \quad \text{neon} &= (19.99245 \times 0.9092) + (20.99396 \times 0.00260) + (21.99139 \times 0.0882) \\ &= 20.17 \text{ amu} \end{aligned}$$

The relative **molecular mass** is the sum of the atomic masses for each atom in the molecule. For  $\text{H}_2\text{SO}_4 = (1 \times 2) + 32 + (16 \times 4) = 98$ .

The **mole** (mol) is simply a unit of quantity, it represents a certain amount of material, i.e. atoms or molecules. The numerical value of one mole is  $6.023 \times 10^{23}$  and is referred to as **Avogadro's number**. The mole is defined as the mass, in grams, equal to the atomic mass of an element or molecule. Therefore, 1 mole of carbon weighs 12 grams and contains  $6.023 \times 10^{23}$  carbon atoms. The following formula can be used to find the number of moles:

$$\text{moles} = \frac{\text{mass in grams}}{\text{atomic (or molecular) mass}}$$

### 1.1.2 Quantum Numbers

From quantum mechanics a set of equations called wave equations are obtained. A series of solutions to these equations, called wave functions, gives the four quantum numbers required to describe the placement of the electrons in the hydrogen atom or in other atoms.

The principal quantum number,  $n$ , determines the energy of an orbital and has a value of  $n = 1, 2, 3, 4, \dots$

The angular momentum quantum number,  $\lambda$ , determines the "shape" of the orbital and has a value of 0 to  $(n - 1)$  for every value of  $n$ .

The magnetic quantum number,  $m_l$ , determines the orientation of the orbital in space and has a value of  $-\lambda$  to  $+\lambda$ .

The electron spin quantum number,  $m_s$ , determines the magnetic field generated by the electron and has a value of  $-\frac{1}{2}$  or  $+\frac{1}{2}$ .

Table 1.2. Quantum Numbers and Electron Distribution

| Shell | Principal quantum number $n$ | Angular momentum quantum number $\lambda$ | Orbital designation* | Magnetic quantum number $m_\lambda$ | Spin quantum number $m_s$    | Total number of electrons per orbital |
|-------|------------------------------|-------------------------------------------|----------------------|-------------------------------------|------------------------------|---------------------------------------|
| K     | 1                            | 0                                         | s                    | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ | 2                                     |
| L     | 2                            | 0                                         | s                    | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ | 2                                     |
|       |                              | 1                                         | $p_x$                | -1                                  | $-\frac{1}{2}, +\frac{1}{2}$ | 6                                     |
|       |                              |                                           | $p_y$                | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              |                                           | $p_z$                | +1                                  | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
| M     | 3                            | 0                                         | s                    | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ | 2                                     |
|       |                              | 1                                         | $p_x$                | -1                                  | $-\frac{1}{2}, +\frac{1}{2}$ | 6                                     |
|       |                              |                                           | $p_y$                | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              |                                           | $p_z$                | +1                                  | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              | 2                                         | $d_{xy}$             | -2                                  | $-\frac{1}{2}, +\frac{1}{2}$ | 10                                    |
|       |                              |                                           | $d_{xz}$             | -1                                  | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              |                                           | $d_{yz}$             | 0                                   | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              |                                           | $d_{z^2}$            | +1                                  | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |
|       |                              |                                           | $d_{x^2-y^2}$        | +2                                  | $-\frac{1}{2}, +\frac{1}{2}$ |                                       |

The following is a summary in which the quantum numbers are used to fill the atomic orbitals:

1. No two electrons can have the same four quantum numbers. This is the Pauli exclusion principle.
2. Orbitals are filled in the order of increasing energy.
3. Each orbital can only be occupied by a maximum of two electrons and must have different spin quantum numbers (opposite spins).
4. The most stable arrangement of electrons in orbitals is the one that has the greatest number of equal spin quantum numbers (parallel spins). This is Hund's rule.

Also note that the energy of an electron also depends on the angular momentum quantum number as well as the principal quantum number. Therefore the order that the orbitals get filled does not strictly follow the principal quantum number. The order in which orbitals are filled is given in figure 1.1.

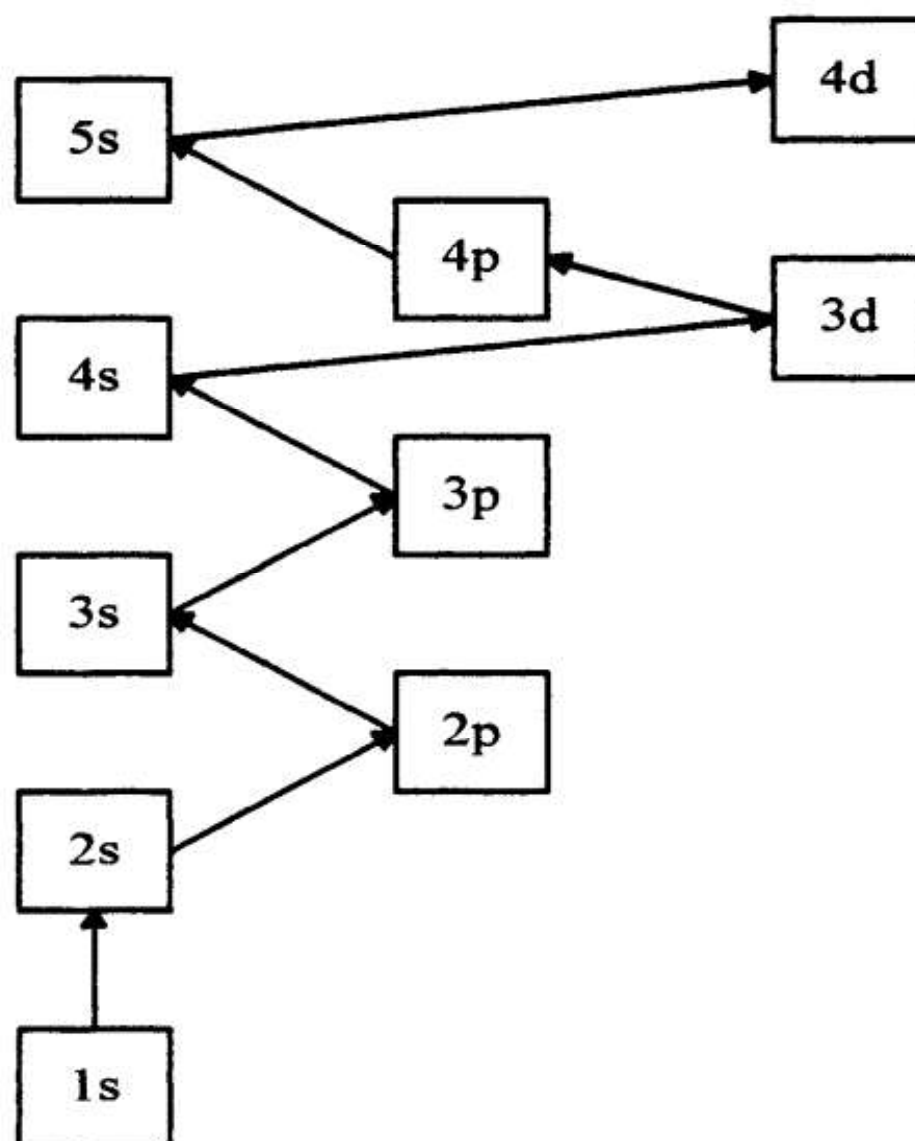


Figure 1.1 Filling Order and Relative Energy Levels of Orbitals

### 1.1.3 Atomic Orbitals

The quantum numbers mentioned earlier were obtained as solutions to a set of wave equations. These wave equations cannot tell precisely where an electron is at any given moment or how fast it is moving. But rather it states the probability of finding the electron at a particular place. An orbital is a region of space where the electron is most likely to be found. An orbital has no definite boundary to it, but can be thought of as a cloud with a specific shape. Also, the orbital is not uniform throughout, but rather densest in the region where the probability of finding the electron is highest.

The shape of an orbital represents 90% of the probability of finding the electron within that space. As the quantum numbers change so do the shapes

and direction of the orbitals. Figure 1.2 show the shapes for principal quantum number  $n = 1, 2$ , and 3.

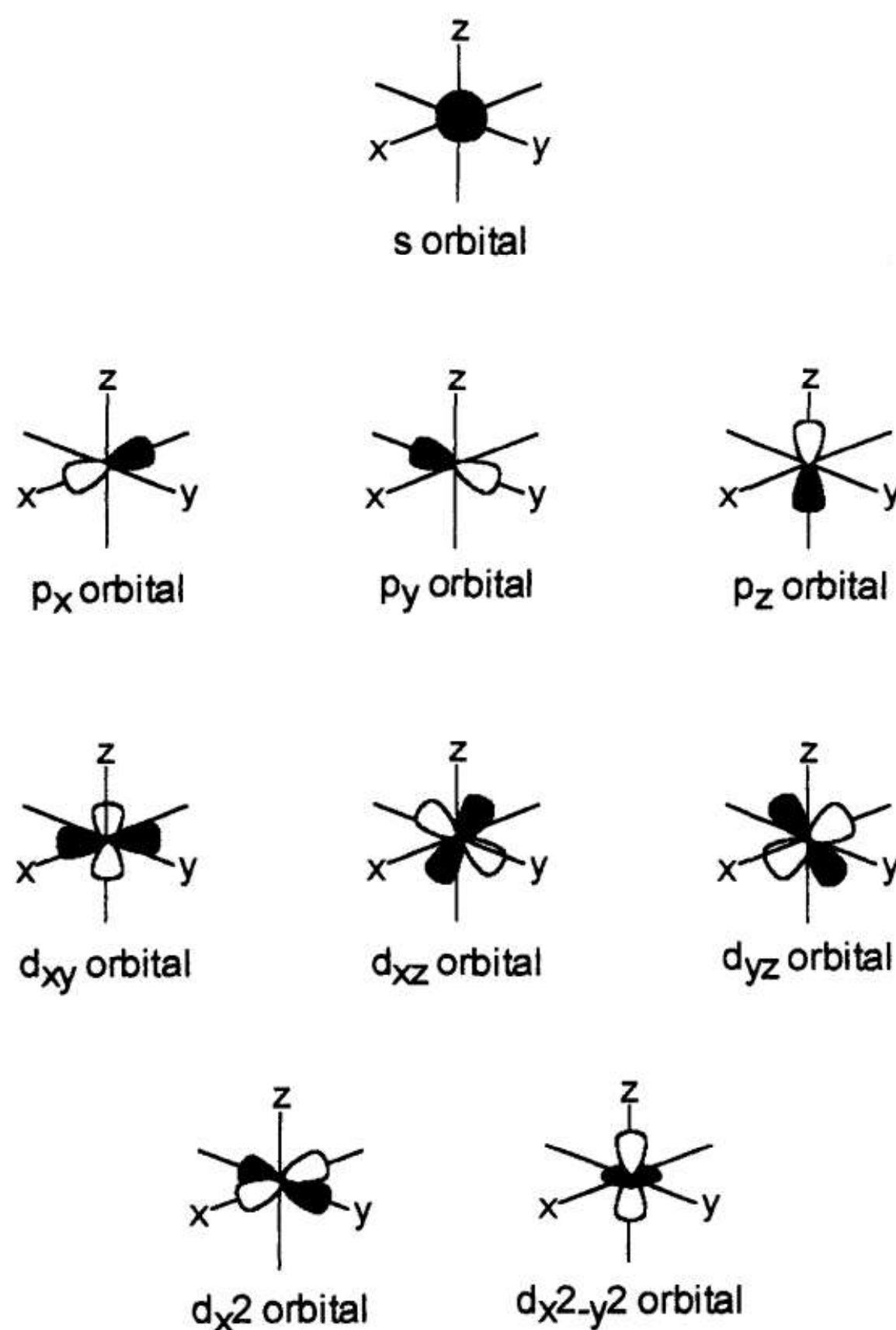


Figure 1.2 Representation of Atomic Orbitals

Another type of orbital is one that originates from the mixing of the different atomic orbitals and is called a hybrid orbital. Hybridization (mixing) of atomic orbitals results in a new set of orbitals with different

shapes and orientations. The orbitals are designated according to which of the separate atomic orbitals have been mixed. For instance, an s orbital mixing with a single p orbital is designated sp. An s orbital mixing with two separate p orbitals ( $p_x + p_y$  or  $p_x + p_z$  or  $p_y + p_z$ ) is designated  $sp^2$  and a s orbital mixing with three separate p orbitals is designated  $sp^3$ . Combinations of other orbitals can occur as well. Table 1.3 lists some of the possible hybrid orbitals.

Table 1.3. Hybrid Orbitals

| Hybrid orbital      | Atomic orbitals hybridized                                                     | Number of hybrid orbitals | Angle of hybrid orbital | Geometry | Example                                                  |
|---------------------|--------------------------------------------------------------------------------|---------------------------|-------------------------|----------|----------------------------------------------------------|
| sp<br>dp            | s + p<br>d + p                                                                 | 2<br>2                    | 180°<br>180°            |          | CO <sub>2</sub><br>HgCl <sub>2</sub>                     |
| $sp^2$              | s +<br>$p_x + p_y$                                                             | 3                         | 120°                    |          | PCl <sub>3</sub><br>SO <sub>3</sub><br>H <sub>2</sub> CO |
| $sp^3$              | s +<br>$p_x + p_y + p_z$                                                       | 4                         | 109°28'                 |          | CH <sub>4</sub><br>AlCl <sub>3</sub>                     |
| $dsp^2$<br>$d^2p^2$ | 1 + $p_x + p_y +$<br>$d_{x^2-y^2}$<br>$d_{x^2-y^2} + d_{z^2} +$<br>$p_x + p_y$ | 4<br>4                    | 90°<br>90°              |          | XeF <sub>4</sub>                                         |
| $dsp^3$             | s +<br>$p_x + p_y + p_z +$<br>$d_{x^2-y^2}$                                    | 5                         | 90°<br>120°<br>180°     |          | PCl <sub>5</sub><br>PF <sub>5</sub>                      |
| $d^2sp^3$           | s +<br>$p_x + p_y + p_z +$<br>$d_{x^2-y^2} + d_{z^2}$                          | 6                         | 90°<br>180°             |          | SF <sub>6</sub><br>XeF <sub>6</sub><br>MoF <sub>6</sub>  |

## 1.1.4 Electronic Configuration of the Elements

Table 1.4. Electronic Configuration of the Elements

|    | Shells     | K  | L  |    | M  |    |    | N  |    |    |    | O  |    |    |    | P  |    |    |    | Q  |
|----|------------|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|----|
|    | Sub-Levels | 1s | 2s | 2p | 3s | 3p | 3d | 4s | 4p | 4d | 4f | 5s | 5p | 5d | 5f | 6s | 6p | 6d | 6f | 7s |
| 1  | Hydrogen   | 1  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 2  | Helium     | 2  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 3  | Lithium    | 2  | 1  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 4  | Beryllium  | 2  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 5  | Boron      | 2  | 2  | 1  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 6  | Carbon     | 2  | 2  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 7  | Nitrogen   | 2  | 2  | 3  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 8  | Oxygen     | 2  | 2  | 4  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 9  | Fluorine   | 2  | 2  | 5  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 10 | Neon       | 2  | 2  | 6  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 11 | Sodium     | 2  | 2  | 6  | 1  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 12 | Magnesium  | 2  | 2  | 6  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 13 | Aluminum   | 2  | 2  | 6  | 2  | 1  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 14 | Silicon    | 2  | 2  | 6  | 2  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 15 | Phosphorus | 2  | 2  | 6  | 2  | 3  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 16 | Sulfur     | 2  | 2  | 6  | 2  | 4  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 17 | Chlorine   | 2  | 2  | 6  | 2  | 5  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 18 | Argon      | 2  | 2  | 6  | 2  | 6  |    |    |    |    |    |    |    |    |    |    |    |    |    |    |
| 19 | Potassium  | 2  | 2  | 6  | 2  | 6  |    | 1  |    |    |    |    |    |    |    |    |    |    |    |    |
| 20 | Calcium    | 2  | 2  | 6  | 2  | 6  |    | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 21 | Scandium   | 2  | 2  | 6  | 2  | 6  | 1  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 22 | Titanium   | 2  | 2  | 6  | 2  | 6  | 2  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 23 | Vanadium   | 2  | 2  | 6  | 2  | 6  | 3  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 24 | Chromium   | 2  | 2  | 6  | 2  | 6  | 5  | 1  |    |    |    |    |    |    |    |    |    |    |    |    |
| 25 | Manganese  | 2  | 2  | 6  | 2  | 6  | 5  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 26 | Iron       | 2  | 2  | 6  | 2  | 6  | 6  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 27 | Cobalt     | 2  | 2  | 6  | 2  | 6  | 7  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 28 | Nickel     | 2  | 2  | 6  | 2  | 6  | 8  | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 29 | Copper     | 2  | 2  | 6  | 2  | 6  | 10 | 1  |    |    |    |    |    |    |    |    |    |    |    |    |
| 30 | Zinc       | 2  | 2  | 6  | 2  | 6  | 10 | 2  |    |    |    |    |    |    |    |    |    |    |    |    |
| 31 | Gallium    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 1  |    |    |    |    |    |    |    |    |    |    |    |
| 32 | Germanium  | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 2  |    |    |    |    |    |    |    |    |    |    |    |
| 33 | Arsenic    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 3  |    |    |    |    |    |    |    |    |    |    |    |
| 34 | Selenium   | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 4  |    |    |    |    |    |    |    |    |    |    |    |
| 35 | Bromine    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 5  |    |    |    |    |    |    |    |    |    |    |    |
| 36 | Krypton    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  |    |    |    |    |    |    |    |    |    |    |    |
| 37 | Rubidium   | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  |    |    | 1  |    |    |    |    |    |    |    |    |
| 38 | Strontium  | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  |    |    | 2  |    |    |    |    |    |    |    |    |
| 39 | Yttrium    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  | 1  |    | 2  |    |    |    |    |    |    |    |    |
| 40 | Zirconium  | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  | 2  |    | 2  |    |    |    |    |    |    |    |    |
| 41 | Niobium    | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  | 4  |    | 1  |    |    |    |    |    |    |    |    |
| 42 | Molybdenum | 2  | 2  | 6  | 2  | 6  | 10 | 2  | 6  | 5  |    | 1  |    |    |    |    |    |    |    |    |



|     | Shells       | K  | L     | M        | N           | O           | P           | Q  |
|-----|--------------|----|-------|----------|-------------|-------------|-------------|----|
|     | Sub-Levels   | 1s | 2s 2p | 3s 3p 3d | 4s 4p 4d 4f | 5s 5p 5d 5f | 6s 6p 6d 6f | 7s |
| 87  | Francium     | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10      | 2 6         | 1  |
| 88  | Radium       | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10      | 2 6         | 2  |
| 89  | Actinium     | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10      | 2 6 1       | 2  |
| 90  | Thorium      | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10      | 2 6 2       | 2  |
| 91  | Protactinium | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 2    | 2 6 1       | 2  |
| 92  | Uranium      | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 3    | 2 6 1       | 2  |
| 93  | Neptunium    | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 4    | 2 6 1       | 2  |
| 94  | Plutonium    | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 6    | 2 6         | 2  |
| 95  | Americium    | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 7    | 2 6         | 2  |
| 96  | Curium       | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 7    | 2 6 1       | 2  |
| 97  | Berkelium    | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 9    | 2 6         | 2  |
| 98  | Californium  | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 10   | 2 6         | 2  |
| 99  | Einsteinium  | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 11   | 2 6 1       | 2  |
| 100 | Fermium      | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 12   | 2 6 1       | 2  |
| 101 | Mendelevium  | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 13   | 2 6 1       | 2  |
| 102 | Nobelium     | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 1       | 2  |
| 103 | Lawrencium   | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 1       | 2  |
| 104 | Unnilquadium | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 2       | 2  |
| 105 | Unnilpentium | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 3       | 2  |
| 106 | Unnilhexium  | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 4       | 2  |
| 107 | Unnilseptium | 2  | 2 6   | 2 6 10   | 2 6 10 14   | 2 6 10 14   | 2 6 5       | 2  |
| 108 |              |    |       |          |             |             |             |    |

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### 1.1.6 Ionization Energy

Ionization energy is the minimum amount of energy needed to remove an electron from a gaseous atom or ion, and is expressed in electron volts (eV).

Going across the periodic table the I.E. increases due to the fact that the principal energy level (principal quantum number) remains the same while the number of electrons increase, thereby enhancing the electrostatic attraction between the protons in the nucleus and the electrons. Going down the table the I.E. decreases because the outer electrons are now further from the nucleus and the protons.

Table 1.6 shows the first ionization energy for the elements.



Table 1.6. First Ionization Energy (in eV)

| Z  | Element    | I.E.  | Z  | Element    | I.E.  | Z  | Element      | I.E.  |
|----|------------|-------|----|------------|-------|----|--------------|-------|
| 1  | Hydrogen   | 13.59 | 30 | Zinc       | 9.39  | 59 | Praseodymium | 5.40  |
| 2  | Helium     | 24.58 | 31 | Gallium    | 6.00  | 60 | Neodymium    | 5.49  |
| 3  | Lithium    | 5.39  | 32 | Germanium  | 7.88  | 61 | Promethium   | 5.55  |
| 4  | Beryllium  | 9.32  | 33 | Arsenic    | 9.81  | 62 | Samarium     | 5.61  |
| 5  | Boron      | 8.30  | 34 | Selenium   | 9.75  | 63 | Europium     | 5.64  |
| 6  | Carbon     | 11.26 | 35 | Bromine    | 11.84 | 64 | Gadolinium   | 6.26  |
| 7  | Nitrogen   | 14.53 | 36 | Krypton    | 14.00 | 65 | Terbium      | 5.89  |
| 8  | Oxygen     | 13.61 | 37 | Rubidium   | 4.18  | 66 | Dysprosium   | 5.82  |
| 9  | Fluorine   | 17.42 | 38 | Strontium  | 5.69  | 67 | Holmium      | 5.89  |
| 10 | Neon       | 21.56 | 39 | Yttrium    | 6.38  | 68 | Erbium       | 5.95  |
| 11 | Sodium     | 5.14  | 40 | Zirconium  | 6.84  | 69 | Thulium      | 6.03  |
| 12 | Magnesium  | 7.64  | 41 | Niobium    | 6.88  | 70 | Ytterbium    | 6.04  |
| 13 | Aluminum   | 5.98  | 42 | Molybdenum | 7.10  | 71 | Lutetium     | 5.32  |
| 14 | Silicon    | 8.15  | 43 | Technetium | 7.28  | 72 | Hafnium      | 7.00  |
| 15 | Phosphorus | 10.48 | 44 | Ruthenium  | 7.36  | 73 | Tantalum     | 7.88  |
| 16 | Sulfur     | 10.36 | 45 | Rhodium    | 7.46  | 74 | Tungsten     | 7.98  |
| 17 | Chlorine   | 12.97 | 46 | Palladium  | 8.33  | 75 | Rhenium      | 7.87  |
| 18 | Argon      | 15.76 | 47 | Silver     | 7.57  | 76 | Osmium       | 8.73  |
| 19 | Potassium  | 4.34  | 48 | Cadmium    | 8.99  | 77 | Iridium      | 9.1   |
| 20 | Calcium    | 6.11  | 49 | Indium     | 5.79  | 78 | Platinum     | 8.96  |
| 21 | Scandium   | 6.54  | 50 | Tin        | 7.34  | 79 | Gold         | 9.22  |
| 22 | Titanium   | 6.82  | 51 | Antimony   | 8.64  | 80 | Mercury      | 10.43 |
| 23 | Vanadium   | 6.74  | 52 | Tellurium  | 9.01  | 81 | Thallium     | 6.11  |
| 24 | Chromium   | 6.87  | 53 | Iodine     | 10.45 | 82 | Lead         | 7.42  |
| 25 | Manganese  | 7.43  | 54 | Xenon      | 12.13 | 83 | Bismuth      | 7.29  |
| 26 | Iron       | 7.87  | 55 | Cesium     | 3.89  | 84 | Polonium     | 8.43  |
| 27 | Cobalt     | 7.86  | 56 | Barium     | 5.21  | 85 | Astatine     | 9.5   |
| 28 | Nickel     | 7.63  | 57 | Lanthanum  | 5.61  | 86 | Radon        | 10.75 |
| 29 | Copper     | 7.72  | 58 | Cerium     | 6.54  |    |              |       |

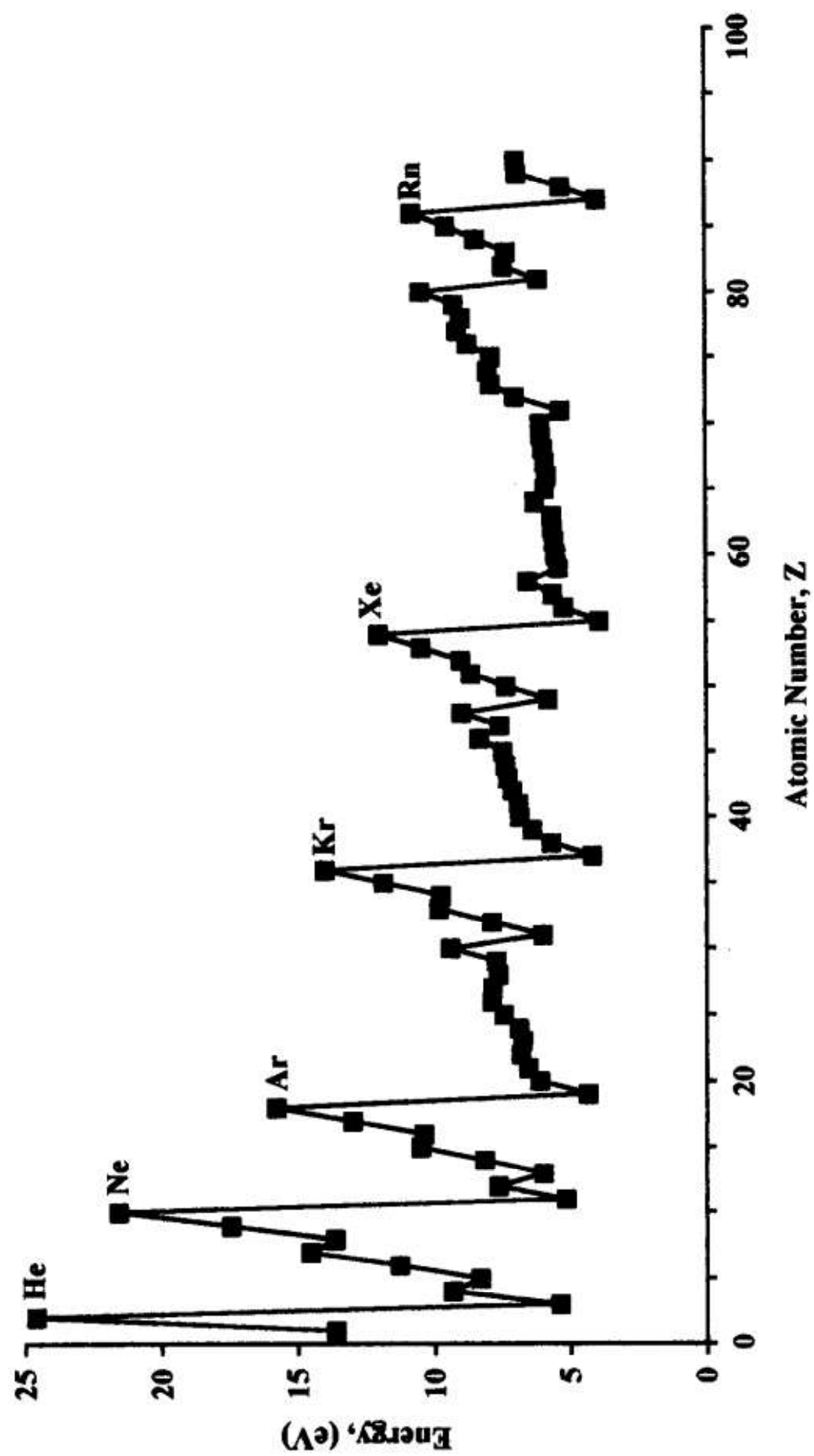


Figure 1.3. First ionization energy

### 1.1.7 Electronegativity

Electronegativity ( $X$ ) is the relative attraction of an atom for an electron in a covalent bond. But due to the complexity of a covalent bond it is not possible to define precise electronegativity values. Originally the element fluorine, whose atoms have the greatest attraction for an electron, was given an arbitrary value of 4.0. All other electronegativity values are based on this.

Note that the greater the difference in electronegativities the more ionic in nature is the bond, and the smaller the difference the more covalent is the bond.

Going across the periodic table the electronegativity increases because the principal energy level remain the same and the electrostatic attraction increases. The atoms also have a desire to have the most stable configuration which is that of the noble gas configuration. Going down the table the electronegativity decreases due to the increased distance from the nucleus.

Table 1.7 lists relative electronegativities for the elements.

Table 1.7. Relative Electronegativities

| Z  | Element    | $X$ | Z  | Element    | $X$ | Z  | Element      | $X$ |
|----|------------|-----|----|------------|-----|----|--------------|-----|
| 1  | Hydrogen   | 2.2 | 27 | Cobalt     | 1.9 | 53 | Iodine       | 2.5 |
| 2  | Helium     | --- | 28 | Nickel     | 1.9 | 54 | Xenon        | --- |
| 3  | Lithium    | 1.0 | 29 | Copper     | 1.9 | 55 | Cesium       | 0.7 |
| 4  | Beryllium  | 1.5 | 30 | Zinc       | 1.6 | 56 | Barium       | 0.9 |
| 5  | Boron      | 2.0 | 31 | Gallium    | 1.6 |    |              |     |
| 6  | Carbon     | 2.5 | 32 | Germanium  | 1.8 | 72 | Hafnium      | 1.3 |
| 7  | Nitrogen   | 3.0 | 33 | Arsenic    | 2.0 | 73 | Tantalum     | 1.5 |
| 8  | Oxygen     | 3.5 | 34 | Selenium   | 2.4 | 74 | Tungsten     | 1.7 |
| 9  | Fluorine   | 4.0 | 35 | Bromine    | 2.8 | 75 | Rhenium      | 1.9 |
| 10 | Neon       | --- | 36 | Krypton    | --- | 76 | Osmium       | 2.2 |
| 11 | Sodium     | 0.9 | 37 | Rubidium   | 0.8 | 77 | Iridium      | 2.2 |
| 12 | Magnesium  | 1.2 | 38 | Strontium  | 1.0 | 78 | Platinum     | 2.2 |
| 13 | Aluminum   | 1.5 | 39 | Yttrium    | 1.2 | 79 | Gold         | 2.4 |
| 14 | Silicon    | 2.8 | 40 | Zirconium  | 1.4 | 80 | Mercury      | 1.9 |
| 15 | Phosphorus | 2.1 | 41 | Niobium    | 1.6 | 81 | Thallium     | 1.8 |
| 16 | Sulfur     | 2.5 | 42 | Molybdenum | 1.8 | 82 | Lead         | 1.9 |
| 17 | Chlorine   | 3.0 | 43 | Technetium | 1.9 | 83 | Bismuth      | 1.9 |
| 18 | Argon      | --- | 44 | Ruthenium  | 2.2 | 84 | Polonium     | 2.0 |
| 19 | Potassium  | 0.8 | 45 | Rhodium    | 2.2 | 85 | Astatine     | 2.2 |
| 20 | Calcium    | 1.0 | 46 | Palladium  | 2.2 | 86 | Radon        | --- |
| 21 | Scandium   | 1.3 | 47 | Silver     | 1.9 | 87 | Francium     | 0.7 |
| 22 | Titanium   | 1.5 | 48 | Cadmium    | 1.7 | 88 | Radium       | 0.9 |
| 23 | Vanadium   | 1.6 | 49 | Indium     | 1.7 | 89 | Actinium     | 1.1 |
| 24 | Chromium   | 1.6 | 50 | Tin        | 1.8 | 90 | Thorium      | 1.3 |
| 25 | Manganese  | 1.5 | 51 | Antimony   | 1.9 | 91 | Protactinium | 1.4 |
| 26 | Iron       | 1.8 | 52 | Tellurium  | 2.1 | 92 | Uranium      | 1.4 |

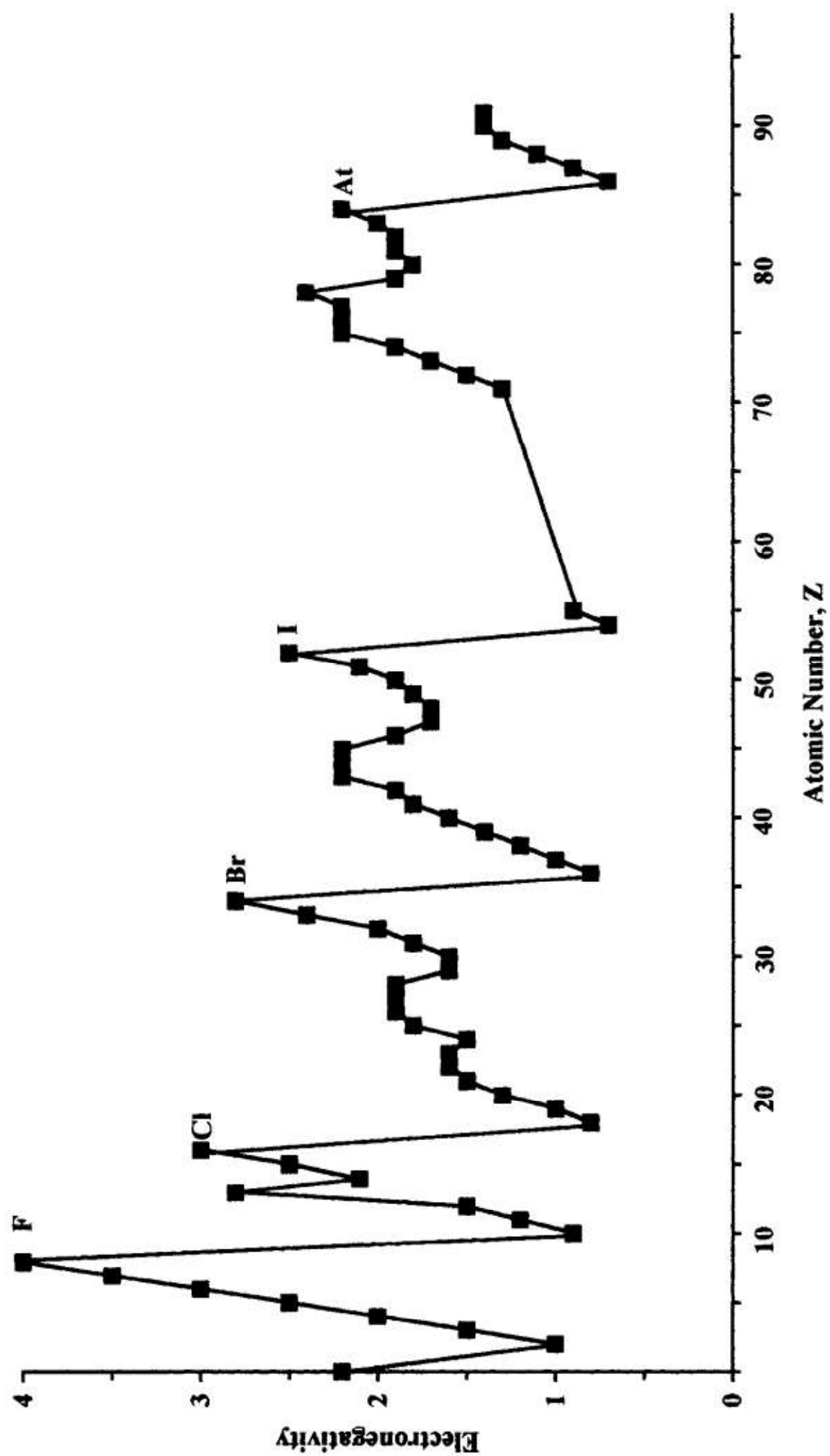


Figure 1.4. Electronegativity

### 1.1.8 Radius of Atoms

The radius of an atom can be estimated by taking half the distance between the nucleus of two of the same atoms. For example, the distance between the nuclei of  $I_2$  is 2.66 Å, half that distance would be the radius of atomic iodine or 1.33 Å. Using this method the atomic radius of nearly all the elements can be estimated.

Note that going across the periodic table, the atomic radius decreases. This is due to the fact that the principal energy level (principal quantum number) remains the same, but the number of electrons increase. The increase in the number of electrons causes an increase in the electrostatic attraction which causes the radius to decrease. However, going down the periodic table the principal energy level increases and hence the atomic radius increases.

Table 1.8 lists the atomic radii of some of the elements.

Table 1.8. Atomic Radii (in Å)

| Z  | Element    | <i>X</i> | Z  | Element    | <i>X</i> | Z  | Element   | <i>X</i> |
|----|------------|----------|----|------------|----------|----|-----------|----------|
| 1  | Hydrogen   | 0.37     | 25 | Manganese  | 1.29     | 49 | Indium    | 1.62     |
| 2  | Helium     | ----     | 26 | Iron       | 1.26     | 50 | Tin       | 1.40     |
| 3  | Lithium    | 1.52     | 27 | Cobalt     | 1.26     | 51 | Antimony  | 1.41     |
| 4  | Beryllium  | 1.12     | 28 | Nickel     | 1.24     | 52 | Tellurium | 1.37     |
| 5  | Boron      | 0.88     | 29 | Copper     | 1.28     | 53 | Iodine    | 1.33     |
| 6  | Carbon     | 0.77     | 30 | Zinc       | 1.33     | 54 | Xenon     | ----     |
| 7  | Nitrogen   | 0.70     | 31 | Gallium    | 1.22     | 55 | Cesium    | 2.62     |
| 8  | Oxygen     | 0.66     | 32 | Germanium  | 1.22     | 56 | Barium    | 2.17     |
| 9  | Fluorine   | 0.64     | 33 | Arsenic    | 1.21     |    |           |          |
| 10 | Neon       | ----     | 34 | Selenium   | 1.17     | 72 | Hafnium   | 1.57     |
| 11 | Sodium     | 1.86     | 35 | Bromine    | 1.14     | 73 | Tantalum  | 1.43     |
| 12 | Magnesium  | 1.60     | 36 | Krypton    | ----     | 74 | Tungsten  | 1.37     |
| 13 | Aluminum   | 1.43     | 37 | Rubidium   | 2.41     | 75 | Rhenium   | 1.37     |
| 14 | Silicon    | 1.17     | 38 | Strontium  | 2.15     | 76 | Osmium    | 1.34     |
| 15 | Phosphorus | 1.10     | 39 | Yttrium    | 1.80     | 77 | Iridium   | 1.35     |
| 16 | Sulfur     | 1.04     | 40 | Zirconium  | 1.57     | 78 | Platinum  | 1.38     |
| 17 | Chlorine   | 0.99     | 41 | Niobium    | 1.43     | 79 | Gold      | 1.44     |
| 18 | Argon      | ----     | 42 | Molybdenum | 1.36     | 80 | Mercury   | 1.50     |
| 19 | Potassium  | 2.31     | 43 | Technetium | 1.30     | 81 | Thallium  | 1.71     |
| 20 | Calcium    | 1.97     | 44 | Ruthenium  | 1.33     | 82 | Lead      | 1.75     |
| 21 | Scandium   | 1.60     | 45 | Rhodium    | 1.34     | 83 | Bismuth   | 1.46     |
| 22 | Titanium   | 1.46     | 46 | Palladium  | 1.38     | 84 | Polonium  | 1.40     |
| 23 | Vanadium   | 1.31     | 47 | Silver     | 1.44     | 85 | Astatine  | 1.40     |
| 24 | Chromium   | 1.25     | 48 | Cadmium    | 1.49     | 86 | Radon     | ----     |

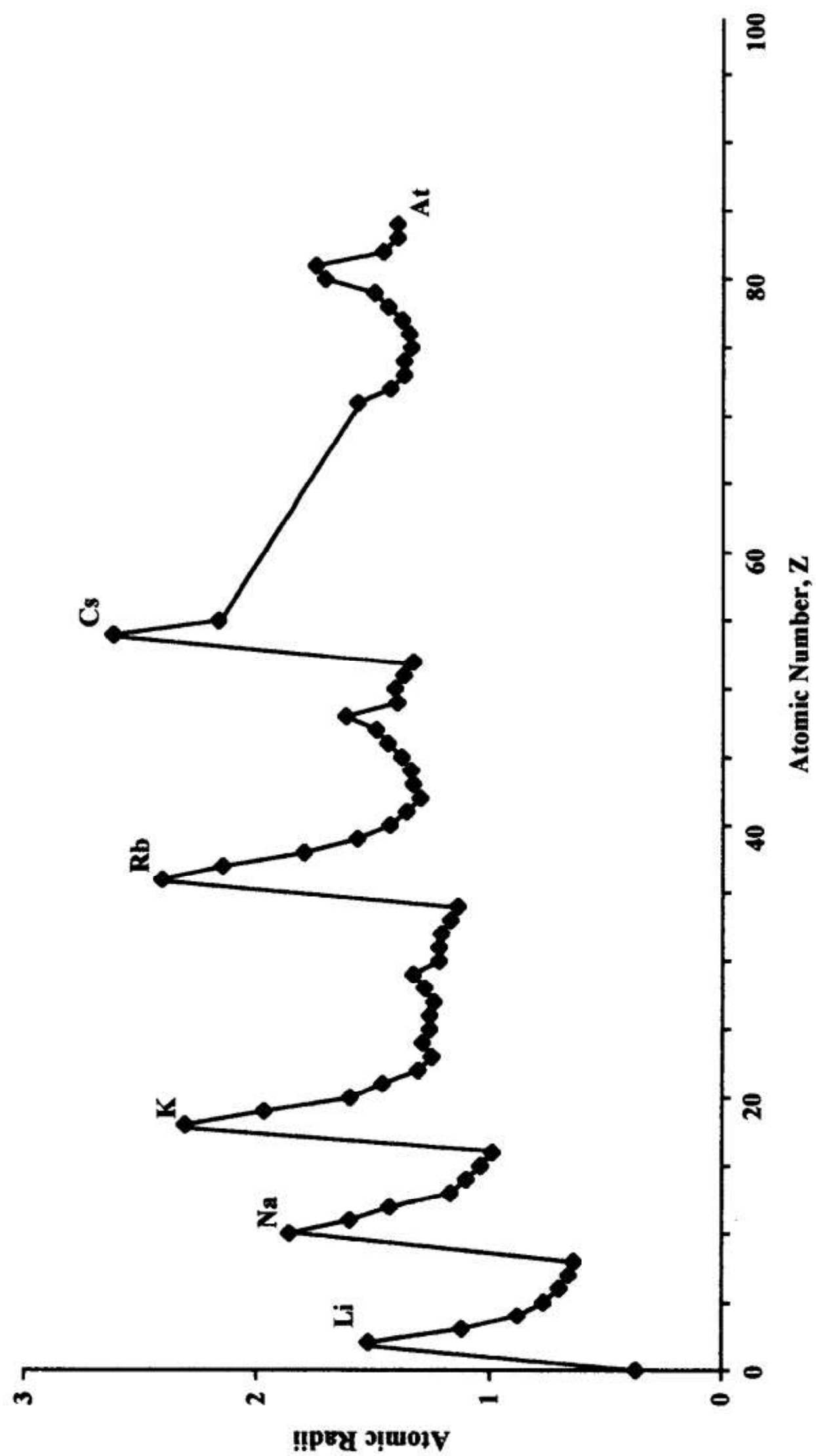


Figure 1.5. Atomic Radii

**1.1.9 Atomic Weights***Table 1.9. Atomic Weights*

| Name        | Symbol | Atomic Wt  | Name         | Symbol | Atomic Wt  |
|-------------|--------|------------|--------------|--------|------------|
| Actinium    | Ac     | 227.0278   | Neodymium    | Nd     | 144.24     |
| Aluminum    | Al     | 26.9815    | Neon         | Ne     | 20.183     |
| Americium   | Am     | (243.0614) | Neptunium    | Np     | 237.0482   |
| Antimony    | Sb     | 121.75     | Nickel       | Ni     | 58.71      |
| Argon       | Ar     | 39.948     | Niobium      | Nb     | 92.906     |
| Arsenic     | As     | 74.9216    | Nitrogen     | N      | 14.0067    |
| Astatine    | At     | (209.9871) | Nobelium     | No     | (259.1009) |
| Barium      | Ba     | 137.34     | Osmium       | Os     | 190.2      |
| Berkelium   | Bk     | (247.0703) | Oxygen       | O      | 15.9994    |
| Beryllium   | Be     | 9.0122     | Palladium    | Pd     | 106.4      |
| Bismuth     | Bi     | 208.980    | Phosphorus   | P      | 30.9738    |
| Boron       | B      | 10.811     | Platinum     | Pt     | 195.09     |
| Bromine     | Br     | 79.909     | Plutonium    | Pu     | (244.0642) |
| Cadmium     | Cd     | 12.401     | Polonium     | Po     | (208.9824) |
| Calcium     | Ca     | 40.08      | Potassium    | K      | 39.102     |
| Californium | Cf     | (251.0796) | Praseodymium | Pr     | 140.907    |
| Carbon      | C      | 12.01115   | Promethium   | Pm     | (144.9127) |
| Cerium      | Ce     | 140.12     | Protactinium | Pa     | 231.0359   |
| Cesium      | Cs     | 132.905    | Radium       | Ra     | 226.0254   |
| Chlorine    | Cl     | 35.453     | Radon        | Rn     | (222.0176) |
| Chromium    | Cr     | 51.996     | Rhenium      | Re     | 186.2      |
| Cobalt      | Co     | 58.9332    | Rhodium      | Rh     | 102.905    |
| Copper      | Cu     | 63.546     | Rubidium     | Rb     | 85.47      |
| Curium      | Cm     | (247.0703) | Ruthenium    | Ru     | 101.07     |
| Dysprosium  | Dy     | 162.50     | Samarium     | Sm     | 150.35     |
| Einsteinium | Es     | (252.083)  | Scandium     | Sc     | 44.956     |
| Erbium      | Er     | 167.26     | Selenium     | Se     | 78.96      |
| Europium    | Eu     | 151.96     | Silicon      | Si     | 28.086     |
| Fermium     | Fm     | (257.0951) | Silver       | Ag     | 107.870    |
| Fluorine    | F      | 18.9984    | Sodium       | Na     | 22.9898    |
| Francium    | Fr     | (223.0197) | Strontium    | Sr     | 87.62      |
| Gadolinium  | Gd     | 157.25     | Sulfur       | S      | 32.064     |
| Gallium     | Ga     | 69.72      | Tantalum     | Ta     | 180.948    |
| Germanium   | Ge     | 72.59      | Technetium   | Tc     | 98.906     |
| Gold        | Au     | 196.967    | Tellurium    | Te     | 127.60     |
| Hafnium     | Hf     | 178.49     | Terbium      | Tb     | 158.924    |
| Helium      | He     | 4.0026     | Thallium     | Tl     | 204.37     |
| Holmium     | Ho     | 164.930    | Thorium      | Th     | 232.038    |
| Hydrogen    | H      | 1.00797    | Thulium      | Tm     | 168.934    |
| Indium      | In     | 114.82     | Tin          | Sn     | 118.69     |
| Iodine      | I      | 126.9044   | Titanium     | Ti     | 47.90      |
| Iridium     | Ir     | 192.2      | Tungsten     | W      | 183.85     |
| Iron        | Fe     | 55.847     | Unnilquadium | Unq    | (261.11)   |

Table 1.9. (Continued)

|             |    |          |              |     |           |
|-------------|----|----------|--------------|-----|-----------|
| Krypton     | Kr | 83.80    | Unnilpentium | Unp | (62.114)  |
| Lanthanum   | La | 183.91   | Unnilhexium  | Unh | (263.118) |
| Lawrencium  | Lr | (262.11) | Unnilseptium | Uns | (262.12)  |
| Lead        | Pb | 207.19   | Uranium      | U   | 238.03    |
| Lithium     | Li | 6.939    | Vanadium     | V   | 50.942    |
| Lutetium    | Lu | 174.97   | Xenon        | Xe  | 131.30    |
| Magnesium   | Mg | 24.312   | Ytterbium    | Yb  | 173.04    |
| Manganese   | Mn | 54.9380  | Yttrium      | Y   | 88.905    |
| Mendelevium | Md | (258.10) | Zinc         | Zn  | 65.37     |
| Mercury     | Hg | 200.59   | Zirconium    | Zr  | 91.22     |
| Molybdenum  | Mo | 95.94    |              |     |           |

## 1.2 Chemical Bonding

### 1.2.1 Covalent Bonding

A **covalent bond** is a bond in which a pair of electrons is shared between two atoms. Depending on the atoms electronegativity the bond is either polar or non-polar.

A pair of atoms with the same electronegativity would form a **non-polar covalent bond**, such as:

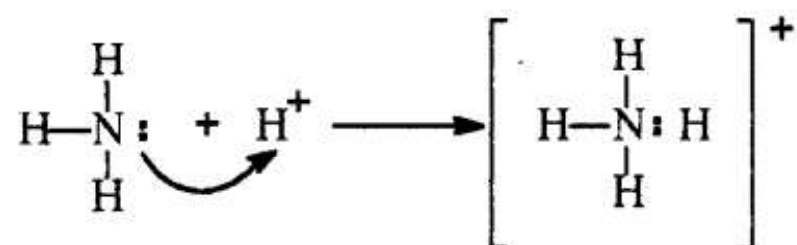


A **polar covalent bond** is one in which the atoms have different electronegativities, such as:



### 1.2.2 Coordinate Covalent Bond (Dative Bond)

A **coordinate covalent bond** is a bond in which both pairs of electrons are donated by one atom and are shared between the two, for example:



### 1.2.3 Ionic Bonding

An **ionic bond** is one in which one or more electrons are transferred from one atom's valence shell (becoming a positively charged ion, called a **cation**) to the other's valence shell (becoming a negatively charged ion, called an **anion**). The resulting electrostatic attraction between oppositely charged ions results in the formation of the ionic bond.



Not all compounds will be either purely covalent or purely ionic, most are somewhere in between. As a rule of thumb, if a compound has less than 50% ionic character it is considered covalent and more than 50%, ionic. The **ionic character** can be related to the difference in electronegativities of the bonded atoms. If the electronegativity difference is 1.7, the bond is about 50% ionic.

### 1.2.4 Dipole-Dipole Bonding

A **dipole-dipole bond** occurs between polar molecules and is a weak electrostatic attraction.

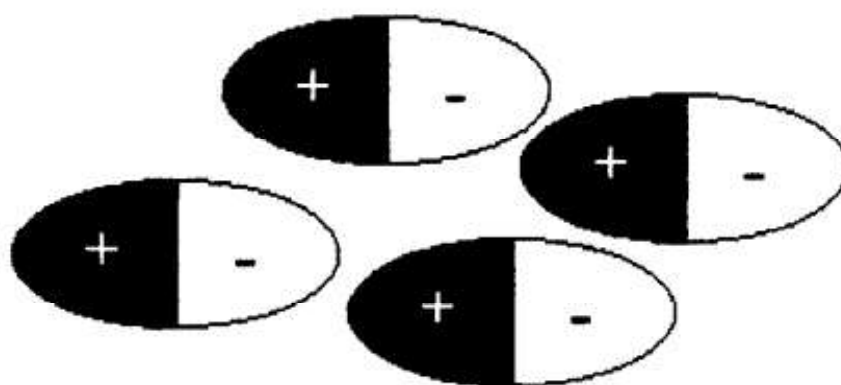


Figure 1.6. Dipole-dipole attraction

### 1.2.5 Ion-Dipole Bonding (Solvation)

An **ion-dipole bond** is another electrostatic attraction between an ion and several polar molecules. When an ionic substance is dissolved in a polar solvent, it is this kind of interaction that takes place. The negative ends of the solvent align themselves to the positive charge, and the positive ends align with the negative charge. This process is **solvation**. When the solvent is water the process is the same but called **hydration**.

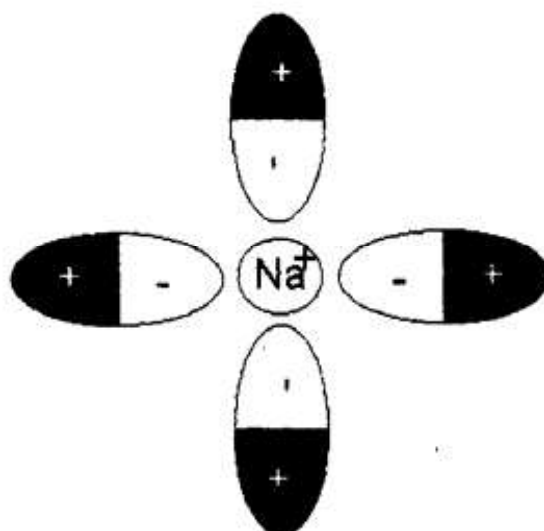


Figure 1.7. Ion-dipole attraction

### 1.2.6 Hydrogen Bonding

When hydrogen is bonded covalently to a small electronegative atom the electron cloud around the hydrogen is drawn to the electronegative atom and a strong dipole is created. The positive end of the dipole approaches close to the negative end of the neighboring dipole and a uniquely strong dipole-dipole bond forms, this is referred to as a **hydrogen bond**.

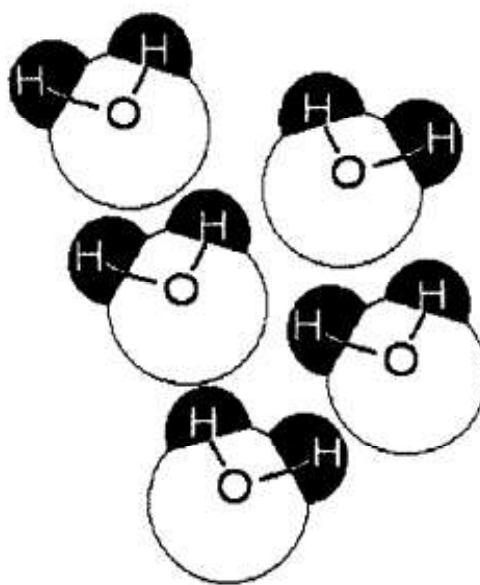


Figure 1.8. Hydrogen bonding

### 1.2.7 van der Waals

When the electron cloud around an atom or molecule shifts (for whatever reason), a temporary dipole is created, this in turn creates an induced dipole in the next molecule. This induced dipole (**van der Waals**) induces another and so on. The induced dipoles now are electrostatically attracted to each other and a weak induced dipole attraction occurs.

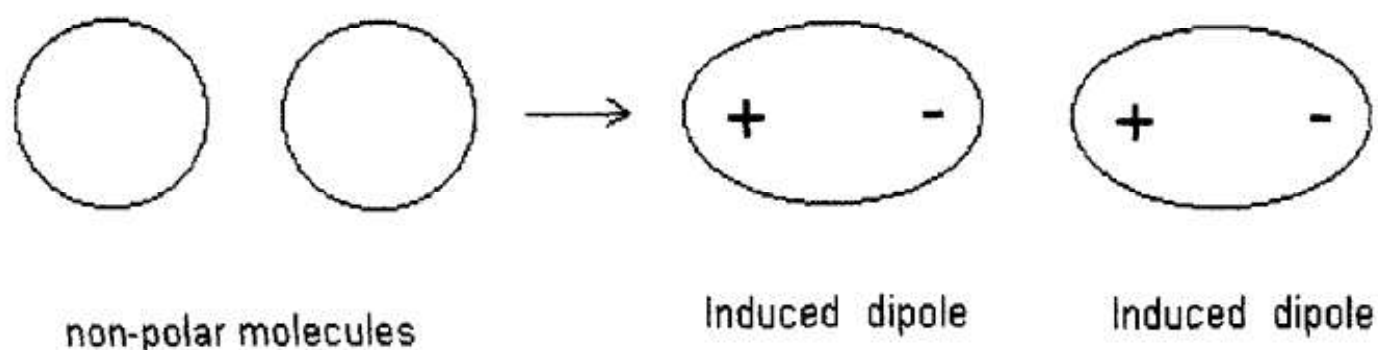


Figure 1.9. van der Waals attraction

### 1.3 Gases

The following laws and equations are for ideal gases. An **ideal gas** is considered to be composed of small particles whose volume is negligible when compared to the whole volume, and the gas particles do not exert any force on one another. Unless otherwise noted:

P - pressure  
V - volume  
T - absolute temperature (Kelvin)  
n - number of moles  
R - gas constant  
8.314 J / mole K

#### 1.3.1 Boyle's Law

For a fixed amount of gas, held at constant temperature, the volume is inversely proportional to the applied pressure.

$$PV = \text{constant}$$

#### 1.3.2 Charles' Law

For a fixed amount of gas, held at constant pressure, the volume is directly proportional to the temperature.

$$V/T = \text{constant}$$

#### 1.3.3 Gay-Lussac's Law

For a fixed amount of gas, held at constant volume, the pressure is directly proportional to the absolute temperature.

$$P/T = \text{constant}$$

### 1.3.4 Avogadro's Law

At constant temperature and pressure, equal volumes of gas contain equal amounts of molecules.

$$V/n = \text{constant}$$

### 1.3.5 Dalton's Law of Partial Pressures

The total pressure exerted by a mixture of several gases is equal to the sum of the gases individual pressure (partial pressure).

$$P_T = p_a + p_b + p_c + \dots$$

$P_T$  pressure of gas a + b + c

$p_a$  pressure of gas a

$p_b$  pressure of gas b

$p_c$  pressure of gas c

### 1.3.6 Ideal Gas Law

Combining the above relationships and Avogadro's principle (under constant pressure and temperature, equal volumes of gas contain the equal numbers of molecules) into one equation we obtain the Ideal Gas Law:

$$PV = nRT$$

### 1.3.7 Equation of State of Real Gases

An ideal gas has negligible volume and exerts no force. However, real gases do have volumes and do exert forces upon one another. When these factors are taken into consideration, the following equation can be obtained:

$$(P + n^2a/V^2) \cdot (V - nb) = nRT$$

**a - proportionality constant**

**b - covolume**

Note that a and b are dependent on the individual gas, since molecular volumes and molecular attractions vary from gas to gas.

Table 1.10. van der Waals constants for real gases.

| Gas              | a (atm liter <sup>2</sup> / mole <sup>2</sup> ) | b (liter / mole) |
|------------------|-------------------------------------------------|------------------|
| He               | 0.034                                           | 0.0237           |
| O <sub>2</sub>   | 1.36                                            | 0.0318           |
| NH <sub>3</sub>  | 4.17                                            | 0.0371           |
| H <sub>2</sub> O | 5.46                                            | 0.0305           |
| CH <sub>4</sub>  | 2.25                                            | 0.0428           |

### 1.3.8 Changes of Pressure, Volume, or Temperature

By combining the equations for Boyle's law, Charles' law, and Gay-Lussac's law, a single equation can be obtained that is useful for many computations:

$$\frac{P_1V_1}{T_1} = \frac{P_2V_2}{T_2}$$

## 1.4 Solutions

### 1.4.1 Mass Percent

The **mass percent** of a solution is the mass of the solute divided by the total mass (solute + solvent) multiplied by 100.

$$\text{percent by mass of solute} = \frac{\text{mass of solute}}{\text{mass of solute} + \text{mass of solvent}} \times 100$$

### 1.4.2 Mole Fraction (*X*)

The **mole fraction (*X*)** is the number of moles of component A divided by the total number of moles of all components.

$$\text{mole fraction of A} = \frac{\text{moles of A}}{\text{moles of all components}}$$

### 1.4.3 Molarity (*M*)

The **molarity (*M*)** of a solution is the number of moles of solute dissolved in 1 liter of solvent.

$$\text{molarity} = \frac{\text{moles of solute}}{\text{liters of solvent}}$$

#### 1.4.4 Molality ( $m$ )

**Molality ( $m$ )** is the number of moles of solute dissolved in 1000 g (1 kg) of solvent.

$$\text{molality} = \frac{\text{moles of solute}}{\text{mass of solvent}}$$

#### 1.4.5 Dilutions

A handy and useful formula when calculating dilutions is:

$$M_{\text{initial}} V_{\text{initial}} = M_{\text{final}} V_{\text{final}}$$

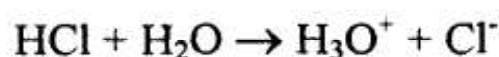
### 1.5 Acids and Bases

#### 1.5.1 Arrhenius Concept

An acid is any species that increases the concentration of **hydronium ions ( $\text{H}_3\text{O}^+$ )**, in aqueous solution.

A base is any species that increases the concentration of **hydroxide ion, ( $\text{OH}^-$ )**, in aqueous solution.

For an acid:



For a base:



However, the drawback with the Arrhenius concept is that it only applies to aqueous solutions.

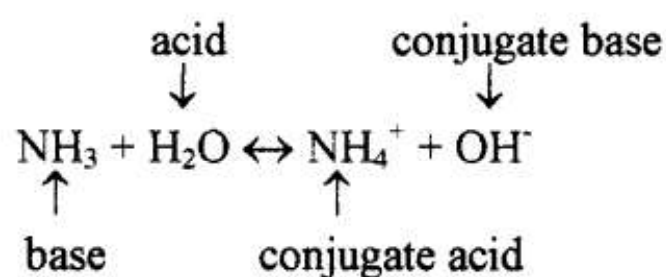
#### 1.5.2 Bronsted-Lowery Concept

An acid is a species which can donate a proton (i.e., a hydrogen ion,  $\text{H}^+$ ) to a proton acceptor.

A base is a species which can accept a proton from a proton donor.

Along with the Bronsted-Lowery concept of a proton donor (acid) and a proton acceptor (base), arises the concept of conjugate acid-base pairs. For

example, when the acid HCl reacts, it donates a proton thereby leaving  $\text{Cl}^-$  (which is now a proton acceptor, or the conjugate base of HCl). Using  $\text{NH}_3$  as the base and  $\text{H}_2\text{O}$  as the acid:



### 1.5.3 Lewis Concept

An acid is a species that can accept a pair of electrons.

A base is a species that can donate a pair of electrons.



## 1.6 Thermodynamics

### 1.6.1 First Law of Thermodynamics

The energy change of a system is equal to the heat absorbed by the system plus the work done by the system. The reason for the minus sign for work,  $w$ , is that any work done by the system results in a loss of energy for the system as a whole.

$$\Delta E = q - w$$

$E$  = internal energy of the system

$q$  = heat absorbed by the system

$w$  = work done by the system

Table 1.11. Thermodynamic Processes

| Process                                    | Sign |
|--------------------------------------------|------|
| work done by system                        | -    |
| work done on system                        | +    |
| heat absorbed by system (endothermic)      | +    |
| heat absorbed by surroundings (exothermic) | -    |

Making a substitution for work, the equation can be expressed as:

$$\Delta E = q - P\Delta V$$

For constant volume, the equation becomes:

$$\Delta E = q_v$$

### 1.6.2 Enthalpy

**Enthalpy, H,** is the heat content of the system at constant pressure.

$$\Delta E = q_p - P\Delta V$$

$$q_p = \Delta E + P\Delta V$$

$$q_p = (E_2 - E_1) + P(V_2 - V_1)$$

$$= (E_2 + PV_2) - (E_1 + PV_1)$$

$$q_p = H_2 - H_1 = \Delta H$$

### 1.6.3 Entropy

**Entropy, S,** is the measure of the degree of randomness of a system.

$$\Delta S = \frac{q_{rev}}{T}$$

T = temperature in °K

### 1.6.4 Gibbs Free Energy

**Gibbs free energy, G,** is the amount of energy available to the system to do useful work.

$$\Delta G = \Delta H - T\Delta S$$

|                |                                            |
|----------------|--------------------------------------------|
| $\Delta G < 0$ | spontaneous process from 1 $\rightarrow$ 2 |
| $\Delta G > 0$ | spontaneous process from 2 $\rightarrow$ 1 |
| $\Delta G = 0$ | equilibrium                                |

### 1.6.5 Standard States

The **standard state** is the standard or normal condition of a species.

Table 1.12. Standard States

| State of Matter | Standard State               |
|-----------------|------------------------------|
| Gas             | 1 atm pressure               |
| Liquid          | Pure liquid                  |
| Solid           | Pure solid                   |
| Element         | Free energy of formation = 0 |
| Solution        | 1 molar concentration        |

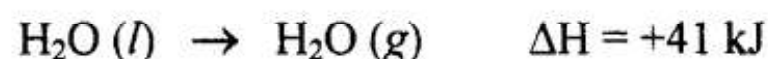
Note also that  $\Delta H^\circ_f$  for an element in its natural state at 25°C and 1 atm is taken to be equal to zero.

### 1.6.6 Hess' Law of Heat Summation

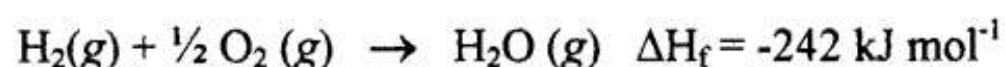
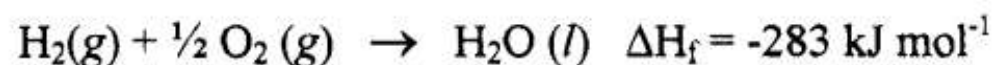
The final value of  $\Delta H$  for the overall process is the sum of all the enthalpy changes.

$$\Delta H^\circ = \Sigma \Delta H^\circ_f (\text{products}) - \Sigma \Delta H^\circ_f (\text{reactants})$$

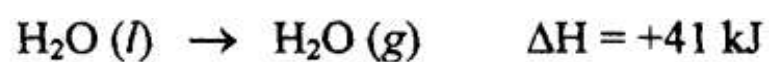
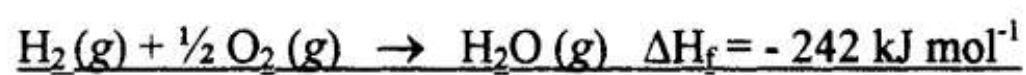
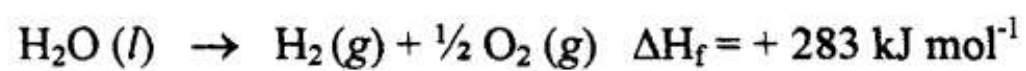
For example, to vaporize 1 mole of  $\text{H}_2\text{O}$  at 100°C and 1 atm, the process absorbs 41 kJ of heat,  $\Delta H = +41$  kJ.



If a different path to the formation of 1 mole of gaseous  $\text{H}_2\text{O}$  is taken, the same amount of net heat will still be absorbed.



Reversing the first reaction, then adding the two reactions together and cancelling common terms, results in the original reaction, and the amount of heat absorbed by the system



Using the Hess' Law of Summation:

$$\Delta H^\circ = \sum \Delta H^\circ_f (\text{products}) - \sum \Delta H^\circ_f (\text{reactants})$$

$$\Delta H^\circ = (-242 \text{ kJ}) - (-283 \text{ kJ}) = +41 \text{ kJ}$$

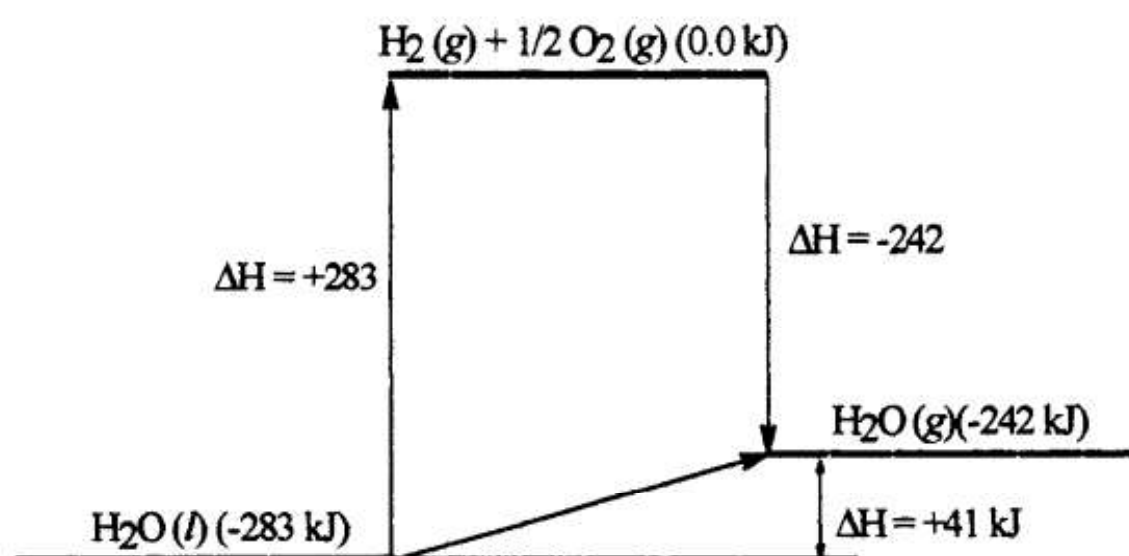


Figure 1.10. Enthalpy Diagram for  $\text{H}_2\text{O} (l) \rightarrow \text{H}_2\text{O} (g)$

## 1.7 Equilibria

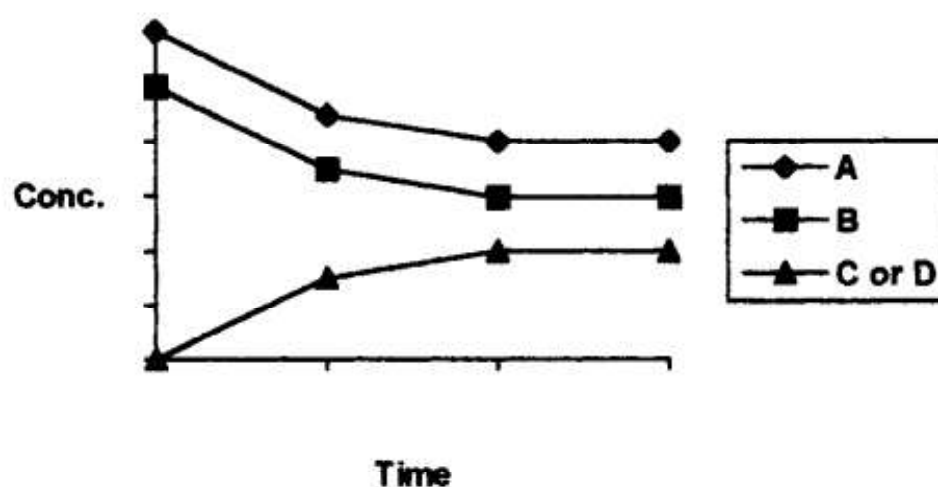
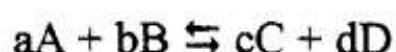


Figure 1.11. Concentrations of reactants and products approaching equilibrium.

When equilibrium is reached in a chemical reaction the rate of the forward reaction is equal to the rate of the reverse reaction, and the concentrations of the reactants and products do not change over time.

### 1.7.1 Homogeneous Equilibrium

**Homogeneous equilibrium** occurs when all reacting species are in the same phase. For the general reaction,



the equation expressing the **law of mass action**, at equilibrium, is:

$$\frac{[C]^c[D]^d}{[A]^a[B]^b} = K_c$$

The quantity,  $K_c$ , is a constant, called the **equilibrium constant** (in this case it denotes the equilibrium constant for species in solution, expressed as moles per liter). The magnitude of  $K_c$  tells us to what extent the reaction proceeds. A large  $K_c$  indicates that the reaction proceeds to the right of the reaction. A low value indicates that the reaction proceeds to the left of the reaction.

For gas-phase equilibrium the expression becomes

$$K_p = \frac{P_C^c P_D^d}{P_A^a P_B^b}$$

where  $P$  is the partial pressures of the species in the reaction.  $K_p$  can be related to  $K_c$  by the following equation,

$$K_p = K_c(0.08206T)^{\Delta n}$$

$T$  = the absolute temperature

$\Delta n$  = moles of product - moles of reactants.

### 1.7.2 Heterogeneous Equilibrium

**Heterogeneous equilibrium** involves reactants and products in different phases. For example, when calcium carbonate is heated in a closed vessel, the following equilibrium reaction occurs:



The reactant is a solid, while the products are in the solid and gas phase. The equilibrium expression is written as the following:

$$K_c' = \frac{[\text{CaO}][\text{CO}_2]}{[\text{CaCO}_3]}$$

In any reaction that includes a solid, the solid concentration will remain constant and therefore is not included in the equilibrium expression. The equilibrium expression now becomes:

$$K_c'' \frac{[\text{CaCO}_3]}{\text{CaO}} = [\text{CO}_2] = K_c$$

### 1.7.3 Le Chatelier's Principle

**Le Chatelier's Principle** states that *when a system is in equilibrium and there is a change in one of the factors which affect the equilibrium, the system reacts in such a way as to cancel out the change and restore equilibrium.*

An increase in temperature will shift the reaction in the direction of heat absorption.

An increase in the pressure will shift the reaction in the direction in which the number of moles is decreased.

An increase or decrease in pressure does not affect a reaction in which there is no variation in the number of moles.

An increase in the concentration of one of the components will cause the reaction to shift so as to decrease the added component.

### 1.7.4 Equilibrium of Water

The reaction for autoionization of water is:



The equilibrium expression is:

$$K = \frac{[\text{H}_3\text{O}^+][\text{OH}^-]}{[\text{H}_2\text{O}][\text{H}_2\text{O}]}$$

Since the concentration of water is a constant ( $\approx 55.55 \text{ M}$ ),  $[\text{H}_2\text{O}]^2$  can be included in the equilibrium constant,  $K$ . this new constant is now called  $K_w$ .

$$K_w = K[\text{H}_2\text{O}]^2 = [\text{H}_3\text{O}^+][\text{OH}^-]$$

$K_w$  is the **ion product constant** for water, also called the **ionization constant** or **dissociation constant** for water. The ionization constant for water at  $25^\circ\text{C}$  has a value of  $1.0 \times 10^{-14}$ . The equilibrium expression now becomes:

$$K_w = 1.0 \times 10^{-14} = [\text{H}_3\text{O}^+][\text{OH}^-]$$

$$\text{Since } [\text{H}_3\text{O}^+] = [\text{OH}^-]$$

$$[\text{H}_3\text{O}^+] = [\text{OH}^-] = 1.0 \times 10^{-7}$$

When the concentration of hydrogen ions equals the concentration of hydroxide ions the solution is said to be neutral.

### 1.7.5 pH

pH is the measure of how strong or weak an acid is, and is defined as the negative of the log of the hydrogen ion concentration, or

$$\text{pH} = -\log[\text{H}_3\text{O}^+]$$

Water has a pH of 7, this is calculated from the dissociation constant for water:

$$[\text{H}_3\text{O}^+] = 1.0 \times 10^{-7}$$

$$\text{pH} = -\log[\text{H}_3\text{O}^+] = -\log(1.0 \times 10^{-7})$$

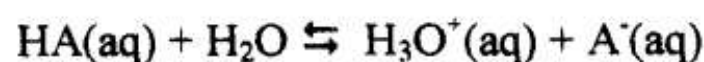
$$\text{pH} = 7$$

The concept of pH can be applied to any system in which hydrogen ions are produced. An acidic solution would have an excess of hydrogen ions, a basic solution would have an excess of hydroxide ions, and a neutral solution the hydrogen ions would equal the hydroxide ions. Since pH is a measure of the hydrogen ion concentration, acidic and basic solutions can be distinguished on the basis of their pH.

acidic solutions:  $[\text{H}_3\text{O}^+] > 10^{-7} \text{ M}$ ,  $\text{pH} < 7$   
 basic solutions:  $[\text{H}_3\text{O}^+] < 10^{-7} \text{ M}$ ,  $\text{pH} > 7$   
 neutral solutions:  $[\text{H}_3\text{O}^+] = 10^{-7} \text{ M}$ ,  $\text{pH} = 7$

### 1.7.6 Ionic Equilibrium

For a monoprotic acid HA, the equilibrium reaction is:



and the equilibrium expression is:

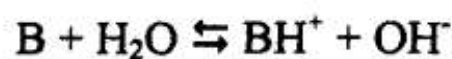
$$K_a = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$$

The equilibrium constant,  $K_a$ , is called the **acid dissociation constant**.

Similarly for a polyprotic acid (i.e. phosphoric acid), the equilibrium reactions are:



For a base the equilibrium reaction is:

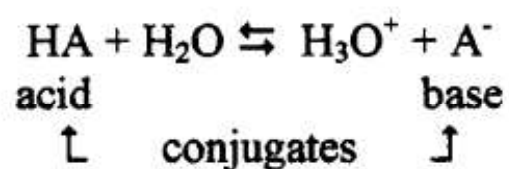


and the equilibrium expression is:

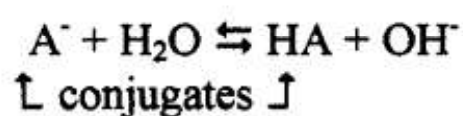
$$K_b = \frac{[\text{BH}^+][\text{OH}^-]}{[\text{B}]}$$

The equilibrium constant,  $K_b$ , is called the **base dissociation constant**.

### 1.7.7 Relationship between $K_a$ and $K_b$ Conjugate Pair



$$K_a = \frac{[\text{H}_3\text{O}^+][\text{A}^-]}{[\text{HA}]}$$



$$K_b = \frac{[\text{HA}][\text{OH}^-]}{[\text{A}^-]}$$

$$K_a K_b = [\text{H}_3\text{O}^+][\text{OH}^-] = 10^{-14}$$

$$\text{p}K_a + \text{p}K_b = 14$$

### 1.7.8 Hydrolysis

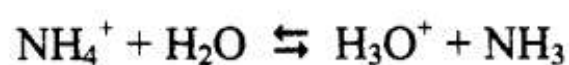
Hydrolysis is the reaction between water and the ions of a salt.

#### 1.7.8.1 Salt of a strong acid - strong base.

Consider NaCl, the salt of a strong acid and a strong base. The hydrolysis of this salt would yield NaOH and HCl. Since both species would completely dissociate into their respective ions yielding equivalent amounts of  $\text{H}_3\text{O}^+$  and  $\text{OH}^-$ , the overall net effect would be that no hydrolysis takes place. Since  $[\text{H}_3\text{O}^+] = [\text{OH}^-]$ , the pH would be 7, a neutral solution.

#### 1.7.8.2 Salt of a strong acid - weak base.

Consider the hydrolysis of  $\text{NH}_4\text{Cl}$ :

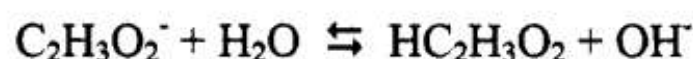


$$K_h = \frac{[\text{H}_3\text{O}^+][\text{NH}_3]}{[\text{NH}_4^+]}$$

$$K_h = \frac{K_w}{K_b} = \frac{[\text{H}_3\text{O}^+][\text{OH}^-]}{[\text{NH}_4^+][\text{OH}^-]/[\text{NH}_3]} = \frac{[\text{H}_3\text{O}^+][\text{NH}_3]}{[\text{NH}_4^+]}$$

### 1.7.8.3 Salt of a weak acid - strong base.

Consider the hydrolysis of  $\text{NaC}_2\text{H}_3\text{O}_2$ :

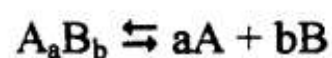


$$K_h = \frac{[\text{HC}_2\text{H}_3\text{O}_2][\text{OH}^-]}{[\text{C}_2\text{H}_3\text{O}_2^-]}$$

$$K_h = \frac{K_w}{K_a} = \frac{[\text{H}_3\text{O}^+][\text{OH}^-]}{[\text{H}_3\text{O}^+][\text{C}_2\text{H}_3\text{O}_2^-]/[\text{HC}_2\text{H}_3\text{O}_2]} = \frac{[\text{HC}_2\text{H}_3\text{O}_2][\text{OH}^-]}{[\text{C}_2\text{H}_3\text{O}_2^-]}$$

### 1.7.9 Solubility Product

In the case for which a solid is being dissolved, the general chemical reaction becomes:



and the equilibrium expression is:

$$K = \frac{[\text{A}]^a[\text{B}]^b}{[\text{A}_a\text{B}_b]}$$

the denominator in the expression  $[\text{A}_a\text{B}_b]$  represents the concentration of the pure solid and is constant, therefore it can be incorporated into the equilibrium constant,  $K$ . The expression now becomes:

$$K_{sp} = [\text{A}]^a[\text{B}]^b$$

For example, a saturated solution of AgCl, would have the following equilibrium:



$$K_{sp} = [\text{Ag}^+][\text{Cl}^-]$$

The value of the  $K_{sp}$  for AgCl is  $1.7 \times 10^{-10}$

$$1.7 \times 10^{-10} = [\text{Ag}^+][\text{Cl}^-]$$

If the ion product is equal to or less than the  $K_{sp}$ , no precipitate will form. If the ion product is greater than the  $K_{sp}$  value, the material will precipitate out of solution so that the ion product will be equal to the  $K_{sp}$ .

Table 1.13. Solubility Products

| Compound          | $K_{sp}$              |
|-------------------|-----------------------|
| AgCl              | $1.7 \times 10^{-10}$ |
| AgBr              | $5.0 \times 10^{-13}$ |
| BaSO <sub>4</sub> | $1.5 \times 10^{-9}$  |
| CuS               | $8.5 \times 10^{-36}$ |
| PbCl <sub>2</sub> | $1.6 \times 10^{-5}$  |
| HgS               | $1.6 \times 10^{-54}$ |

### 1.7.10 Common Ion Effect

The common ion is when an ion common to one of the salt ions is introduced to the solution. The introduction of a common ion produces an effect on the equilibrium of the solution and according to Le Chatelier's principle, i.e. the equilibrium is shifted so as to reduce the effect of the added ion. This is referred to as the **common ion effect**.

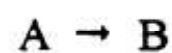
In the case of a solution of AgCl, if NaCl is added, the common ion being Cl<sup>-</sup>, the equilibrium would be shifted to the left so that the ion product will preserve the value of the  $K_{sp}$ .

## 1.8 Kinetics

**Kinetics** deals with the rate (how fast) that a chemical reaction proceeds with. The reaction rate can be determined by following the concentration of either the reactants or products. The rate is also dependent on the concentrations, temperature, catalysts, and nature of reactants and products.

### 1.8.1 Zero-Order Reactions

Zero-order reactions are independent of the concentrations of reactants.



$$\text{rate} = -\frac{\Delta[A]}{\Delta t} = k[A]^0 = k$$

### 1.8.2 First-Order Reactions

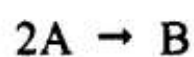
First-order reactions are dependent on the concentration of the reactant.



$$\text{rate} = k[A]^1 = k[A]$$

### 1.8.3 Second-Order Reactions

There are two type of second-order reactions. The first kind involves a single kind of reactant.



$$\text{rate} = k[A]^2$$

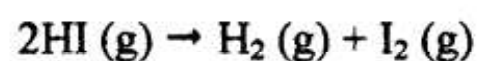
The second kind of reaction involves two different kind of reactants.



$$\text{rate} = k[A][B]$$

### 1.8.4 Collision Theory

Consider the decomposition of HI.



In order for the decomposition of HI to take place, two molecules of HI must collide with each other with the proper orientation as shown in Figure 1.12. If the molecules collide without the proper orientation then no decomposition takes place.

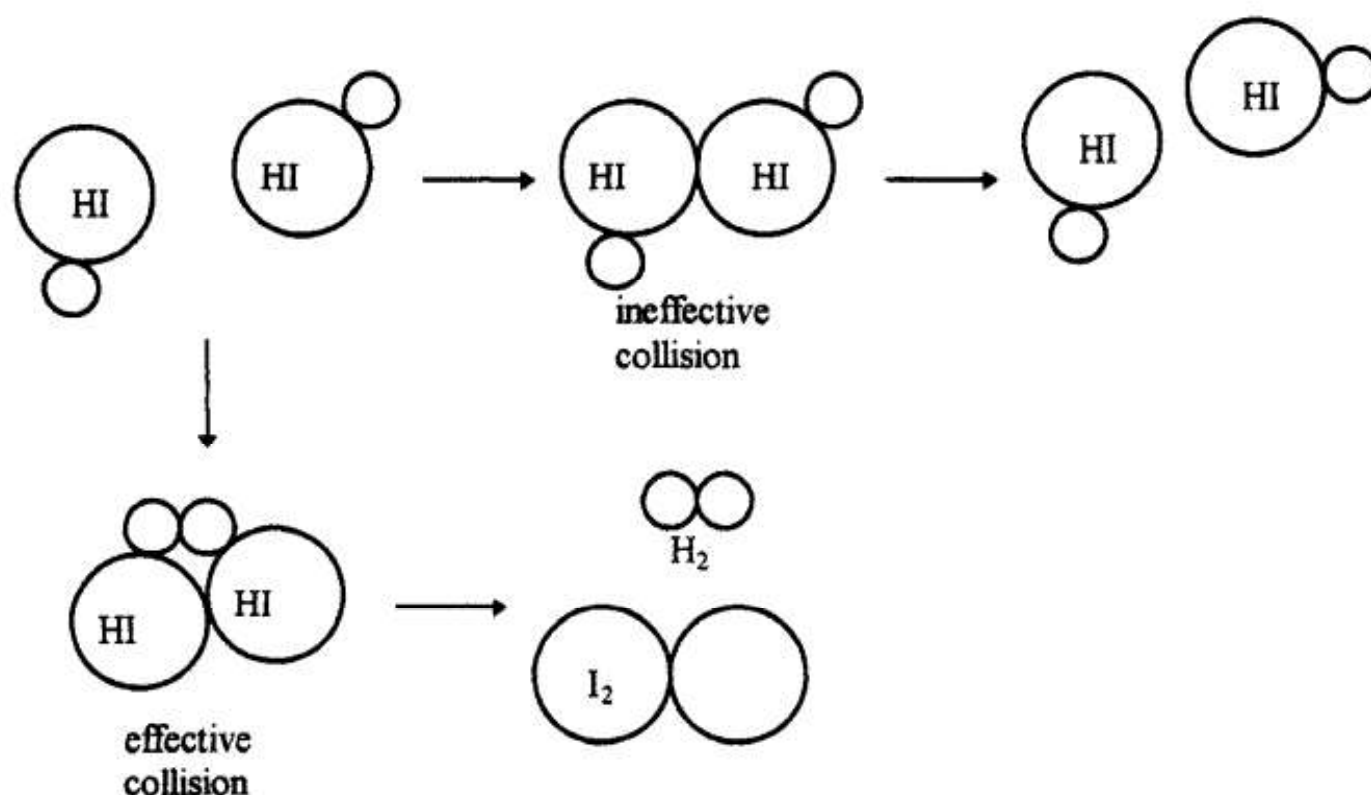


Figure 1.12. Effective and Ineffective collisions

Not all collisions with the proper orientation will react. Only those collisions with the proper orientation and sufficient energy to allow for the breaking and forming of bonds will react. The minimum energy available in a collision which will allow a reaction to occur is called the **activation energy**.

### 1.8.5 Transition State Theory

When a collision with the proper orientation and sufficient activation energy occurs, an intermediate state exists before the products are formed. This intermediate state, also called an **activated complex** or **transition state**, is neither the reactant or product, but rather a highly unstable combination of both, as represented in Figure 1.13 for the decomposition of HI.

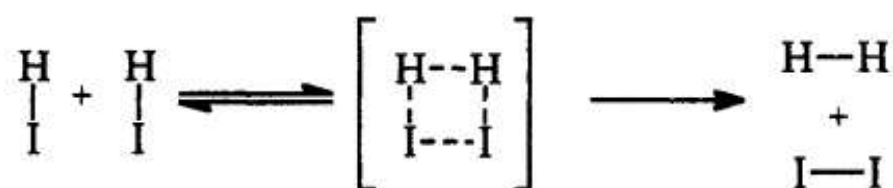


Figure 1.13. Transition state or activated complex

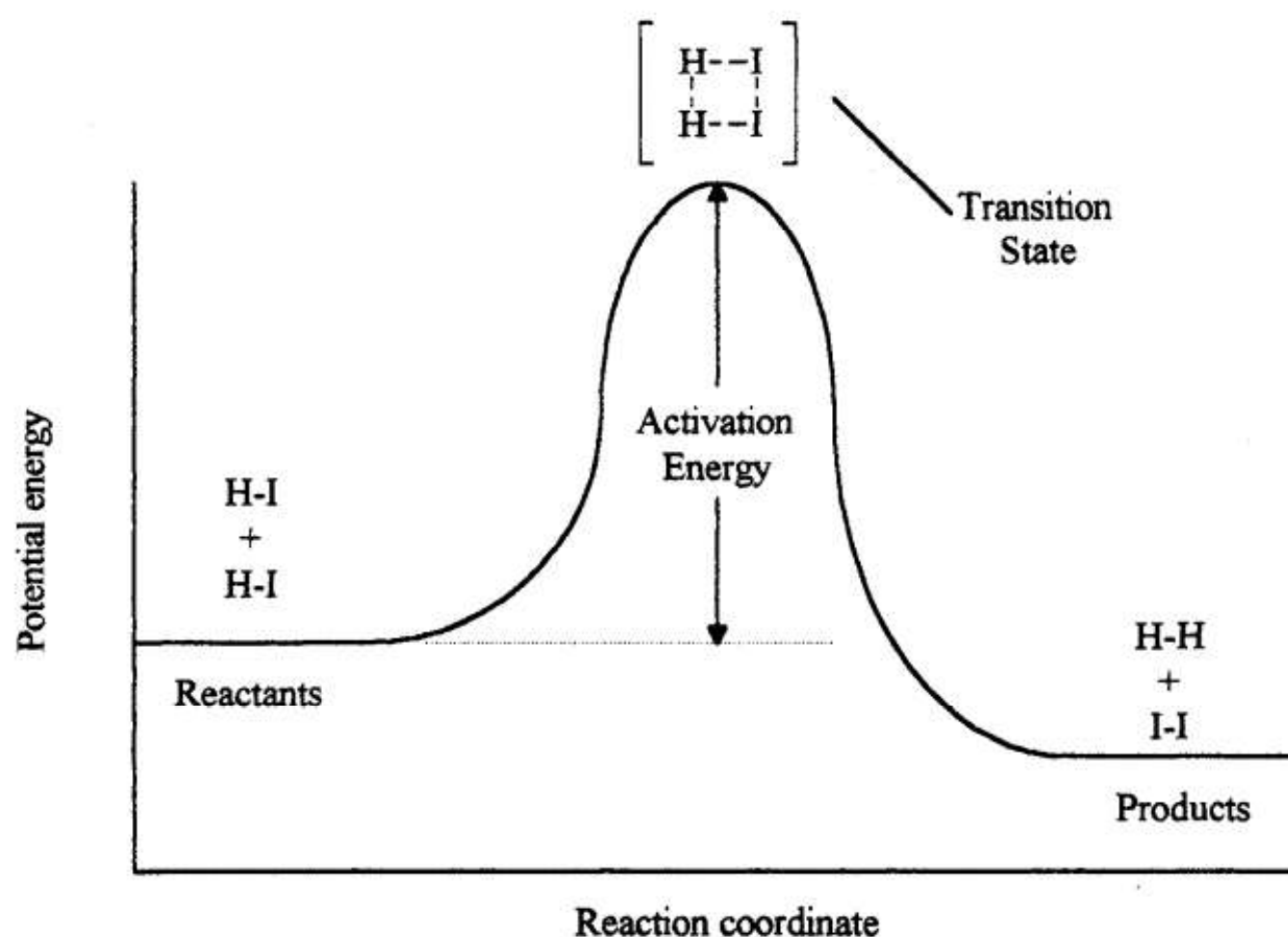


Figure 1.14. Potential energy diagram for the decomposition of HI.

Figure 1.14 shows the potential energy diagram for the decomposition of HI. As can be seen, in order to reach the activated complex or transition state the proper orientation and sufficient collision energy must be achieved. Once these requirements are achieved the reaction continues on to completion and the products are formed.

### 1.8.6 Catalysts

A **catalyst** is a substance that affects the rate of a chemical reaction without itself being consumed or chemically altered. The catalyst takes part in the reaction by providing an alternative route to the production of products. The catalyzed reaction has a lower activation energy than that of the uncatalyzed reaction, as shown in Figure 1.15. By lowering the activation energy there are more molecules with sufficient energy that can react and thus the rate of the reaction is affected.

A **homogeneous catalyst** is in the same phase as the reactants. The catalyst and the reactants form a reactive intermediate.

A **heterogeneous catalyst** is not in the same phase as the reactants. The reactants are absorbed on the surface of the heterogeneous catalyst and the reaction then takes place.

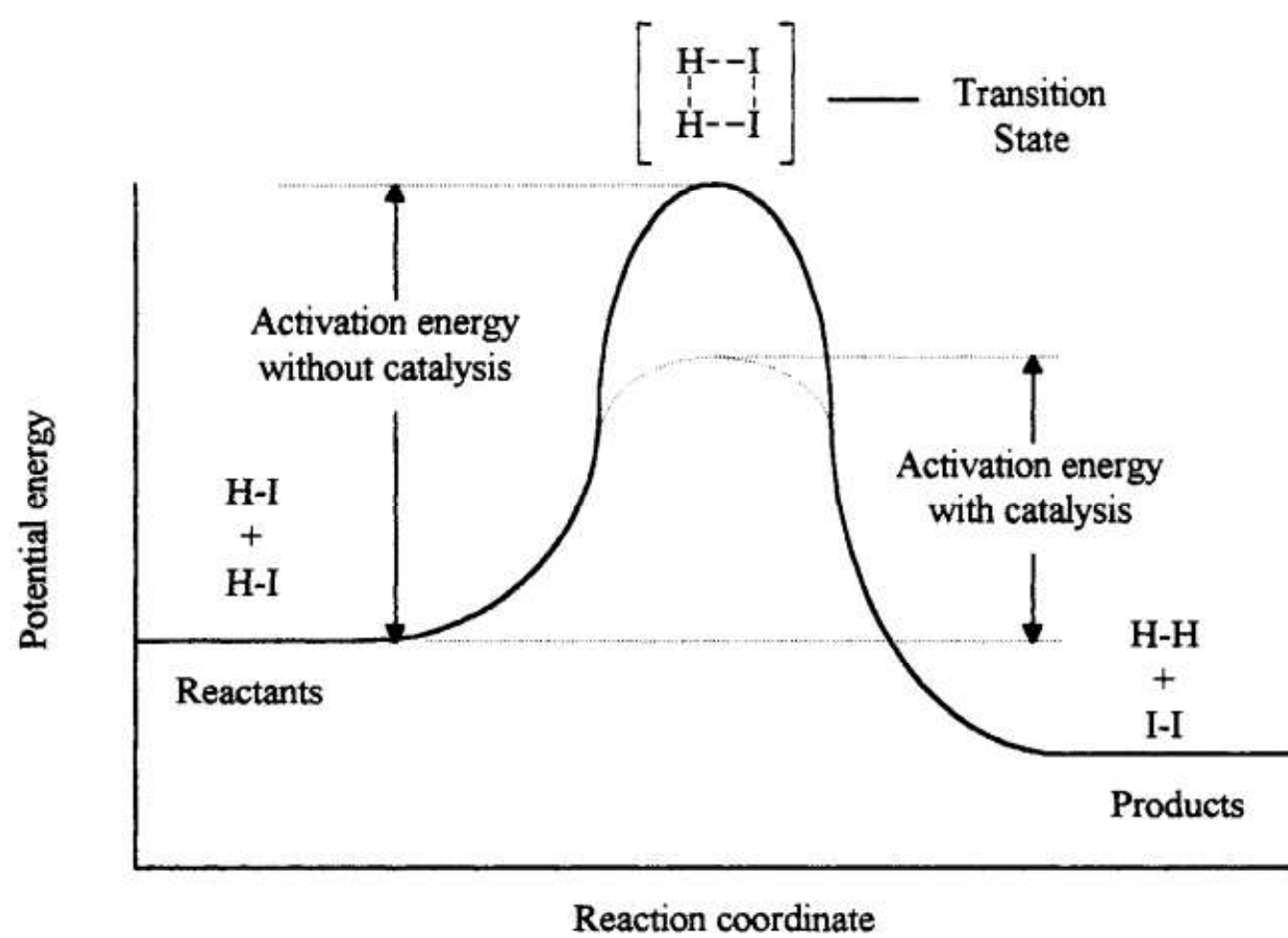


Figure 1.15. Energy diagram for a reaction with and without a catalysts

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## Chapter 2

### **Inorganic Chemistry**

*2.1 Group IA Elements*

*2.2 Group IIA Elements*

*2.3 Group IIIA Elements*

*2.4 Group IVA Elements*

*2.5 Group VA Elements*

*2.6 Group VIA Elements*

*2.7 Group VIIA Elements*

*2.8 Group VIIIA Elements*

*2.9 Transition Elements*

*2.10 Ionic Solids*

*2.11 Coordination Numbers*

*2.12 Ionic Crystal Systems*

*2.13 Crystal Lattice Packing*

*2.14 Crystal Lattice Types*

*2.15 Crystal Lattice Energy*

*2.16 Complexes*

## 2.1 Group IA Elements

Alkali Metals -Li, Na, K, Rb, Cs, Fr

Table 2.1. Group IA Properties

| Element                        | Li     | Na     | K      | Rb     | Cs     | Fr     |
|--------------------------------|--------|--------|--------|--------|--------|--------|
| Electronic configuration       | [He]2s | [Ne]3s | [Ar]4s | [Kr]5s | [Xe]6s | [Rn]7s |
| M.P. (°K)                      | 453.7  | 371.0  | 336.35 | 312.64 | 301.55 | 300    |
| B.P. (°K)                      | 1615   | 1156   | 1032   | 961    | 944    | 950    |
| Pauling's<br>Electronegativity | 0.98   | 0.93   | 0.82   | 0.82   | 0.79   | 0.7    |
| Atomic radius (Å)              | 2.05   | 2.23   | 2.77   | 2.98   | 3.34   | -      |
| Covalent radius (Å)            | 1.23   | 1.54   | 2.03   | 2.16   | 2.35   | -      |
| Ionic radius (Å)(+1)           | 0.68   | 0.98   | 1.33   | 1.48   | 1.67   | 1.8    |
| Ionization enthalpy (eV)       | 5.392  | 5.139  | 4.341  | 4.177  | 3.894  | -      |
| Crystal Structure              | bcc    | bcc    | bcc    | bcc    | bcc    | bcc    |

Table 2.2. Group IA Compounds

|                                             | Li | Na | K | Rb | Cs | Fr |
|---------------------------------------------|----|----|---|----|----|----|
| H <sup>-</sup>                              | x  | x  | x | x  | x  | -  |
| X <sup>-</sup>                              | x  | x  | x | x  | x  | -  |
| CH <sub>3</sub> COO <sup>-</sup>            | x  | x  | x | x  | x  | -  |
| HCO <sub>3</sub> <sup>-</sup>               | x  | x  | x | x  | x  | -  |
| ClO <sup>-</sup>                            | -  | x  | x | -  | -  | -  |
| ClO <sub>3</sub> <sup>-</sup>               | x  | x  | x | x  | x  | -  |
| ClO <sub>4</sub> <sup>-</sup>               | x  | x  | x | x  | x  | -  |
| OH <sup>-</sup>                             | x  | x  | x | x  | x  | -  |
| NO <sub>3</sub> <sup>-</sup>                | x  | x  | x | x  | x  | -  |
| NO <sub>2</sub> <sup>-</sup>                | x  | x  | x | -  | x  | -  |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> | x  | x  | x | -  | -  | -  |
| HSO <sub>4</sub> <sup>-</sup>               | x  | x  | x | x  | x  | -  |
| HSO <sub>3</sub> <sup>-</sup>               | -  | x  | x | -  | -  | -  |
| CO <sub>3</sub> <sup>-2</sup>               | x  | x  | x | x  | x  | -  |
| C <sub>2</sub> O <sub>4</sub> <sup>-2</sup> | x  | x  | x | -  | x  | -  |
| HPO <sub>4</sub> <sup>-2</sup>              | -  | x  | x | -  | -  | -  |
| SO <sub>4</sub> <sup>-2</sup>               | x  | x  | x | x  | x  | -  |
| SO <sub>3</sub> <sup>-2</sup>               | x  | x  | x | -  | -  | -  |
| PO <sub>3</sub> <sup>-3</sup>               | x  | x  | x | -  | -  | -  |
| PO <sub>4</sub> <sup>-3</sup>               | x  | x  | x | -  | -  | -  |
| N <sup>-3</sup>                             | x  | x  | x | -  | -  | -  |

## 2.2 Group IIA Elements

Alkaline Earth Metals -Be, Mg, Ca, Sr, Ba, Ra

Table 2.3. Group IIA Properties

| Element                        | Be                  | Mg                  | Ca                  | Sr                  | Ba                  | Ra                  |
|--------------------------------|---------------------|---------------------|---------------------|---------------------|---------------------|---------------------|
| Electronic configuration       | [He]2s <sup>2</sup> | [Ne]3s <sup>2</sup> | [Ar]4s <sup>2</sup> | [Kr]5s <sup>2</sup> | [Xe]6s <sup>2</sup> | [Rn]7s <sup>2</sup> |
| M.P. (°K)                      | 1560                | 922                 | 1112                | 1041                | 1002                | 973                 |
| B.P. (°K)                      | 2745                | 1363                | 1757                | 1650                | 2171                | 1809                |
| Pauling's<br>Electronegativity | 1.57                | 1.31                | 1.00                | 0.95                | 0.89                | 0.9                 |
| Atomic radius (Å)              | 1.40                | 1.72                | 2.223               | 2.45                | 2.78                | -                   |
| Covalent radius (Å)            | 0.90                | 1.36                | 1.74                | 1.91                | 1.98                | -                   |
| Ionic radius (Å)(+2)           | 0.35                | 0.66                | 1.18                | 1.112               | 1.34                | 1.43                |
| Ionization enthalpy (eV)       | 9.322               | 7.646               | 6.113               | 5.695               | 5.212               | 5.279               |
| Crystal Structure              | hex                 | hex                 | fcc                 | fcc                 | bcc                 | bcc                 |

Table 2.4. Group IIA Compounds

|                                             | Be | Mg | Ca | Sr | Ba | Ra |
|---------------------------------------------|----|----|----|----|----|----|
| H <sup>+</sup>                              | x  | x  | x  | x  | x  | -  |
| X <sup>-</sup>                              | x  | x  | x  | x  | x  | -  |
| CH <sub>3</sub> COO <sup>-</sup>            | x  | x  | x  | x  | x  | -  |
| HCO <sub>3</sub> <sup>-</sup>               | -  | -  | -  | -  | -  | -  |
| ClO <sup>-</sup>                            | -  | -  | x  | -  | x  | -  |
| ClO <sub>3</sub> <sup>-</sup>               | -  | x  | x  | x  | x  | -  |
| ClO <sub>4</sub> <sup>-</sup>               | -  | x  | x  | x  | x  | -  |
| OH <sup>-</sup>                             | x  | x  | x  | x  | x  | -  |
| NO <sub>3</sub> <sup>-</sup>                | x  | x  | x  | x  | x  | -  |
| NO <sub>2</sub> <sup>-</sup>                | -  | x  | x  | x  | x  | -  |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> | -  | -  | x  | -  | x  | -  |
| HSO <sub>4</sub> <sup>-</sup>               | -  | -  | -  | x  | -  | -  |
| HSO <sub>3</sub> <sup>-</sup>               | -  | -  | x  | -  | -  | -  |
| CO <sub>3</sub> <sup>-2</sup>               | x  | x  | x  | x  | x  | -  |
| C <sub>2</sub> O <sub>4</sub> <sup>-2</sup> | x  | x  | x  | x  | x  | -  |
| HPO <sub>4</sub> <sup>-2</sup>              | -  | x  | x  | x  | x  | -  |
| SO <sub>4</sub> <sup>-2</sup>               | x  | x  | x  | x  | x  | -  |
| SO <sub>3</sub> <sup>-2</sup>               | -  | x  | x  | x  | x  | -  |
| PO <sub>3</sub> <sup>-3</sup>               | -  | -  | x  | -  | x  | -  |
| PO <sub>4</sub> <sup>-3</sup>               | x  | x  | x  | -  | x  | -  |
| N <sup>-3</sup>                             | x  | x  | x  | x  | x  | -  |

## 2.3 Group IIIA Elements

Boron group - B, Al, Ga, In, Tl

Table 2.5. Group IIIA Properties

| Element                        | B                      | Al                     | Ga                                         | In                                         | Tl                                                          |
|--------------------------------|------------------------|------------------------|--------------------------------------------|--------------------------------------------|-------------------------------------------------------------|
| Electronic configuration       | [He]2s <sup>2</sup> 2p | [Ne]3s <sup>2</sup> 3p | [Ar]3d <sup>10</sup><br>4s <sup>2</sup> 4p | [Kr]4d <sup>10</sup><br>5s <sup>2</sup> 5p | [Xe]4f <sup>14</sup><br>5d <sup>10</sup> 6s <sup>2</sup> 6p |
| M.P. (°K)                      | 2300                   | 933.25                 | 301.90                                     | 429.76                                     | 577                                                         |
| B.P. (°K)                      | 4275                   | 2793                   | 2478                                       | 2346                                       | 1746                                                        |
| Pauling's<br>Electronegativity | 2.04                   | 1.61                   | 1.81                                       | 1.78                                       | 2.04                                                        |
| Atomic radius (Å)              | 1.17                   | 1.82                   | 1.81                                       | 2.00                                       | 2.08                                                        |
| Covalent radius (Å)            | 0.82                   | 1.18                   | 1.26                                       | 1.44                                       | 1.48                                                        |
| Ionic radius (Å)(+3)           | 0.23                   | 0.51                   | 0.81                                       | 0.81                                       | 0.95                                                        |
| Ionization enthalpy (eV)       | 8.298                  | 5.986                  | 5.999                                      | 5.786                                      | 6.108                                                       |
| Crystal Structure              | rhomb                  | fcc                    | orthorho                                   | tetrag                                     | hex                                                         |

Table 2.6. Group IIIA Compounds

|                                             | B | Al | Ga | In | Tl |
|---------------------------------------------|---|----|----|----|----|
| H <sup>-</sup>                              | x | -  | x  | -  | -  |
| X <sup>-</sup>                              | x | x  | x  | x  | x  |
| CH <sub>3</sub> COO <sup>-</sup>            | - | x  | x  | -  | x  |
| HCO <sub>3</sub> <sup>-</sup>               | - | -  | -  | -  | -  |
| ClO <sup>-</sup>                            | - | -  | -  | -  | -  |
| ClO <sub>3</sub> <sup>-</sup>               | - | -  | -  | -  | x  |
| ClO <sub>4</sub> <sup>-</sup>               | - | -  | x  | x  | x  |
| OH <sup>-</sup>                             | - | x  | x  | x  | x  |
| NO <sub>3</sub> <sup>-</sup>                | - | x  | x  | x  | x  |
| NO <sub>2</sub> <sup>-</sup>                | - | -  | -  | -  | x  |
| H <sub>2</sub> PO <sub>4</sub> <sup>-</sup> | - | -  | -  | -  | x  |
| HSO <sub>4</sub> <sup>-</sup>               | - | -  | -  | -  | x  |
| HSO <sub>3</sub> <sup>-</sup>               | - | -  | -  | -  | x  |
| CO <sub>3</sub> <sup>-2</sup>               | - | -  | -  | -  | x  |
| C <sub>2</sub> O <sub>4</sub> <sup>-2</sup> | - | x  | x  | -  | x  |
| HPO <sub>4</sub> <sup>-2</sup>              | - | -  | -  | -  | -  |
| SO <sub>4</sub> <sup>-2</sup>               | - | x  | x  | x  | x  |
| SO <sub>3</sub> <sup>-2</sup>               | - | -  | -  | -  | x  |
| PO <sub>3</sub> <sup>-3</sup>               | - | x  | -  | -  | -  |
| PO <sub>4</sub> <sup>-3</sup>               | - | x  | -  | -  | x  |
| N <sup>-3</sup>                             | x | x  | x  | -  | -  |

## 2.4 Group IVA Elements

Carbon group - C, Si, Ge, Sn, Pb

Table 2.7. Group IVA Properties

| Element                        | C                                      | Si                                     | Ge                                                      | Sn                                                      | Pb                                                                          |
|--------------------------------|----------------------------------------|----------------------------------------|---------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------------------------------------|
| Electronic configuration       | [He]2s <sup>2</sup><br>2p <sup>2</sup> | [Ne]3s <sup>2</sup><br>3p <sup>2</sup> | [Ar]3d <sup>10</sup><br>4s <sup>2</sup> 4p <sup>2</sup> | [Kr]4d <sup>10</sup><br>5s <sup>2</sup> 5p <sup>2</sup> | [Xe]4f <sup>14</sup><br>5d <sup>10</sup> 6s <sup>2</sup><br>6p <sup>2</sup> |
| M.P. (°K)                      | 4100                                   | 1685                                   | 1210.4                                                  | 505.06                                                  | 600.6                                                                       |
| B.P. (°K)                      | 4470                                   | 3540                                   | 3107                                                    | 2876                                                    | 2023                                                                        |
| Pauling's<br>Electronegativity | 2.55                                   | 1.90                                   | 2.01                                                    | 1.96                                                    | 2.33                                                                        |
| Atomic radius (Å)              | 0.91                                   | 1.46                                   | 1.52                                                    | 1.72                                                    | 1.81                                                                        |
| Covalent radius (Å)            | 0.77                                   | 1.11                                   | 1.22                                                    | 1.41                                                    | 1.47                                                                        |
| Ionic radius (Å)(xx)           |                                        |                                        |                                                         |                                                         |                                                                             |
| Ionization enthalpy (eV)       | 11.260                                 | 8.151                                  | 7.899                                                   | 7.344                                                   | 7.416                                                                       |
| Crystal Structure              | hex                                    | fcc                                    | orthorho                                                | tetrag                                                  | fcc                                                                         |

## 2.5 Group VA Elements

Nitrogen group - N, P, As, Sb, Bi

Table 2.8. Group VA Properties

| Element                        | N                                      | P                                      | As                                                       | Sb                                                      | Bi                                                                          |
|--------------------------------|----------------------------------------|----------------------------------------|----------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------------------------------------|
| Electronic configuration       | [He]2s <sup>2</sup><br>2p <sup>3</sup> | [Ne]3s <sup>2</sup><br>3p <sup>3</sup> | [Ar] 3d <sup>10</sup><br>4s <sup>2</sup> 4p <sup>3</sup> | [Kr]4d <sup>10</sup><br>5s <sup>2</sup> 5p <sup>3</sup> | [Xe]4f <sup>14</sup><br>5d <sup>10</sup> 6s <sup>2</sup><br>6p <sup>3</sup> |
| M.P. (°K)                      | 63.14                                  | 317.3                                  | 1081                                                     | 904                                                     | 544.52                                                                      |
| B.P. (°K)                      | 77.35                                  | 550                                    | 876 (sub)                                                | 1860                                                    | 1837                                                                        |
| Pauling's<br>Electronegativity | 3.04                                   | 2.19                                   | 2.18                                                     | 2.05                                                    | 2.02                                                                        |
| Atomic radius (Å)              | 0.75                                   | 1.23                                   | 1.33                                                     | 1.53                                                    | 1.63                                                                        |
| Covalent radius (Å)            | 0.75                                   | 1.06                                   | 1.20                                                     | 1.40                                                    | 1.46                                                                        |
| Ionic radius (Å)(xx)           |                                        |                                        |                                                          |                                                         |                                                                             |
| Ionization enthalpy (eV)       | 14.534                                 | 10.486                                 | 9.81                                                     | 8.641                                                   | 7.289                                                                       |
| Crystal Structure              | hex                                    | monoclini                              | rhomb                                                    | rhomb                                                   | rhomb                                                                       |

## 2.6 Group VIA Elements

Oxygen group - O, S, Se, Te, Po

Table 2.9. Group VIA Properties

| Element                        | O                                      | S                                      | Se                                                       | Te                                                      | Po                                                                          |
|--------------------------------|----------------------------------------|----------------------------------------|----------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------------------------------------|
| Electronic configuration       | [He]2s <sup>2</sup><br>2p <sup>4</sup> | [Ne]3s <sup>2</sup><br>3p <sup>4</sup> | [Ar] 3d <sup>10</sup><br>4s <sup>2</sup> 4p <sup>4</sup> | [Kr]4d <sup>10</sup><br>5s <sup>2</sup> 5p <sup>4</sup> | [Xe]4f <sup>14</sup><br>5d <sup>10</sup> 6s <sup>2</sup><br>6p <sup>4</sup> |
| M.P. (°K)                      | 50.35                                  | 388.36                                 | 494                                                      | 722.65                                                  | 527                                                                         |
| B.P. (°K)                      | 90.18                                  | 717.75                                 | 958                                                      | 1261                                                    | 1235                                                                        |
| Pauling's<br>Electronegativity | 3.44                                   | 2.58                                   | 2.55                                                     | 2.1                                                     | 2.0                                                                         |
| Atomic radius (Å)              | 0.65                                   | 1.09                                   | 1.22                                                     | 1.42                                                    | 1.53                                                                        |
| Covalent radius (Å)            | 0.73                                   | 1.02                                   | 1.16                                                     | 1.36                                                    | 1.46                                                                        |
| Ionic radius (Å)(-2)           | 1.32                                   | 1.84                                   | 1.91                                                     | 2.11                                                    | -                                                                           |
| Ionization enthalpy (eV)       | 13.618                                 | 10.360                                 | 9.752                                                    | 9.009                                                   | 8.42                                                                        |
| Crystal Structure              | cubic                                  | orthorho                               | hex                                                      | hex                                                     | monoclin                                                                    |

## 2.7 Group VIIA Elements

Halogens - F, Cl, Br, I, At

Table 2.10. Group VIIA Properties

| Element                        | F                                      | Cl                                     | Br                                                       | I                                                       | At                                                                          |
|--------------------------------|----------------------------------------|----------------------------------------|----------------------------------------------------------|---------------------------------------------------------|-----------------------------------------------------------------------------|
| Electronic configuration       | [He]2s <sup>2</sup><br>2p <sup>5</sup> | [Ne]3s <sup>2</sup><br>3p <sup>5</sup> | [Ar] 3d <sup>10</sup><br>4s <sup>2</sup> 4p <sup>5</sup> | [Kr]4d <sup>10</sup><br>5s <sup>2</sup> 5p <sup>5</sup> | [Xe]4f <sup>14</sup><br>5d <sup>10</sup> 6s <sup>2</sup><br>6p <sup>5</sup> |
| M.P. (°K)                      | 53.48                                  | 172.16                                 | 265.90                                                   | 386.7                                                   | 575                                                                         |
| B.P. (°K)                      | 84.95                                  | 239.1                                  | 332.25                                                   | 458.4                                                   | 610                                                                         |
| Pauling's<br>Electronegativity | 3.98                                   | 3.16                                   | 2.96                                                     | 2.66                                                    | 2.2                                                                         |
| Atomic radius (Å)              | 0.57                                   | 0.97                                   | 1.12                                                     | 1.32                                                    | 1.43                                                                        |
| Covalent radius (Å)            | 0.72                                   | 0.99                                   | 1.14                                                     | 1.33                                                    | 1.45                                                                        |
| Ionic radius (Å)(-1)           | 1.33                                   | 1.81                                   | 1.96                                                     | 2.20                                                    | -                                                                           |
| Ionization enthalpy (eV)       | 17.411                                 | 112.967                                | 11.814                                                   | 10.451                                                  | -                                                                           |
| Crystal Structure              | cubic                                  | orthorho                               | orthorho                                                 | orthorho                                                | -                                                                           |

## 2.8 Group VIIIA Elements

Noble (Inert) Gases - He, Ne, Ar, Kr, Xe, Rn

Table 2.11. Group VIIIA Properties

| Element                     | He     | Ne                      | Ar                      | Kr                              | Xe                              | Rn                                      |
|-----------------------------|--------|-------------------------|-------------------------|---------------------------------|---------------------------------|-----------------------------------------|
| Electronic configuration    | $1s^2$ | $[\text{He}] 2s^2 2p^6$ | $[\text{Ne}] 3s^2 3p^6$ | $[\text{Ar}] 3d^{10} 4s^2 4p^6$ | $[\text{Kr}] 4d^{10} 5s^2 5p^6$ | $[\text{Xe}] 4f^{14} 5d^{10} 6s^2 6p^6$ |
| M.P. (°K)                   | 0.95   | 24.553                  | 83.81                   | 115.78                          | 165.03                          | 202                                     |
| B.P. (°K)                   | 4.215  | 27.096                  | 87.30                   | 119.80                          | 161.36                          | 211                                     |
| Pauling's Electronegativity | 0      | 0                       | 0                       | 0                               | 0                               | 0                                       |
| Atomic radius (Å)           | 0.49   | 0.51                    | 0.88                    | 1.03                            | 1.24                            | 1.34                                    |
| Covalent radius (Å)         | 0.93   | 0.71                    | 0.98                    | 1.12                            | 1.31                            | -                                       |
| Ionic radius (Å)            | -      | -                       | -                       | -                               | -                               | -                                       |
| Ionization enthalpy (eV)    | 24.58  | 21.56                   | 15.75                   | 13.99                           | 12.13                           | 10.74                                   |
| Crystal Structure           | hex    | fcc                     | fcc                     | fcc                             | fcc                             | fcc                                     |

Table 2.12. Some Group VIIIA Compounds

| Oxidation State | Compound                  | Form    | Mp (°C) | Structure   |
|-----------------|---------------------------|---------|---------|-------------|
| II              | $\text{XeF}_2$            | Crystal | 129     | Linear      |
| IV              | $\text{XeF}_4$            | Crystal | 117     | Square      |
| VI              | $\text{XeF}_6$            | Crystal | 49.6    |             |
|                 | $\text{Cs}_2\text{XeF}_8$ | Solid   |         |             |
|                 | $\text{XeOF}_4$           | Liquid  | -46     | Sq. Pyramid |
|                 | $\text{XeO}_3$            | Crystal |         | Pyramidal   |
| VIII            | $\text{XeO}_4$            | Gas     |         | Tetrahedral |
|                 | $\text{XeO}_6^{4-}$       | Salts   |         | Octahedral  |

## 2.9 Transition Metal Elements

Table 2.13. Transition Elements Properties

| Element | Elec.<br>conf.                   | M.P.<br>(°C) | B.P.<br>(°C) | Density<br>(g/cm <sup>3</sup> ) | Atomic<br>Radius | Ionic Radius (Å) |      |      |      |
|---------|----------------------------------|--------------|--------------|---------------------------------|------------------|------------------|------|------|------|
|         |                                  |              |              |                                 |                  | +2               | +3   | +4   | +X   |
| Sc      | 3d <sup>1</sup> 4s <sup>2</sup>  | 1540         | 2730         | 3.0                             | 1.61             |                  | 0.81 |      |      |
| Y       | 4d <sup>1</sup> 5s <sup>2</sup>  | 1500         | 2927         | 4.472                           | 1.8              |                  | 0.92 |      |      |
| La      | 5d <sup>1</sup> 6s <sup>2</sup>  | 920          | 3470         | 6.162                           | 1.86             |                  | 1.14 |      |      |
| Ti      | 3d <sup>2</sup> 4s <sup>2</sup>  | 1670         | 3260         | 4.5                             | 1.45             | 0.90             | 0.87 | 0.68 |      |
| Zr      | 4d <sup>2</sup> 5s <sup>2</sup>  | 1850         | 3580         | 6.4                             | 1.60             |                  |      | 0.79 |      |
| Hf      | 5d <sup>2</sup> 6s <sup>2</sup>  | 2000         | 5400         | 13.2                            | -                |                  |      | 0.78 |      |
| V       | 3d <sup>3</sup> 4s <sup>2</sup>  | 1900         | 3450         | 5.8                             | 1.32             | 0.88             | 0.74 |      | X=5  |
| Nb      | 4d <sup>4</sup> 5s <sup>1</sup>  | 2420         | 4930         | 8.57                            | 1.45             |                  |      |      | 0.59 |
| Ta      | 5d <sup>3</sup> 6s <sup>2</sup>  | 3000         | -            | -                               | 1.45             |                  |      |      | 0.69 |
|         |                                  |              |              |                                 |                  |                  |      |      | 0.68 |
| Cr      | 3d <sup>5</sup> 4s <sup>1</sup>  | 1900         | 2640         | 7.2                             | 1.37             | 0.88             | 0.63 |      | X=6  |
| Mo      | 4d <sup>5</sup> 5s <sup>1</sup>  | 2610         | 5560         | 10.2                            | 1.36             |                  |      |      | 0.52 |
| W       | 5d <sup>4</sup> 6s <sup>2</sup>  | 3410         | 5930         | 19.3                            | 1.37             |                  |      |      | 0.62 |
|         |                                  |              |              |                                 |                  |                  |      |      | 0.62 |
| Mn      | 3d <sup>5</sup> 4s <sup>2</sup>  | 1250         | 2100         | 7.4                             | 1.37             | 0.80             | 0.66 |      | X=7  |
| Tc      | 4d <sup>5</sup> 5s <sup>2</sup>  | 2140         | -            | -                               | 1.36             |                  |      |      | 0.46 |
| Re      | 5d <sup>5</sup> 6s <sup>2</sup>  | 3180         | -            | 21                              | 1.37             |                  |      |      | 0.56 |
| Fe      | 3d <sup>6</sup> 4s <sup>2</sup>  | 1540         | 3000         | 7.9                             | 1.24             | 0.76             | 0.64 |      |      |
| Ru      | 4d <sup>7</sup> 5s <sup>1</sup>  | 2300         | 3900         | 12.2                            | 1.33             |                  |      | 0.67 |      |
| Os      | 5d <sup>6</sup> 6s <sup>2</sup>  | 3000         | 5500         | 22.4                            | 1.34             |                  |      | 0.69 |      |
| Co      | 3d <sup>7</sup> 4s <sup>2</sup>  | 1490         | 2900         | 8.9                             | 1.25             | 0.74             | 0.63 |      |      |
| Rh      | 4d <sup>8</sup> 5s <sup>1</sup>  | 1970         | 3730         | 12.4                            | 1.34             | 0.86             | 0.68 |      |      |
| Ir      | 5d <sup>7</sup> 6s <sup>2</sup>  | 2450         | 4500         | 22.5                            | 1.36             |                  |      | 0.68 |      |
| Ni      | 3d <sup>8</sup> 4s <sup>2</sup>  | 1450         | 2730         | 8.9                             | 1.25             | 0.72             | 0.62 |      |      |
| Pd      | 4d <sup>10</sup>                 | 1550         | 3125         | 12.0                            | 1.38             | 0.80             |      | 0.65 |      |
| Pt      | 5d <sup>9</sup> 6s <sup>1</sup>  | 1770         | 3825         | 21.4                            | 1.39             | 0.80             |      | 0.65 |      |
| Cu      | 3d <sup>10</sup> 4s <sup>1</sup> | 1083         | 2600         | 8.9                             | 1.28             | 0.69             |      |      | X=1  |
| Ag      | 4d <sup>10</sup> 5s <sup>1</sup> | 961          | 2210         | 10.5                            | 1.44             | 0.89             |      |      | 0.96 |
| Au      | 5d <sup>10</sup> 6s <sup>1</sup> | 1063         | 2970         | 19.3                            | 1.44             |                  | 0.85 |      | 1.26 |
|         |                                  |              |              |                                 |                  |                  |      |      | 1.37 |
| Zn      | 3d <sup>10</sup> 4s <sup>2</sup> | 419          | 906          | 7.3                             | 1.33             | 0.74             |      |      |      |
| Cd      | 4d <sup>10</sup> 5s <sup>2</sup> | 321          | 765          | 8.64                            | 1.49             | 0.97             |      |      |      |
| Hg      | 5d <sup>10</sup> 6s <sup>2</sup> | -39          | 357          | 13.54                           | 1.52             | 1.10             |      |      |      |

Table 2.14. Oxidation States of Transition Elements

| Sc   | Ti   | V    | Cr   | Mn   | Fe   | Co   | Ni   | Cu  | Zn  |
|------|------|------|------|------|------|------|------|-----|-----|
| +III | +III | +II  | +II  | +II  | +II  | +II  | +II  | +I  | +II |
|      | +IV  | +III | +III | +III | +III | +III | +III | +II |     |
|      |      | +IV  | +VI  | +IV  | +IV  |      |      |     |     |
|      |      | +V   |      | +VI  | +VI  |      |      |     |     |
|      |      |      |      | +VII |      |      |      |     |     |

| Ce   | Mo   | Ru   | Rh   | Pd  | Ag  | Cd  |
|------|------|------|------|-----|-----|-----|
| +III | +III | +II  | +III | +II | +I  | +II |
| +IV  | +IV  | +III | +IV  | +IV | +II |     |
|      | +V   | +IV  |      |     |     |     |
|      | +VI  | +VI  |      |     |     |     |

| W   | Os    | Ir   | Pt  | Au   | Hg  |
|-----|-------|------|-----|------|-----|
| +IV | +IV   | +III | +II | +I   | +I  |
| +V  | +VI   | +IV  | +IV | +III | +II |
| +VI | +VIII | +VI  |     |      |     |

## 2.10 Ionic Solids

**Ionic solids** are mostly inorganic compounds, which are held together by ionic bonds (Chapter 1.2.3). The ions are treated as though they were hard spheres with either positive (cations) or negative (anions) charges. Using this model the ionic solids or **crystals**, are found to be arranged in a very specific order called a **crystal lattice**. The crystal lattice consists of repeating units called unit cells (see below).

## 2.11 Coordination Number

For ionic compounds the **coordination number** is the number of anions that are arranged about the cation in an organized structure. For example, NaCl has a coordination number of 6. In other words, 6  $\text{Cl}^-$  atoms surround 1  $\text{Na}^+$  atom. The number of anions that can surround a cation is dependent (but not entirely) on the relative sizes of the ions involved. Table 2.15 illustrates the ratios of the radii of the ions and their coordination number.

Table 2.15. Radius Ratios and Coordination Number

| Coordination Number | Geometry              | Ratio (+/-)   |
|---------------------|-----------------------|---------------|
| 2                   | Linear                | 0.000 - 0.155 |
| 3                   | Trigonal              | 0.155 - 0.225 |
| 4                   | Tetrahedral           | 0.225 - 0.414 |
| 4/6                 | Sq. Planar/Octahedral | 0.414 - 0.732 |
| 8                   | Cubic                 | 0.732 - 1.000 |
| 12                  | Dodecahedral          | 1.000 -       |

Taking NaCl, the radii of  $\text{Na}^+$  ion is  $0.95\text{\AA}$  and  $\text{Cl}^-$  is  $1.81\text{\AA}$ . Their ratio would be as follows:

$$\frac{r_{\text{cation}}}{r_{\text{anion}}} = \frac{r_{\text{Na}}}{r_{\text{Cl}}} = \frac{0.95}{1.81} = 0.52$$

forming the sodium chloride lattice with coordination number 6.

## 2.12 Ionic Crystal Systems

A crystal lattice can be broken down to a small repeating unit called a unit cell. There are only seven distinct unit cells possible, and are shown in Figure 2.1.

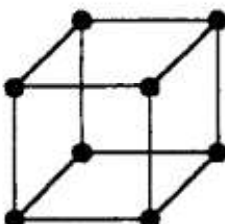
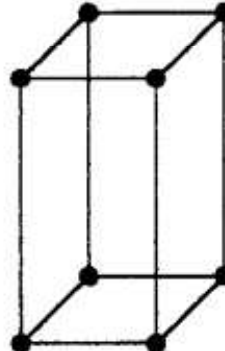
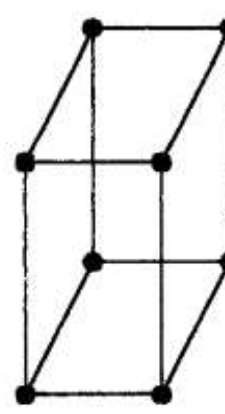
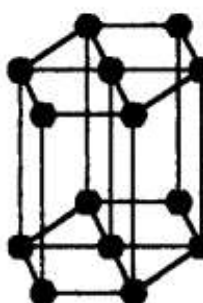
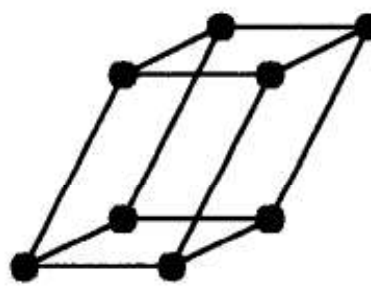
|                       | All Edges Equal                                                                                                                                                                    | Two Edges Equal                                                                                                                                                                                        | No Edges Equal                                                                                                                                                                                               |
|-----------------------|------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| All $90^\circ$ Angles | <p>cubic</p>  <p><math>a = b = c</math><br/><math>\alpha = \beta = \gamma = 90^\circ</math></p> | <p>tetragonal</p>  <p><math>a = b \neq c</math><br/><math>\alpha = \beta = \gamma = 90^\circ</math></p>           | <p>orthorhombic</p>  <p><math>a \neq b \neq c</math><br/><math>\alpha = \beta = \gamma = 90^\circ</math></p>            |
| Two $90^\circ$ angles |                                                                                                                                                                                    | <p>hexagonal</p>  <p><math>a = b \neq c</math><br/><math>\alpha = \beta = 90^\circ; \gamma = 120^\circ</math></p> | <p>monoclinic</p>  <p><math>a \neq b \neq c</math><br/><math>\alpha = \gamma = 90^\circ; \beta \neq 90^\circ</math></p> |

Figure 2.1. Unit Cells

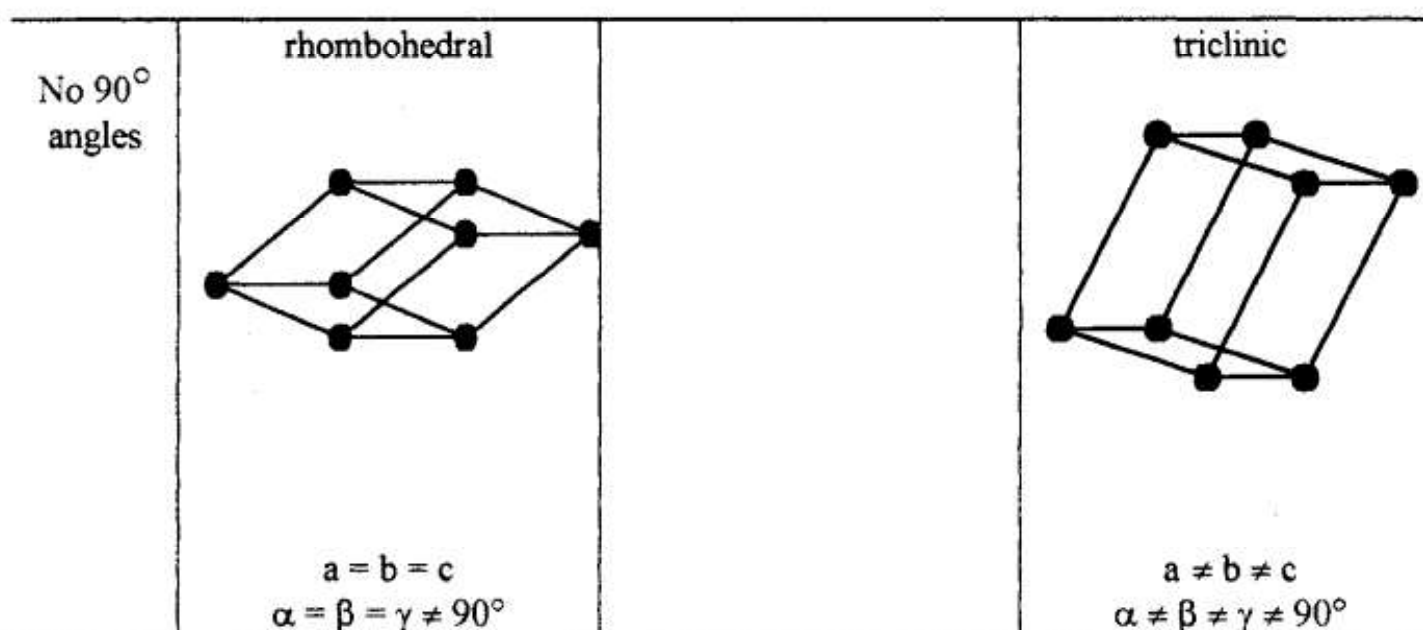


Figure 2.1. Unit Cells

### 2.13 Crystal Lattice Packing

When a crystal lattice forms the ions are arranged in the most efficient way of packing spheres into the smallest possible space. Starting with a single layer as in figure 2.2a, a second layer can be placed on top of it in the hollows of the first Figure 2.2b. At this point a third layer can be placed. If the third layer is placed directly over the first, Figure 2.2c, the structure is **hexagonal close-packed (hcp)**. The layering in hexagonal close-packed is ABABAB. If the third layer is placed so it is not directly over the first a different arrangement is obtained. This structure is **cubic close-packed (ccp)**. The layering in cubic close-packed is ABCABC.

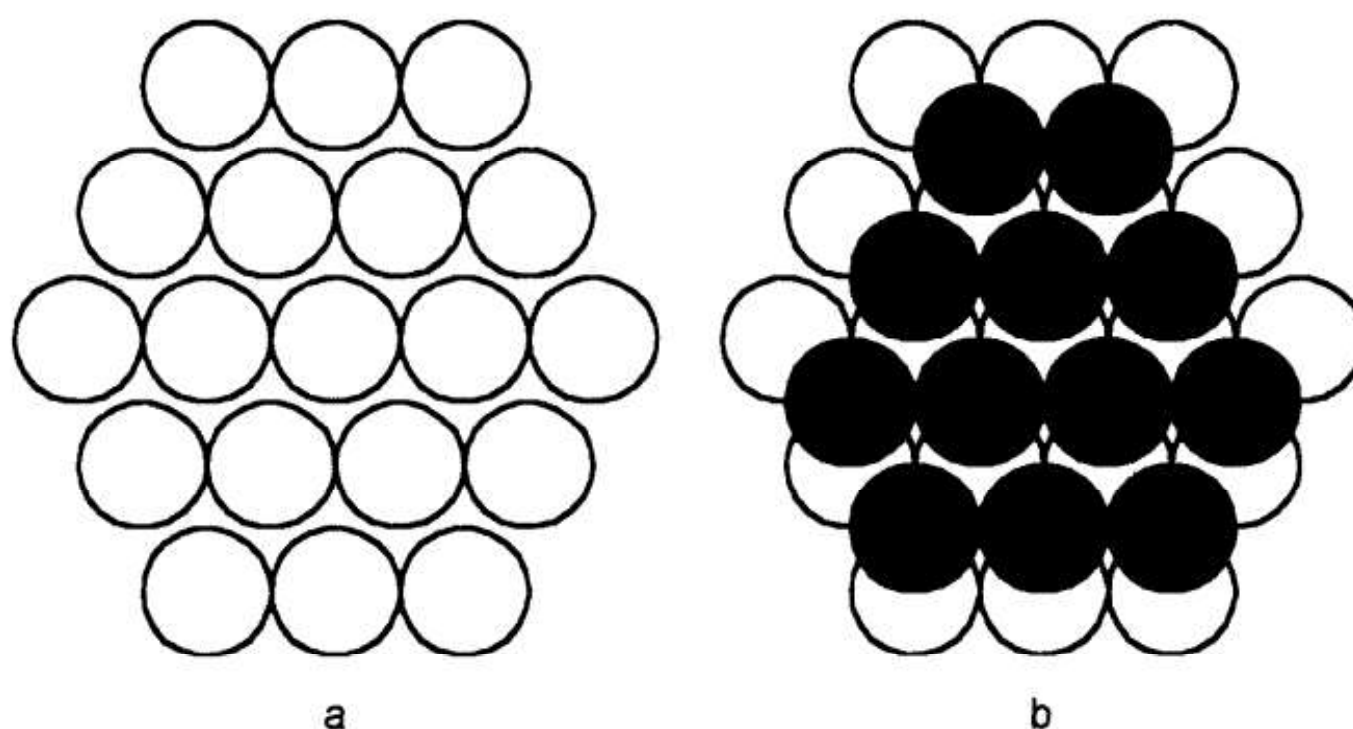


Figure 2.2. Close Packing of Atoms

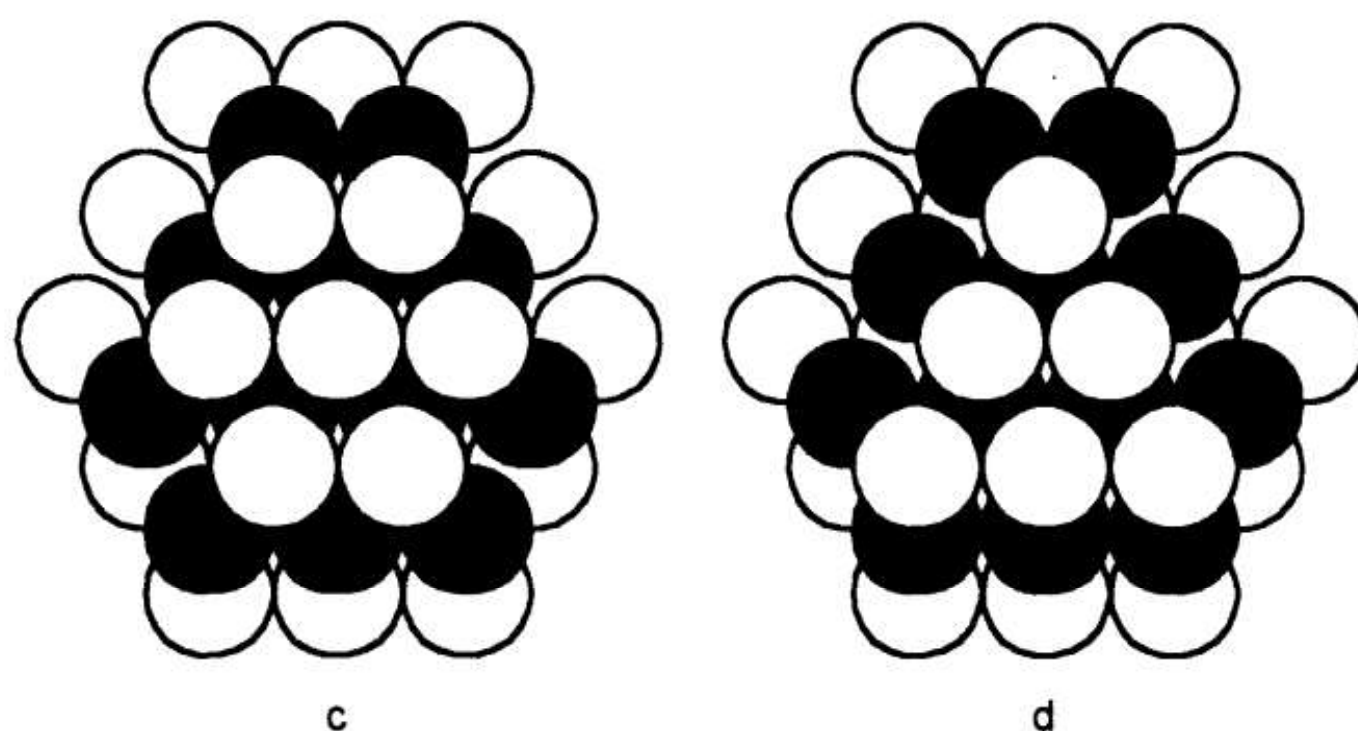


Figure 2.2. Close Packing of Atoms

## 2.14 Crystal Lattice Types

Shown below are commonly encountered crystal lattice structures. The lattice type depends on the radius ratio favoring a particular coordination number for the structure type.

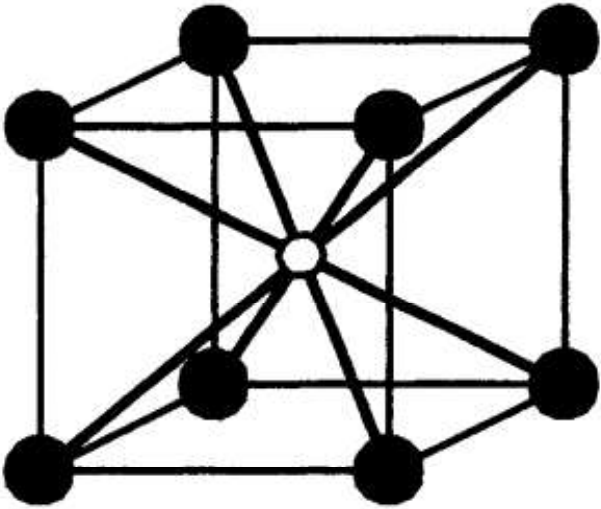
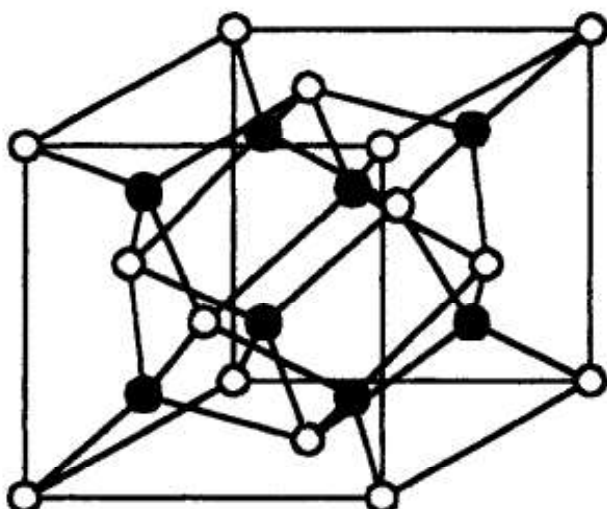
| Structure Type                                                                                                                                                     |                                                                                                                                                                 |
|--------------------------------------------------------------------------------------------------------------------------------------------------------------------|-----------------------------------------------------------------------------------------------------------------------------------------------------------------|
| AB                                                                                                                                                                 | AB <sub>2</sub>                                                                                                                                                 |
|  <p>Cesium Chloride<br/>Coordination 8<br/><math>r_{+/-} = 0.732 - 1</math></p> |  <p>Fluorite<br/>Coordination 8:4<br/><math>r_{+/-} = 0.732 - 1</math></p> |

Figure 2.3. Common Lattice Types

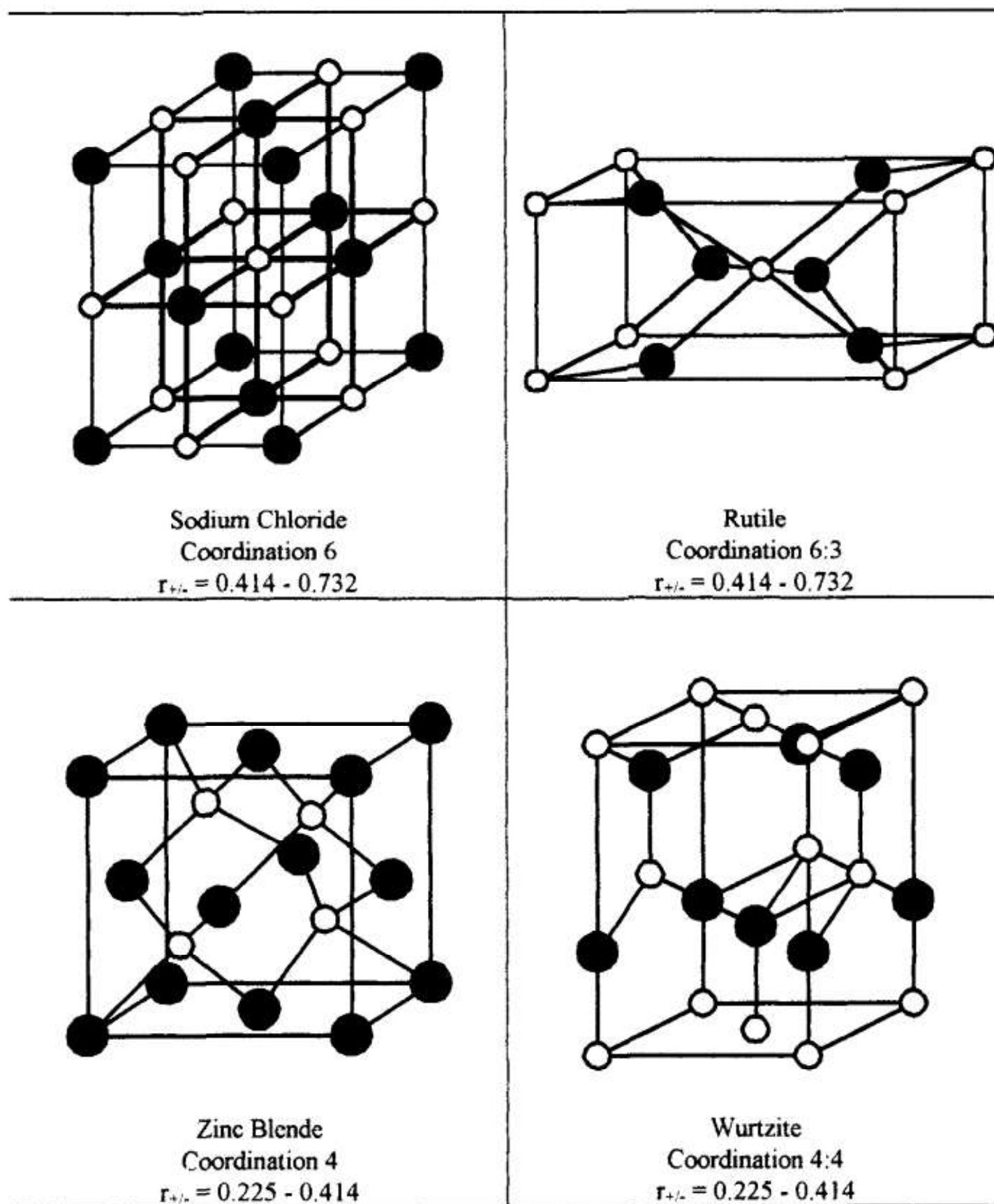


Figure 2.3. Common Lattice Types

## 2.15 Crystal Lattice Energy

### 2.15.1 Born-Haber Cycle

An important property of an ionic crystal is the energy required to break the crystal apart into individual ions, this is the **crystal lattice energy**. It can be measured by a thermodynamic cycle, called the **Born-Haber cycle**.

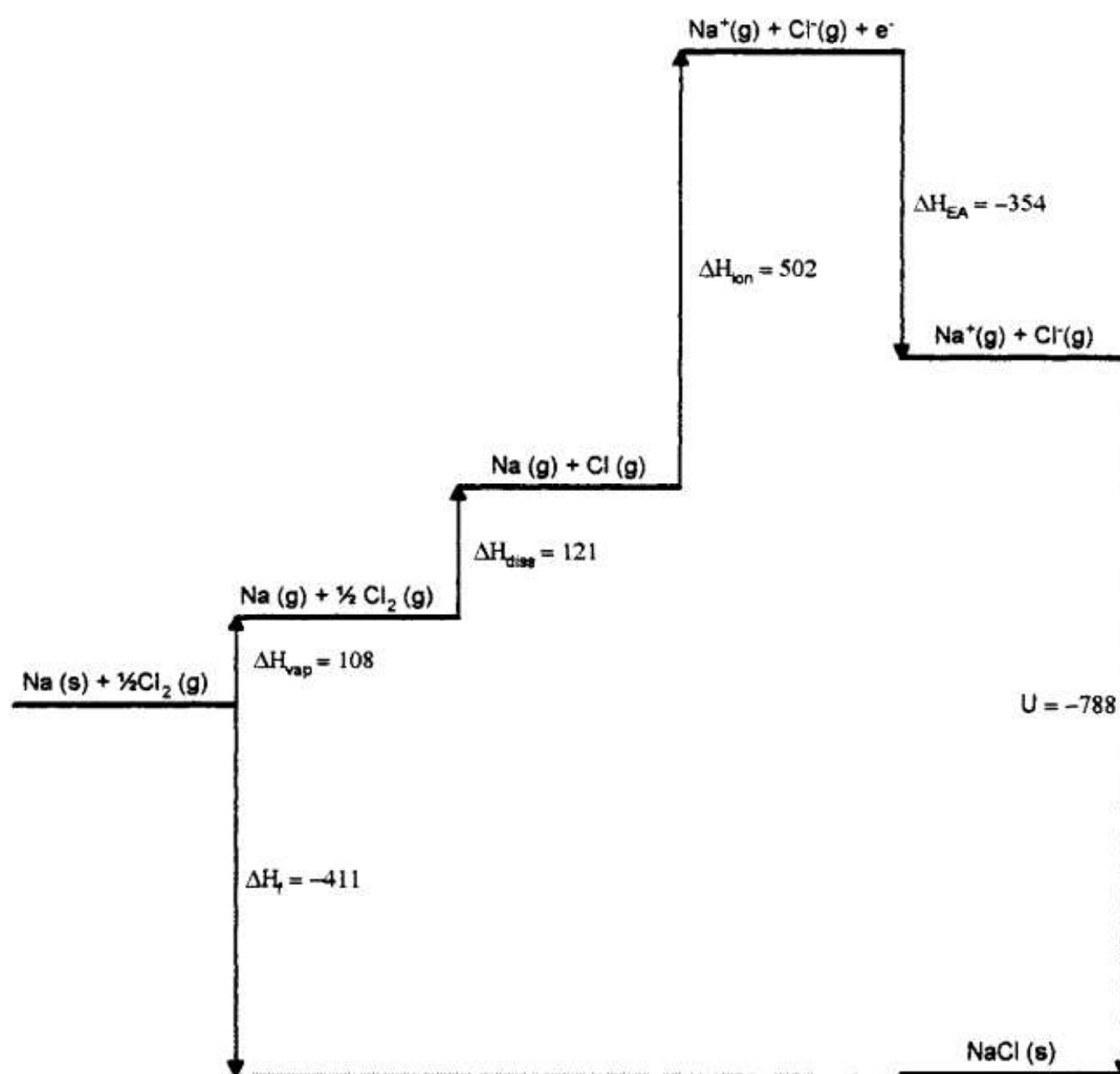


Figure 2.4. Born-Haber Cycle

The Born-Haber cycle follows the Law of Conservation of Energy, that is when a system goes through a series of changes and is returned to its initial state the sum of the energy changes is equal to zero. Thus the equation:

$$0 = \Delta h_f + \Delta h_{\text{vap}} + \frac{1}{2} \Delta h_{\text{diss}} + \Delta H_{\text{ion}} + \Delta H_{\text{EA}} + U$$

From this the crystal lattice energy,  $U$ , can be calculated from the following enthalpies:

|                                                                          |                                        |            |
|--------------------------------------------------------------------------|----------------------------------------|------------|
| enthalpy of formation                                                    | $(\Delta h_f)$                         | -411       |
| vaporization of sodium                                                   | $(\Delta h_{\text{vap}})$              | -108       |
| dissociation of $\text{Cl}_2 \text{ (g)}$ into gaseous atoms             | $(\frac{1}{2} \Delta h_{\text{diss}})$ | -121       |
| ionization of $\text{Na (g)}$ to $\text{Na}^+ \text{ (g)}$               | $(\Delta h_{\text{ion}})$              | -502       |
| electron attachment to $\text{Cl (g)}$ to give $\text{Cl}^- \text{ (g)}$ | $(\Delta H_{\text{EA}})$               | 354        |
| crystal lattice energy                                                   | $U$                                    | -788kJ/mol |

### 2.15.2 Madelung Constant

The crystal lattice energy can be estimated from a simple electrostatic model. When this model is applied to an ionic crystal only the electrostatic charges and the shortest anion-cation internuclear distance need be considered. The summation of all the geometrical interactions between the ions is called the **Madelung constant**. From this model an equation for the crystal lattice energy is derived:

$$U = -1389 \frac{M}{r} \left( 1 - \frac{1}{n} \right)$$

$U$  = crystal lattice energy

$M$  = Madelung constant

$r$  = shortest internuclear distance

$n$  = Born exponent

The Madelung constant is unique for each crystal structure and is defined only for those whose interatomic vectors are fixed by symmetry. The **Born exponent**,  $n$ , can be estimated for alkali halides by the noble-gas-like electron configuration of the ion. It can also be estimated from the compressibility of the crystal system. For NaCl,  $n$  equals 9.1.

Table 2.16. Madelung Constants

| Structure Type   | M       |
|------------------|---------|
| NaCl             | 1.74756 |
| CsCl             | 1.76267 |
| CaF <sub>2</sub> | 5.03878 |
| Zinc Blende      | 1.63805 |
| Wurtzite         | 1.64132 |

Table 2.17. Born Exponents

| Configuration | n  |
|---------------|----|
| He            | 5  |
| Ne            | 7  |
| Ar            | 9  |
| Kr            | 10 |
| Xe            | 12 |

For NaCl, substituting in the appropriate values into the equation we obtain:

$$U = -1389 \frac{1.747}{2.82} \left( 1 - \frac{1}{9.1} \right)$$

$$U = -860 + 95 = -765 \text{ kJ mol}^{-1}$$

As can be seen the result is close (within 3%) of the value of  $U$  obtained from using the Born-Haber cycle. More accurate calculations can be obtained

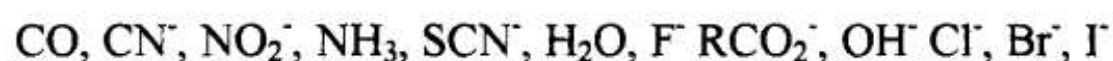
if other factors are taken into account, such as, van der Waals repulsion, zero-point energy, etc....

## 2.16 Complexes

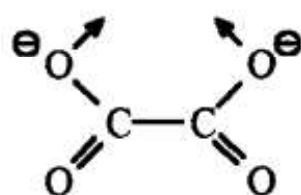
Transition and non-transition metal ions form a great many complex ions and molecules. Bonding is achieved by an ion or molecule donating a pair of electrons to the metal ion. This type of bond is an coordinate covalent bond (section 1.2.2), the resulting complexes are called **coordination complexes**. The species donating the electron pair is called a **ligand**. More than one type of ligand can bond to the same metal ion, i.e.  $\text{K}_2\text{PtCl}_6$ . In addition a ligand can bond to more than one site on the metal ion, a phenomenon called **chelation**.

The bonding involved in the formation of coordination complexes involve the d orbitals (section 1.1.3) of the metal ion. The electron pair being donated occupies the empty d orbitals and accounts for the geometry of the complex.

### 2.16.1 Unidentate Ligands



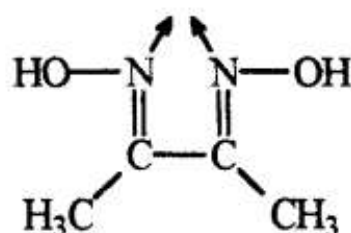
### 2.16.2 Bidentate Ligands



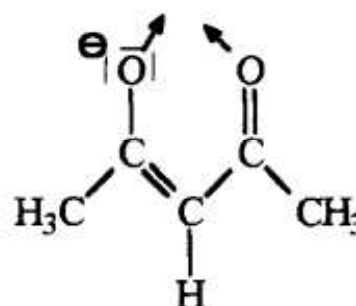
Oxalate Ion



Ethylenediamine

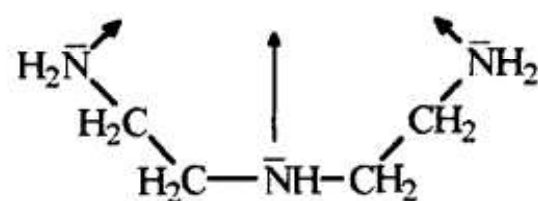


Diacetyldioxime



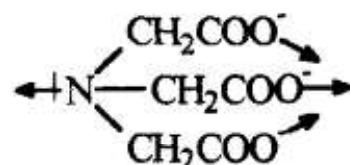
Acetylacetonate

## 2.16.3 Tridentate Ligands



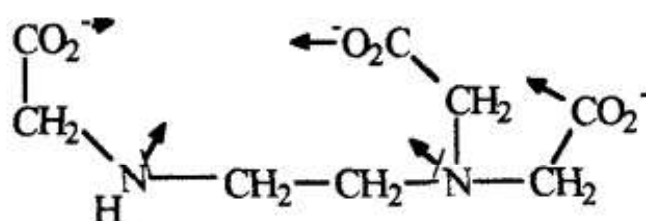
Diethylenetriamine

## 2.16.4 Quadridentate Ligands



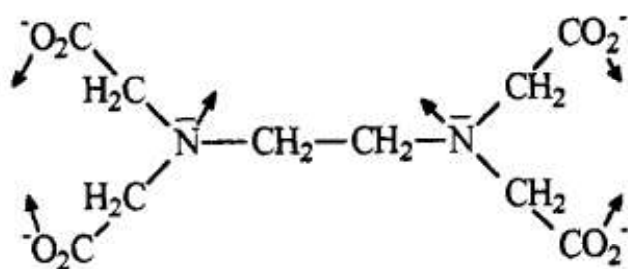
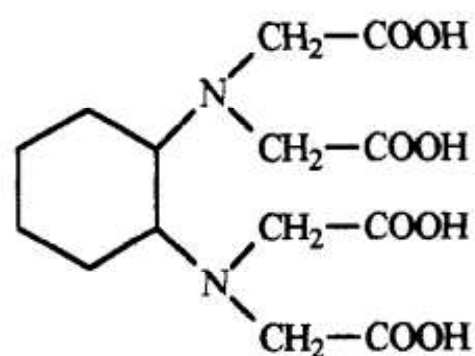
Tricarboxymethylamine

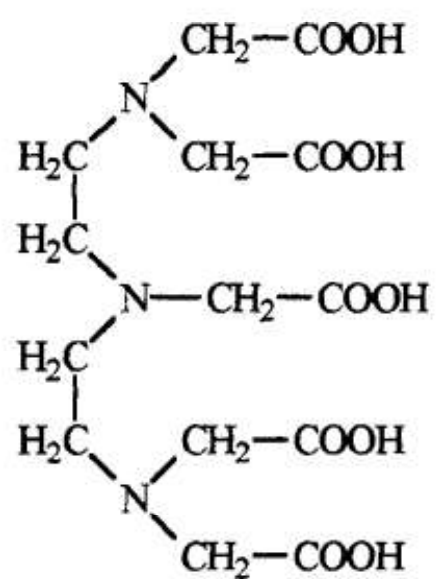
## 2.16.5 Pentadentate Ligands



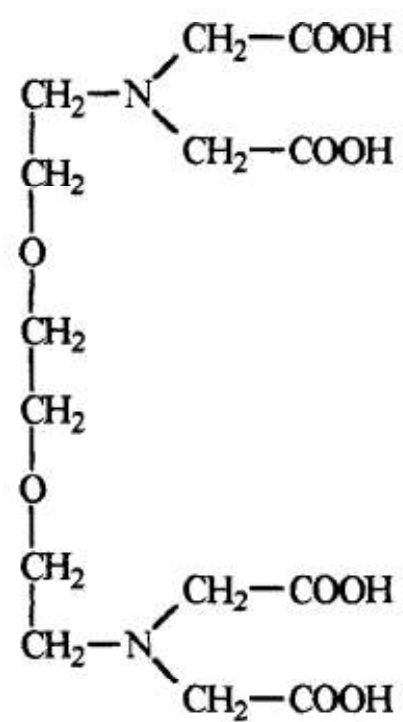
Ethylenediaminetriacetic acid

## 2.16.6 Hexadentate Ligands

Ethylenediaminetetraacetic acid  
- EDTADiaminocyclohexanetetraacetic  
acid - CDTA



Diethylenetriaminepentaacetic  
acid - DTPA



Dioxaoctamethylenedinitriolo  
tetraacetic acid - PGTA

## Chapter 3

### **Organic Chemistry**

3.1 *Classification of Organic Compounds*

3.2 *Alkanes*

3.3 *Alkenes*

3.4 *Dienes*

3.5 *Alkynes*

3.6 *Benzene*

3.7 *Alkylbenzenes*

3.8 *Alkenylbenzenes*

3.9 *Alkyl Halides*

3.10 *Aryl Halides*

3.11 *Alcohols*

3.12 *Phenols*

3.13 *Ethers*

3.14 *Epoxides*

3.15 *Aldehydes and Ketones*

3.16 *Carboxylic Acids*

3.17 *Acid Chlorides*

3.18 *Esters*

3.19 *Acid Anhydrides*

3.20 *Amides*

3.21 *Amines*

3.22 *Alicyclic Compounds*

3.23 *Heterocyclic Compounds*

3.24 *Isomers*

3.25 *Polymer Structures*

### 3.1 Classification Of Organic Compounds

#### 3.1.1 General Classification

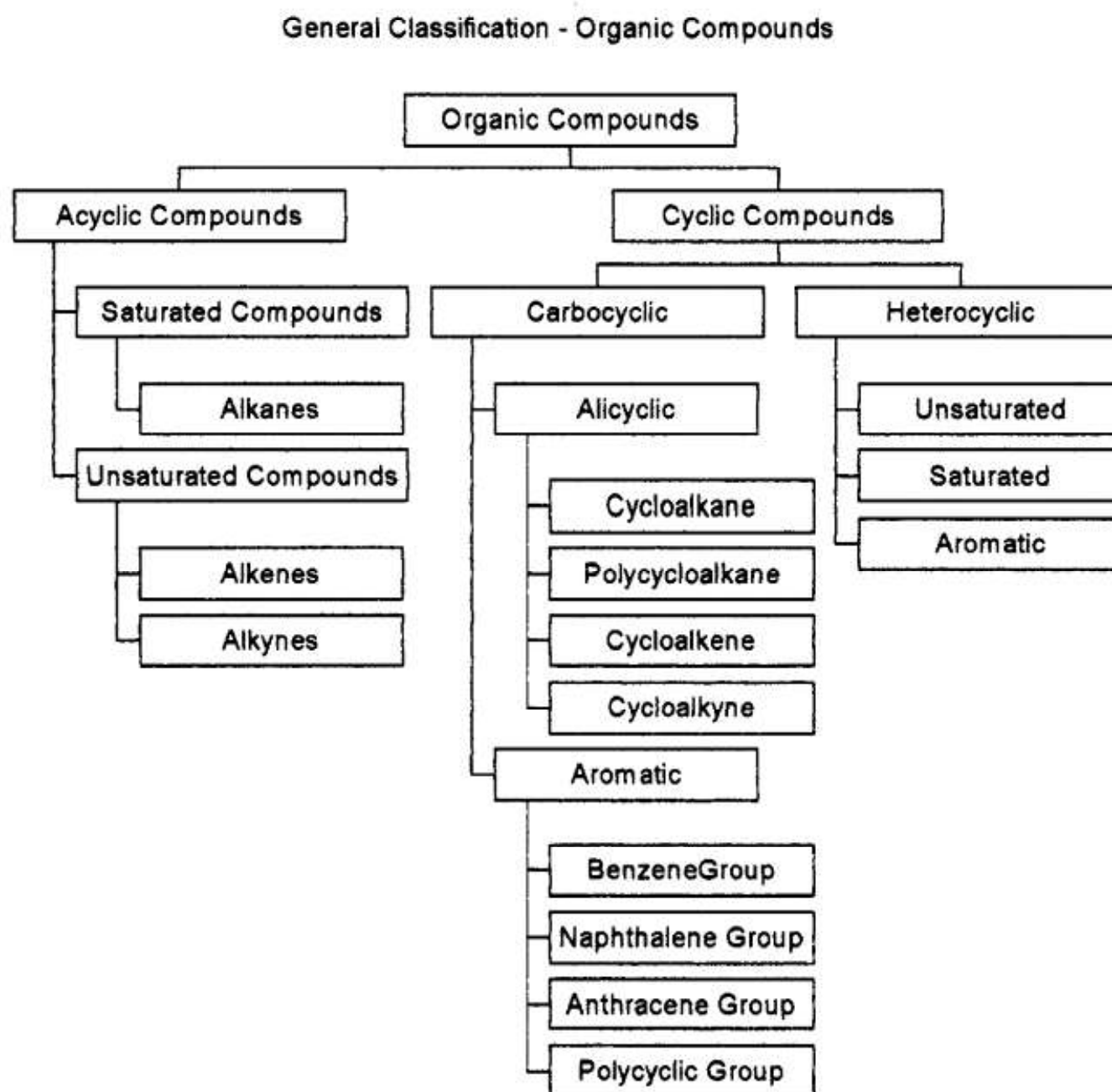


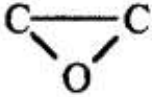
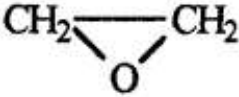
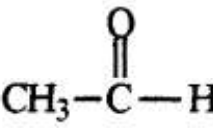
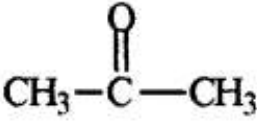
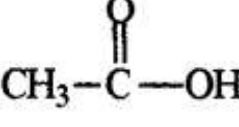
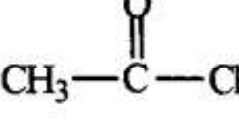
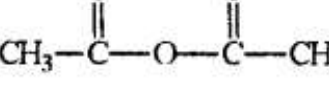
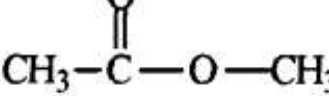
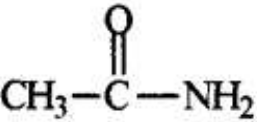
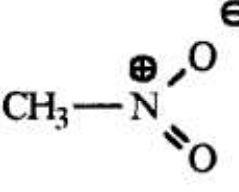
Figure 3.1. General Classification of Organic Compounds

#### 3.1.2 Classification by Functional Group

Table 3.1. Organic Functional Groups

| Type    | Functional Group | Example                                                            | Name        |
|---------|------------------|--------------------------------------------------------------------|-------------|
| Alkane  | R-H              | CH <sub>3</sub> CH <sub>2</sub> CH <sub>3</sub>                    | propane     |
| Alkene  | R=R              | CH <sub>2</sub> =CHCH <sub>3</sub>                                 | propene     |
| Diene   | R=R-R=R          | CH <sub>2</sub> =CH-CH=CH <sub>2</sub>                             | 1,4-butene  |
| Alkyne  | R≡R              | CH≡CH                                                              | ethyne      |
| Halide  | R-X              | CH <sub>3</sub> CH <sub>2</sub> -Br                                | bromoethane |
| Alcohol | R-OH             | CH <sub>3</sub> CH <sub>2</sub> -OH                                | ethanol     |
| Ether   | R-O-R            | CH <sub>3</sub> CH <sub>2</sub> -O-CH <sub>2</sub> CH <sub>3</sub> | ethoxyether |

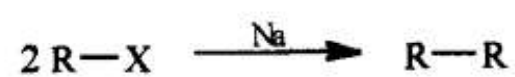
Table 3.1. (Continued)

|                 |                                                                                   |                                                                                       |                  |
|-----------------|-----------------------------------------------------------------------------------|---------------------------------------------------------------------------------------|------------------|
| Epoxide         |  |    | ethylene oxide   |
| Aldehyde        | R-CHO                                                                             |    | ethanal          |
| Ketone          | R-CO-R                                                                            |   | 2-propanone      |
| Carboxylic Acid | R-CO <sub>2</sub> H                                                               |  | ethanoic acid    |
| Acid Chloride   | R-CO-Cl                                                                           |  | acetyl chloride  |
| Acid Anhydride  | (RCO) <sub>2</sub> O                                                              |  | acetic anhydride |
| Ester           | R-CO <sub>2</sub> R                                                               |  | methyl ethanoate |
| Amide           | R-CONH <sub>2</sub>                                                               |  | ethanamide       |
| Amine 1°        | R-NH <sub>2</sub>                                                                 | CH <sub>3</sub> CH <sub>2</sub> -NH <sub>2</sub>                                      | ethanamine       |
| Amine 2°        | R-NH-R                                                                            | CH <sub>3</sub> CH <sub>2</sub> -NH-CH <sub>2</sub> CH <sub>3</sub>                   | diethanamine     |
| Amine 3°        | R <sub>3</sub> -N                                                                 | (CH <sub>3</sub> CH <sub>2</sub> ) <sub>3</sub> -N                                    | triethanamine    |
| Nitro Compound  | R-NO <sub>2</sub>                                                                 |  | nitromethane     |
| Nitrile         | R-C≡N                                                                             | CH <sub>3</sub> C≡N                                                                   | ethanenitrile    |
| Thiol           | R-SH                                                                              | CH <sub>3</sub> CH <sub>2</sub> -SH                                                   | ethanethiol      |

## 3.2 Alkanes

### 3.2.1 Preparation of Alkanes

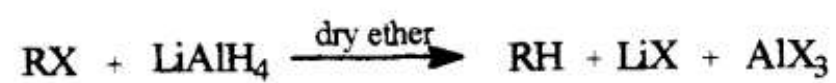
#### 3.2.1.1 Wurtz Reaction



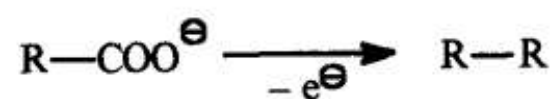
#### 3.2.1.2 Grignard Reduction



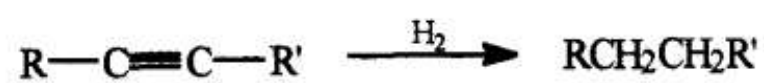
#### 3.2.1.3 Reduction



#### 3.2.1.4 Kolbe Reaction



#### 3.2.1.5 Hydrogenation

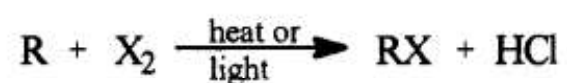


### 3.2.2 Reactions of Alkanes

#### 3.2.2.1 Combustion



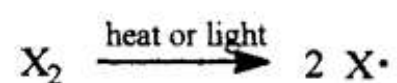
### 3.2.2.2 Halogenation



Reactivity X:  $Cl_2 > Br_2$

H:  $3^\circ > 2^\circ > 1^\circ > CH_3-H$

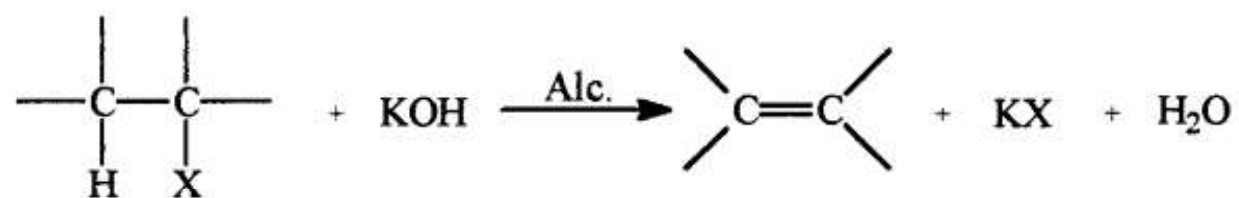
### 3.2.2.3 Free Radical Substitution



## 3.3 Alkenes

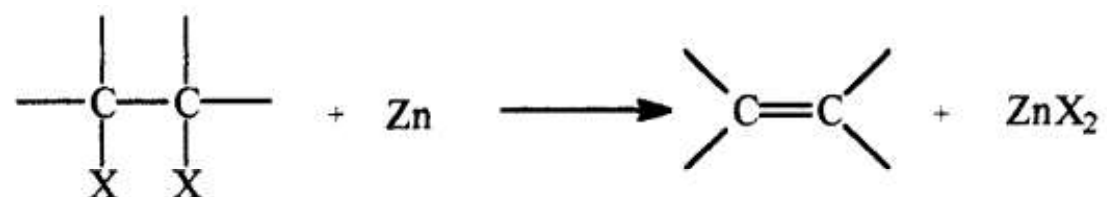
### 3.3.1 Preparation of Alkenes

#### 3.3.1.1 Dehydrohalogenation of Alkyl Halides

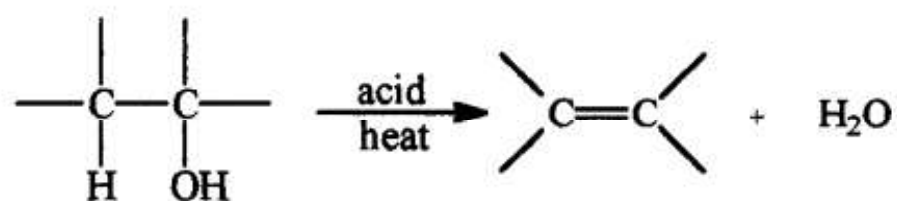


Ease of dehydrohalogenation  $3^\circ > 2^\circ > 1^\circ$

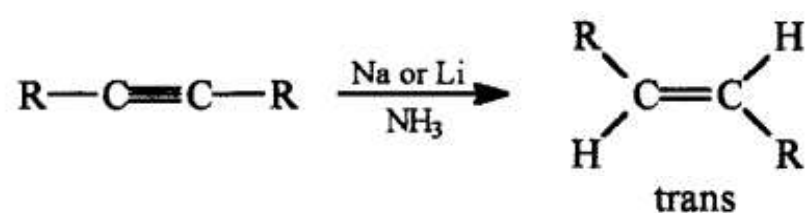
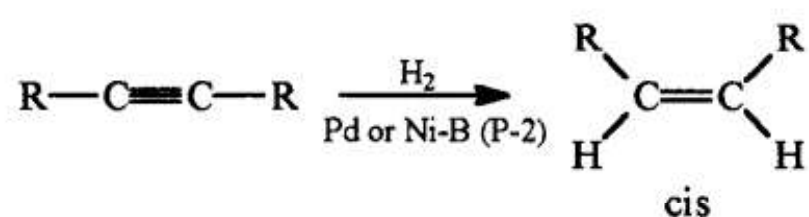
#### 3.3.1.2 Dehalogenation of Vicinal Dihalides



### 3.3.1.3 Dehydration of Alcohols

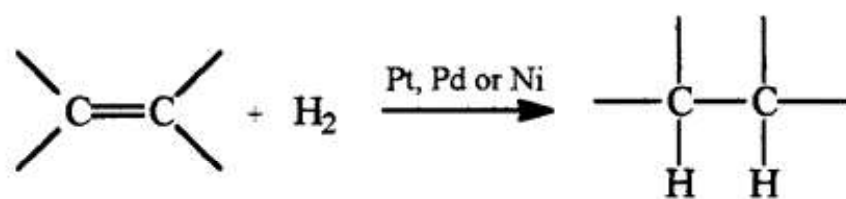


### 3.3.1.4 Reduction of Alkynes

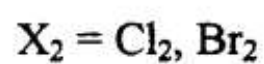
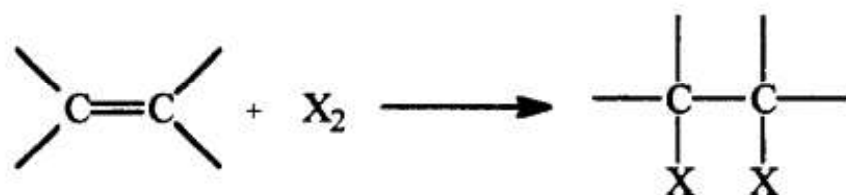


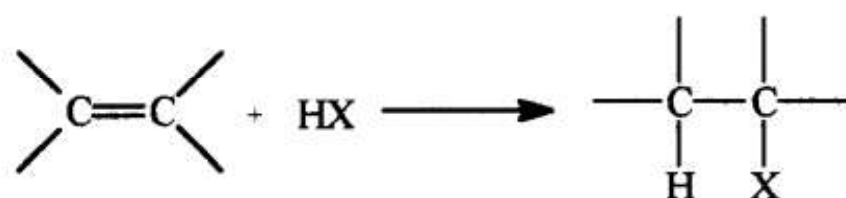
## 3.3.2 Reactions of Alkenes

### 3.3.2.1 Hydrogenation



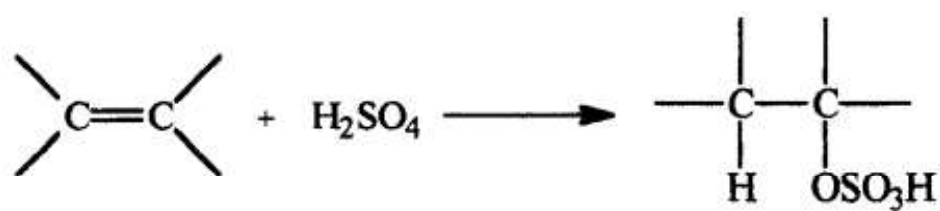
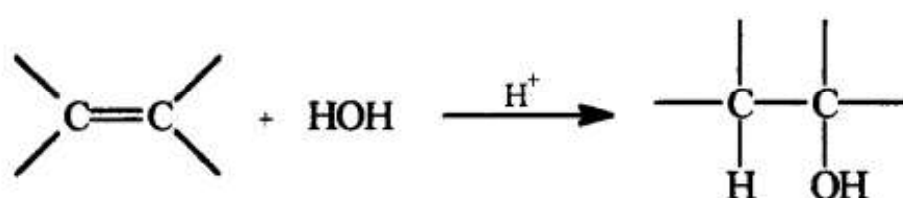
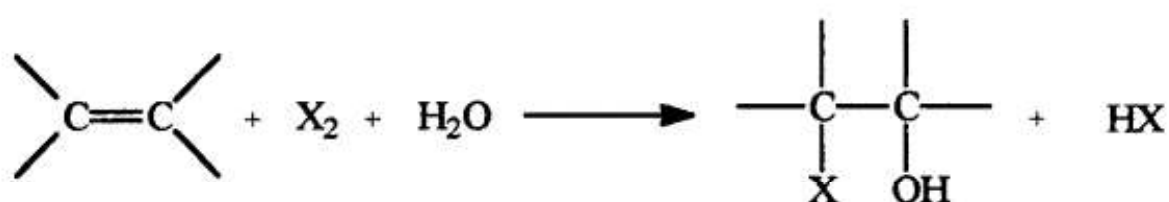
### 3.3.2.2 Halogenation



**3.3.2.3 Addition of Hydrogen Halide**

HX = HCl, HBr, HI

**Markovnikov's rule:** The hydrogen of the acid attaches itself to the carbon atom which already has the greatest number of hydrogens. In the presence of peroxide, HBr will undergo anti-Markovnikov addition.

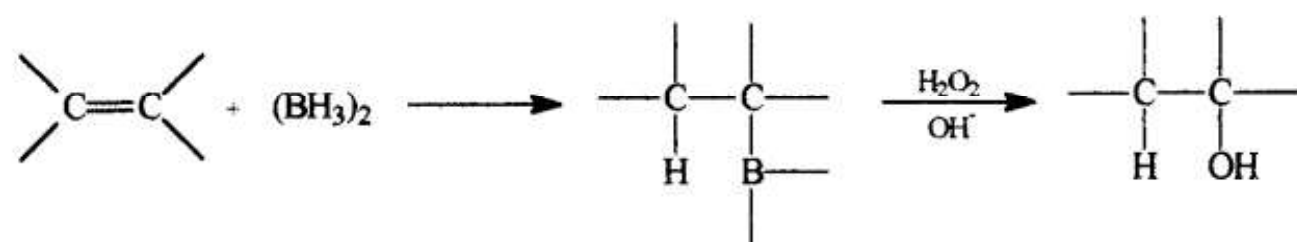
**3.3.2.4 Addition of Sulfuric Acid****3.3.2.5 Addition of Water****3.3.2.6 Halohydrin Formation**

X<sub>2</sub> = Cl<sub>2</sub>, Br<sub>2</sub>

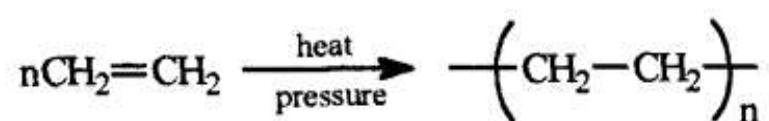
### 3.3.2.7 Oxymercuration-Demercuration



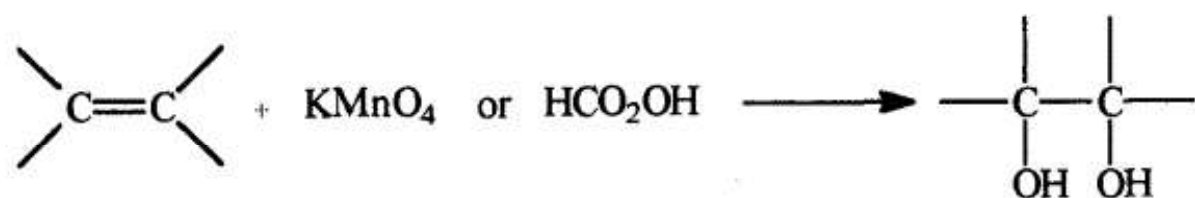
### 3.3.2.8 Hydroboration-Oxidation



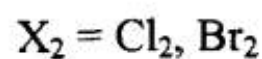
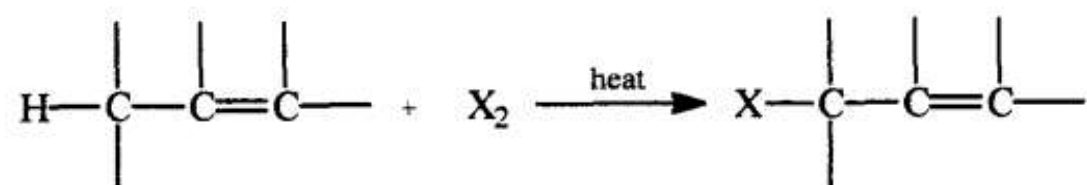
### 3.3.2.9 Polymerization



### 3.3.2.10 Hydroxylation



### 3.3.2.11 Halogenation - Allylic Substitution

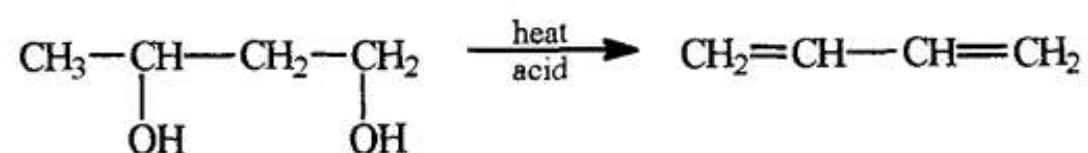


## 3.4 Dienes

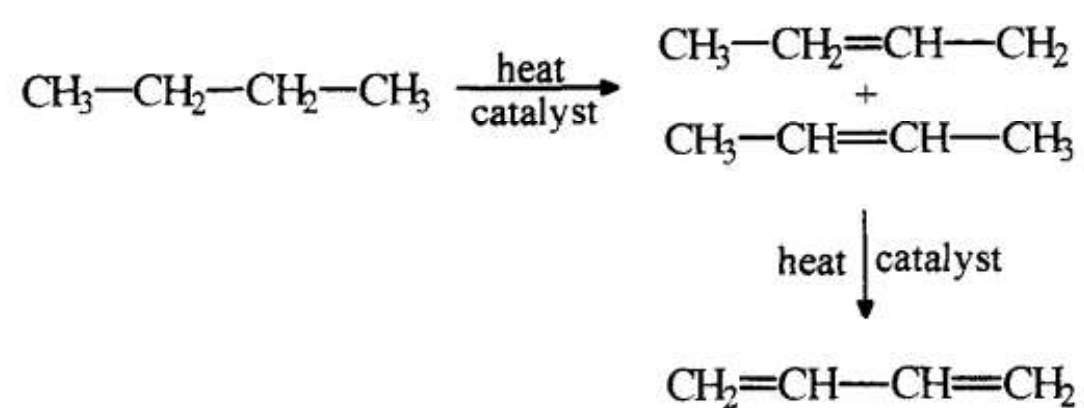
Isolated dienes can be prepared following the methods for alkanes using difunctional starting materials.

### 3.4.1 Preparation of Conjugated Dienes

#### 3.4.1.1 Dehydration of 1,3-Diol

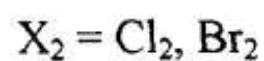
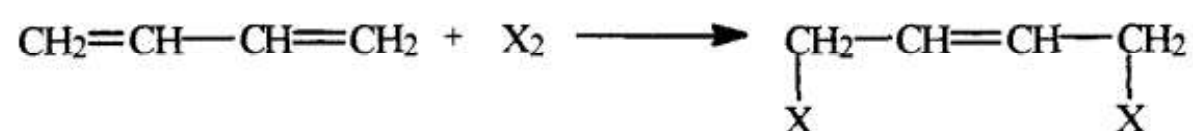


#### 3.4.1.2 Dehydrogenation

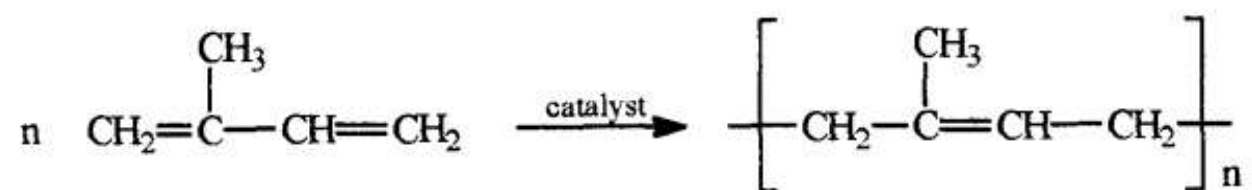


### 3.4.2 Reactions of Dienes

#### 3.4.2.1 1,4-Addition



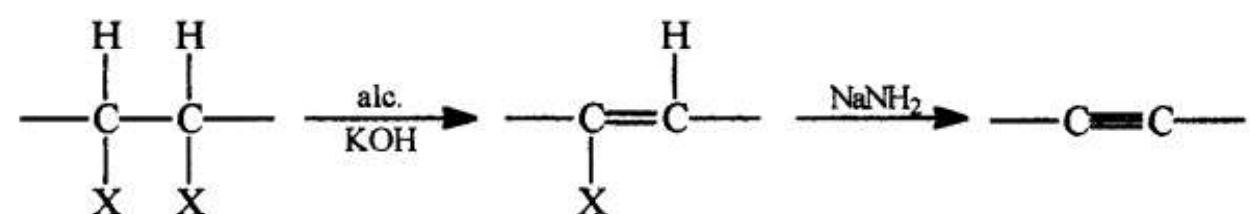
#### 3.4.2.2 Polymerization



## 3.5 Alkynes

### 3.5.1 Preparation of Alkynes

#### 3.5.1.1 Dehydrohalogenation of Alkyl Dihalides



#### 3.5.1.2 Dehalogenation of Tetrahalides

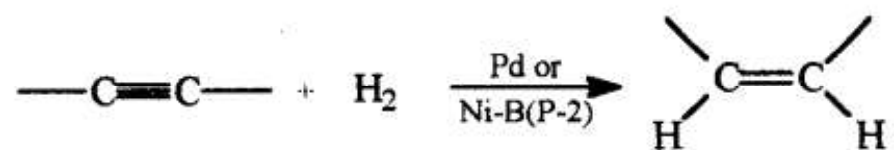


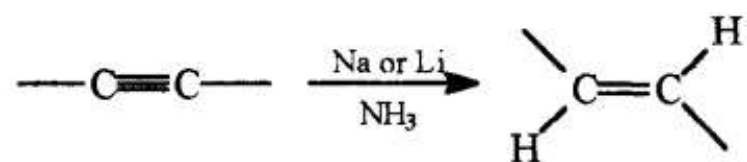
#### 3.5.1.3 Reaction of Water and Calcium Carbide



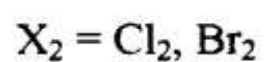
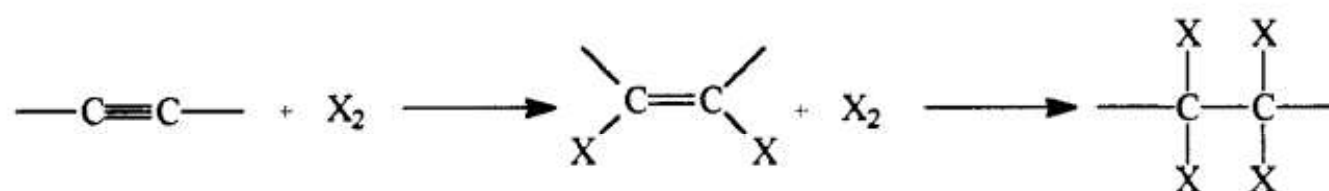
### 3.5.2 Reactions of Alkynes

#### 3.5.2.1 Hydrogenation

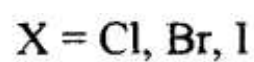
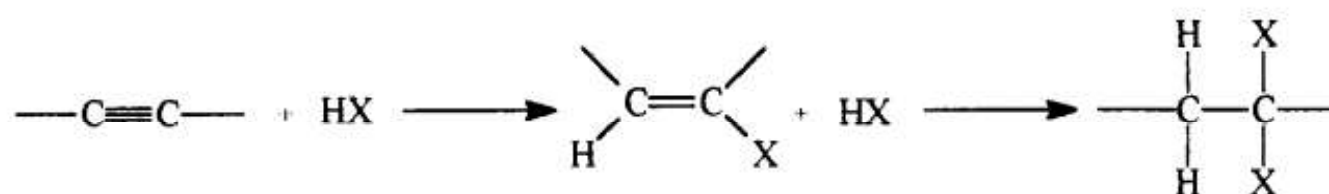




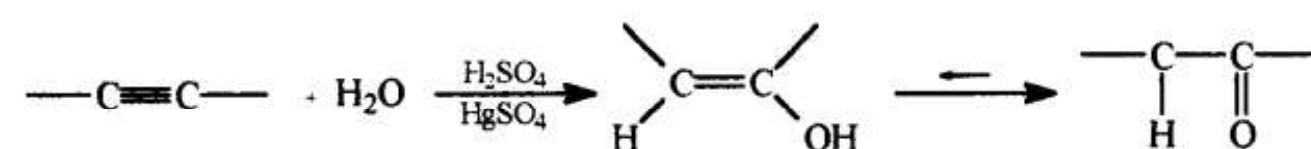
### 3.5.2.2 Halogenation



### 3.5.2.3 Addition of Hydrogen Halide



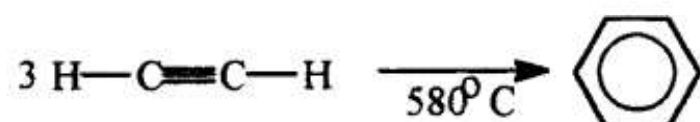
### 3.5.2.4 Addition of Water (Hydration)



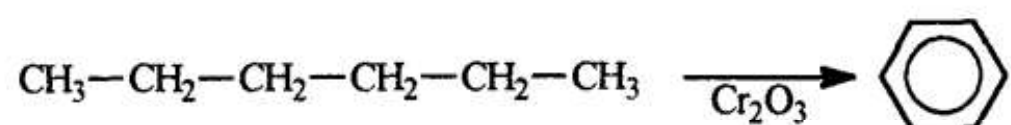
## 3.6 Benzene

### 3.6.1 Preparation of Benzene

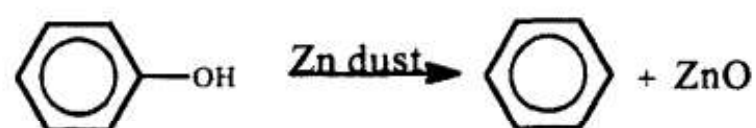
#### 3.6.1.1 Ring Formation



### 3.6.1.2 Cyclization



### 3.6.1.3 Elimination

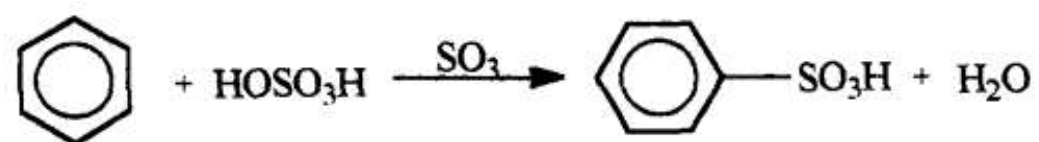


## 3.6.2 Reactions of Benzenes

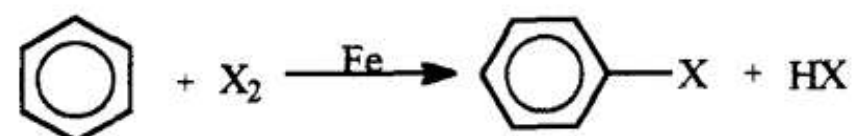
### 3.6.2.1 Nitration



### 3.6.2.2 Sulfonation

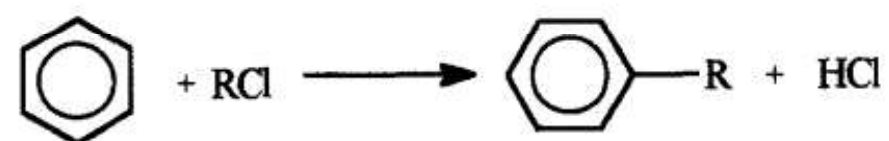


### 3.6.2.3 Halogenation

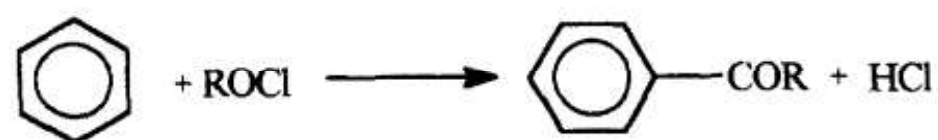


X = Cl, Br

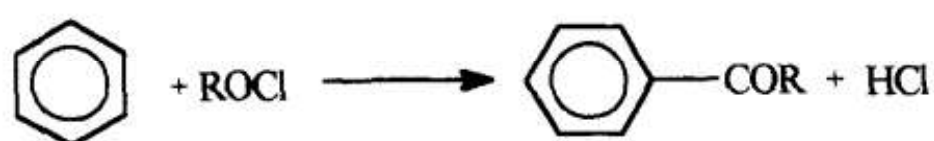
### 3.6.2.4 Friedel-Crafts Alkylation



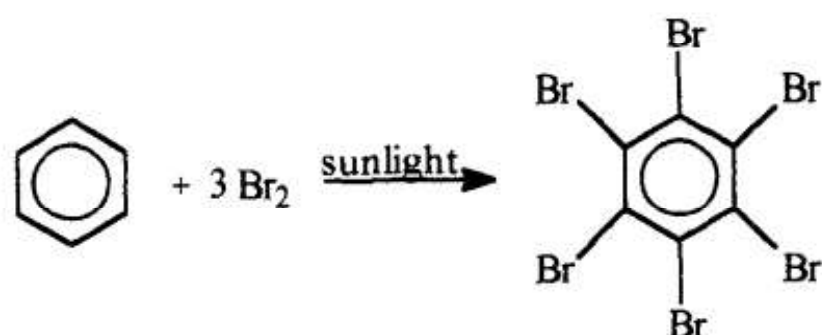
### 3.6.2.5 Friedel-Crafts Acylation



### 3.6.2.6 Hydrogenation



### 3.6.2.7 Bromination



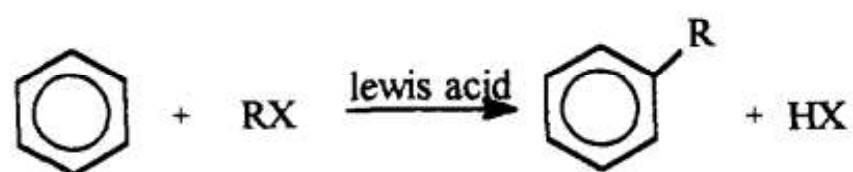
### 3.6.2.8 Combustion



## 3.7 Alkylbenzenes

### 3.7.1 Preparation of Alkylbenzenes

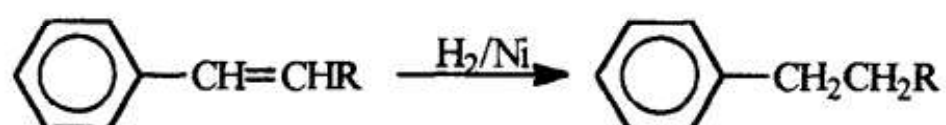
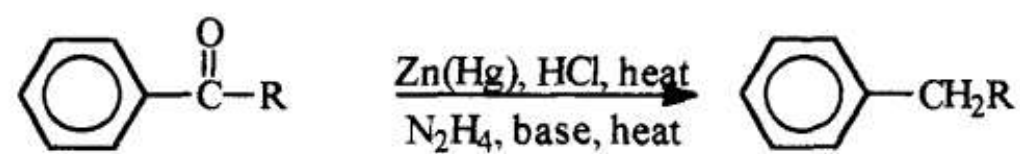
#### 3.7.1.1 Freidel-Crafts Alkylation



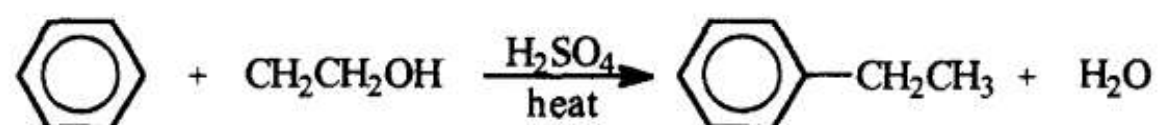
Lewis acid:  $\text{AlCl}_3$ ,  $\text{BF}_3$ ,  $\text{HF}$

Ar-H cannot be used in place of R-X

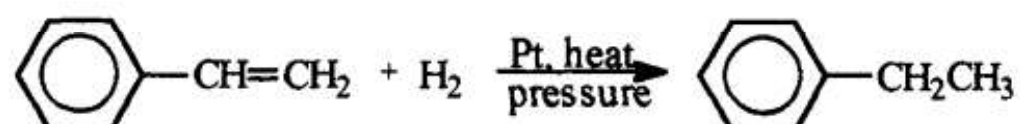
### 3.7.1.2 Side Chain Conversion



### 3.7.1.3 Electrophilic Aromatic Substitution

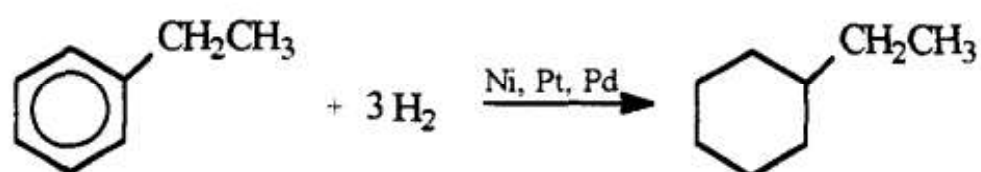


### 3.7.1.4 Hydrogenation

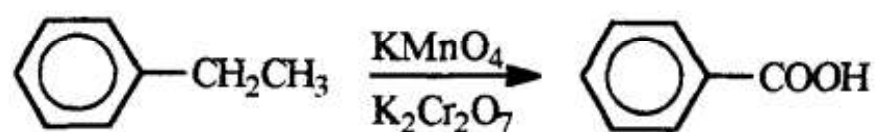


## 3.7.2 Reactions of Alkylbenzenes

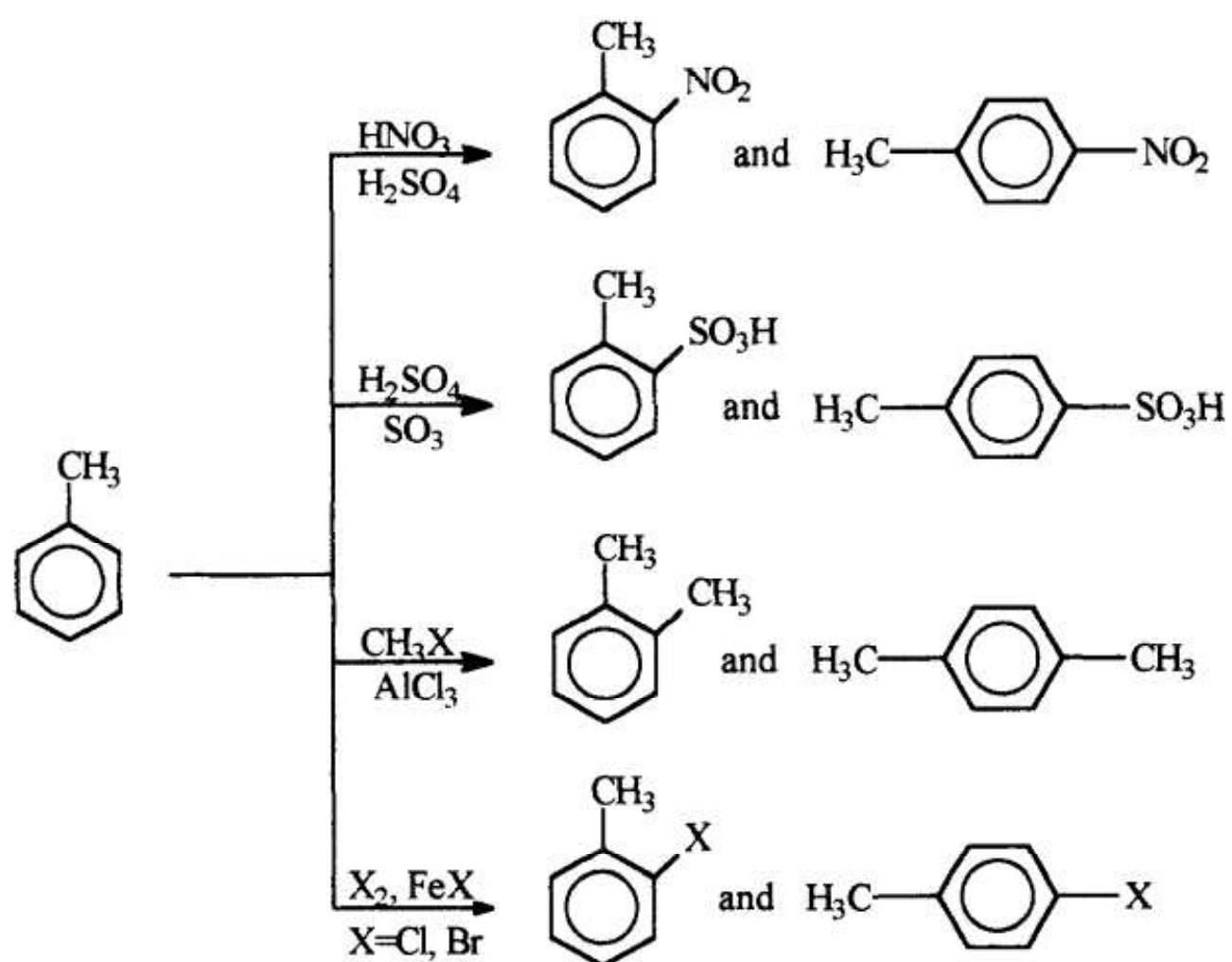
### 3.7.2.1 Hydrogenation



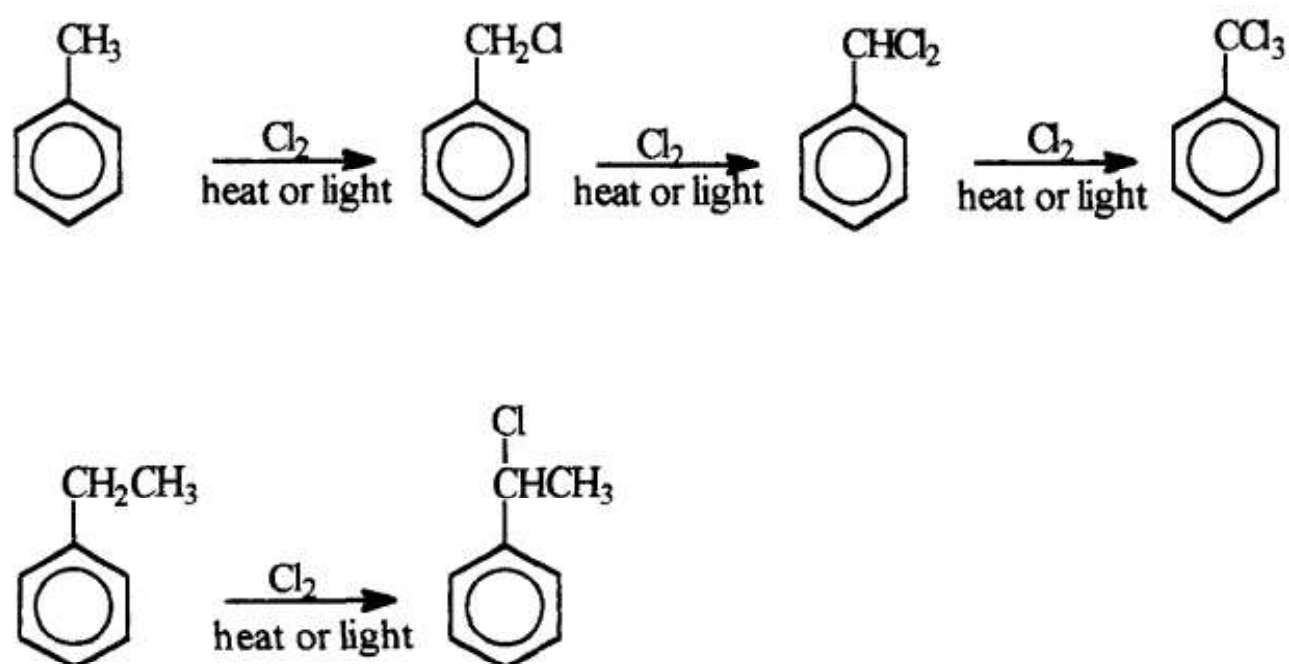
### 3.7.2.2 Oxidation



## 3.7.2.3 Substitution in ring - electrophilic aromatic substitution



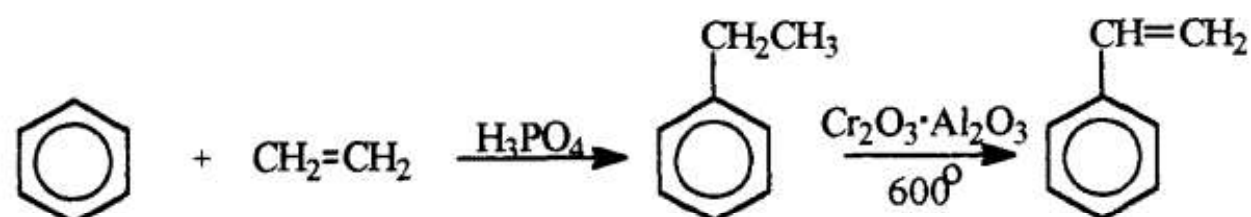
## 3.7.2.4 Substitution in the side chain



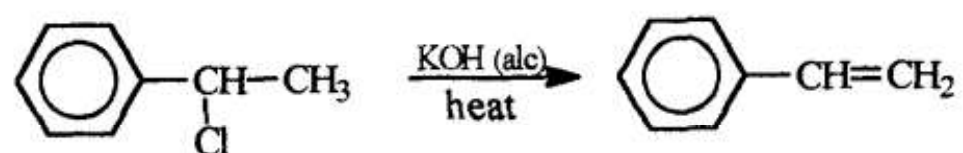
### 3.8 Alkenylbenzenes

#### 3.8.1 Preparation of Alkenylbenzenes

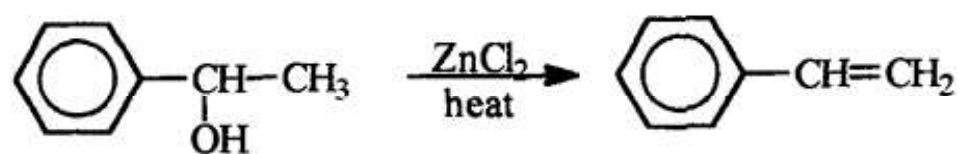
##### 3.8.1.1 Dehydrogenation



##### 3.8.1.2 Dehydrohalogenation

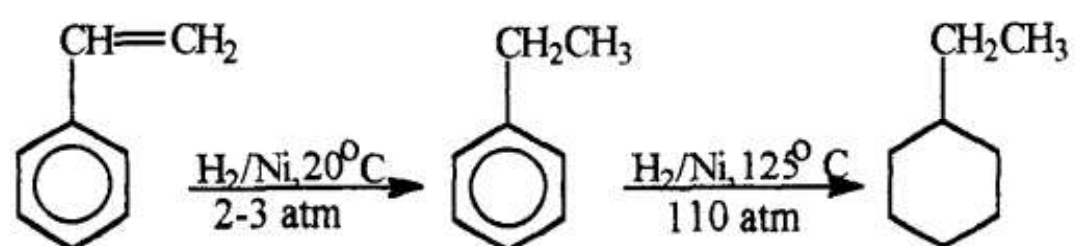


##### 3.8.1.3 Dehydration

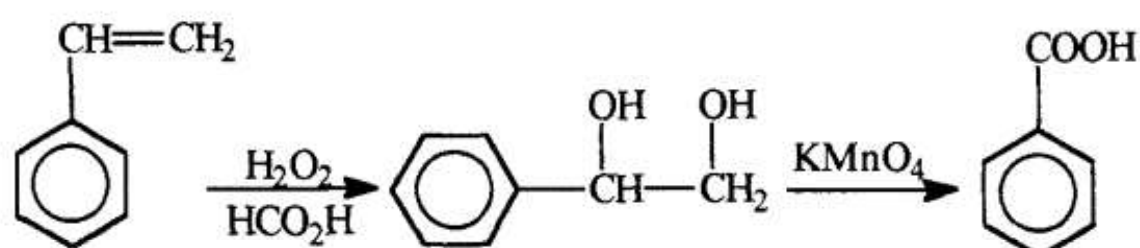


#### 3.8.2 Reactions of Alkenylbenzenes

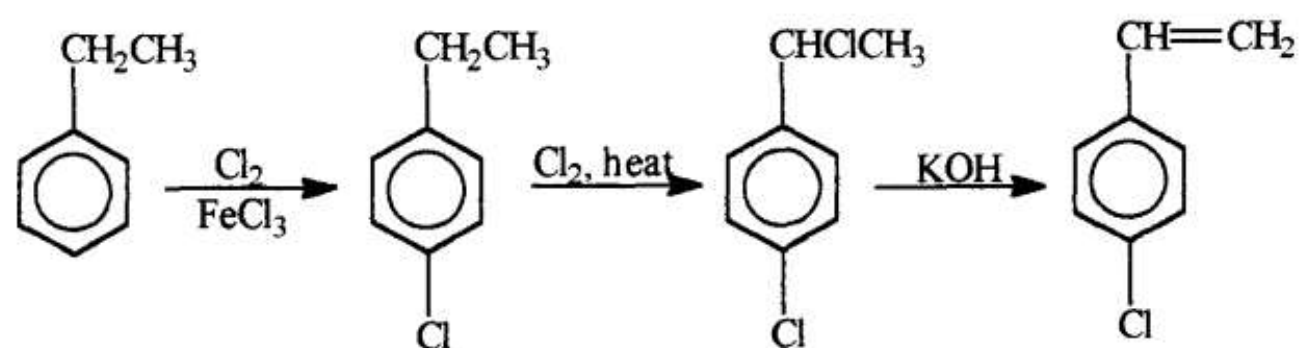
##### 3.8.2.1 Catalytic Hydrogenation



## 3.8.2.2 Oxidation



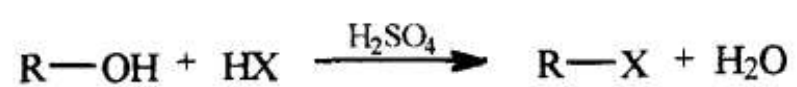
## 3.8.2.3 Ring Halogenation



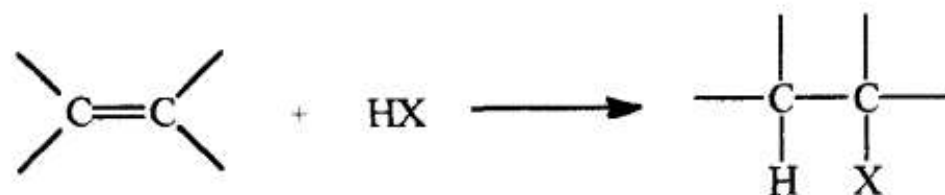
## 3.9 Alkyl Halides

## 3.9.1 Preparation of Alkyl Halides

## 3.9.1.1 From Alcohols



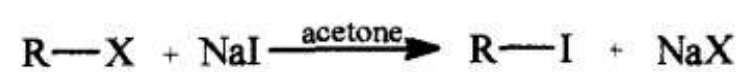
## 3.9.1.2 Addition of Hydrogen Halide to Alkenes



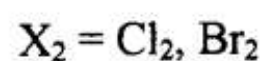
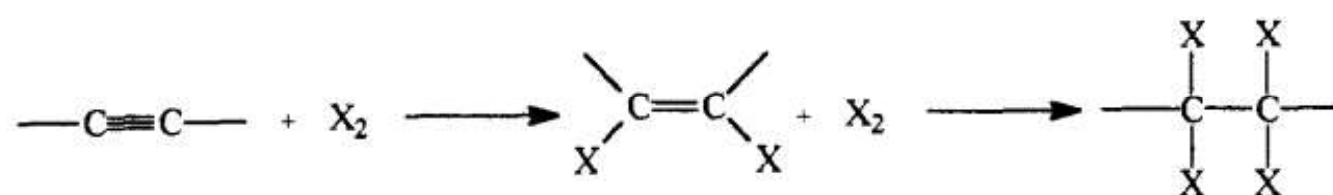
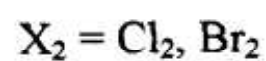
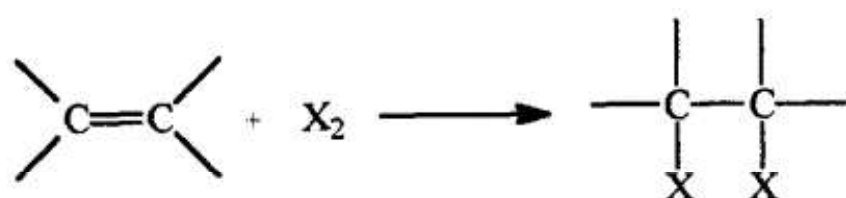
## 3.9.1.3 Halogenation of Alkanes



### 3.9.1.4 Halide Exchange



### 3.9.1.5 Halogenation of Alkenes and Alkynes



## 3.9.2 Reactions of Alkyl Halides

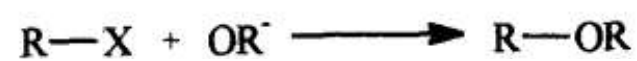
### 3.9.2.1 Addition of Hydroxide

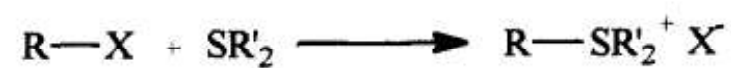


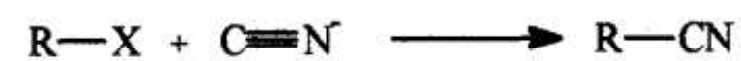
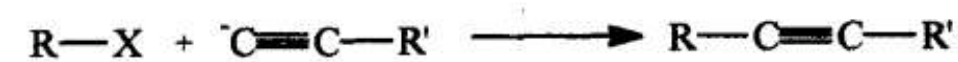
### 3.9.2.2 Addition of Water

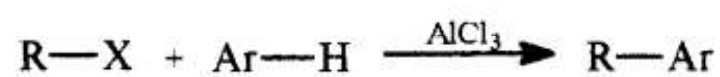
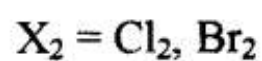
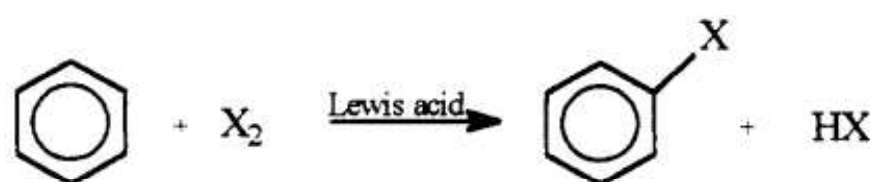


### 3.9.2.3 Addition of Alkoxide

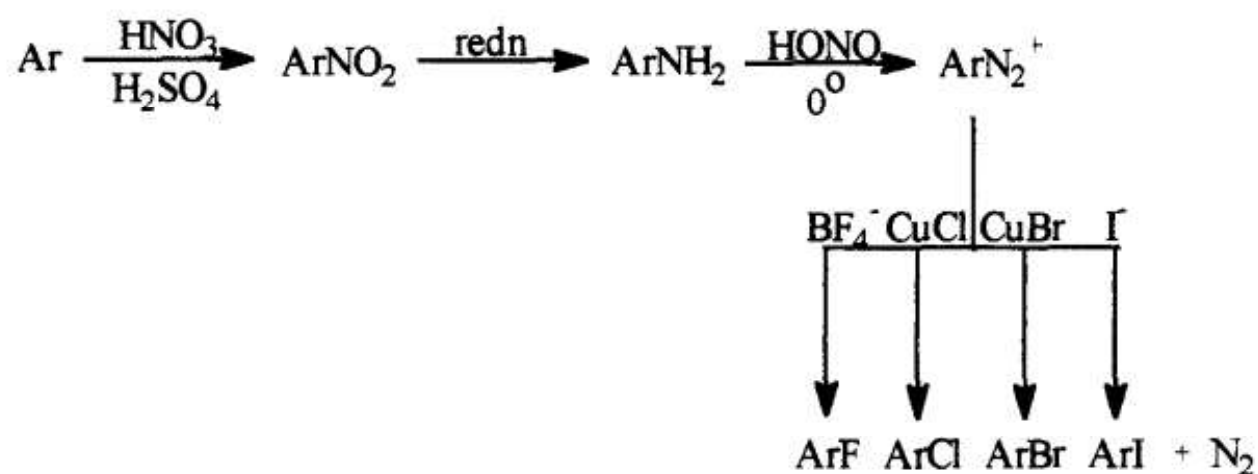


**3.9.2.4 Addition of Carboxylate****3.9.2.5 Addition of Hydrosulfide****3.9.2.6 Addition of Thioalkoxide****3.9.2.7 Addition of Sulfide****3.9.2.8 Addition of Thiocyanide****3.9.2.9 Addition of Iodide****3.9.2.10 Addition of Amide****3.9.2.11 Addition of Ammonia**

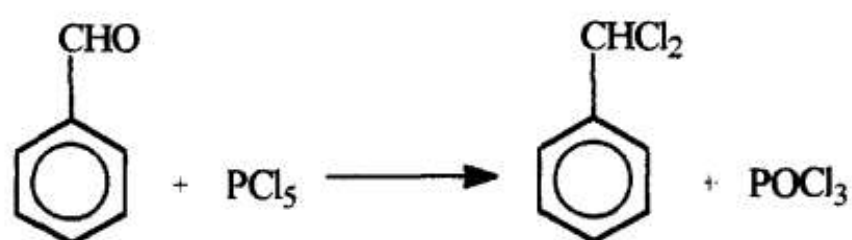
**3.9.2.12 Addition of 1° Amine****3.9.2.13 Addition of 2° Amine****3.9.2.14 Addition of 3° Amine****3.9.2.15 Addition of Azide****3.9.2.16 Addition of Nitrite****3.9.2.17 Addition of Phosphine****3.9.2.18 Addition of Cyanide****3.9.2.19 Addition of Alkynyl Anion**

**3.9.2.20 Addition of Carbanion****3.10 Aryl Halides****3.10.1 Preparation of Aryl Halides****3.10.1.1 Halogenation by Substitution****3.10.1.2 From Arylthallium Compounds**

## 3.10.1.3 From Diazonium Salt

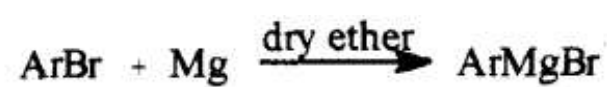


## 3.10.1.4 Halogenation by Addition

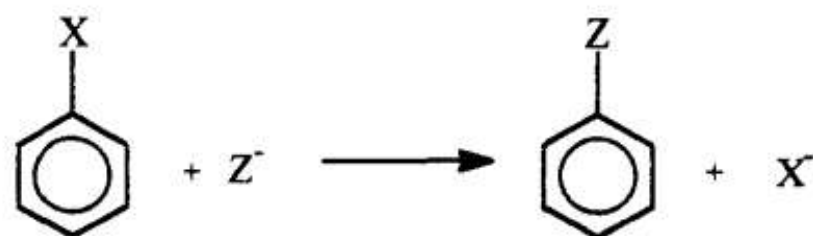


## 3.10.2 Reactions of Aryl Halides

## 3.10.2.1 Grignard Reagent Formation

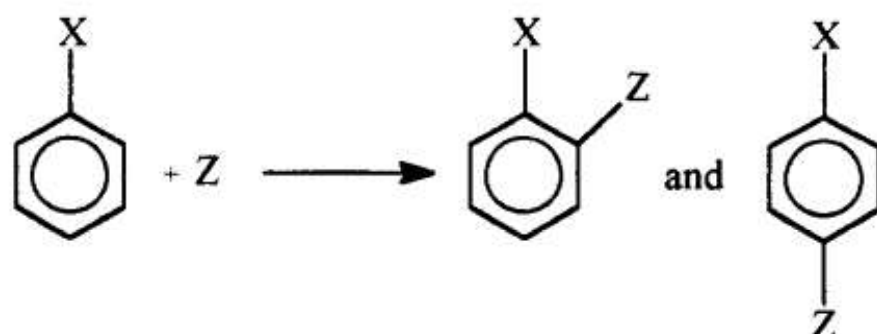


## 3.10.2.2 Nucleophilic Aromatic Substitution



Z = strong base

### 3.10.2.3 Electrophilic Aromatic Substitution



X deactivates and directs ortho, para in electrophilic aromatic substitution.

## 3.11 Alcohols

### 3.11.1 Preparation of Alcohols

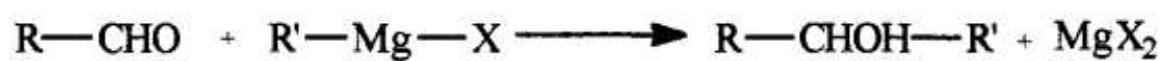
#### 3.11.1.1 Addition of Hydroxide



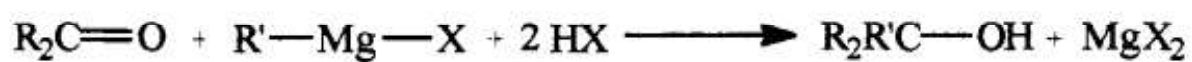
#### 3.11.1.2 Grignard Synthesis



primary alcohol



secondary alcohol

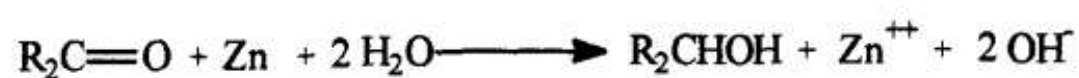


tertiary alcohol

## 3.11.1.3 Reduction of Carbonyl Compounds

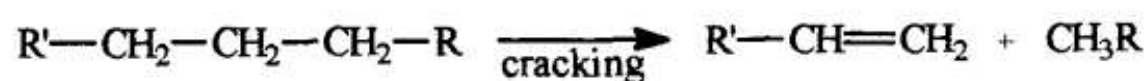
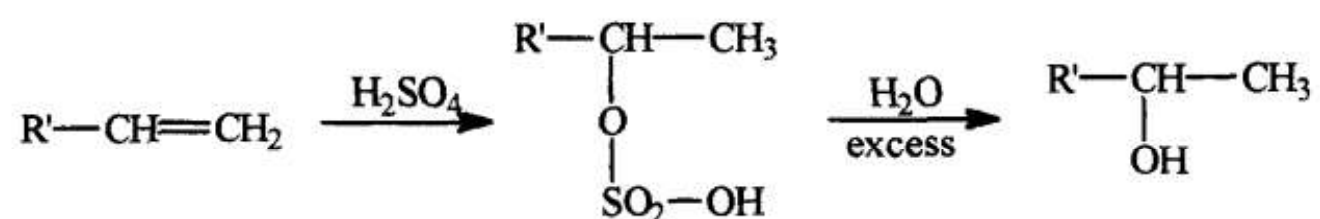


primary alcohol

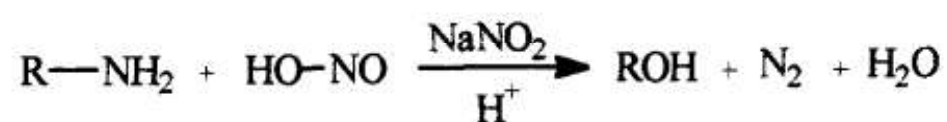


secondary alcohol

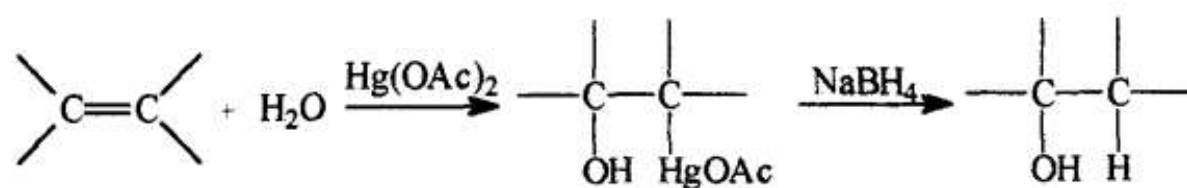
## 3.11.1.4 Hydration of Alkenes

 $R > R'$ 

## 3.11.1.5 Reaction of Amines with Nitrous Acid

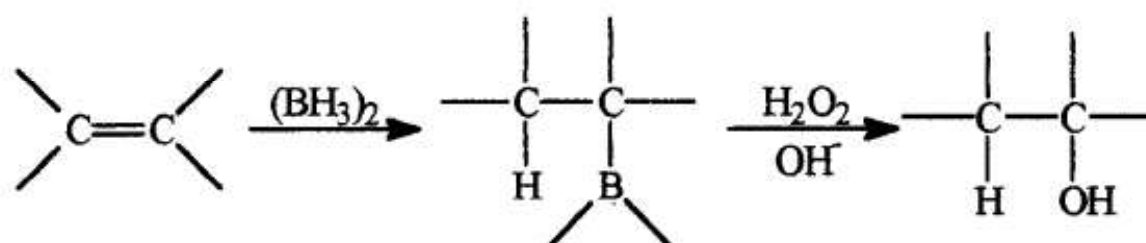


## 3.11.1.6 Oxymercuration-Demercuration



Markovnikov addition

## 3.11.1.7 Hydroboration-Oxidation



Anti-Markovnikov addition

## 3.11.2 Reactions of Alcohols

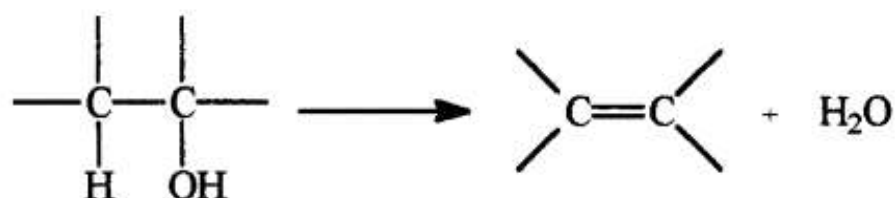
## 3.11.2.1 Reaction with Hydrogen Halides

Reactivity of HX:  $\text{HI} > \text{HBr} > \text{HCl}$ Reactivity of ROH:  $\text{allyl, benzyl} > 3^\circ > 2^\circ > 1^\circ$ 

## 3.11.2.2 Reaction with Phosphorus Trihalide



## 3.11.2.3 Dehydration



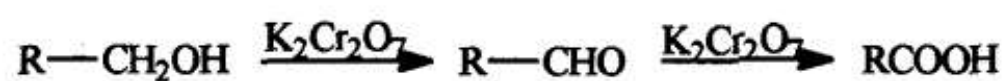
## 3.11.2.4 Ester Formation



## 3.11.2.5 Reaction with Active Metals



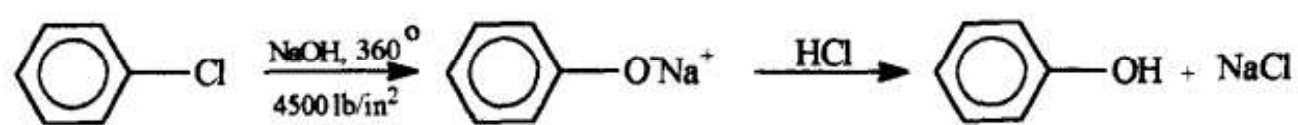
## 3.11.2.6 Oxidation



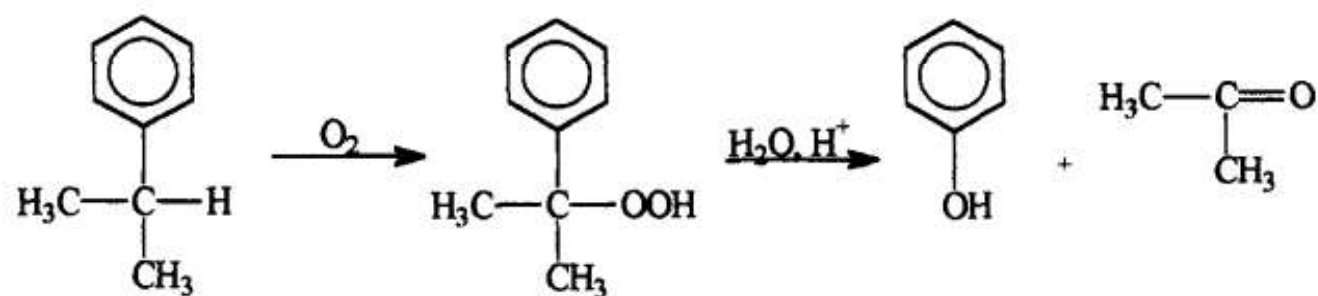
## 3.12 Phenols

## 3.12.1 Preparation of Phenols

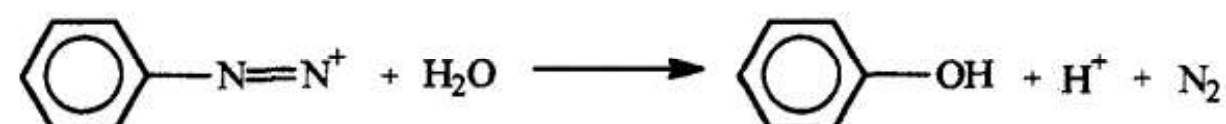
## 3.12.1.1 Nucleophilic Displacement of Halides



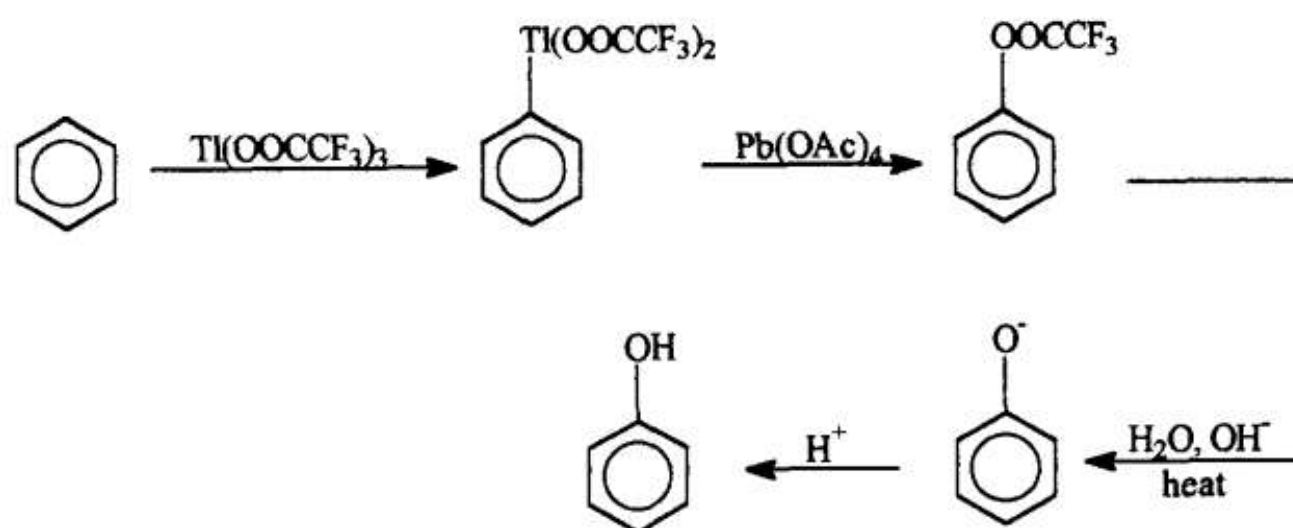
## 3.12.1.2 Oxidation of Cumene



## 3.12.1.3 Hydrolysis of Diazonium Salts



## 3.12.1.4 Oxidation of Arylthallium Compounds

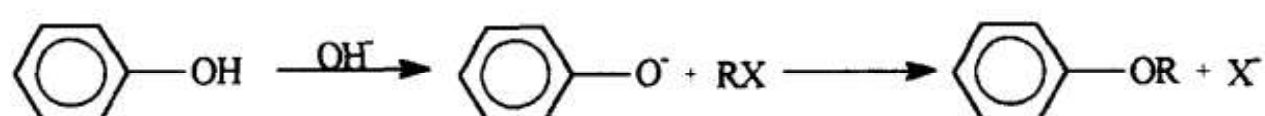


## 3.12.2 Reactions of Phenols

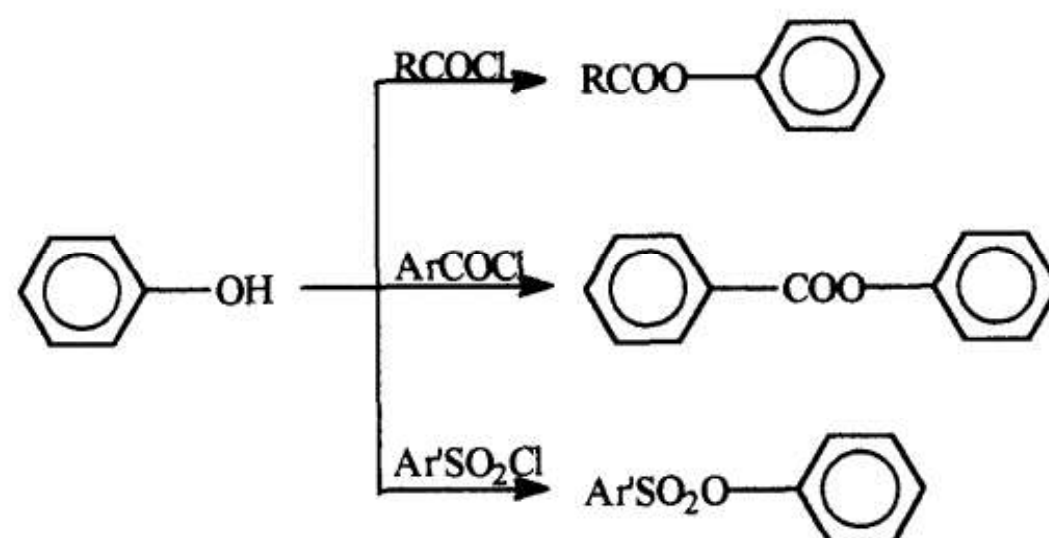
## 3.12.2.1 Salt Formation



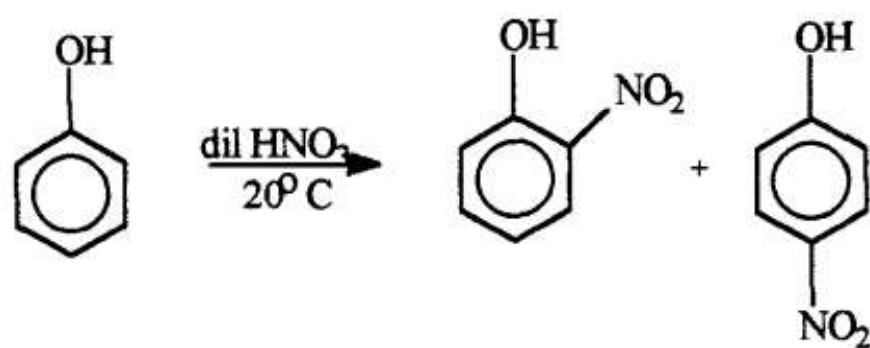
## 3.12.2.2 Ether Formation - Williamson Synthesis



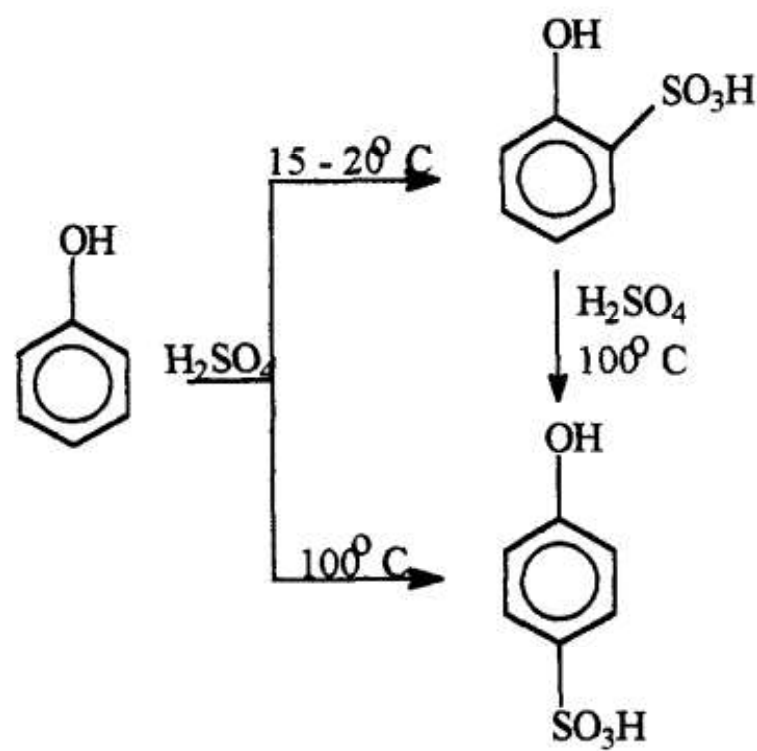
## 3.12.2.3 Ester Formation



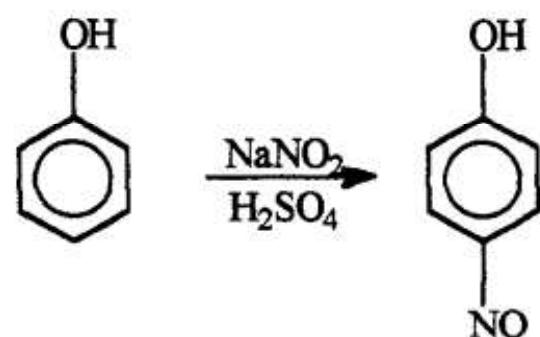
## 3.12.2.4 Ring Substitution - Nitration



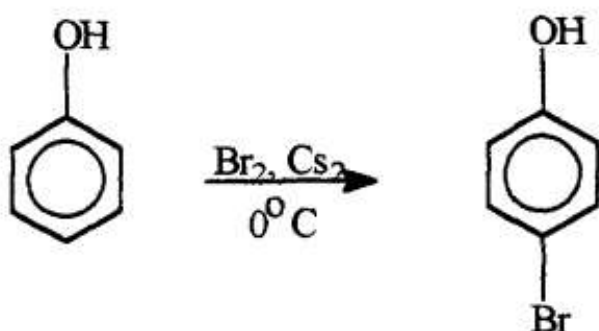
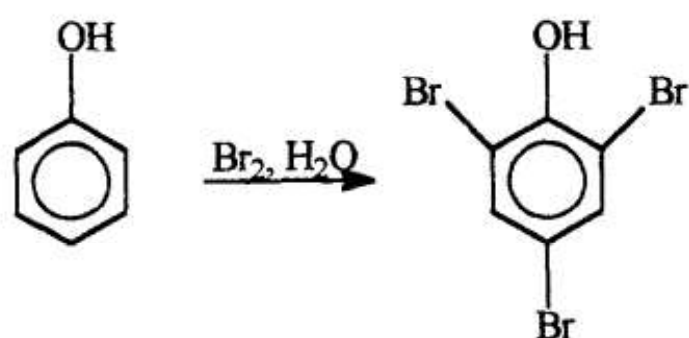
## 3.12.2.5 Ring Substitution - Sulfonation



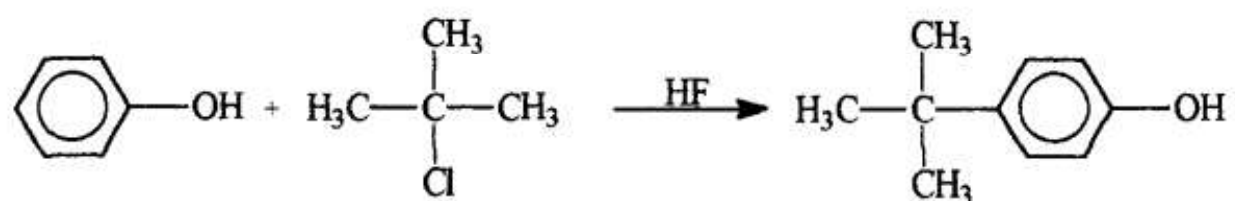
## 3.12.2.6 Ring Substitution - Nitrosation



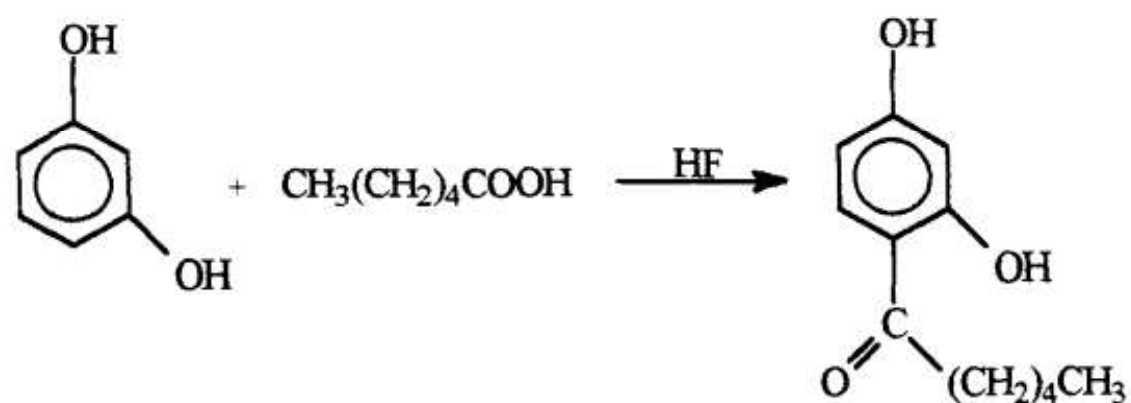
## 3.12.2.7 Ring Substitution - Halogenation



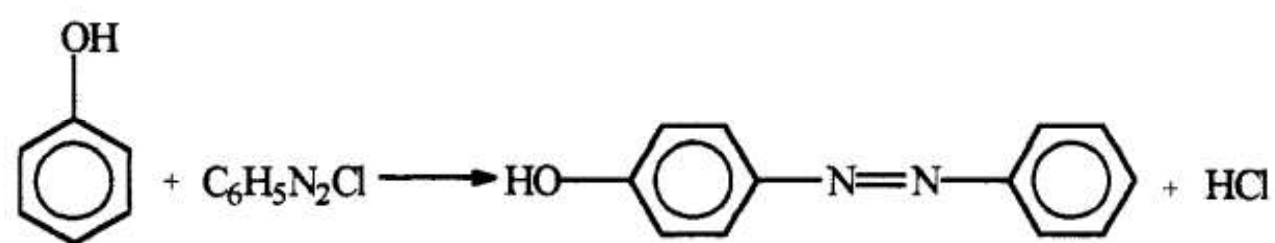
## 3.12.2.8 Ring Substitution - Friedel-Crafts Alkylation



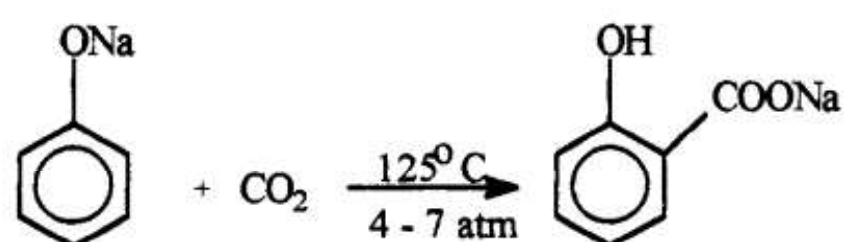
## 3.12.2.9 Ring Substitution - Friedel-Crafts Acylation



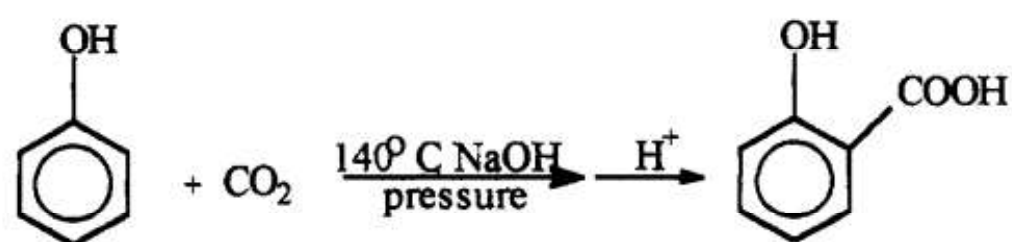
## 3.12.2.10 Coupling with Diazonium Salts



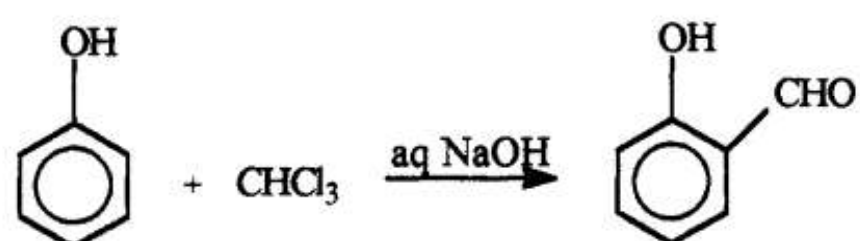
## 3.12.2.11 Carbonation. Kolbe Reaction



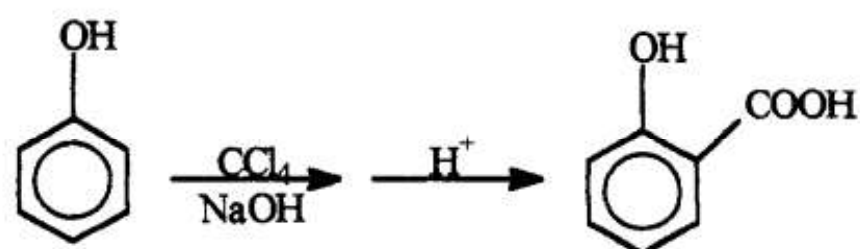
## 3.12.2.12 Carboxylation. Kolbe Reaction



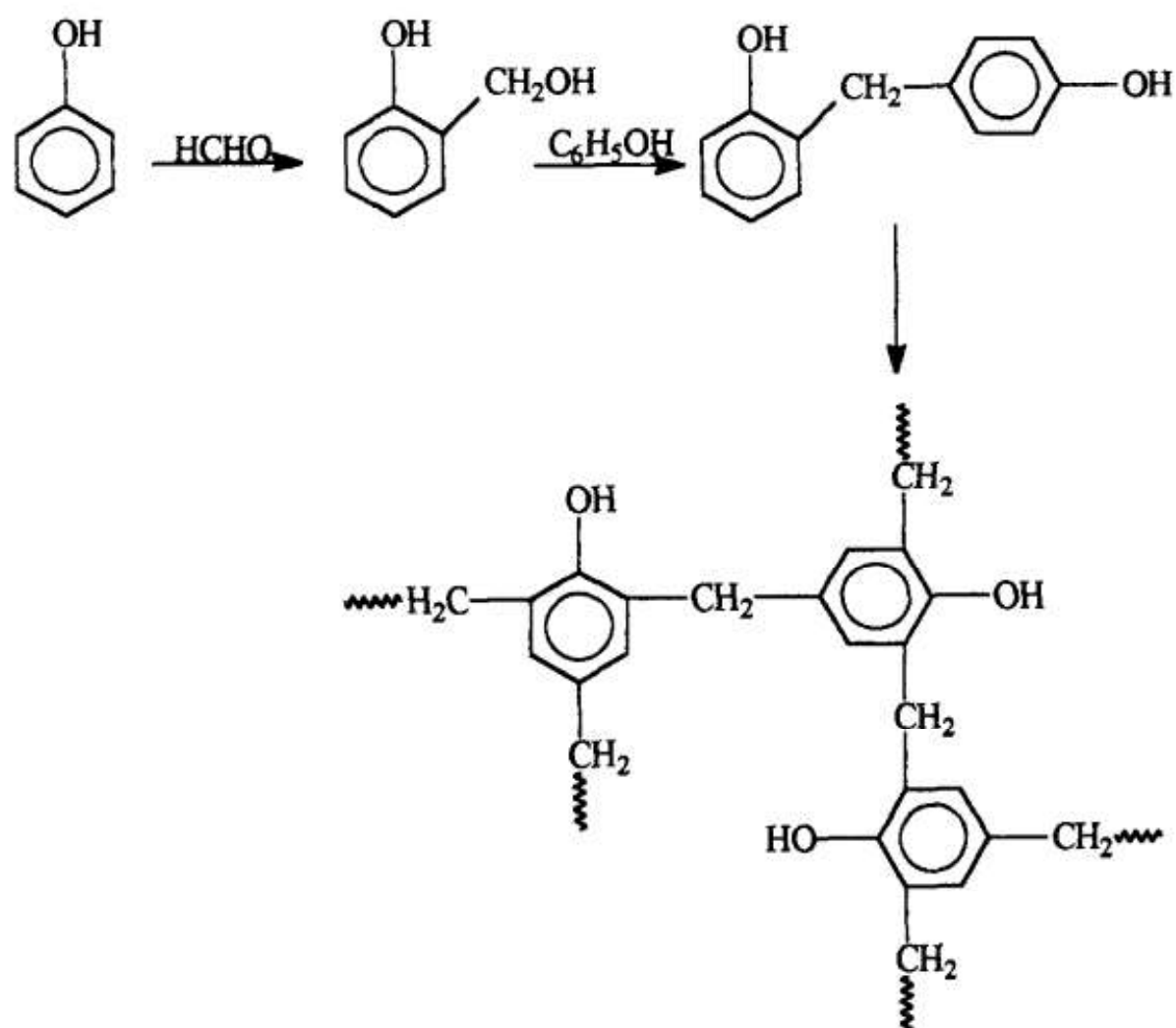
## 3.12.2.13 Aldehyde Formation. Reimer-Tiemann Reaction



## 3.12.2.14 Carboxylic Acid Formation. Reimer-Tiemann Reaction



## 3.12.2.15 Reaction with Formaldehyde



## 3.13 Ethers

## 3.13.1 Preparation of Ethers

## 3.13.1.1 Williamson Synthesis

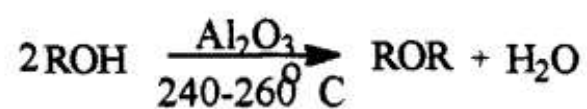


$\text{R}' = \text{alkyl or aryl}$

## 3.13.1.2 Oxymercuration-Demercuration

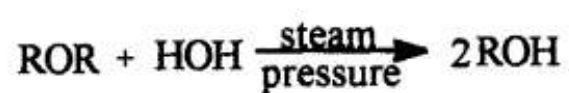
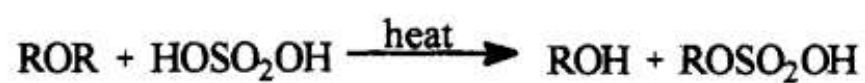


## 3.13.1.3 Dehydration of Alcohols

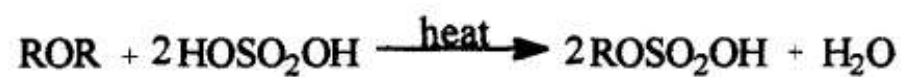
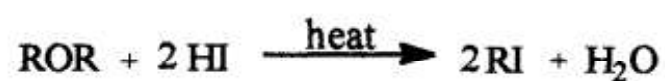
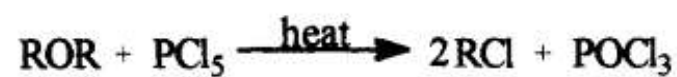


## 3.13.2 Reactions of Ethers

## 3.13.2.1 Single Cleavage by Acids



## 3.13.2.2 Double Cleavage by Acids



## 3.13.2.3 Substitution on the Hydrocarbon Chain

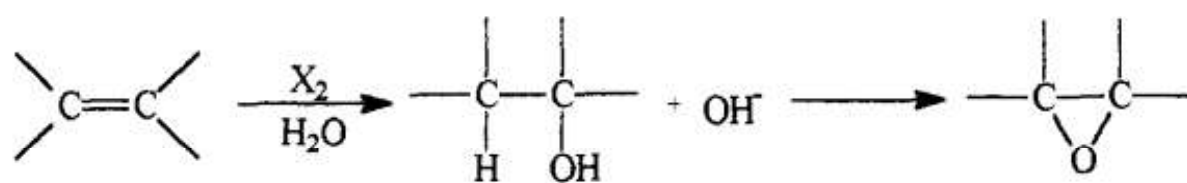


HX = Cl, Br

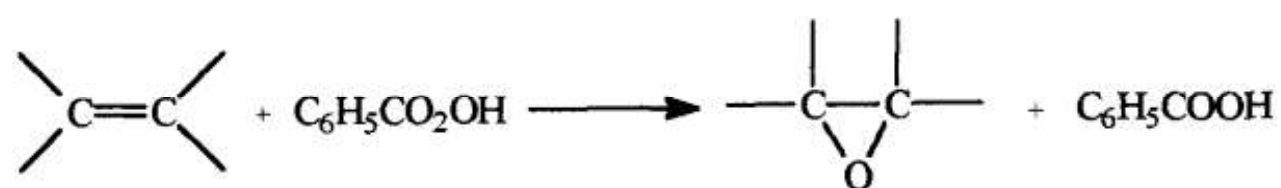
## 3.14 Epoxides

## 3.14.1 Preparation of Epoxides

## 3.14.1.1 Halohydrin Reaction

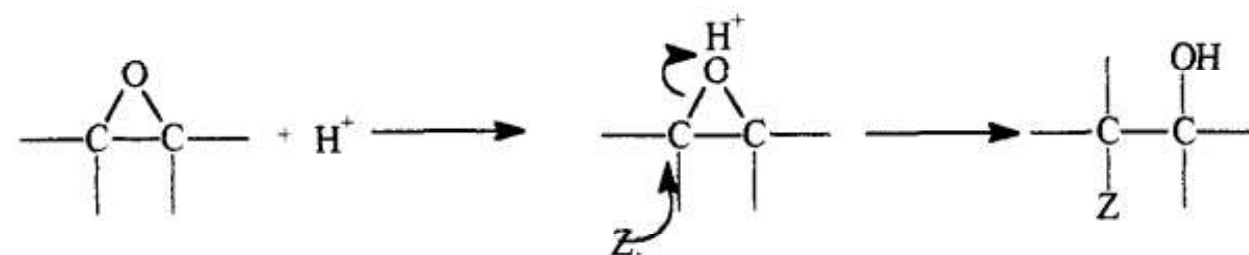


## 3.14.1.2 Peroxidation

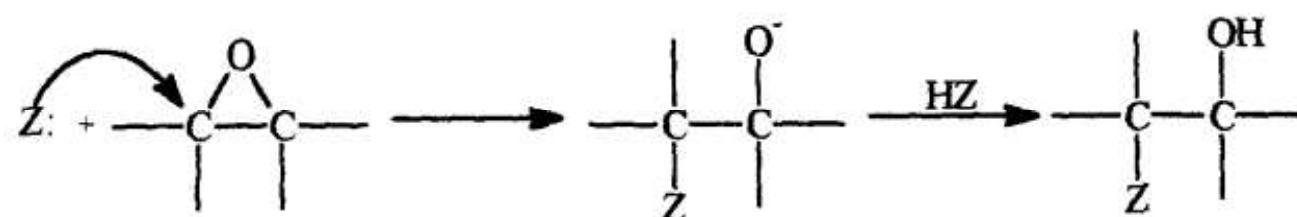


## 3.14.2 Reactions of Epoxides

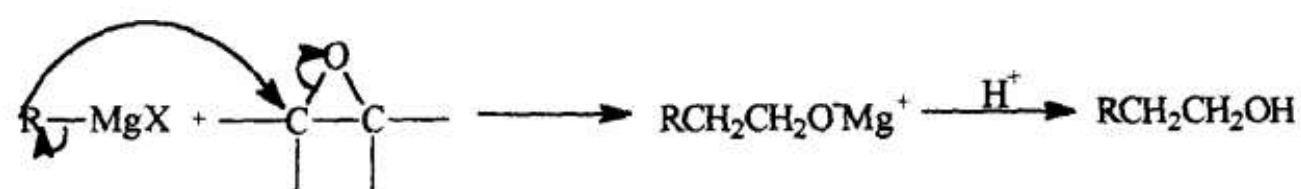
## 3.14.2.1 Acid-Catalyzed Cleavage



## 3.14.2.2 Base-Catalyzed Cleavage



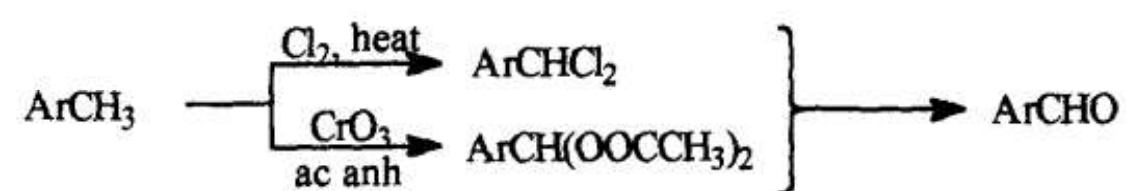
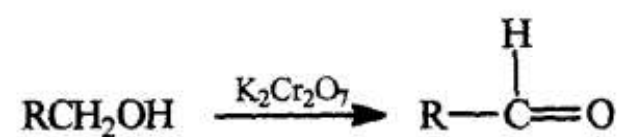
## 3.14.2.3 Grignard Reaction



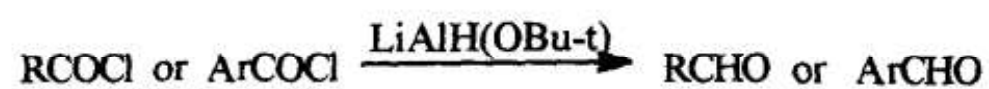
## 3.15 Aldehydes And Ketones

## 3.15.1 Preparation of Aldehydes

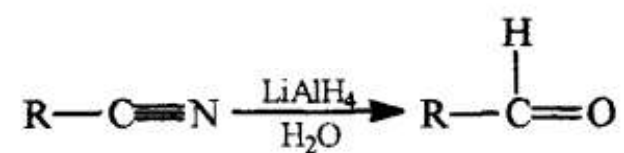
## 3.15.1.1 Oxidation



## 3.15.1.2 Reduction

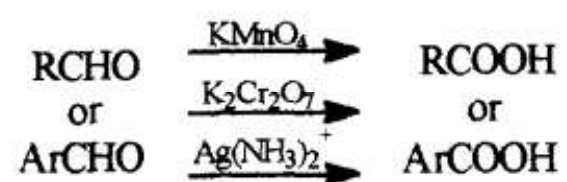


## 3.15.1.3 Reduction

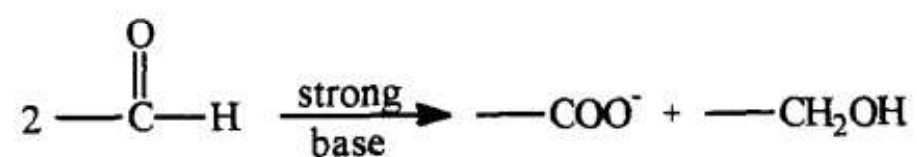


## 3.15.2 Reactions Specific to Aldehydes

## 3.15.2.1 Oxidation

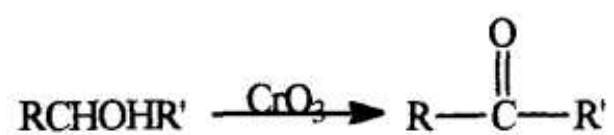


## 3.15.2.2 Cannizzaro Reaction

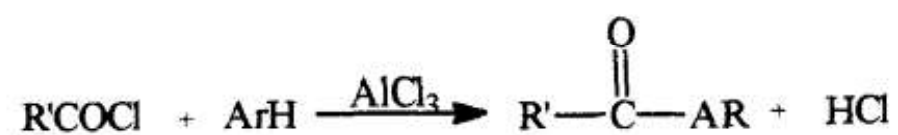


## 3.15.3 Preparation of Ketones

## 3.15.3.1 Oxidation



## 3.15.3.2 Friedel-Crafts Acylation



R' = aryl or alkyl

### 3.15.3.3 Grignard Reaction

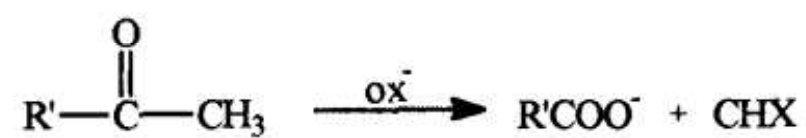


### 3.15.4 Reactions Specific to Ketones

#### 3.15.4.1 Halogenation

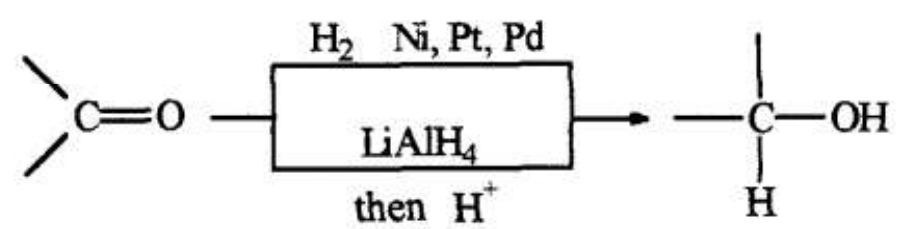


#### 3.15.4.2 Oxidation

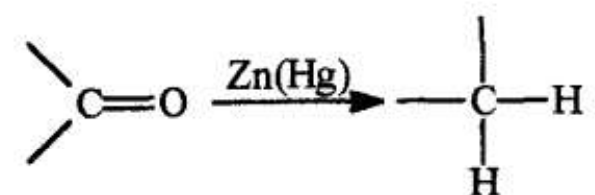


### 3.15.5 Reactions Common to Aldehydes And Ketones

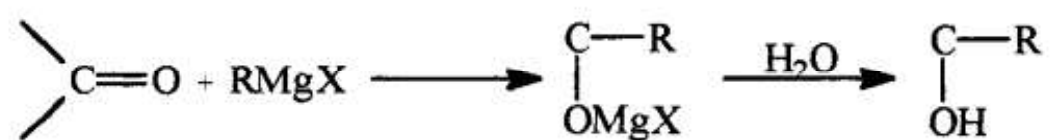
#### 3.15.5.1 Reduction to Alcohol



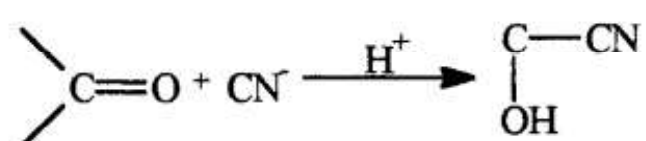
#### 3.15.5.2 Reduction to Hydrocarbon



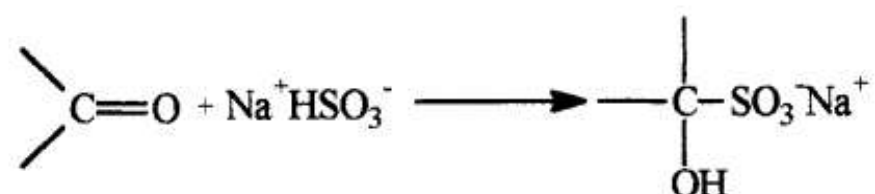
## 3.15.5.3 Grignard Reaction



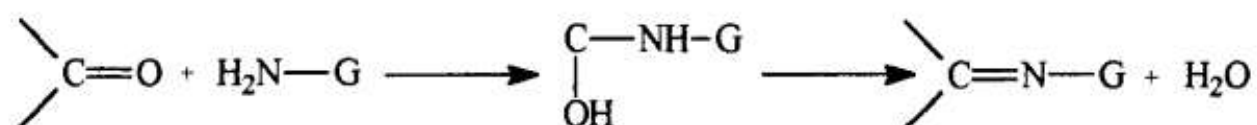
## 3.15.5.4 Cyanohydrin Formation



## 3.15.5.5 Addition of Bisulfite

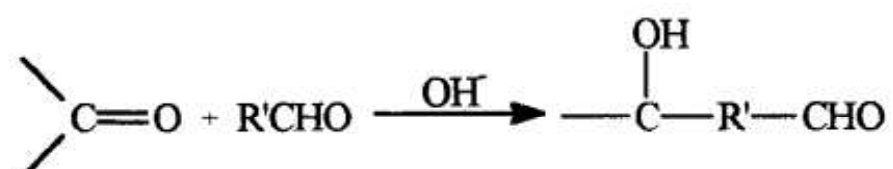


## 3.15.5.6 Addition of Ammonia Derivatives

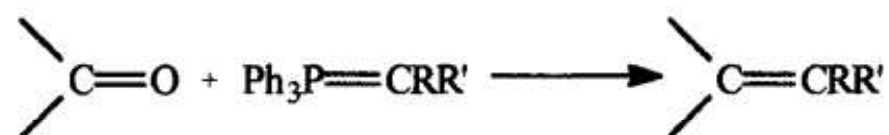


| G                               | Product                           |
|---------------------------------|-----------------------------------|
| R                               | =NR                               |
| OH                              | =NOH                              |
| NH <sub>2</sub>                 | =NNH <sub>2</sub>                 |
| NHC <sub>6</sub> H <sub>5</sub> | =NNHC <sub>6</sub> H <sub>5</sub> |
| NHCONH <sub>2</sub>             | =NNHCONH <sub>2</sub>             |

## 3.15.5.7 Aldol Condensation



### 3.15.5.8 Wittig Reaction



### 3.15.5.9 Acetal Formation



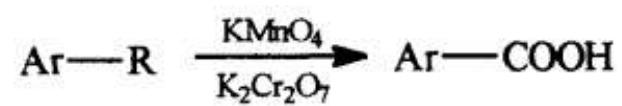
## 3.16 Carboxylic Acids

### 3.16.1 Preparation of Carboxylic Acids

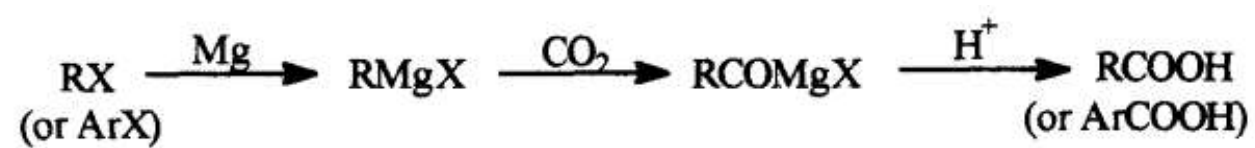
#### 3.16.1.1 Oxidation of Primary Alcohols



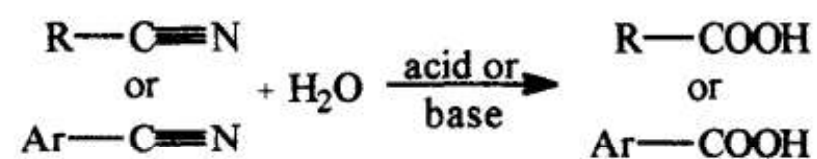
#### 3.16.1.2 Oxidation of Alkylbenzenes



#### 3.16.1.3 Carbonation of Grignard Reagents

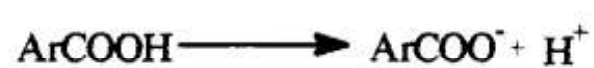


#### 3.16.1.4 Hydrolysis of Nitriles

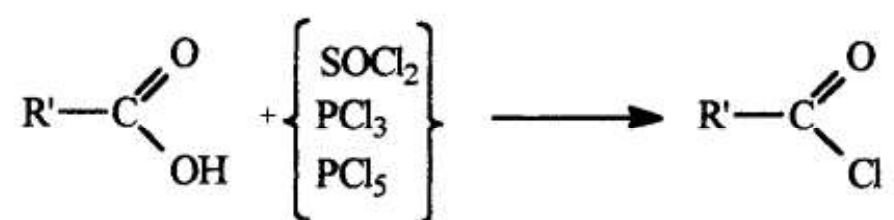


### 3.16.2 Reactions of Carboxylic Acids

#### 3.16.2.1 Acidity Salt Formation

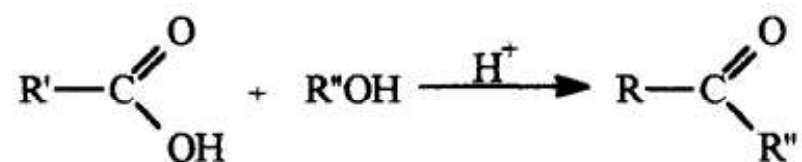


#### 3.16.2.2 Conversion to Acid Chloride



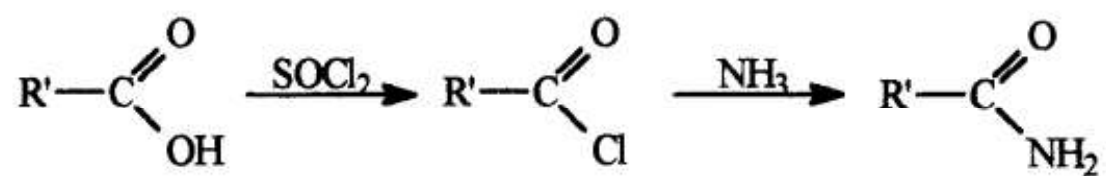
R' = alkyl or aryl

#### 3.16.2.3 Conversion to Esters



R = alkyl or aryl

#### 3.16.2.4 Conversion to Amides



R' = alkyl or aryl

### 3.16.2.5 Reduction

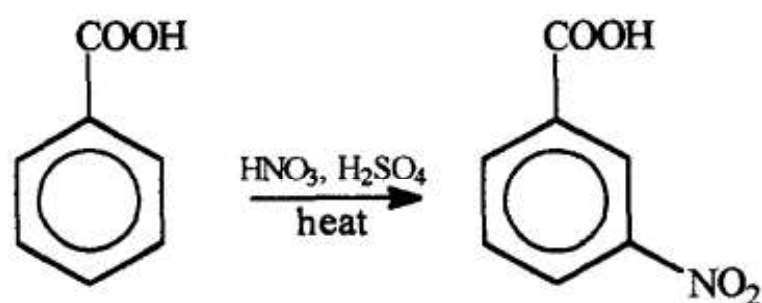


R' = alkyl or aryl

### 3.16.2.6 Alpha-Halogenation of Aliphatic Acids

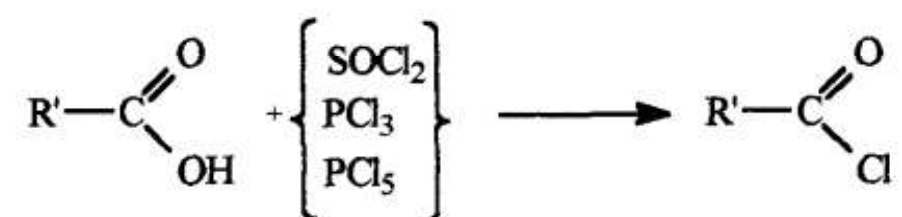


### 3.16.2.7 Ring Substitution in Aromatic Acids



## 3.17 Acid Chlorides

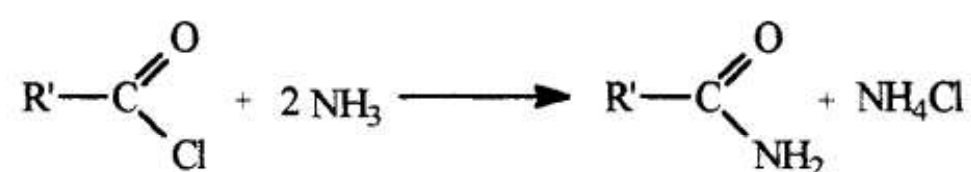
### 3.17.1 Preparation of Acid Chlorides



R' = alkyl or aryl

**3.17.2 Reactions of Acid Chlorides****3.17.2.1 Hydrolysis (Acid Formation)**

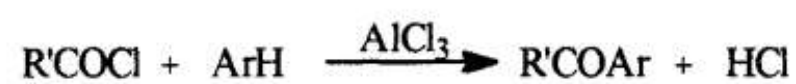
R' = alkyl or aryl

**3.17.2.2 Ammonolysis (Amide Formation)**

R' = alkyl or aryl

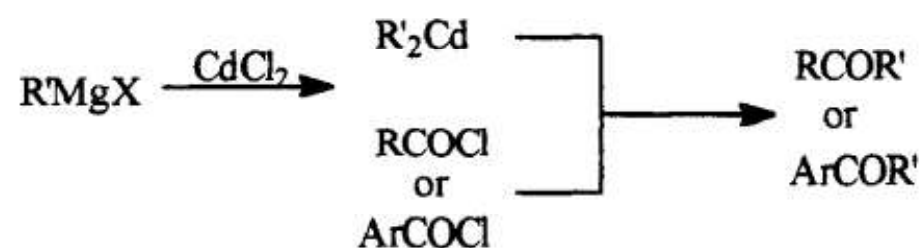
**3.17.2.3 Alcoholysis (Ester Formation)**

R' = alkyl or aryl

**3.17.2.4 Friedel-Crafts Acylation (Ketone Formation)**

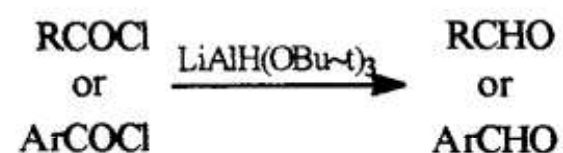
R' = alkyl or aryl

### 3.17.2.5 Ketone Formation by Reaction with Organocadmium Compounds

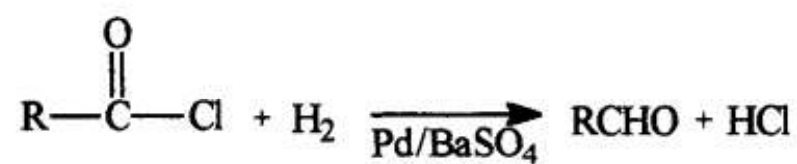


R' must be an acyl or primary alkyl alcohol

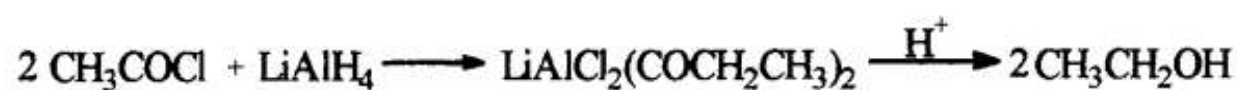
### 3.17.2.6 Aldehyde Formation by Reduction



### 3.17.2.7 Rosenmund Reduction



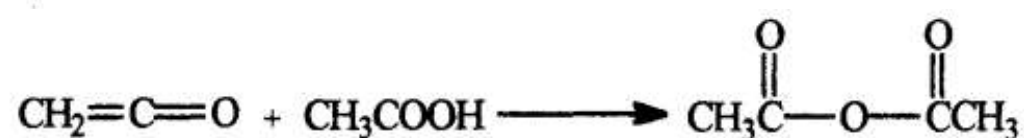
### 3.17.2.8 Reduction to Alcohols



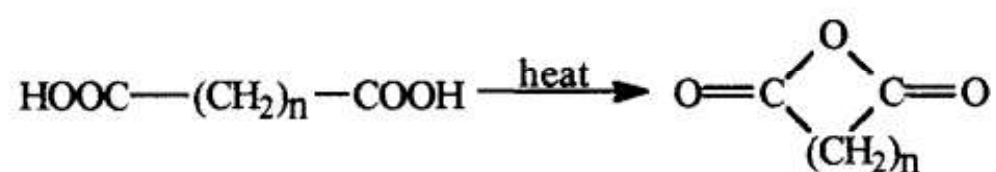
## 3.18 Acid Anhydrides

### 3.18.1 Preparation of Acid Anhydrides

#### 3.18.1.1 Ketene Reaction



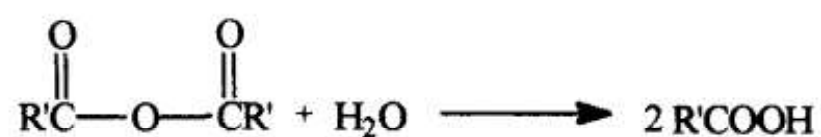
### 3.18.1.2 Dehydration of Dicarboxylic Acids



$n = 2, 3, 4$

## 3.18.2 Reactions of Acid Anhydrides

### 3.18.2.1 Hydrolysis (Acid Formation)



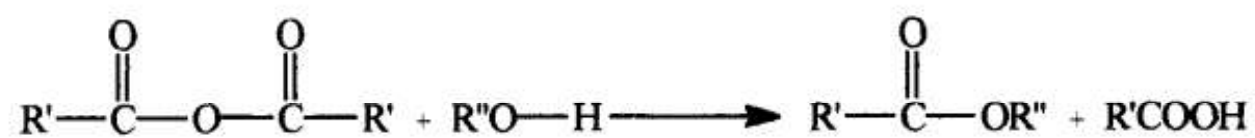
$\text{R}' = \text{alkyl or aryl}$

### 3.18.2.2 Ammonolysis (Amide Formation)



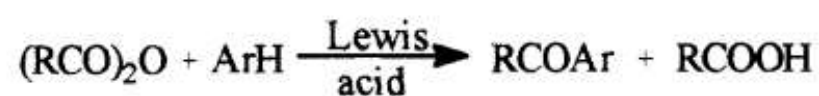
$\text{R}' = \text{alkyl or aryl}$

### 3.18.2.3 Alcoholysis (Ester Formation)



$\text{R}' = \text{alkyl or aryl}$

### 3.18.2.4 Friedel-Crafts Acylation (Ketone Formation)



### 3.19 Esters

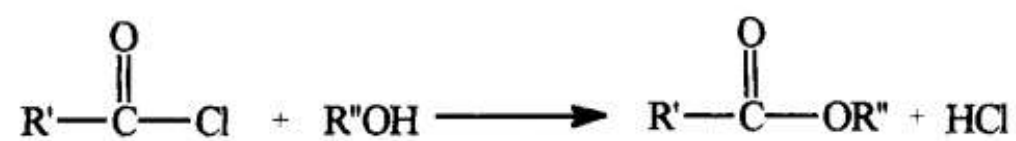
#### 3.19.1 Preparation of Esters

##### 3.19.1.1 From Acids



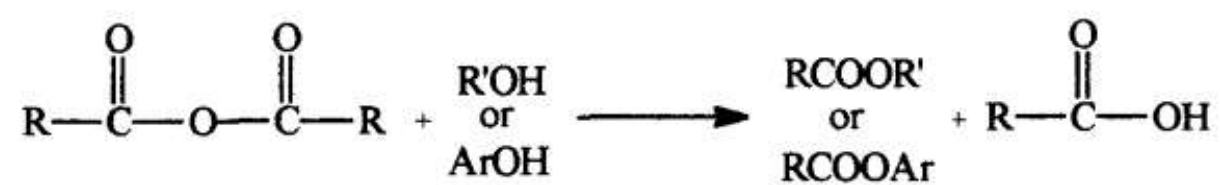
R' = alkyl or aryl

##### 3.19.1.2 From Acid Chlorides



R' = alkyl or aryl

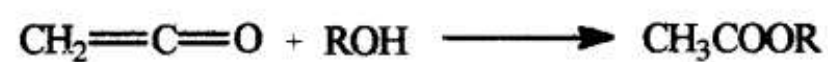
##### 3.19.1.3 From Acid Anhydrides

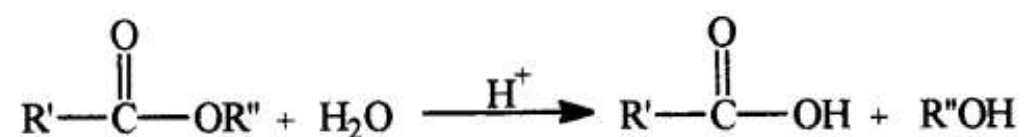


##### 3.19.1.4 Transesterification

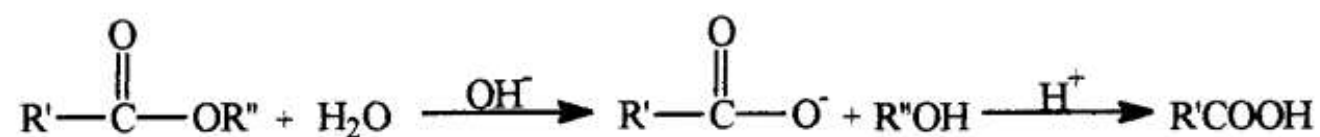


##### 3.19.1.5 From Ketene and Alcohols

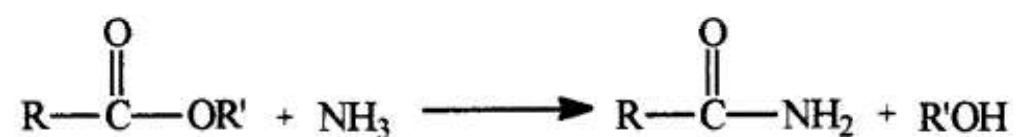
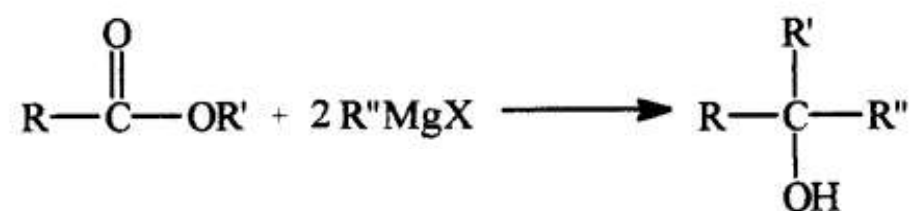


**3.19.2 Reactions of Esters****3.19.2.1 Hydrolysis**

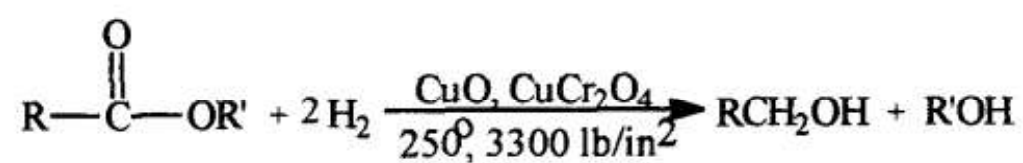
R' = alkyl or aryl

**3.19.2.2 Saponification**

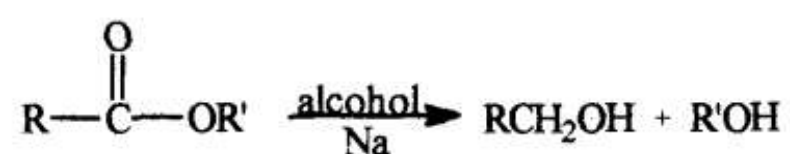
R' = alkyl or aryl

**3.19.2.3 Ammonolysis****3.19.2.4 Transesterification****3.19.2.5 Grignard Reaction**

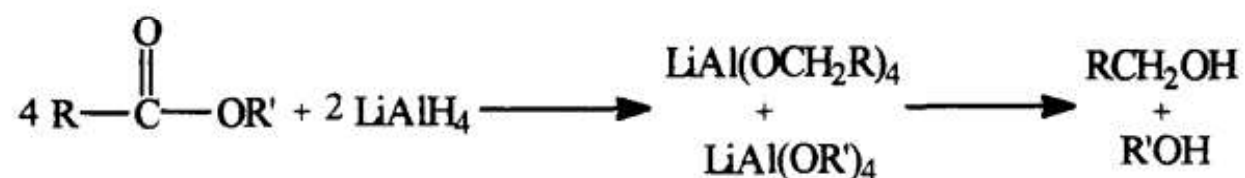
## 3.19.2.6 Hydrogenolysis



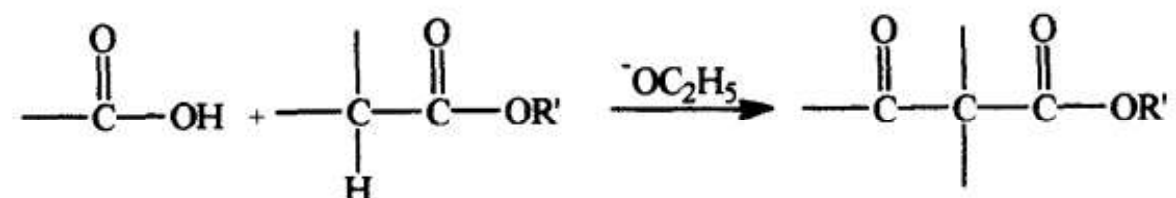
## 3.19.2.7 Bouvauelt - Blanc Method



## 3.19.2.8 Chemical Reduction



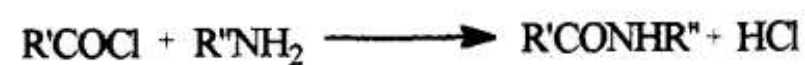
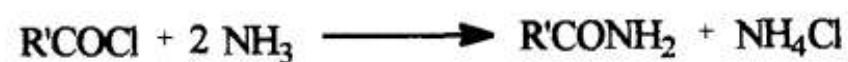
## 3.19.2.9 Claisen Condensation



## 3.20 Amides

## 3.20.1 Preparation of Amides

## 3.20.1.1 From Acid Chlorides





R' = alkyl or aryl

### 3.20.1.2 From Acid Anhydrides



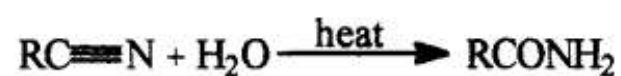
### 3.20.1.3 From Esters by Ammonolysis



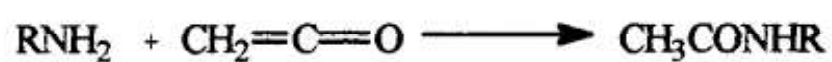
### 3.20.1.4 From Carboxylic Acids



### 3.20.1.5 From Nitriles

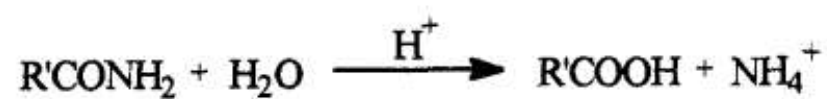


### 3.20.1.6 From Ketenes and Amines



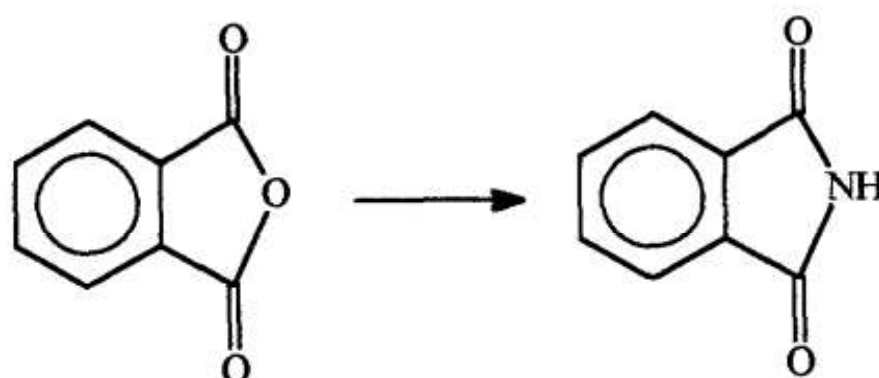
### 3.20.2 Reactions of Amides

#### 3.20.2.1 Hydrolysis



R' = alkyl or aryl

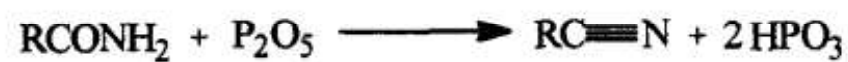
#### 3.20.2.2 Conversion to Imides



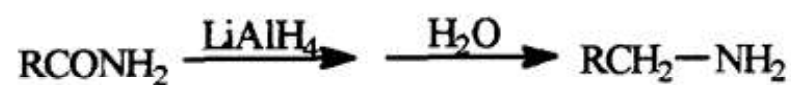
#### 3.20.2.3 Reaction with Nitrous Acid



#### 3.20.2.4 Dehydration



#### 3.20.2.5 Reduction



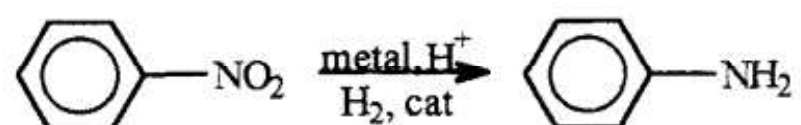
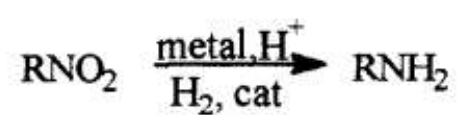
#### 3.20.2.6 Hoffman Degradation



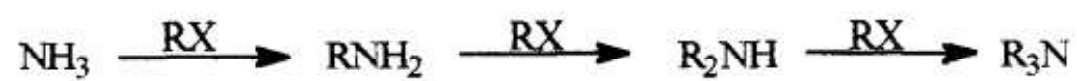
## 3.21 Amines

### 3.21.1 Preparation of Amines

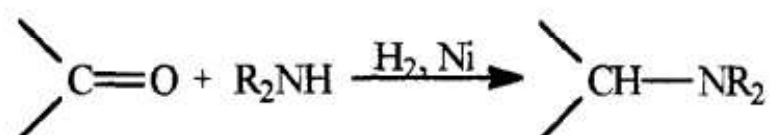
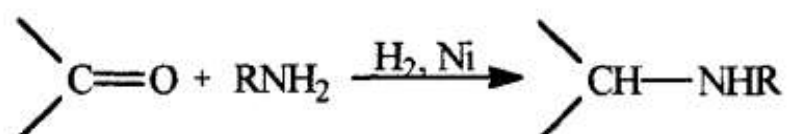
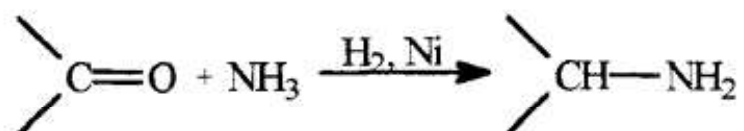
#### 3.21.1.1 Reduction of Nitro Compounds



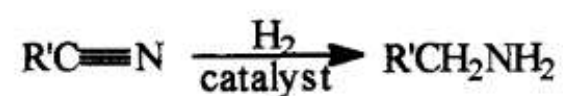
#### 3.21.1.2 Reaction of Ammonia with Halides



#### 3.21.1.3 Reductive Amination

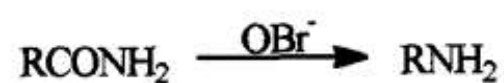


### 3.21.1.4 Reduction of Nitriles



R' = alkyl or aryl

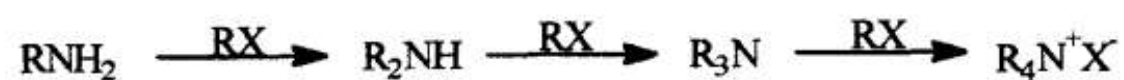
### 3.21.1.5 Hofmann Degradation



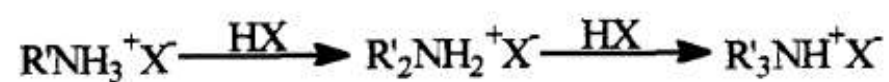
R' = alkyl or aryl

## 3.21.2 Reactions of Amines

### 3.21.2.1 Alkylation

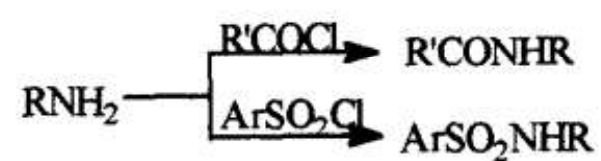


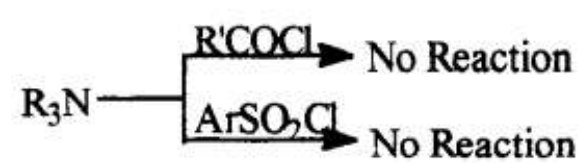
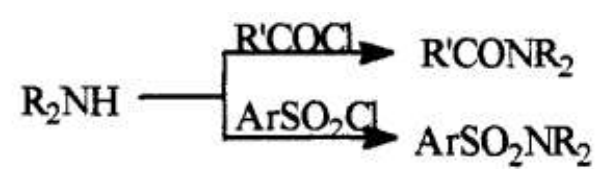
### 3.21.2.2 Salt Formation



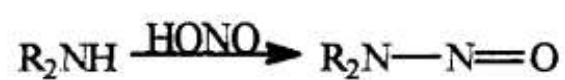
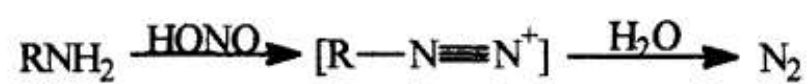
R' = alkyl or aryl

### 3.21.2.3 Amide Formation





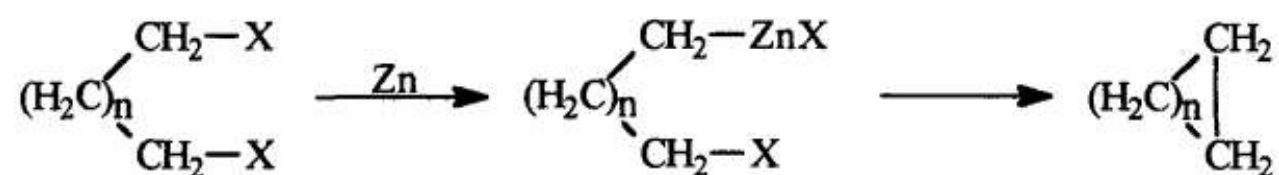
#### 3.21.2.4 Reaction of Amines with Nitrous Acid



## 3.22 Alicyclic Compounds

### 3.22.1 Preparation of Alicyclic Compounds

#### 3.22.1.1 Cyclization

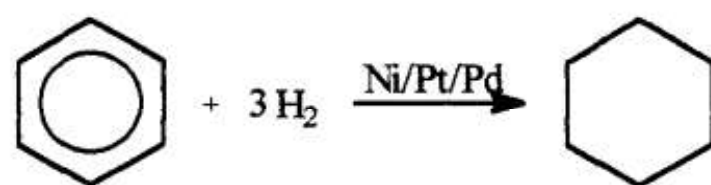


When  $n = 1$  cyclopropane

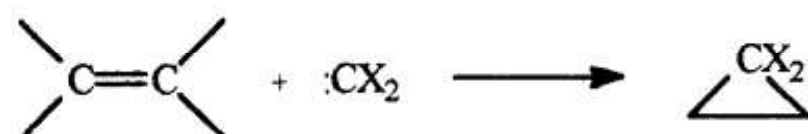
$n = 2$  cyclobutane

$n = 3$  cyclopentane

#### 3.22.1.2 Hydrogenation



#### 3.22.1.3 Cycloaddition



$\text{X} = \text{H}, \text{Cl}, \text{Br}$

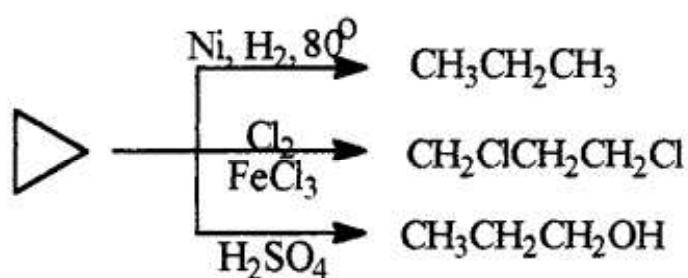
### 3.22.2 Reactions of Alicyclic Compounds

#### 3.22.2.1 Free Radical Addition





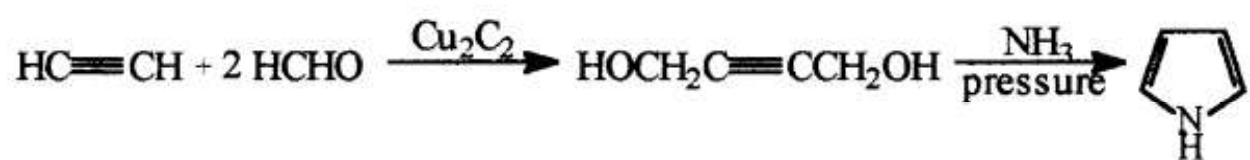
### 3.22.2.2 Addition Reaction



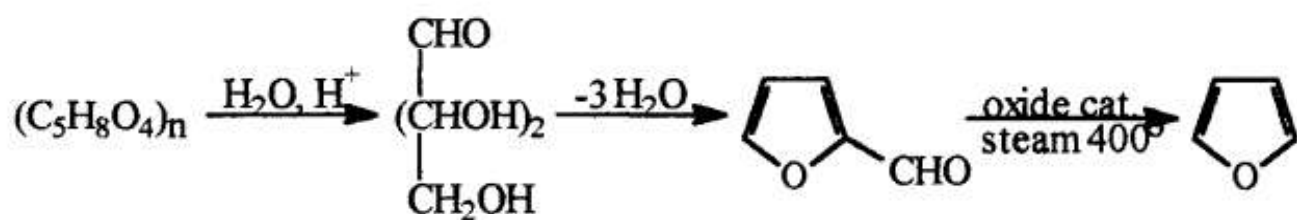
## 3.23 Heterocyclic Compounds

### 3.23.1 Preparation of Pyrrole, Furan, and Thiophene

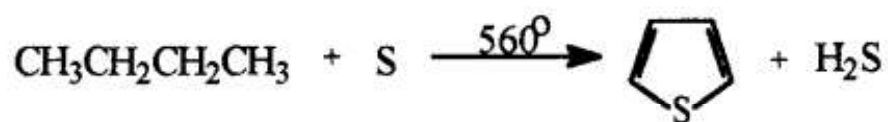
#### 3.23.1.1 Pyrrole



#### 3.23.1.2 Furan

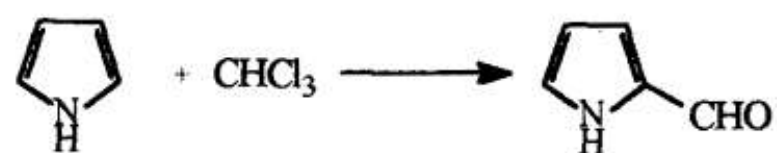
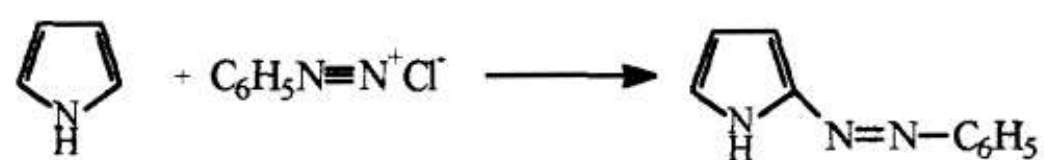


#### 3.23.1.3 Thiophene

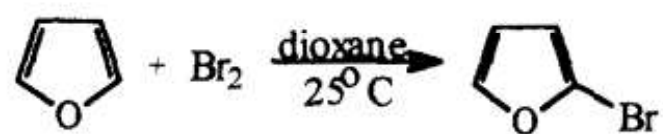
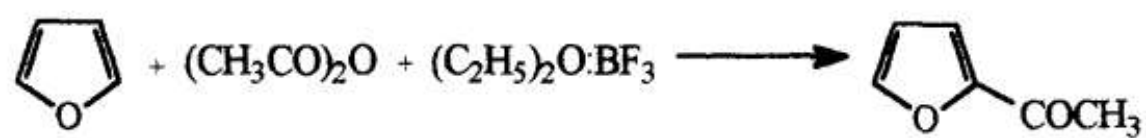
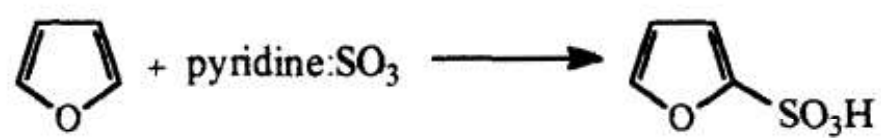


### 3.23.2 Reactions of Pyrrole, Furan, and Thiophene

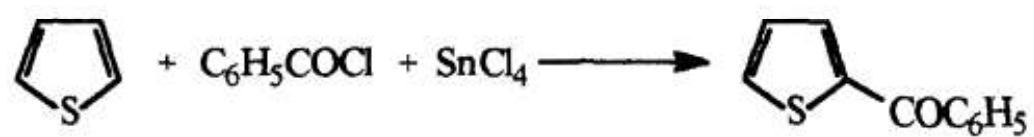
#### 3.23.2.1 Pyrrole

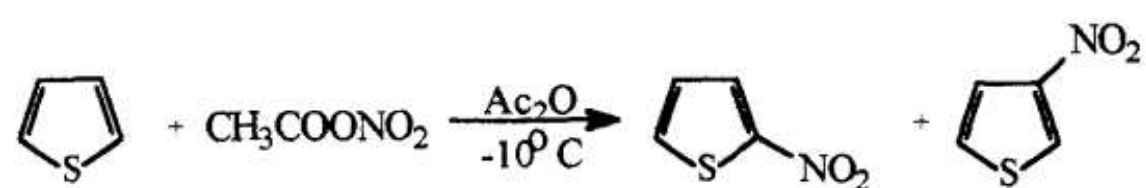
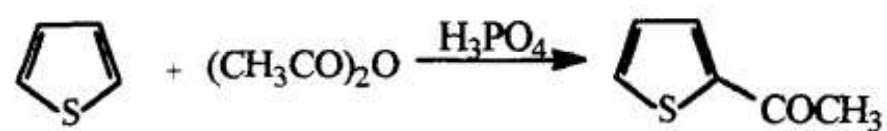
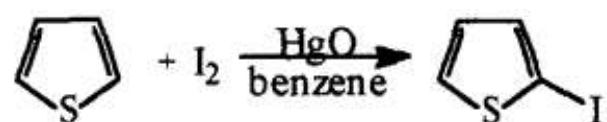


#### 3.23.2.2 Furan



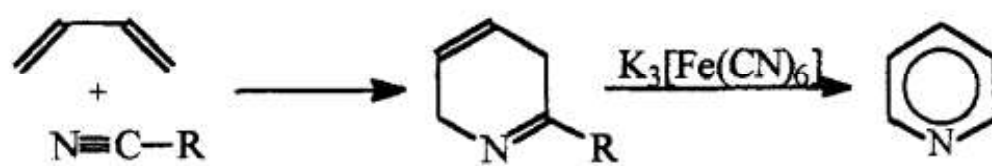
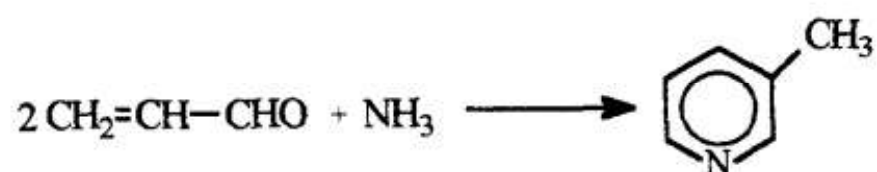
#### 3.23.2.3 Thiophene



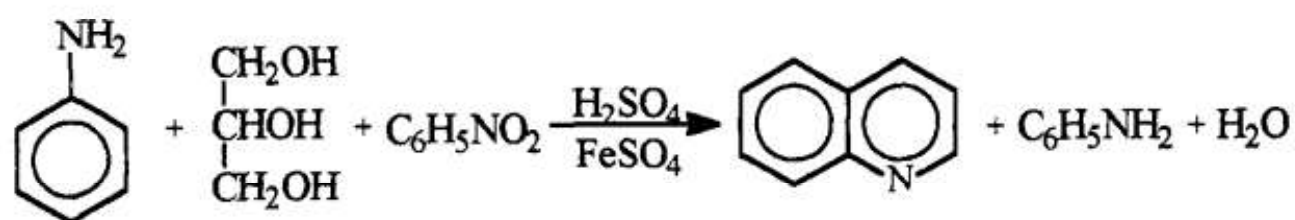


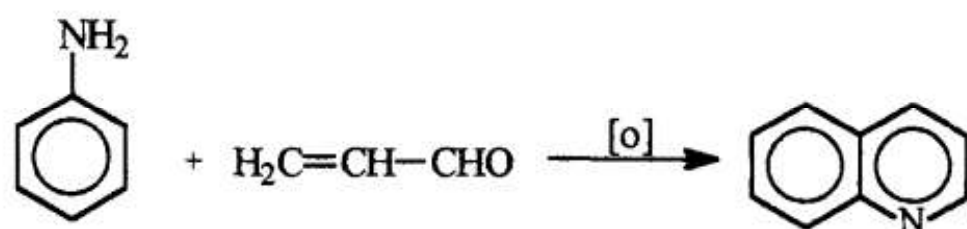
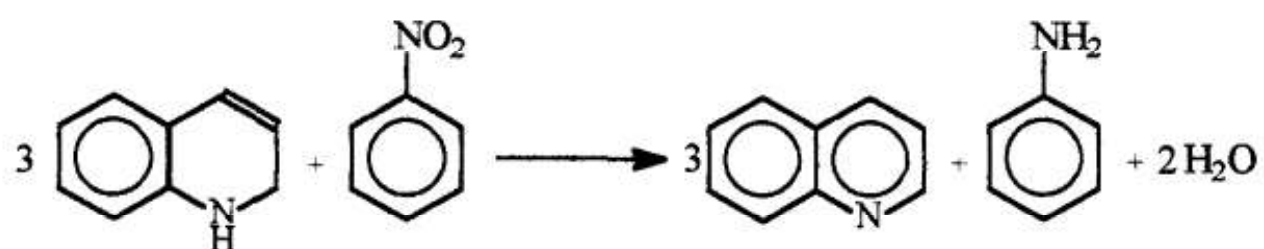
### 3.23.3 Preparation of Pyridine, Quinoline, and Isoquinoline

#### 3.23.3.1 Pyridine

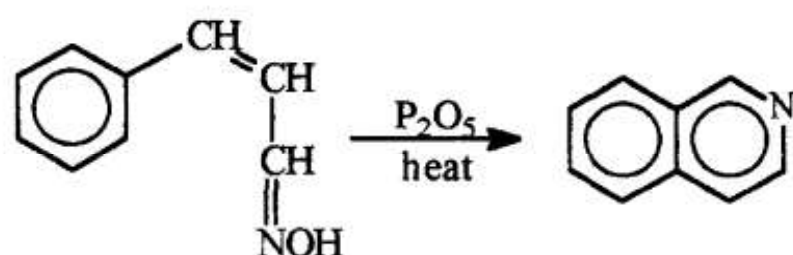


#### 3.23.3.2 Quinoline



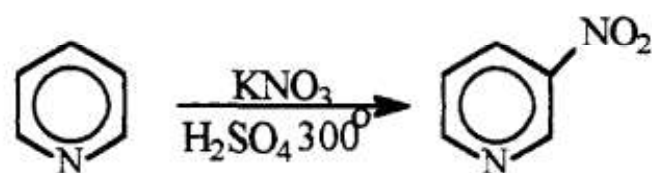
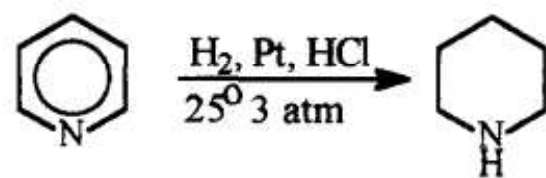


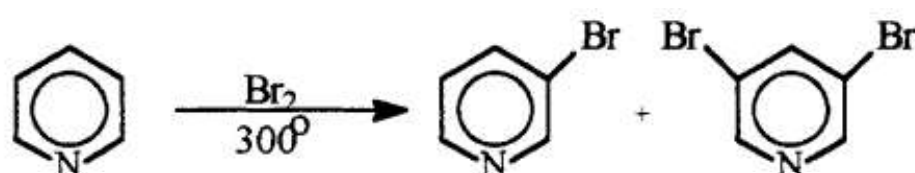
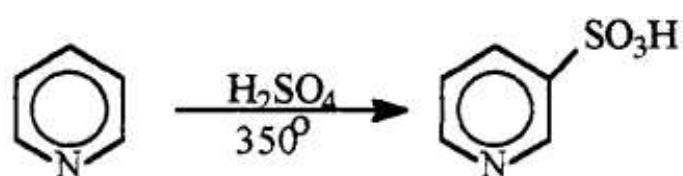
### 3.23.3.3 Isoquinoline



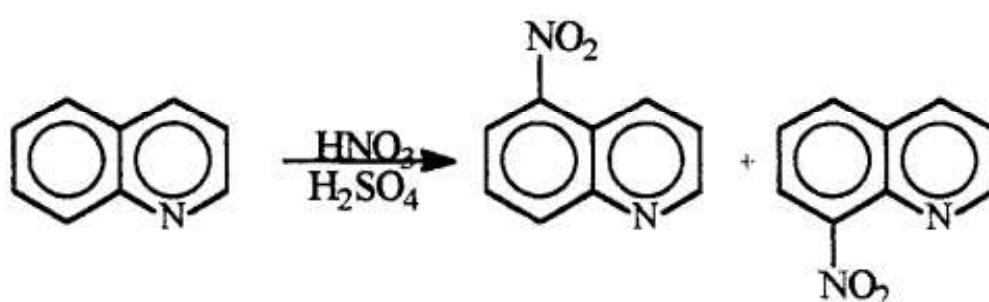
## 3.23.4 Reactions of Pyridine, Quinoline, and Isoquinoline

### 3.23.4.1 Pyridine

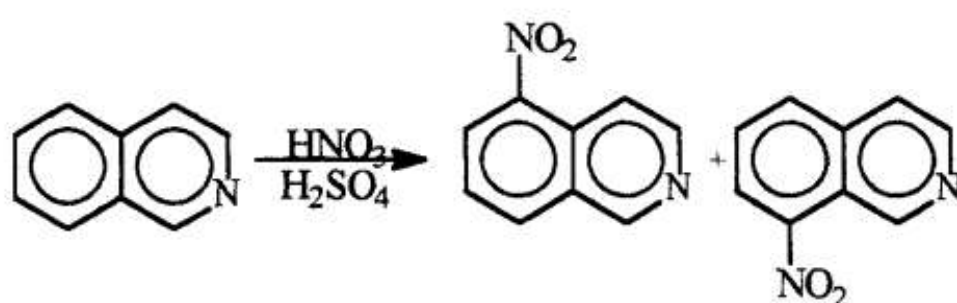




#### 3.23.4.2 Quinoline



#### 3.23.4.3 Isoquinoline



### 3.24 Isomers

#### 3.24.1 Isomers and Stereoisomers

Organic compounds that have the same chemical formula but are attached to one another in different ways are called **isomers**. Isomers that have the same chemical formula and are attached to one another in same way but whose orientation to one another differ are called **Stereoisomers**. There are several different types of isomers that are encountered in organic chemistry.

To represent three dimensional structures on paper the chiral center of a molecule is taken at the cross point of a cross and the groups are attached at

the ends. The horizontal line represents the bonds projecting out of the plane of the paper. The vertical line represents the bonds projecting into the plane of the paper.

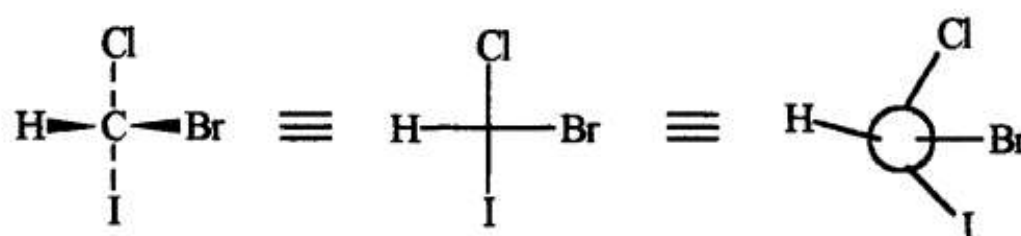


Figure 3.2. Three Dimensional Representations

### 3.24.2 Optical Activity

In addition to having different arrangements of atoms, certain organic compounds exhibit a unique property of rotating **plane-polarized light** (light that has its amplitude in one plane). Compounds that rotate light are said to be **optically active**. Optically active compounds that rotate light to the right are called dextrorotatory and are symbolized by D or +. Compounds that rotate light to the left are called levorotatory and are symbolized by L or -.

### 3.24.3 Enantiomers

Enantiomers are stereoisomers that are non-superimposable mirror images of each other. Enantiomers have identical physical and chemical (except towards optically active reagents) properties except for the direction in which plane-polarized light is rotated. Enantiomers account for a compound's optical activity.

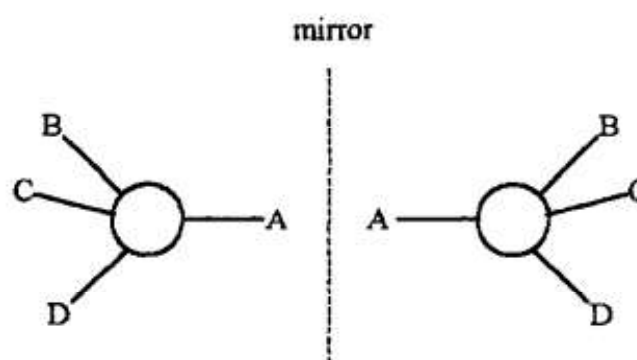


Figure 3.3. Enantiomers

### 3.24.4 Chirality

Molecules that are not superimposable on their mirror images are **chiral**. Chiral molecules exist as enantiomers but achiral molecules cannot exist as enantiomers. A carbon atom to which four different groups are attached is a **chiral center**. Not all molecules that contain a chiral center are chiral. Not all chiral molecules contain a chiral center.

### 3.24.5 Racemic Mixture

A mixture of equal parts of enantiomers is called a **racemic mixture**. A racemic mixture contains equal parts of D and L components and therefore, the mixture is optically inactive.

### 3.24.6 Diastereomers

**Diastereomers** are stereoisomers that are not mirror images of each other. Diastereomers have different physical properties. And they may be dextrorotatory, levorotatory or inactive.

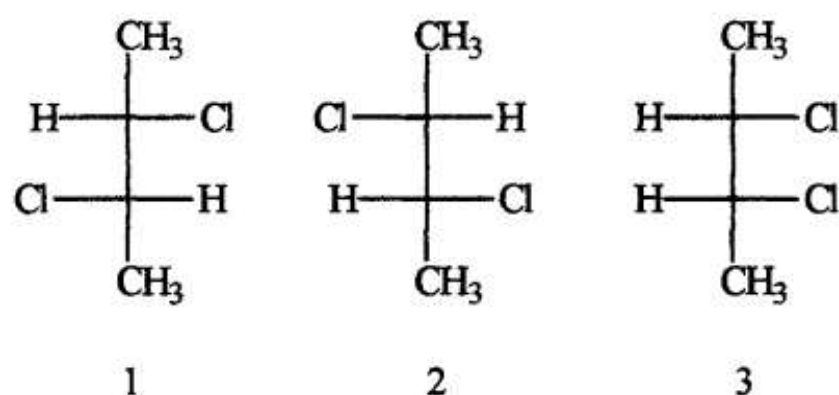


Figure 3.4 Enantiomers and Diastereomers

Structures 1 and 2 are enantiomers, structure 3 is a diastereomer of structures 1 and 2.

### 3.24.7 Meso Compounds

Meso compounds are superimposable mirror images of each other, even though they contain a chiral center.

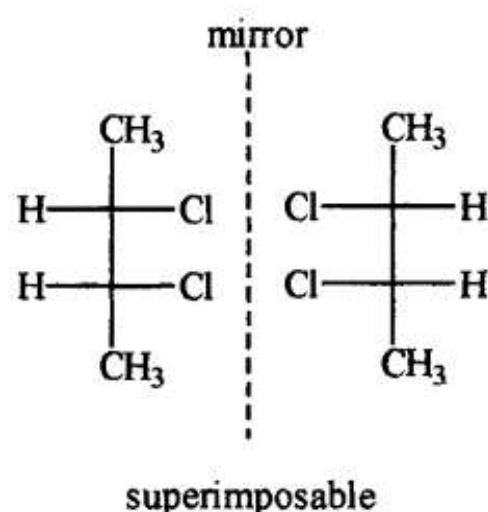


Figure 3.5. Meso Compound

Meso compounds can be recognized by the fact that half the molecule is a mirror image of the other half.

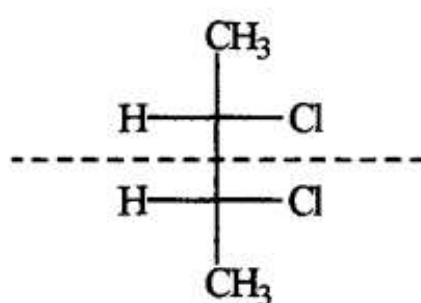


Figure 3.6. Plane of symmetry of a meso compound

The upper half of the molecule is a non-superimposable mirror image of the lower half, making the top half an enantiomer of the lower half. However, since the two halves are in the same molecule the rotation of plane-polarized light by the upper half is cancelled by the lower half and the compound is optically inactive.

### 3.24.8 Positional Isomers

**Positional isomers** are compounds that have the same number and kind of atoms but are arranged (or bonded) in a different order. They also have different physical and chemical properties. Butane (figure 3.1) can have two different structures, n-butane and 2-methylpropane:

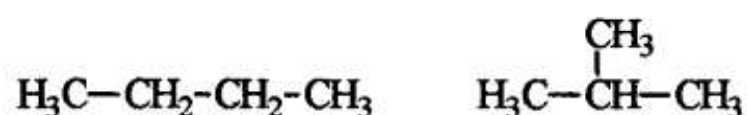


Figure 3.7. n-butane and 2-methylpropane

### 3.24.9 Geometric Isomers

**Geometric isomers** or cis-trans isomerism can exist in compounds that contain a double bond or a ring structure. In order for this type of isomerism to exist the groups coming off the same end of the double bond must be different. For example bromoethene does not have cis-trans isomerism.

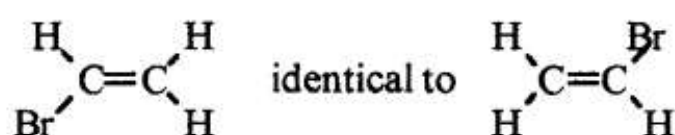


Figure 3.8. Bromoethene structure

However, 1,2-dibromoethene can exist as cis-1,2-dibromoethene and trans-1,2-dibromoethene

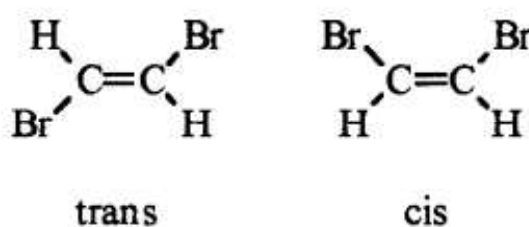


Figure 3.9. Trans and cis butene

Ring structures confer restricted rotation around the bonds and thereby give rise to geometric isomer. In trans-1,3-dichlorocyclopentane one chlorine is above the plane of the ring and the other is below. In cis-1,3-dichlorocyclopentane both chlorines are above the plane of the ring.

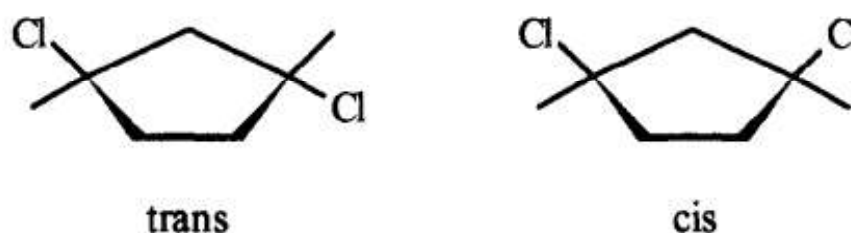


Figure 3.10. Trans and cis- 1,3-cyclopentane

### 3.24.10 Conformational Isomers

**Conformational isomers** deal with the orientations within a molecule. The free rotation around a single bond accounts for the different

conformations that can exist within a molecule. For example, n-butane can have the following conformations:

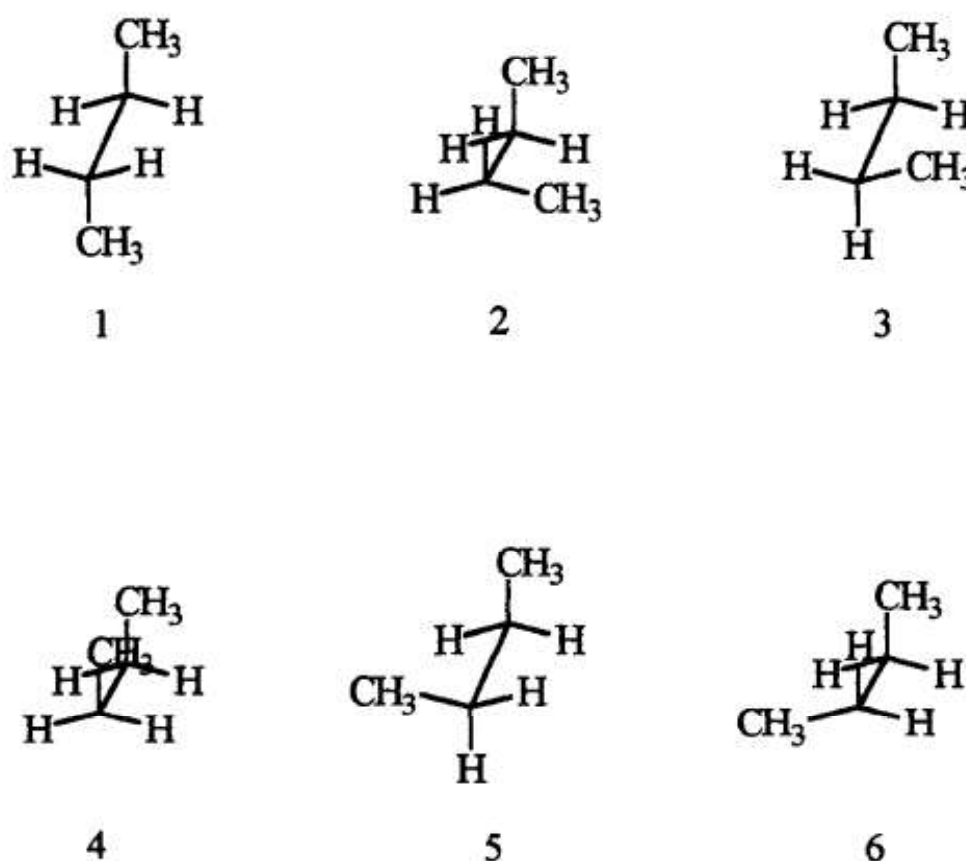


Figure 3.11. Conformational isomers of butane

Figure 1 has a *staggered* or *anti* conformation. Since in figure 1, the two methyl groups are farthest apart, this form is referred to as *anti*. Figures 3 and 5 have *staggered* or *gauche* conformations. Figures 2, 4, and 6 have an *eclipsed* conformation.

A different type of projection used to view isomers, called Newman projections, is sometimes used. The following figures are the same as above:

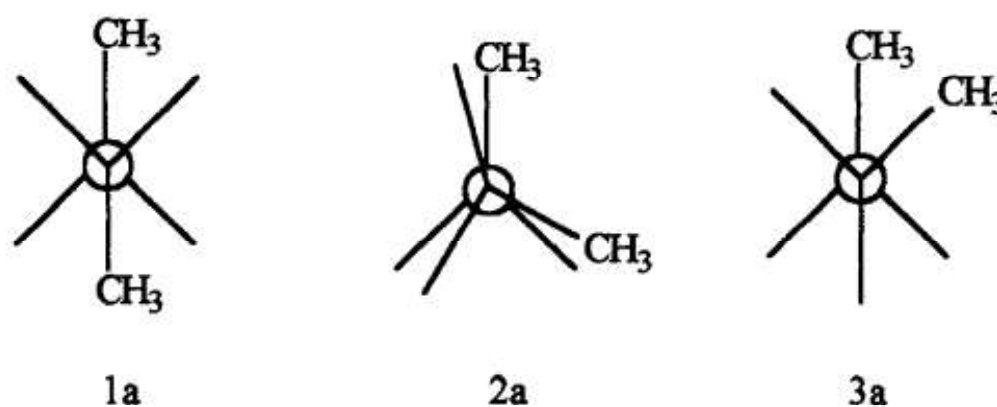


Figure 3.12. Newman projections

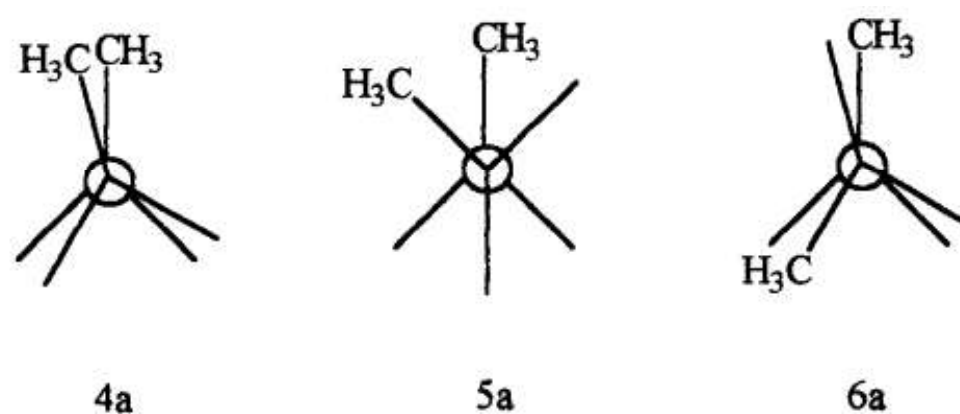


Figure 3.12. Newman projections

Although cyclohexane is a ring structure it does have free rotation around single bonds. Cyclohexane has two main conformations. The most stable form is called the chair form, the less stable is called the boat form:



Figure 3.13. Chair and boat conformations of cyclohexane

The bonds in cyclohexane occupy two kinds of position, six hydrogens lie in the plane and six hydrogens lie either above or below the plane. Those that are in the plane of the ring lie in the "equator" of it, and are called the **equatorial bonds**. Those bonds that are above or below are pointed along the axis perpendicular to the plane and are called **axial bonds**.

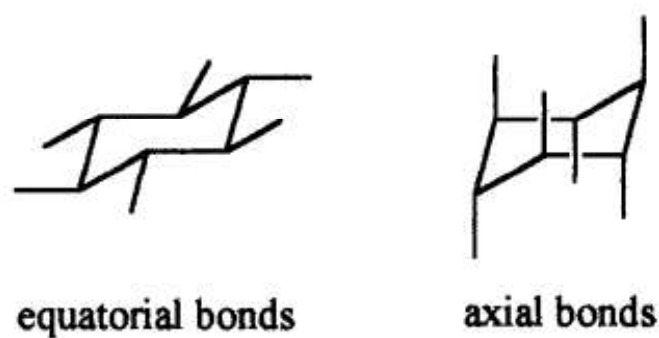


Figure 3.14. Equatorial and axial bonds of cyclohexane

### 3.24.11 Configurational Isomers

The arrangement of atoms that characterizes a certain stereoisomer is called its configuration. In general, optically active compounds can have more than one configuration. Determination of the Configuration can be determined by the following two steps:

Step 1. Following a set of sequence rule we assign a sequence of priority to the four atoms attached to the chiral center.

Step 2. The molecule is oriented so that the group of lowest priority is directed away from us. The arrangement of the remaining groups is then observed. If the sequence of highest priority to lowest priority is clockwise, the configuration is designated R. If the sequence is counterclockwise, the configuration is designated S.

From these steps a set of sequence rules can be formulated that will allow a configuration to be designated as either R or S.

Sequence 1. If the four atoms attached to the chiral center are all different, priority depends on the atomic number, with the atom of higher atomic number getting higher priority.

Sequence 2. If the relative priority of two groups cannot be decided by Sequence 1, it shall be determined by a similar comparison of the atoms attached to it.

For example, bromochloriodomethane,  $\text{CHClBrI}$ , has two possible configurations as shown in figure 3.8. Using the sequence rules, the order of the atoms for the configuration is I, Br, Cl, H. However, the figure on the left has a different sequence than the one on the right. Hence, (R)-bromochloriodomethane and (S)-bromochloriodomethane

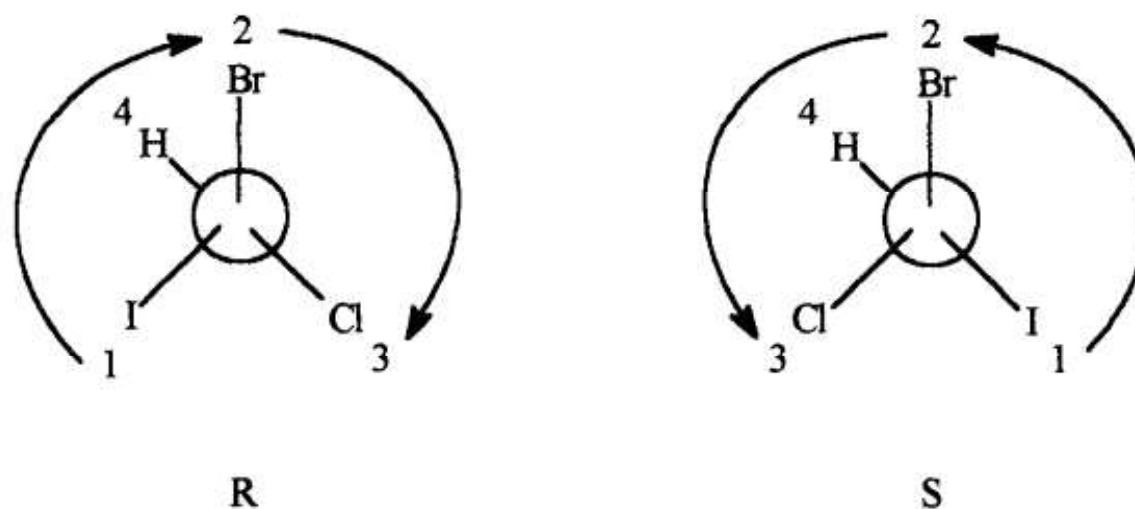
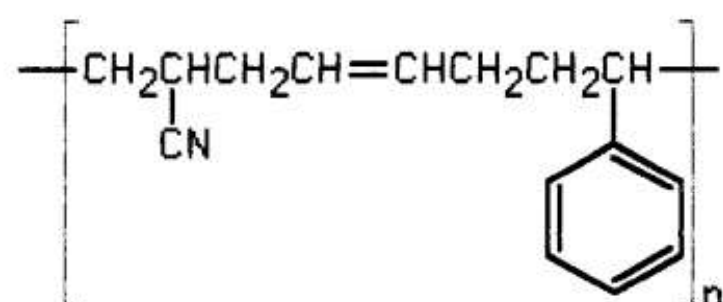


Figure 3.15. R and S configuration

### 3.25 Polymer Structures

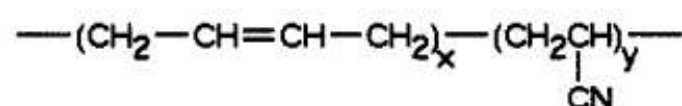
The following listing of common polymers provides respective structure. The reader should note that the name of the polymer often provides the key to its representative structure. There are, however, names such as polycarbonate that can represent a variety of polymeric materials.

Acrylonitrile-butadiene-styrene terpolymer (ABS):



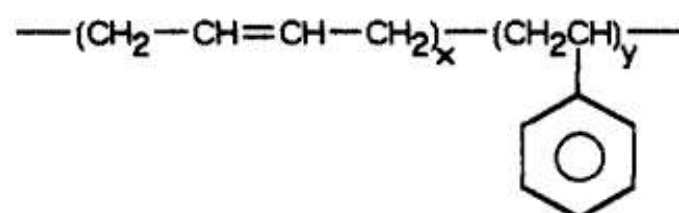
Buna-N:

Elastomeric copolymer of butadiene and acrylonitrile.

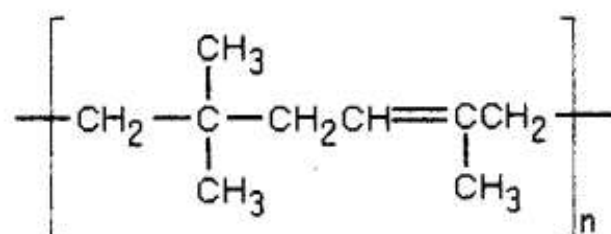


Buna-S:

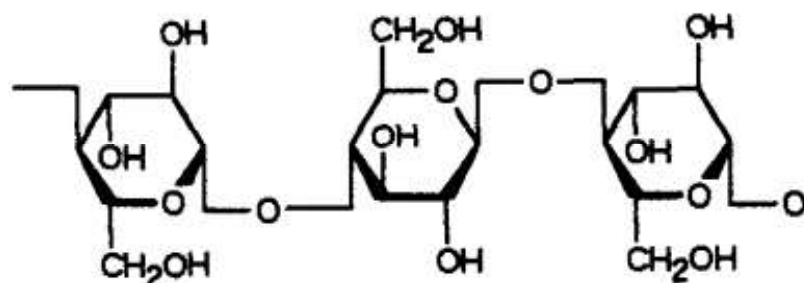
Elastomeric copolymer of butadiene and styrene.



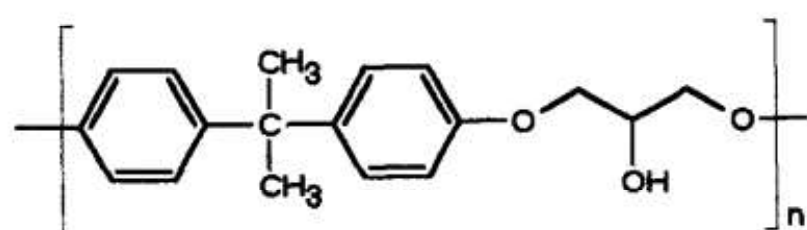
Butyl rubber:



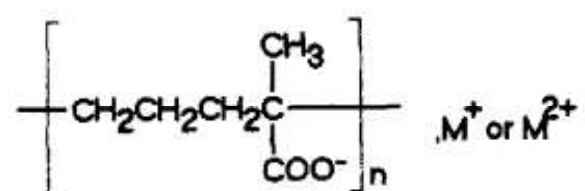
Cellulose:



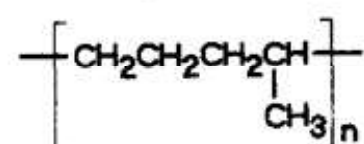
Epoxy resins:



Ethylene-methacrylic acid copolymers (ionomers):

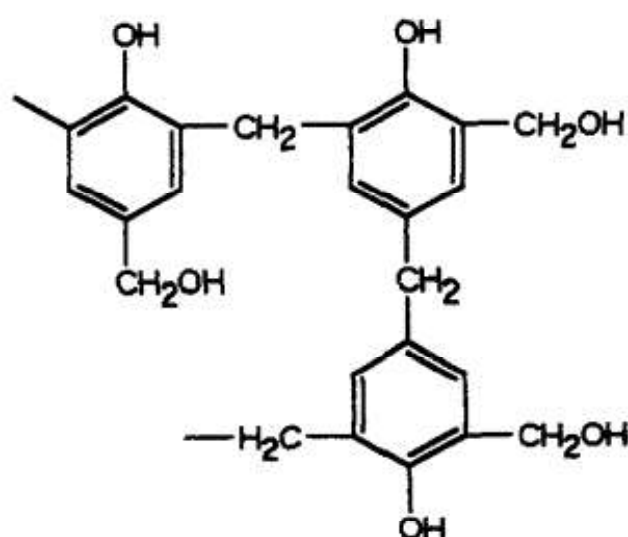


Ethylene-propylene elastomers:

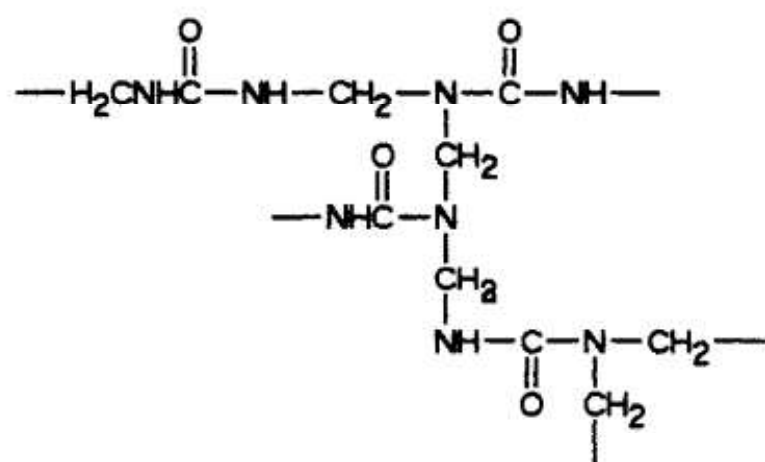


Formaldehyde resins:

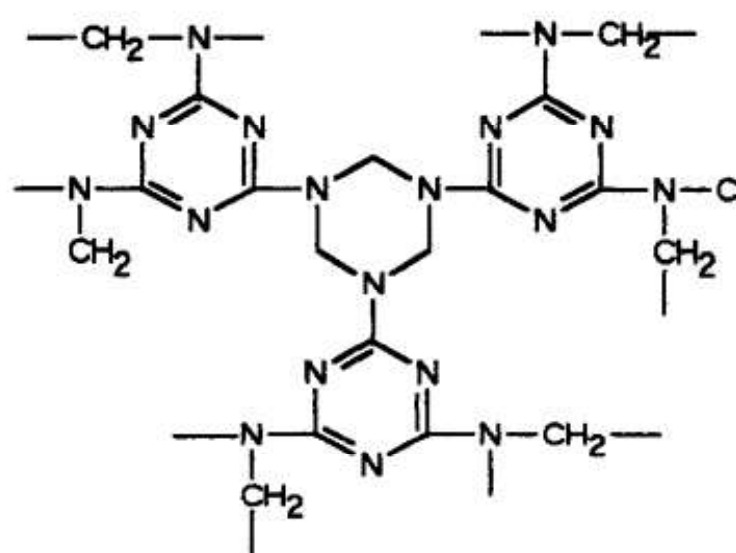
*Phenol-formaldehyde (PF):*



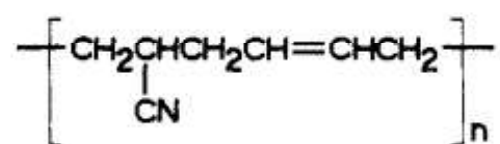
*Urea-formaldehyde (UF):*



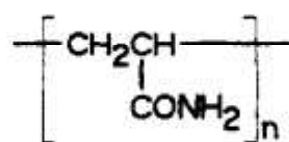
*Melamine-formaldehyde (MF):*



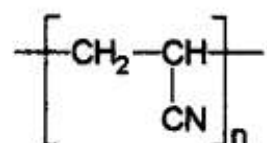
Nitrile rubber (NBR):



Polyacrylamide:

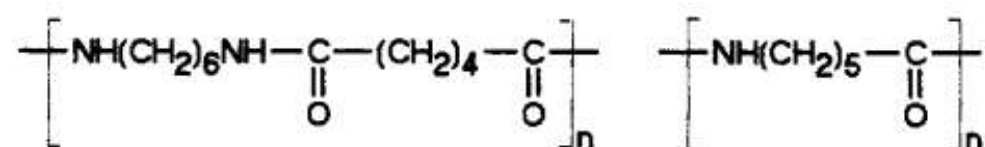


Polyacrylonitrile:



Polyamides (nylons):

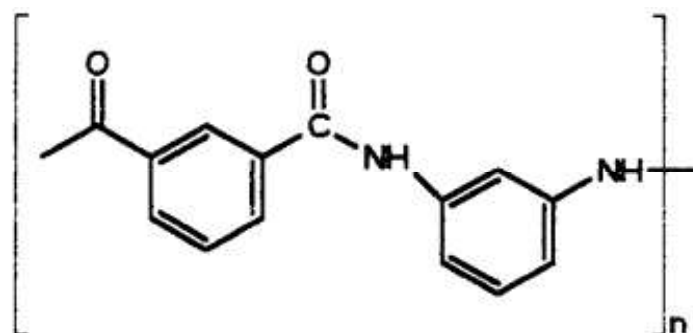
*Nylon 6,6 and nylon 6:*



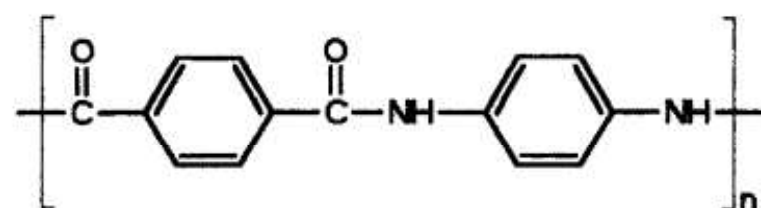
nylon 6,6

nylon 6

*Aromatic polyamides:*

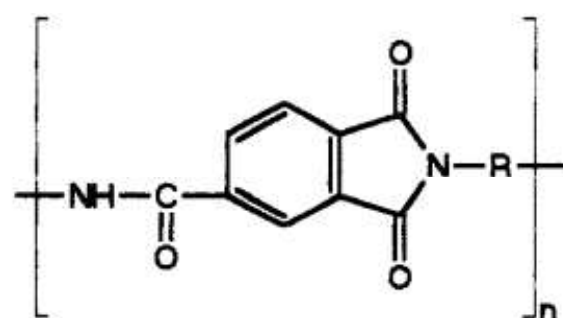


Nomex

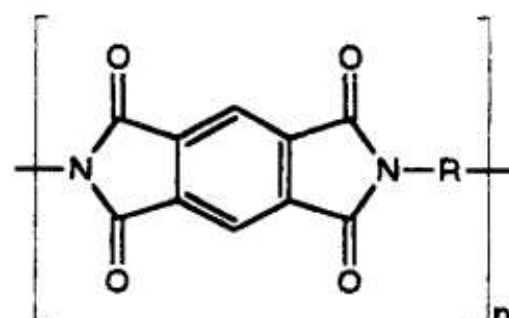


Kevlar

*Polyamide imides and polyimides:*

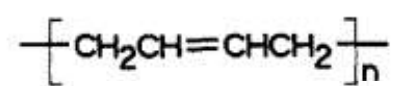


poly(amide imides)

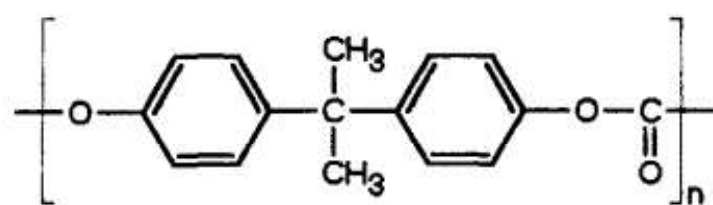


polyimides

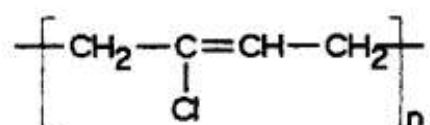
Polybutadiene (butadiene rubber, BR):



Polycarbonate (PC):

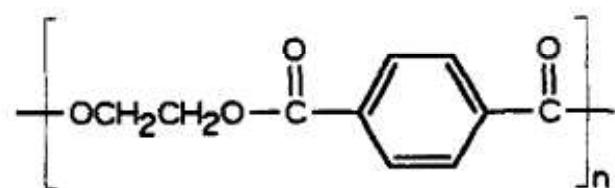


Polychloroprene:

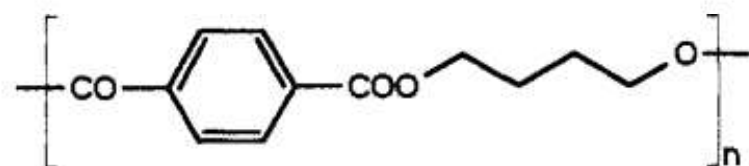


Polyesters:

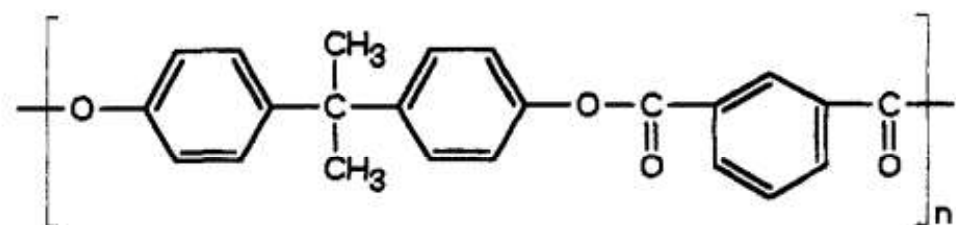
*Poly(ethylene terephthalate) (PET):*



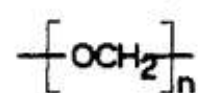
*Poly(butylene terephthalate) (PBT):*



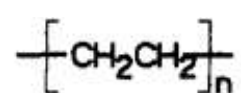
*Aromatic polyesters:*



Polyether (polyoxymethylene; polyacetal):



Polyethylene (PE):



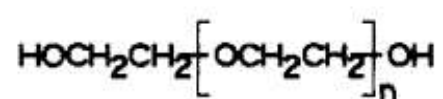
*Low-density polyethylene (LDPE).*

*High-density polyethylene (HDPE).*

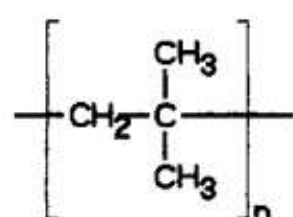
*Linear low-density polyethylene (LLDPE).*

*Ultrahigh molecular weight polyethylene (UMWPE).*

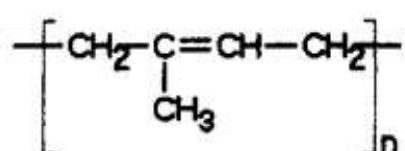
Poly(ethylene glycol) (PEG):



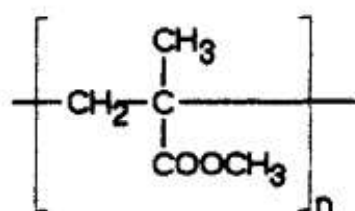
Polyisobutylene (PIB):



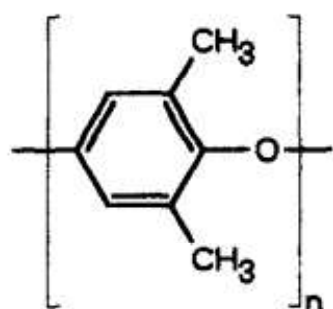
Polyisoprene:



Poly(methyl methacrylate) (PMMA):

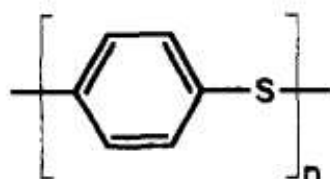


Poly(phenylene oxide) (PPO):

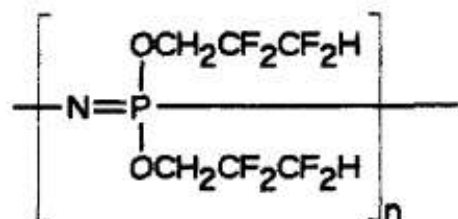


**poly(2,6-dimethyl-p-phenylene ether)**

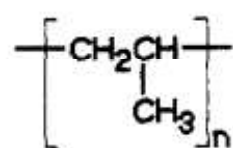
Poly(phenylene sulfide) (PPS):



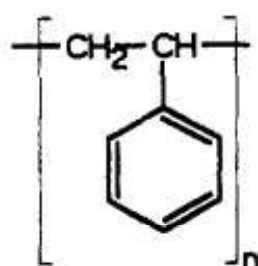
Polyphosphazenes:



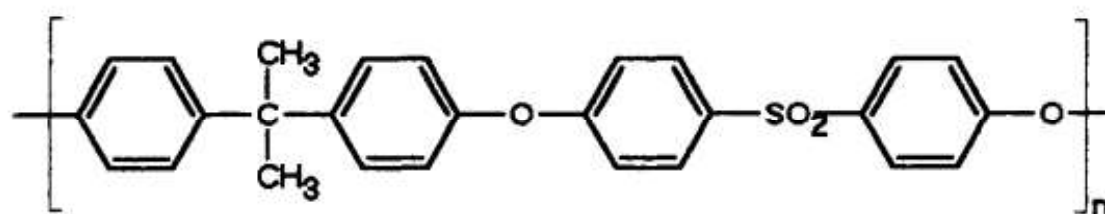
Polypropylene (PP):



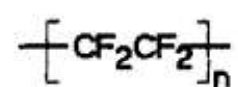
Polystyrene (PS):



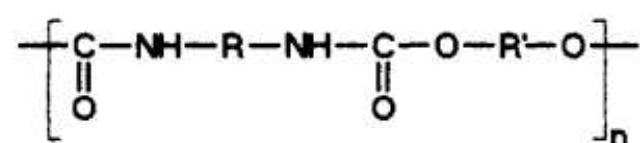
Poly sulfone:



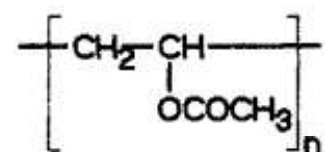
Polytetrafluoroethylene (PTFE):



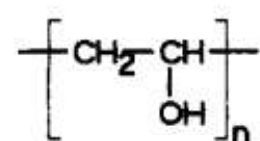
Polyurethane:



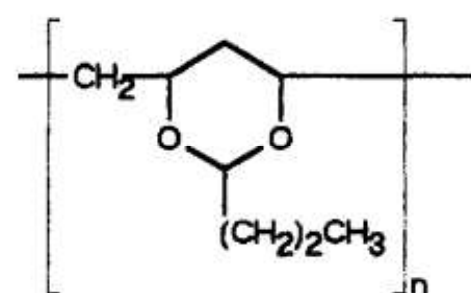
Poly(vinyl acetate) (PVA):



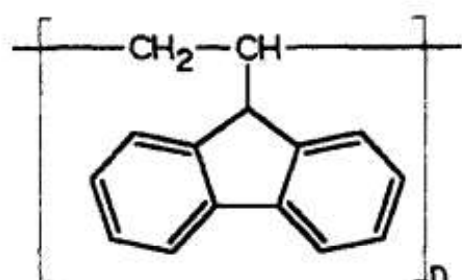
Poly(vinyl alcohol) (PVAL):



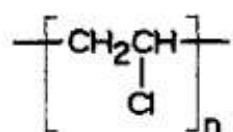
Poly(vinyl butyral) (PVB):



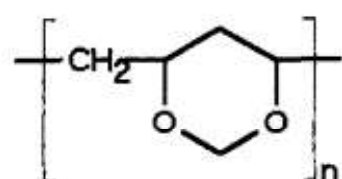
Poly(vinyl carbazole):



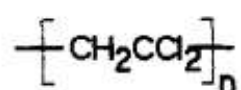
Poly(vinyl chloride) (PVC):



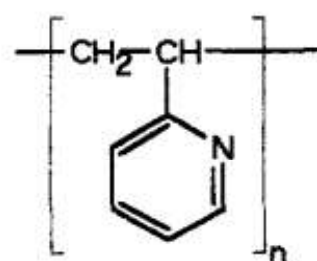
Poly(vinyl formal) (PVF):



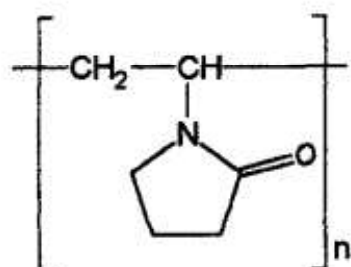
Poly(vinylidene chloride):



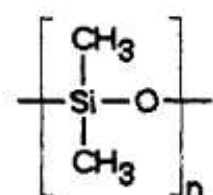
Poly(vinyl pyridine):



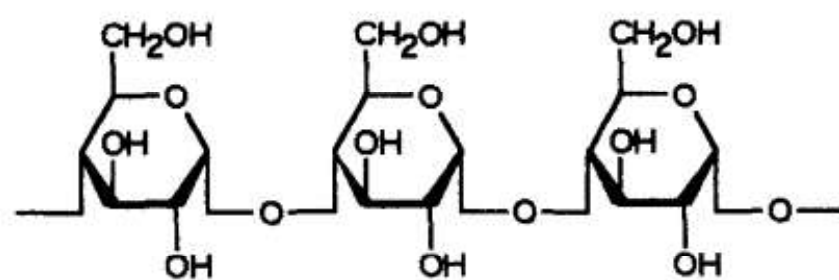
Poly(vinyl pyrrolidone):



Silicones (siloxanes):

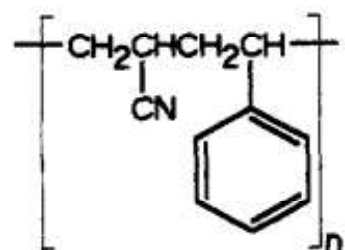


Starch:

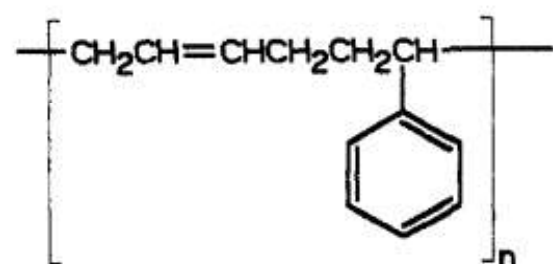


linear amylose

Styrene-acrylonitrile copolymer (SAN):



Styrene-butadiene rubber (SBR):



## Chapter 4

### **Instrumental Analysis**

#### *4.1 The Electromagnetic Spectrum*

#### *4.2 Ultraviolet-Visible Spectrum*

#### *4.3 Infrared Spectrum*

#### *4.4 Nuclear Magnetic Resonance*

#### *4.5 Mass Spectroscopy*

### **4.1 The Electromagnetic Spectrum**

#### **4.1.1 The Electromagnetic Spectrum**

The various regions of the electromagnetic spectrum are somewhat arbitrary and not very sharply defined. Each region overlaps at both ends the adjacent regions. The units defining the different regions can be in frequency (Hz,  $\text{cm}^{-1}$ ), energy (kcal/mole, eV) and wavelengths (**m and  $\lambda$** , "official" or most common unit used for a given region). Some useful relationships and constants are the following: 1 nanometer (nm) = 1 millimicron (**m $\mu$** ),  $=10^{-9}$  m; 1  $\mu\text{m}$  (formerly micron) =  $10^{-6}$  m = 10 mm; 1 angstrom ( $\text{\AA}$ ) = 0.1 nm =  $10^{-8}$  cm; 1 eV = 23.06 kcal/mole = 8063  $\text{cm}^{-1}$ . Energy,  $E = h\nu$  [ $h$  = Planck's constant =  $9.534 \times 10^{-14}$  kcal-sec/mole =  $1.583 \times 10^{-34}$  cal-sec/molecule;  $\nu$  in Hz (cycles/sec)].  $E$  in kcal/mole =  $2.8635/\lambda$  ( $\lambda$  in  $\mu\text{m}$ );  $E$  in eV =  $12,3451$  ( $\lambda$  in  $\text{\AA}$ ).

Table 4.1 The Electromagnetic Spectrum

| Region         | Spectral Use                                                 | Hz                   | cm-1                 | kcal/mole             | eV                    | m                    | $\lambda$                      |
|----------------|--------------------------------------------------------------|----------------------|----------------------|-----------------------|-----------------------|----------------------|--------------------------------|
| Cosmic rays    |                                                              | $10^{22}$            | $3 \times 10^{11}$   | $9.5 \times 10^8$     | $4.1 \times 10^7$     | $3 \times 10^{-14}$  | $3 \times 10^{-4} \text{ \AA}$ |
| Gamma rays     | Nuclear transitions                                          | $10^{19}$            | $3 \times 10^7$      | $9.5 \times 10^5$     | $4.1 \times 10^4$     | $3 \times 10^{-10}$  | 3 \AA                          |
| Soft X-rays    | Inner electron transitions                                   | $10^{17}$            | $1 \times 10^5$      | $9.5 \times 10^3$     | $4.1 \times 10^2$     | $3 \times 10^{-8}$   | 300 \AA                        |
| Vacuum uv      | Valence electron transitions                                 | $1.5 \times 10^{15}$ | $5 \times 10^4$      | 143                   | 6.2                   | $2 \times 10^{-7}$   | 200 nm                         |
| Quartz uv      | (electronic spectra)                                         | $7.5 \times 10^{14}$ | $2.5 \times 10^4$    | 71.5                  | 3.1                   | $4 \times 10^{-7}$   | 400 nm                         |
| Visible        |                                                              | $3.8 \times 10^{14}$ | $1.2 \times 10^4$    | 36.2                  | 1.6                   | $8 \times 10^{-7}$   | 800 nm                         |
| Near ir        | Vibrational ir overtone and combination region               | $1.2 \times 10^{14}$ | $4 \times 10^3$      | 12                    | 0.52                  | $2.5 \times 10^{-6}$ | 2.5 $\mu\text{m}$              |
| Vibrational ir | Fundamental region                                           | $2.5 \times 10^{13}$ | $8 \times 10^2$      | 2.4                   | 0.10                  | $1.2 \times 10^{-5}$ | 12.5 $\mu\text{m}$             |
| Far ir         | Skeletal, ring torsional, solid state (lattice) deformations | $10^{12}$            | 33                   | $9.5 \times 10^{-2}$  | $4.1 \times 10^{-3}$  | $3 \times 10^{-4}$   | 300 $\mu\text{m}$              |
| Microwave      | Molecular rotations; bond torsions                           | $10^9$               | $3.3 \times 10^{-2}$ | $9.5 \times 10^{-5}$  | $4.1 \times 10^{-6}$  | $3 \times 10^{-1}$   | 300 mm                         |
| Short Radio    | Spin orientations                                            | $1.5 \times 10^6$    | $5 \times 10^{-5}$   | $1.4 \times 10^{-7}$  | $6.1 \times 10^{-9}$  | $2 \times 10^2$      | 200 m                          |
| Broadcast      | Radio, tv, etc.                                              | $5.5 \times 10^5$    | $1.8 \times 10^{-5}$ | $5.2 \times 10^{-8}$  | $2.2 \times 10^{-9}$  | $5.6 \times 10^2$    | 550 m                          |
| Long Radio     | Induction heating; longwave communication                    | $3 \times 10^3$      | $10^{-7}$            | $2.9 \times 10^{-10}$ | $1.3 \times 10^{-11}$ | $10^5$               | $10^5 \text{ m}$               |
| Electric Power | Commercial power and light                                   | $3 \times 10^{-1}$   | $10^{-11}$           | $2.9 \times 10^{-14}$ | $1.3 \times 10^{-14}$ | $10^9$               | $10^9 \text{ m}$               |

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## 4.2 Ultraviolet-Visible Spectroscopy

### 4.2.1 Solvents

Table 4.2. UV-Vis Solvents

| Substance              | Formula             | BP (°C) | Cut-off (nm) |       |
|------------------------|---------------------|---------|--------------|-------|
|                        |                     |         | 1 mm         | 10 mm |
| 2-Methylbutane         | $C_4H_9CH_3$        | 28      | ---          | 210   |
| Pentane                | $C_5H_{12}$         | 36      | ---          | 200   |
| Hexane                 | $C_6H_{14}$         | 69      | 190          | 200   |
| Heptane                | $C_7H_{16}$         | 96      | ---          | 195   |
| <i>i</i> -Octane       | $C_8H_{18}$         | 98      | 190          | 205   |
| Cyclopentane           | $C_5H_{10}$         | 49      | ---          | 210   |
| Methylcyclopentane     | $C_5H_9CH_3$        | 72      | ---          | 200   |
| Cyclohexane            | $C_6H_{12}$         | 81      | 190          | 195   |
| Methylcyclohexane      | $C_6H_{11}CH_3$     | 101     | ---          | 205   |
| Benzene                | $C_6H_6$            | 80      | 275          | 280   |
| Toluene                | $C_6H_5CH_3$        | 110     | 280          | 285   |
| <i>m</i> -Xylene       | $C_6H_4(CH_3)_2$    | 139     | 285          | 290   |
| Decalin                | $C_{10}H_{18}$      | 190     | ---          | 200   |
| Water                  | HOH                 | 100     | 187          | 191   |
| Methanol               | $CH_3OH$            | 65      | 200          | 205   |
| Ethanol                | $CH_3CH_2OH$        | 78      | 200          | 205   |
| 2-Propanol             | $CH_3CH(OH)CH_3$    | 81      | 200          | 210   |
| Glycerol               | $(HOCH_2)_2CH(OH)$  | 290d    | 200          | 205   |
| Sulfuric acid          | 96% $H_2SO_4$       | 300     | ---          | 210   |
| Diethyl ether          | $Et_2O$             | 35      | 205          | 215   |
| THF                    | $CH_2CH_2CH_2CH_2O$ | 67      | ---          | 220   |
| 1,4-Dioxan             | $(OCH_2CH_2)_2$     | 102     | 210          | 220   |
| Dibutyl ether          | $(C_4H_9)_2O$       | 142     | ---          | 210   |
| Carbon disulfide       | $CS_2$              | 46      | ---          | 380   |
| Chloroform             | $CHCl_3$            | 60      | 230          | 245   |
| Carbon tetrachloride   | $CCl_4$             | 76      | 245          | 260   |
| Methylene chloride     | $CH_2Cl_2$          | 40      | 220          | 230   |
| 1,1-Dichloroethane     | $ClCH_2CH_2Cl$      | 84      | 220          | 230   |
| 1,1,2,2-Dichloroethene | $Cl_2C=CCl_2$       | 120     | 280          | 290   |
| Tribromomethane        | $CHBr_3$            | 150     | 315          | 330   |
| Bromotrichloromethane  | $BrCCl_3$           | 105     | 320          | 340   |
| Acetonitrile           | $CH_3CN$            | 81      | 190          | 195   |
| Methylnitrite          | $CH_3NO_2$          | 100     | 360          | 380   |
| Pyridine               | $C_5H_5N$           | 112     | 300          | 305   |
| N,N-DMF                | $HCON(CH_3)_2$      | 152     | ---          | 270   |
| DMSO                   | $(CH_3)_2SO$        | 189d    | 250          | 265   |
| Acetone                | $CH_3COCH_3$        | 56      | 320          | 330   |

## 4.2.2 Woodward's Rules for Diene Absorption

|                                                |     |
|------------------------------------------------|-----|
| Parent heteroannular diene                     | 214 |
| Parent homoannular diene                       | 253 |
| Add for each substituent:                      |     |
| Double bond extending conjugation              | 30  |
| Alkyl substituent, ring residue, etc.          | 5   |
| Exocyclic double bond                          | 5   |
| N(alkyl) <sub>2</sub>                          | 60  |
| S(alkyl)                                       | 30  |
| O(alkyl)                                       | 6   |
| OAc                                            | 0   |
| $\lambda_{\text{calc max}} = \text{TOTAL, nm}$ |     |

## 4.2.3 Selected UV-Vis Tables

Table 4.3. Characteristics of Simple Chromophoric Groups

| Chromophore        | Example                              | $\lambda_{\text{max}}$ , m $\mu$ | $\epsilon_{\text{max}}$ | Solvent  |
|--------------------|--------------------------------------|----------------------------------|-------------------------|----------|
| C=C                | Ethylene                             | 171                              | 15,530                  | Vapor    |
|                    | 1-Octene                             | 177                              | 12,600                  | Heptane  |
| C $\equiv$ C       | 2-Octyne                             | 178                              | 10,000                  | Heptane  |
|                    |                                      | 196                              | 2,100                   | Heptane  |
|                    |                                      | 223                              | 160                     | Heptane  |
|                    |                                      |                                  |                         |          |
| C=O                | Acetaldehyde                         | 160                              | 20,000                  | Vapor    |
|                    |                                      | 180                              | 10,000                  | Vapor    |
|                    |                                      | 290                              | 17                      | Hexane   |
|                    | Acetone                              | 166                              | 16,000                  | Vapor    |
|                    |                                      | 189                              | 900                     | Hexane   |
|                    |                                      | 279                              | 15                      | Hexane   |
| -CO <sub>2</sub> H | Acetic acid                          | 208                              | 32                      | Ethanol  |
| -COCl              | Acetyl chloride                      | 220                              | 100                     | Hexane   |
| -CONH <sub>2</sub> | Acetamide                            | 178                              | 9,500                   | Hexane   |
|                    |                                      | 220                              | 63                      | Water    |
| -CO <sub>2</sub> R | Ethyl acetate                        | 211                              | 57                      | Ethanol  |
| -NO <sub>2</sub>   | Nitromethane                         | 201                              | 5,000                   | Methanol |
|                    |                                      | 274                              | 17                      | Methanol |
| -ONO <sub>2</sub>  | Butyl nitrate                        | 270                              | 17                      | Ethanol  |
| -ONO               | Butyl nitrite                        | 220                              | 14,500                  | Hexane   |
|                    |                                      | 356                              | 87                      | Hexane   |
| -NO                | Nitrosobutane                        | 300                              | 100                     | Ether    |
|                    |                                      | 665                              | 20                      | Ether    |
| C=N                | <i>neo</i> -Pentylidene n-butylamine | 235                              | 100                     | Ethanol  |
| -C $\equiv$ N      | Acetonitrile                         | 167                              | weak                    | Vapor    |
| -N <sub>3</sub>    | Azidoacetic ester                    | 285                              | 20                      | Ethanol  |
| =N <sub>2</sub>    | Diazomethane                         | 410                              | 3                       | Vapor    |
| -N=N-              | Azomethane                           | 338                              | 4                       | Ethanol  |

Table 4.4. Characteristics of Simple Conjugated Chromophoric Groups

| Chromophore                         | Example                         | $\lambda_{\max}$ , m $\mu$ | $\epsilon_{\max}$ | Solvent |
|-------------------------------------|---------------------------------|----------------------------|-------------------|---------|
| C=C-C=C                             | Butadiene                       | 217                        | 20,900            | Hexane  |
| C=C-C $\equiv$ C                    | Vinylacetylene                  | 219                        | 7,600             | Hexane  |
|                                     |                                 | 228                        | 7,800             | Hexane  |
| C=C-C=O                             | Crotonaldehyde                  | 218                        | 18,000            | Ethanol |
|                                     |                                 | 320                        | 30                | Ethanol |
|                                     | 3-Penten-2-one                  | 224                        | 9,750             | Ethanol |
|                                     |                                 | 314                        | 38                | Ethanol |
| -C $\equiv$ C-C=O                   | 1-Hexyn-3-one                   | 214                        | 4,500             | Ethanol |
|                                     |                                 | 308                        | 20                | Ethanol |
| C=C-CO <sub>2</sub> H               | <i>cis</i> -Crotonic acid       | 206                        | 13,500            | Ethanol |
|                                     |                                 | 242                        | 250               | Ethanol |
| -C $\equiv$ C-CO <sub>2</sub> H     | <i>n</i> -Butylpropionic acid   | 210                        | 6,000             | Ethanol |
| C=C-C=N-                            | <i>N-n</i> -Butylcrotonaldimine | 219                        | 25,000            | Hexane  |
| C=C-C $\equiv$ N                    | Methacrylonitrile               | 215                        | 680               | Ethanol |
| C=C-NO <sub>2</sub>                 | 1-Nitro-1-propene               | 229                        | 9,400             | Ethanol |
|                                     |                                 | 235                        | 9,800             | Ethanol |
| HO <sub>2</sub> C-CO <sub>2</sub> H | Oxalic acid                     | 185                        | 4,000             | Water   |

Table 4.5. Ultraviolet Absorption of Some Monosubstituted Benzenes (in Water)

| C <sub>6</sub> H <sub>5</sub> X  | Primary Band               |                   | Secondary Band             |                   |
|----------------------------------|----------------------------|-------------------|----------------------------|-------------------|
|                                  | $\lambda_{\max}$ , m $\mu$ | $\epsilon_{\max}$ | $\lambda_{\max}$ , m $\mu$ | $\epsilon_{\max}$ |
| -H                               | 203.5                      | 7,400             | 254                        | 204               |
| -NH <sub>3</sub>                 | 203                        | 7,500             | 254                        | 169               |
| -CH <sub>3</sub>                 | 206.5                      | 7,000             | 261                        | 225               |
| -I                               | 207                        | 7,000             | 257                        | 700               |
| -Cl                              | 209.5                      | 7,400             | 263.5                      | 190               |
| -Br                              | 210                        | 7,900             | 261                        | 192               |
| -OH                              | 210.5                      | 6,200             | 270                        | 1,450             |
| -OCH <sub>3</sub>                | 217                        | 6,400             | 269                        | 1,480             |
| -SO <sub>2</sub> NH <sub>2</sub> | 217.5                      | 9,700             | 264.5                      | 740               |
| -CN                              | 224                        | 13,000            | 271                        | 1,000             |
| -CO <sub>2</sub> <sup>-</sup>    | 224                        | 8,700             | 268                        | 560               |
| -CO <sub>2</sub> H               | 230                        | 11,600            | 273                        | 970               |
| -NH <sub>2</sub>                 | 230                        | 8,600             | 280                        | 1,430             |
| -O <sup>-</sup>                  | 235                        | 9,400             | 287                        | 2,600             |
| -NHCOCH <sub>3</sub>             | 238                        | 10,500            | ---                        | ---               |
| -COCH <sub>3</sub>               | 245.5                      | 9,800             | ---                        | ---               |
| -CHO                             | 249.5                      | 11,400            | ---                        | ---               |
| -NO <sub>2</sub>                 | 268.5                      | 7,800             | ---                        | ---               |

## 4.3 Infrared Spectroscopy

### 4.3.1 Infrared Media

Table 4.6. IR media

| Substance                                   | Usable Regions of the Spectrum: $\text{cm}^{-1}$ ( $\mu\text{m}$ ) |                                                               |                                |
|---------------------------------------------|--------------------------------------------------------------------|---------------------------------------------------------------|--------------------------------|
|                                             | Near IR <sup>1</sup>                                               | Mid IR                                                        | Far IR                         |
| KBr                                         | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 250 (12.5-40)            |
| KCl                                         | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 526 (12.5-19)            |
| CsBr                                        | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 250 (12.5-40)            |
| CsI                                         | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 130 (12.5-77)            |
| AgCl                                        | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 530 (12.5-19)            |
| TlCl                                        | 10000 - 3333 (1-3)                                                 | 5000 - 667 (2-15)                                             | 800 - 530 (12.5-19)            |
| Polyethylene                                | 10000 - 3333 (1-3) <sup>2</sup>                                    | 2500 - 1540 (4-6.5)<br>1250 - 741 (8-13.5)                    | 625 - 278 (16-36)              |
| Polystyrene                                 |                                                                    |                                                               | 400 - 278 (25-36) <sup>3</sup> |
| Teflon                                      |                                                                    | 5000 - 1333 (2-7.5) <sup>4</sup><br>1111 - 690 (9-14.5)       |                                |
| Kel-F                                       |                                                                    | 5000 - 1333 (2-7.5)<br>870 - 690 (11.5-14.5)                  |                                |
| Nujol <sup>5</sup>                          |                                                                    | 5000 - 3333 (2-3)<br>2500 - 1540 (4-6.5)<br>1250 - 667 (8-15) | 667 - 286 (15-35)              |
| Fluorolube <sup>6</sup>                     |                                                                    | 5000 - 1430 (2-7)                                             |                                |
| C <sub>4</sub> Cl <sub>6</sub> <sup>7</sup> |                                                                    | 5000 - 1667 (2-6)<br>1430 - 1250 (7-8)                        |                                |

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1. Very little work has been reported for near ir spectra of pellets or mulls; most measurements are made in solution.
2. For a 0.1 mm sheet when compensated; otherwise, interfering bands occur at 1.9, 2.3, and 2.6 - 2.8  $\mu\text{m}$ .
3. For 0.025 mm sheet.
4. For 0.01 mm thick specimen; Teflon and Kel-F powders are very good for observing details in the OH stretch region.
5. Common brand of heavy mineral oil.
6. A saturated chlorofluorocarbon oil.
7. Hexachloro-1,3-butadiene.

## 4.3.2 Infrared Absorption Frequencies of Functional Groups

Table 4.7. Saturated Compounds sp = sharp, br = broad, (w) = weak, (s) = strong

| Functional Group                                    | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound   |
|-----------------------------------------------------|--------------------------------------|-----------------------------|--------------------|
| <b>SATURATED COMPOUNDS</b>                          |                                      |                             |                    |
| <b>Linear</b>                                       |                                      |                             |                    |
| CH <sub>3</sub> asymmetric                          | 2970-2950                            | 2967                        | <i>n</i> -Octane   |
| CH <sub>3</sub> symmetric                           | 2885-2865                            | 2868                        |                    |
| CH <sub>3</sub> asymmetric                          | 1465-1440                            | 1466                        |                    |
| CH <sub>3</sub> symmetric                           | 1380-1370                            | 1380                        |                    |
| CH <sub>2</sub> asymmetric                          | 2930-2915                            | 2920                        | <i>n</i> -Octane   |
| CH <sub>2</sub> symmetric                           | 2860-2840                            | 2854                        |                    |
| CH <sub>2</sub>                                     | 1480-1450                            | 1470                        |                    |
| (CH <sub>2</sub> ) <sub>n</sub> , n > 4             | 723-720                              | 723                         | <i>n</i> -Octane   |
|                                                     | 735-725                              | 733                         | <i>n</i> -Pentane  |
|                                                     | 755-735                              | 741                         | 2-Methylpentane    |
|                                                     | 800-770                              | 781                         | <i>n</i> -Propane  |
| <b>Branched</b>                                     |                                      |                             |                    |
| CH                                                  | 2890                                 | 2890                        | Triphenylmethane   |
|                                                     | 1340                                 | 1341                        |                    |
| (CH <sub>3</sub> ) <sub>2</sub> -CH-                | 1385-1380                            | 1384                        | 2-Methylheptane    |
|                                                     | 1372-1366                            | 1366                        |                    |
|                                                     | 1175-1165                            |                             |                    |
|                                                     | 1160-1140                            |                             |                    |
|                                                     | 922-917                              |                             |                    |
| (CH <sub>3</sub> ) <sub>3</sub> -C-                 | 1395-1380                            | 1393                        | 2,2-Dimethylhexane |
|                                                     | 1375-1365                            | 1366                        |                    |
|                                                     | 1252-1245                            |                             |                    |
|                                                     | 1225-1195                            |                             |                    |
|                                                     | 930-925                              |                             |                    |
| -C(CH <sub>3</sub> )-C(CH <sub>3</sub> )-           | 1165-1150                            | 1160                        | 3,4-Dimethylhexane |
|                                                     | 1130-1120                            | 1122                        |                    |
|                                                     | 1080-1065                            | 1071                        |                    |
| (CH <sub>3</sub> ) <sub>2</sub> -C-R <sub>2</sub>   | 1391-1381                            | 1389                        | 3,3-Dimethylhexane |
|                                                     | 1220-1190                            | 1192                        |                    |
|                                                     | 1195-1185                            | 1189                        |                    |
| (C <sub>2</sub> H <sub>5</sub> ) <sub>2</sub> -CH-R | 1250                                 | 1250                        | 3-Ethylhexane      |
|                                                     | 1150                                 | 1155                        |                    |
|                                                     | 1130                                 | 1131                        |                    |
| C-C(CH <sub>3</sub> )-C                             | 1160-1150                            |                             |                    |

Table 4.7. (Continued)

|                          |                        |      |              |
|--------------------------|------------------------|------|--------------|
| <b>Cyclic Compounds</b>  |                        |      |              |
| Cyclopropane derivatives | 3100-3072              | 3075 | Cyclopropane |
|                          | 3033-2995              | 3028 |              |
|                          | 1030-1000              | 1024 |              |
| Cyclobutane derivatives  | 3000-2975              | 2974 | Cyclobutane  |
|                          | 2924-2874              | 2896 |              |
|                          | 1000-960 or<br>930-890 | 901  |              |
| Cyclopentane derivatives | 2959-2952              | 2951 | Cyclopentane |
|                          | 2870-2853              | 2871 |              |
|                          | 1000-960               | 968  |              |
|                          | 930-890                | 894  |              |
| Cyclohexane derivatives  | 1055-1000              | 1038 | Cyclohexane  |
|                          | 1015-950               | 1014 |              |

Table 4.8. Unsaturated Compounds

| Functional Group                                    | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound     |
|-----------------------------------------------------|-----------------------------------------|--------------------------------|----------------------|
| <b>UNSATURATED COMPOUNDS</b>                        |                                         |                                |                      |
| <b>Isolated -C=C- bonds</b><br>CH <sub>2</sub> =CH- | 3095-3075                               | 3096                           | 1-Butene             |
|                                                     | 3030-2990                               | 2994                           |                      |
|                                                     | 1648-1638                               | 1645                           |                      |
|                                                     | 1420-1410                               | 1420                           |                      |
|                                                     | 1000-980                                | 994                            |                      |
|                                                     | 915-905                                 | 912                            |                      |
| CH <sub>2</sub> =C                                  | 3095-3075                               | 3096                           | Methylpropene        |
|                                                     | 1660-1640                               | 1661                           |                      |
|                                                     | 1420-1410                               | 1420                           |                      |
|                                                     | 895-885                                 | 887                            |                      |
| -CH=C                                               | 3040-3010                               | 3037                           | 3-Methyl-2-pentene   |
|                                                     | 1680-1665                               | 1675                           |                      |
|                                                     | 1350-1340                               | 1351                           |                      |
|                                                     | 840-805                                 | 812                            |                      |
| -CH=CH- ( <i>cis</i> )                              | 3040-3010                               | 3030                           | <i>cis</i> -2-Butene |
|                                                     | 1660-1640                               | 1661                           |                      |
|                                                     | 1420-1395                               | 1406                           |                      |
|                                                     | 730-675                                 | 675                            |                      |

Table 4.8. (Continued)

|                                   |                                                |                             |                        |
|-----------------------------------|------------------------------------------------|-----------------------------|------------------------|
| -CH=CH-( <i>trans</i> )           | 3040-3010<br>1700-1670<br>1310-1295<br>980-960 | 3021<br>1701<br>1302<br>964 | <i>trans</i> -2-Butene |
| <b>Conjugated -C=C- bonds</b>     |                                                |                             |                        |
| -C=C-C=C-                         | 1629-1590<br>1820-1790                         | 1592<br>1821                | 1,3-Butadiene          |
| <b>Allenic -C=C- bonds</b>        |                                                |                             |                        |
| -C=C=C-                           | 1960-1940<br>1070-1060                         |                             |                        |
| <b>-C≡C- bonds</b>                |                                                |                             |                        |
| -C≡C-                             | 2270-2250                                      | 2268                        | 2-Pentyne              |
| <b>-C≡CH groups</b>               |                                                |                             |                        |
| CH (stretch)                      | 3320-3300*                                     | 3320                        | 1-Butyne               |
| -C≡C-                             | 2140-2100                                      | 2122                        |                        |
| CH (bend)                         | 700-600                                        |                             |                        |
| * CCl <sub>4</sub> Solutions only |                                                |                             |                        |

Table 4.9. Aromatic Compounds

| Functional Group          | Absorption Range (cm <sup>-1</sup> )                      | Example (cm <sup>-1</sup> )                | Example Compound |
|---------------------------|-----------------------------------------------------------|--------------------------------------------|------------------|
| <b>AROMATIC COMPOUNDS</b> |                                                           |                                            |                  |
| <b>General</b>            |                                                           |                                            |                  |
| CH                        | 3060-3010                                                 |                                            |                  |
| CH substitution bands     |                                                           |                                            |                  |
| overtones                 | 2000-1650 (w)                                             |                                            |                  |
| C=C                       | 1620-1590 sp<br>1590-1560 sp                              |                                            |                  |
| CH                        | 1510-1480 sp<br>1450 sp                                   |                                            |                  |
| <b>Mono-substitution</b>  |                                                           |                                            |                  |
|                           | 1175-1125<br>1110-1070<br>1070-1000<br>765-725<br>720-690 | 1170<br>1088<br>1032<br>728 (s)<br>693 (s) | Toluene          |
| <b>Di-substitution</b>    |                                                           |                                            |                  |
| <i>ortho</i>              | 1225-1175<br>1125-1090<br>1070-1000<br>765-735            | 1185<br>1121<br>1053<br>741 (s)            | <i>o</i> -Xylene |
| <i>meta</i>               | 1175-1125<br>1110-1070<br>1070-1000<br>900-770<br>710-690 | 1171<br>1095<br>1039<br>769 (s)<br>690 (s) | <i>m</i> -Xylene |

Table 4.9. (Continued)

|                                   |                                                          |                                            |                        |
|-----------------------------------|----------------------------------------------------------|--------------------------------------------|------------------------|
| <i>para</i>                       | 1225-1175<br>1125-1090<br>1070-1000<br>855-790           | 1219<br>1120<br>1043<br>796 (s)            | <i>p</i> -Xylene       |
| <b>Tri-substitution</b><br>1,2,3- | 1175-1125<br>1110-1070<br>1000-960<br>800-755<br>740-695 | 1162<br>1095<br>1009<br>765 (s)<br>710 (s) | 1,2,3-Trimethylbenzene |
| 1,2,4-                            | 1225-1175<br>1130-1090<br>1000-960<br>900-865<br>855-800 | 1156<br>1130<br>1000<br>873 (s)<br>805 (s) | 1,2,4-Trimethylbenzene |
| 1,3,5-                            | 1175-1125<br>1070-1000<br>860-810<br>705-685             | 1165<br>1039<br>836 (s)<br>690 (s)         | 1,3,5-Trimethylbenzene |

Table 4.10. Alcohol Compounds

| Functional Group                               | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|------------------------------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>ALCOHOLS</b>                                |                                         |                                |                  |
| <b>General</b>                                 |                                         |                                |                  |
| OH unbridged group                             | 3650-3590 sp                            |                                |                  |
| OH inter- and intra-<br>molecularly H - bonded | 3570-3450                               |                                |                  |
| OH intermolecularly<br>H-bonded                | 3400-3200 br                            |                                |                  |
| <b>Primary alcohols</b>                        |                                         |                                |                  |
|                                                | 1350-1260                               | 1339                           |                  |
|                                                | 1065-1020                               | 1028                           | 1-Pentanol       |
| <b>Secondary alcohols</b>                      |                                         |                                |                  |
|                                                | 1370-1260                               | 1369                           |                  |
|                                                | 1120-1080                               | 1111                           | 2-Pentanol       |
| <b>Tertiary alcohols</b>                       |                                         |                                |                  |
|                                                | 1410-1310                               | 1379                           |                  |
|                                                | 1170-1120                               | 1124                           | 2-Methylbutanol  |
| <b>Aromatic ring hydroxy compounds</b>         |                                         |                                |                  |
| OH unbridged                                   | 3617-3599 sp                            |                                |                  |
| OH dimer                                       | 3460-3322 br                            |                                |                  |
| OH polymer                                     | 3370-3322 br                            |                                |                  |
|                                                | 1410-1310                               | 1350                           |                  |
|                                                | 1225-1175                               | 1225                           | Phenol           |

Table 4.11. Peroxide Compounds

| Functional Group | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|------------------|-----------------------------------------|--------------------------------|------------------|
| <b>PEROXIDES</b> |                                         |                                |                  |
| <b>Aliphatic</b> | 1820-1810<br>1800-1780<br>890-820       |                                |                  |
| <b>Aromatic</b>  | 1805-1780<br>1785-1755<br>1020-980      |                                |                  |

Table 4.12. Ether Type Compounds

| Functional Group                     | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|--------------------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>ETHERS</b>                        |                                         |                                |                  |
| <b>Aliphatic</b>                     |                                         |                                |                  |
| O-CH <sub>3</sub>                    | 2830-2815                               |                                |                  |
| C-O-C                                | 1150-1060                               | 1140                           |                  |
| O-(CH <sub>2</sub> ) <sub>4</sub>    | 742-734                                 |                                | Diethyl ether    |
| O-CH <sub>3</sub>                    | 1455                                    |                                |                  |
| <b>Aromatic</b>                      |                                         |                                |                  |
| =C-O-C                               | 1275-1200                               | 1247                           |                  |
| C-O-C                                | 1075-1020                               | 1038                           | Anisol           |
| <b>Cyclic</b>                        |                                         |                                |                  |
| C-O-C                                | 1140-1070                               |                                |                  |
| <b>Epoxides</b>                      |                                         |                                |                  |
| general                              | 1260-1240                               | 1261                           | 1,2-Epoxybutane  |
| <i>trans</i> compounds               | 890                                     |                                |                  |
| <i>cis</i> compounds                 | 830                                     | 826                            | 1,2-Epoxybutane  |
| <b>Tetrahydrofuran derivatives</b>   |                                         |                                |                  |
|                                      | 1098-1075                               | 1076                           | Tetrahydrofuran  |
|                                      | 915-913                                 | 912                            |                  |
| <b>Trioxans</b>                      |                                         |                                |                  |
|                                      | 1175                                    | 1172                           | Trioxan          |
|                                      | 958                                     | 957                            |                  |
| <b>Tetrahydropyran derivatives</b>   |                                         |                                |                  |
|                                      | 1120-1080                               |                                |                  |
|                                      | 1100-900                                |                                |                  |
|                                      | 825-805                                 |                                |                  |
| <b>Dioxan derivatives</b>            |                                         |                                |                  |
|                                      | 1125                                    | 1122                           | Dioxan           |
| <b>KETALS, ACETALS</b>               |                                         |                                |                  |
| R <sub>2</sub> -C-(O-C) <sub>2</sub> | 1190-1158<br>1143-1124<br>1098-1063     |                                |                  |

Table 4.13. Ketone and Aldehyde Compounds

| Functional Group           | Absorption Range (cm <sup>-1</sup> )     | Example (cm <sup>-1</sup> ) | Example Compound    |
|----------------------------|------------------------------------------|-----------------------------|---------------------|
| <b>KETONES</b>             |                                          |                             |                     |
| <b>Aliphatic</b>           |                                          |                             |                     |
|                            | 1725-1705                                | 1727                        | Butanone            |
|                            | 1325-1215                                | 1269                        |                     |
|                            | 1200                                     | 1215                        |                     |
| <b>Unsaturated</b>         |                                          |                             |                     |
| C=C                        | 1650-1620                                | 1618                        | Methyl vinyl ketone |
| C=O                        | 1685-1665                                | 1684                        |                     |
| <b>Aromatic</b>            |                                          |                             |                     |
| Aryl, alkyl                | 1700-1680                                | 1694                        | Acetophenone        |
| Aryl, aryl                 | 1670-1660                                |                             |                     |
| <b>Cyclic</b>              |                                          |                             |                     |
| 4- & 5-membered rings      | 1775-1740                                | 1739                        | Cyclopentanone      |
| 6- & 7-membered rings      | 1725-1700                                | 1703                        | Cycloheptanone      |
| <b>Diketones</b>           |                                          |                             |                     |
| α-Diketones                | 1730-1710                                | 1721                        | Diacyl ketone       |
| β-Diketones                | 1640-1540                                |                             |                     |
| γ-Diketones                | 1725-1705                                |                             |                     |
| <b>Halogen substituted</b> |                                          |                             |                     |
| α,α-Dihalogen substitution | 1765-1745                                |                             |                     |
| α-Dihalogen substitution   | 1745-1725                                |                             |                     |
| <b>ALDEHYDES</b>           |                                          |                             |                     |
| <b>General</b>             |                                          |                             |                     |
| CH                         | 2900-2700 2 band<br>2720-2700<br>975-780 |                             |                     |
| <b>Aliphatic</b>           |                                          |                             |                     |
| C=O                        | 1740-1720                                | 1735                        | Butyraldehyde       |
| CH                         | 1440-1325                                | 1390                        |                     |
| <b>Unsaturated</b>         |                                          |                             |                     |
| C=O                        | 1650-1620                                | 1637                        | Crotonaldehyde      |
| C=O α,β unsaturated        | 1690-1650                                |                             |                     |

Table 4.14. Carboxylic Acid Compounds

| Functional Group         | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound |
|--------------------------|--------------------------------------|-----------------------------|------------------|
| <b>CARBOXYLIC ACIDS</b>  |                                      |                             |                  |
| <b>General</b>           |                                      |                             |                  |
| OH                       | 3200-2500 br                         |                             |                  |
| CH                       | 1440-1396                            |                             |                  |
|                          | 1320-1210                            |                             |                  |
| OH dimer                 | 950-900 br                           | 1718                        | Acetic acid      |
| C=O halogen substitution | 1740-1720                            |                             |                  |
| C=O aliphatic            | 1720-1700                            |                             |                  |
| C=O unsaturated          | 1710-1690                            |                             |                  |
| C=O aromatic             | 1700-1680                            | 1695                        | Benzoic acid     |

Table 4.14. (Continued)

|                        |           |      |               |
|------------------------|-----------|------|---------------|
| C=C                    | 1660-1620 | 1655 | Crotonic acid |
| <b>Carboxylic Ions</b> |           |      |               |
| C=O                    | 1610-1560 |      |               |
| C=O                    | 1420-1300 |      |               |

Table 4.15. Ester Compounds

| Functional Group                  | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound |
|-----------------------------------|--------------------------------------|-----------------------------|------------------|
| <b>ESTERS</b>                     |                                      |                             |                  |
| C=O unsaturated, aryl             | 1800-1770                            |                             |                  |
| C=C unsaturated, aryl             | 1730-1710                            | 1718                        |                  |
| C-O acrylates, fumarate           | 1300-1200                            | 1282                        | Ethyl acetate    |
| C-O                               | 1190-1130                            |                             |                  |
| C=O electronegatively substituted | 1770-1745                            |                             |                  |
| C=O $\alpha,\gamma$ keto          | 1755-1740                            |                             |                  |
| C=O saturated                     | 1750-1735                            | 1744                        | Methyl acetate   |
| C=O $\beta$ keto                  | 1660-1640                            |                             |                  |
| C-O benzoates, phthalates         | 1310-1250                            | 1277                        | Methyl benzoate  |
|                                   | 1150-1100                            | 1108                        |                  |
| C-O acetates                      | 1250-1230                            | 1246                        | Propyl acetate   |
|                                   | 1060-1000                            | 1047                        |                  |
| C-O phenolic acetates             | 1205                                 |                             |                  |
| C-O formate                       | 1200-1180                            | 1190                        | Propyl formate   |
| <b>LACTONES</b>                   |                                      |                             |                  |
| $\beta$ -Lactones                 | 1840-1800                            |                             |                  |
| $\gamma$ -Lactones                | 1780-1760                            | 1776                        | Butyrolactone    |
| $\delta$ -Lactones                | 1750-1730                            |                             |                  |
|                                   | 1280-1150                            | 1168                        |                  |

Table 4.16. Anhydride Compounds

| Functional Group  | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound        |
|-------------------|--------------------------------------|-----------------------------|-------------------------|
| <b>ANHYDRIDES</b> |                                      |                             |                         |
| <b>Aliphatic</b>  |                                      |                             |                         |
| C=O               | 1850-1800                            | 1842                        | Acetic acid anhydride   |
| C=O               | 1785-1760                            | 1783                        |                         |
| C-O               | 1170-1050                            | 1134                        |                         |
| <b>Aromatic</b>   |                                      |                             |                         |
| C=O               | 1880-1840                            | 1866                        | Phthalic acid anhydride |
| C=O               | 1790-1770                            | 1773                        |                         |
| C-O               | 1300-1200                            | 1267                        |                         |
| <b>Cyclic</b>     |                                      |                             |                         |
| C=O               | 1870-1820                            | 1818                        | Glutaric acid anhydride |
| C=O               | 1800-1750                            | 1772                        |                         |

Table 4.17. Amide Compounds

| Functional Group          | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound      |
|---------------------------|-----------------------------------------|--------------------------------|-----------------------|
| <b>AMIDES</b>             |                                         |                                |                       |
| <b>Primary</b>            |                                         |                                |                       |
| NH free                   | 3500                                    |                                |                       |
| NH free                   | 3400                                    |                                |                       |
| NH bridges                | 3350                                    | 3346                           | Butyramide            |
| NH bridged                | 3190                                    | 3191                           |                       |
| C=O                       | 1660-1640                               | 1660                           |                       |
|                           | 1430-1400                               | 1430                           |                       |
| <b>Secondary</b>          |                                         |                                |                       |
| NH free <i>trans</i>      | 3460-3400                               |                                | N-Methylacetamide     |
| NH free <i>cis</i>        | 3440-3420                               |                                |                       |
| NH bridged <i>trans</i>   | 3320-3270                               | 3280                           |                       |
| NH bridged <i>cis</i>     | 3180-3140                               |                                |                       |
| bridged <i>cis, trans</i> | 3100-3070                               | 3090                           |                       |
| C=O                       | 1680-1630                               | 1652                           |                       |
| NH                        | 1570-1510                               | 1564                           |                       |
|                           | 720 br                                  | 725                            |                       |
| <b>Tertiary</b>           |                                         |                                |                       |
| C=O                       | 1670-1630                               | 1670                           | N,N-Dimethyl formamid |

Table 4.18. Amino Acid Compounds

| Functional Group                 | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|----------------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>AMINO ACIDS</b>               |                                         |                                |                  |
| NH                               | 3130-3030 br                            |                                |                  |
|                                  | 2760-2530                               |                                |                  |
|                                  | 2140-2080                               |                                |                  |
| C=O                              | 1720-1680                               |                                |                  |
| ionized form                     | 1600-1560                               |                                |                  |
|                                  | 1300                                    |                                |                  |
| C=O $\alpha$ -amino acids        | 1754-1720                               |                                |                  |
| C=O $\beta, \gamma$ -amino acids | 1730-1700                               |                                |                  |
| Amino acid HCl                   | 3030-2500                               |                                |                  |
| NH amino acid HCl's              | 1660-1590                               |                                |                  |
| NH amino acid HCl's              | 1550-1490                               |                                |                  |

Table 4.19. Amine Compounds

| Functional Group  | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|-------------------|-----------------------------------------|--------------------------------|------------------|
| <b>AMINES</b>     |                                         |                                |                  |
| <b>General</b>    |                                         |                                |                  |
| N-CH <sub>3</sub> | 2820-2730                               |                                |                  |
| N-CH <sub>3</sub> | 1426                                    |                                |                  |
| C-N               | 1410                                    |                                |                  |

Table 4.19. (Continued)

|                             |                                     |                  |                    |
|-----------------------------|-------------------------------------|------------------|--------------------|
| <b>Aliphatic, primary</b>   |                                     |                  |                    |
| NH free                     | 3500-3200<br>(2 bands)              | 3350<br>3210     | Ethylamine         |
| NH                          | 1650-1590<br>1200-1150<br>1120-1030 | 1630<br><br>1100 |                    |
| <b>Aliphatic, secondary</b> |                                     |                  |                    |
| NH free                     | 3500-3200 1 band                    | 3230             | Dipropylamine      |
| NH                          | 1650-1550                           |                  |                    |
| C-N                         | 1200-1120                           | 1126             |                    |
| C-N                         | 1150-1080                           | 1090             |                    |
| <b>Aliphatic, tertiary</b>  |                                     |                  |                    |
| C-N                         | 1230-1130                           | 1175             | Ethyldimethylamine |
| C-N                         | 1130-1030                           | 1070             |                    |
| <b>Aromatic, primary</b>    |                                     |                  |                    |
|                             | 3510-3450                           | 3460             | Aniline            |
|                             | 3420-3380                           | 3413             |                    |
|                             | 1630-1600                           | 1621             |                    |
| <b>Aromatic, secondary</b>  |                                     |                  |                    |
| Free                        | 3450-3430                           |                  |                    |
| Bridged                     | 3400-3300                           | 3400             | N-Methylaniline    |

Table 4.20. Unsaturated Nitrogen Compounds

| Functional Group                      | Absorption Range<br>( $\text{cm}^{-1}$ ) | Example<br>( $\text{cm}^{-1}$ ) | Example Compound |
|---------------------------------------|------------------------------------------|---------------------------------|------------------|
| <b>UNSATURATED NITROGEN COMPOUNDS</b> |                                          |                                 |                  |
| <b>Imines</b>                         |                                          |                                 |                  |
| NH                                    | 3400-3300                                |                                 |                  |
| C=N                                   | 1690-1640                                |                                 |                  |
| <b>Oximes</b>                         |                                          |                                 |                  |
| Liquid                                | 3602-3590                                |                                 |                  |
| Solid                                 | 3250                                     |                                 |                  |
| Solids                                | 3115                                     |                                 |                  |
| Aliphatic                             | 1680-1665                                |                                 |                  |
| Aromatic                              | 1650-1620<br>1300<br>900                 |                                 |                  |

Table 4.21. Cyanide and Isocyanide Compounds

| Functional Group                             | Absorption Range<br>( $\text{cm}^{-1}$ ) | Example<br>( $\text{cm}^{-1}$ ) | Example Compound  |
|----------------------------------------------|------------------------------------------|---------------------------------|-------------------|
| <b>CYANIDES, ISOCYANIDES</b>                 |                                          |                                 |                   |
| C $\equiv$ N unconjugated                    | 2265-2240                                | 2256                            | Ethyl cyanide     |
| C $\equiv$ N conjugated or aromatic          | 2240-2220                                | 2222                            | Benzyl cyanide    |
| C $\equiv$ N cyanide,<br>thiocyanide complex | 2200-2000                                |                                 |                   |
| N $\equiv$ C alkyl isocyanide                | 2183-2150                                | 2166                            | Methyl isocyanide |
| N $\equiv$ C aryl isocyanide                 | 2140-2080                                | 2100                            | Phenyl isocyanide |

Table 4.22. Cyclic Nitrogen Compounds

| Functional Group                 | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|----------------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>CYCLIC NITROGEN COMPOUNDS</b> |                                         |                                |                  |
| <b>Pyridines, quinolines</b>     |                                         |                                |                  |
| CH                               | 3100-3000                               | 3030                           | Pyridine         |
| C=C, C=N                         | 1615-1590                               | 1590                           |                  |
|                                  | 1585-1550                               |                                |                  |
|                                  | 1520-1465                               | 1490                           |                  |
|                                  | 1440-1410                               |                                |                  |
|                                  | 920-690                                 | 707                            |                  |
| <b>Pyrimidines</b>               |                                         |                                |                  |
| CH                               | 3060-3010                               |                                |                  |
| C=C, C=N                         | 1580-1520                               |                                |                  |
| Ring                             | 1000-900                                |                                |                  |

Table 4.23. Unsaturated Nitrogen-Nitrogen Compounds

| Functional Group                               | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|------------------------------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>UNSATURATED NITROGEN-NITROGEN COMPOUNDS</b> |                                         |                                |                  |
| Azo compounds                                  | 1630-1575                               |                                | Phenylazide      |
| N=N azides                                     | 2160-2120                               | 2130                           |                  |
| N=N azides                                     | 1340-1180                               | 1297                           |                  |

Table 4.24. Nitro Compounds

| Functional Group       | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>NITRO COMPOUNDS</b> |                                         |                                |                  |
| <b>Aliphatic</b>       |                                         |                                |                  |
|                        | 1570-1500                               | 1546                           | 2-Nitrobutane    |
|                        | 1385-1365                               | 1362                           |                  |
|                        | 880                                     | 879                            |                  |
| <b>Aromatic</b>        |                                         |                                |                  |
|                        | 1550-1510                               | 1527                           | Nitrobenzene     |
|                        | 1370-1330                               | 1351                           |                  |
|                        | 849                                     | 853                            |                  |

Table 4.25. Phosphorus Compounds

| Functional Group            | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|-----------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>PHOSPHORUS COMPOUNDS</b> |                                         |                                |                  |
| O-H phosphoric acids        | 2700-2560 br                            |                                |                  |
| P-H                         | 2440-2350 sp                            |                                |                  |
| P=O                         | 1350-1250                               |                                |                  |
| P=O                         | 1250-1150                               |                                |                  |
| P-O-C                       | 1240-1190                               |                                |                  |
| P-O-R                       | 1190                                    |                                |                  |
| P-O-C                       | 1170-1150                               |                                |                  |

Table 4.25. (Continued)

|                                                |           |      |                    |
|------------------------------------------------|-----------|------|--------------------|
| P-O-C                                          | 1050-990  |      |                    |
| P-O-P                                          | 970-940   |      |                    |
| P-F                                            | 885       |      |                    |
| P=S                                            | 840-600   |      |                    |
| O-P-H                                          | 865-840   |      |                    |
| O-P-O                                          | 590-520   |      |                    |
| O-P-O                                          | 460-440   |      |                    |
| <b>PHOSPHORUS-CARBON COMPOUNDS</b>             |           |      |                    |
| P-C aromatic                                   | 1450-1435 |      |                    |
| P-C aliphatic                                  | 1320-1280 | 1298 | Trimethylphosphine |
| P-C                                            | 750-650   | 707  |                    |
| PO <sub>4</sub> <sup>-3</sup> aryl phosphates  | 1080-1040 |      |                    |
| PO <sub>4</sub> <sup>-3</sup> alkyl phosphates | 1180-1150 |      |                    |
| PO <sub>4</sub> <sup>-3</sup> alkyl phosphates | 1080      |      |                    |

Table 4.26. Deuterated Compounds

| Functional Group                | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound |
|---------------------------------|--------------------------------------|-----------------------------|------------------|
| <b>DEUTERATED COMPOUNDS</b>     |                                      |                             |                  |
| O-D deuterated alcohols         | 2650-2400                            |                             |                  |
| O-D deuterated carboxylic acids | 675                                  |                             |                  |

Table 4.27. Sulfur Compounds

| Functional Group        | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound     |
|-------------------------|--------------------------------------|-----------------------------|----------------------|
| <b>SULFUR COMPOUNDS</b> |                                      |                             |                      |
| C=S                     | 1400-1300                            | 1357                        | Dithioacetic acid    |
| S=S                     | 1200-1050                            |                             |                      |
| P=S                     | 840-600                              |                             |                      |
| SH mercaptans           | 2600-2550                            | 2580                        | Ethyl mercaptan      |
| C-S mercaptans          | 700-600                              | 665                         |                      |
| C-S-C dialkyl sulfides  | 750-600                              | 726                         | Methyl ethyl sulfide |
|                         | 710-570                              | 676                         |                      |
|                         | 660-630                              | 654                         |                      |
| Aliphatic sulphones     | 1410-1390                            | 1407                        | Dimethylsulphone     |
|                         | 1350-1300                            | 1316                        |                      |
| Sulphonic acids         | 1210-1150                            |                             |                      |
|                         | 1060-1030                            |                             |                      |
|                         | 650                                  |                             |                      |

Table 4.28. Silicon Compounds

| Functional Group                  | Absorption Range (cm <sup>-1</sup> ) | Example (cm <sup>-1</sup> ) | Example Compound |
|-----------------------------------|--------------------------------------|-----------------------------|------------------|
| <b>SILICON COMPOUNDS</b>          |                                      |                             |                  |
| SiH alkylsilanes                  | 2300-2100                            | 2175                        | Dimethylsilane   |
| Si(CH <sub>3</sub> ) <sub>2</sub> | 1265-1258                            | 1262                        |                  |

Table 4.28. (Continued)

|                                   |           |      |                        |
|-----------------------------------|-----------|------|------------------------|
|                                   | 814-800   |      |                        |
|                                   | 800       |      |                        |
| Si(CH <sub>3</sub> ) <sub>3</sub> | 1260-1240 | 1259 | Methoxytrimethylsilane |
|                                   | 850-830   | 844  |                        |
|                                   | 760       | 763  |                        |
| Si-C aromatic                     | 1429      |      |                        |
|                                   | 1130-1090 |      |                        |
| Si-C                              | 860-715   |      |                        |
| Si-O siloxanes                    | 1100-1000 |      |                        |
| Si-O-C open-chain                 | 1090-1020 |      |                        |
| Si-O-Si open-chain                | 1097      |      |                        |
| Si-O-Si cyclic                    | 1080-1010 |      |                        |

Table 4.29. Halogen Compounds

| Functional Group            | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound |
|-----------------------------|-----------------------------------------|--------------------------------|------------------|
| <b>HALOGEN COMPOUNDS</b>    |                                         |                                |                  |
| <b>Iodine Compounds</b>     |                                         |                                |                  |
|                             | 500                                     |                                |                  |
| <b>Bromine Compounds</b>    |                                         |                                |                  |
|                             | 700-500                                 |                                |                  |
| <b>Chlorine Compounds</b>   |                                         |                                |                  |
| Monochloro                  | 800-600                                 |                                |                  |
|                             | 750-700                                 |                                |                  |
| Fully chlorinated compounds | 780-710                                 |                                |                  |
| <b>Fluorine Compounds</b>   |                                         |                                |                  |
|                             | 1400-1000                               |                                |                  |
|                             | 1100-1000                               |                                |                  |
| Fully fluorinated compounds | 745-730                                 |                                |                  |

Table 4.30. Inorganic Compounds

| Functional Group                | Absorption Range<br>(cm <sup>-1</sup> ) | Example<br>(cm <sup>-1</sup> ) | Example Compound  |
|---------------------------------|-----------------------------------------|--------------------------------|-------------------|
| <b>INORGANIC COMPOUNDS</b>      |                                         |                                |                   |
| <b>Sulfates</b>                 |                                         |                                |                   |
|                                 | 1200-1140                               | 1143                           | Potassium sulfate |
|                                 | 1130-1080                               | 1117                           |                   |
|                                 | 680-610                                 | 617                            |                   |
| <b>Nitrates</b>                 |                                         |                                |                   |
|                                 | 1380-1350                               | 1370                           | Potassium nitrate |
|                                 | 840-815                                 | 825                            |                   |
| <b>Nitrites</b>                 |                                         |                                |                   |
|                                 | 840-800                                 |                                |                   |
|                                 | 750                                     |                                |                   |
| <b>Water of Crystallization</b> |                                         |                                |                   |
|                                 | 1630-1615                               |                                |                   |

Table 4.30. (Continued)

|                             |           |      |                    |
|-----------------------------|-----------|------|--------------------|
| <b>Halogen-Oxygen salts</b> |           |      |                    |
| Chlorates                   | 980-930   | 978  | Potassium chlorate |
|                             | 930-910   | 932  |                    |
| Bromates                    | 810-790   | 793  | Potassium bromate  |
| Iodates                     | 785-730   | 756  | Potassium iodate   |
| <b>Carbonates</b>           |           |      |                    |
|                             | 1450-1410 | 1410 | Calcium carbonate  |
|                             | 880-860   | 875  |                    |

## 4.4 Nuclear Magnetic Resonance Spectroscopy

### 4.4.1 Common NMR Solvents

Table 4.31. NMR Solvents

| Compound                           | M.W.    | d <sup>20/4</sup> | m.p. <sup>1</sup> | b.p. <sup>1</sup> | $\delta^2_{\text{H}}(\text{mult})^3$ | $\delta^2_{\text{C}}(\text{mult})^3$ |
|------------------------------------|---------|-------------------|-------------------|-------------------|--------------------------------------|--------------------------------------|
| Acetic Acid-d <sub>4</sub>         | 64.078  | 1.12              | 17                | 118               | 11.53 (1)<br>2.03 (5)                | 178 (br)<br>20.0 (7)                 |
| Acetone-d <sub>6</sub>             | 64.117  | 0.87              | -94               | 57                | 2.04 (5)                             | 206.0 (13)<br>29.8 (7)               |
| Acetonitrile-d <sub>3</sub>        | 44.071  | 0.84              | -45               | 82                | 1.93 (5)                             | 118.2 (br)                           |
| Benzene-d <sub>6</sub>             | 84.152  | 0.95              | 5                 | 80                | 7.15 (br)                            | 128.0 (3)                            |
| Chloroform-d                       | 120.384 | 1.50              | -64               | 62                | 7.24 (1)                             | 77.0 (3)                             |
| Cyclohexane-d <sub>12</sub>        | 96.236  | 0.89              | 6                 | 81                | 1.38 (br)                            | 26.4 (5)                             |
| Deuterium Oxide                    | 20.028  | 1.11              | 3.8               | 101.4             | 4.67 (TSP)                           |                                      |
| 1,2-Dichloroethane-d <sub>4</sub>  | 102.985 | 1.25              | -40               | 84                | 3.72 (br)                            | 43.6 (5)                             |
| Diethyl-d <sub>10</sub> Ether      | 84.185  | 0.82              | -116              | 35                | 3.34 (m)<br>1.07 (m)                 | 65.3 (5)<br>14.5 (7)                 |
| Dimethylformamide-d <sub>7</sub>   | 80.138  | 1.04              | -61               | 153               | 8.01 (br)<br>2.91 (5)<br>2.74 (5)    | 162.7 (3)<br>35.2 (7)<br>30.2 (7)    |
| Dimethyl-d <sub>6</sub> Sulphoxide | 84.170  | 1.18              | 18                | 189               | 2.49 (5)                             | 39.5 (7)                             |
| p-Dioxane-d <sub>8</sub>           | 96.156  | 1.13              | 122               | 101               | 3.53 (m)                             | 66.5 (5)                             |
| Ethyl Alcohol-d <sub>6</sub>       | 52.106  | 0.91              | <-130             | 79                | 5.19 (1)<br>3.55 (br)<br>1.11 (m)    | 56.8 (5)<br>17.2 (7)                 |

Table 4.31. (Continued)

|                                   |         |      |      |     |                        |                        |
|-----------------------------------|---------|------|------|-----|------------------------|------------------------|
| Hexafluoroacetone<br>Deuterate    | 198.067 | 1.71 | 21   |     | 5.26 (1)               | 122.5 (4)<br>92.9 (7)  |
| HMPT-d <sub>18</sub>              | 197.314 | 1.14 | 7    | 106 | 2.53 (2x5)             | 35.8 (7)               |
| Methyl Alcohol-d <sub>4</sub>     | 36.067  | 0.89 | -98  | 65  | 4.78 (1)               | 49.0 (7)               |
| Methylene Chloride-d <sub>2</sub> | 86.945  | 1.35 | -95  | 40  | 5.32 (3)               | 53.8 (5)               |
| Tetrahydrofuran-d <sub>8</sub>    | 80.157  | 0.99 | -109 | 66  | 3.58 (br)<br>1.73 (br) | 67.4 (5)<br>25.3 (br)  |
| Trifluoroacetic Acid-d            | 115.030 | 1.50 | -15  | 72  | 11.50 (1)              | 164.2 (4)<br>116.6 (4) |

1. Melting and boiling points (in °C) are those of the corresponding light compounds. (except for **D<sub>2</sub>O**) and are intended only to indicate the useful liquid range of the materials.
2. Chemical shifts in ppm relative to TMS.
3. The multiplicity br indicates a broad peak without resolvable fine structure, while m indicates one with fine structure.
4. Note that chemical shifts can be dependent on solute, concentration and temperature.

#### 4.4.2 Reference Standards for Proton NMR

Table 4.32. NMR Reference Standards

| Compound (Abbrev.)                                                      | Formula                                                                                                           | m.p.<br>°C    | b.p.<br>°C | Hydrogen bands                                                                                 |                           |                            |
|-------------------------------------------------------------------------|-------------------------------------------------------------------------------------------------------------------|---------------|------------|------------------------------------------------------------------------------------------------|---------------------------|----------------------------|
|                                                                         |                                                                                                                   |               |            | Group <sup>1</sup>                                                                             | δ                         | τ                          |
| Tetramethylsilane<br>(TMS) <sup>2</sup>                                 | (CH <sub>3</sub> ) <sub>4</sub> Si                                                                                |               | 26.5       | CH <sub>3</sub> (s)                                                                            | 0.00                      | 10.00                      |
| Hexamethyl siloxane<br>(HMDS) <sup>3</sup>                              | [(CH <sub>3</sub> ) <sub>3</sub> Si] <sub>2</sub> O                                                               | -59           | 100.4      | CH <sub>3</sub> (s)                                                                            | 0.04                      | 9.96                       |
| Sodium-3-trimethylsilyl-<br>1-propane sulfonate<br>(DSS) <sup>4</sup>   | (CH <sub>3</sub> ) <sub>3</sub> Si-<br>CH <sub>2</sub> -CH <sub>2</sub> -<br>CH <sub>2</sub> -SO <sub>3</sub> -Na | Solid<br>Salt |            | CH <sub>3</sub> (s)<br>1-CH <sub>2</sub> (m)<br>2-CH <sub>2</sub> (m)<br>3-CH <sub>2</sub> (m) | 0.00<br>0.6<br>1.8<br>2.9 | 10.00<br>9.4<br>8.2<br>7.1 |
| Sodium 3-trimethylsilyl<br>propionate-d <sub>4</sub> (TSP) <sup>5</sup> | (CH <sub>3</sub> ) <sub>3</sub> Si-<br>CD <sub>2</sub> -CD <sub>2</sub> -<br>COO-Na                               | Solid<br>Salt |            | CH <sub>3</sub> (s)                                                                            | 0.00                      | 10.00                      |

1. The functional group which produces the observed band. The multiplicity of the band is indicated in parenthesis; s = singlet; m = complex multiplet.
2. Primary reference standard for room temperature and below.
3. Can be used as reference up to 180°C.
4. Reference for water solutions. The **CH<sub>2</sub>** bands can interfere with weak sample bands.
5. Reference for water solutions.

## 4.4.3 NMR Proton Chemical Shift Chart

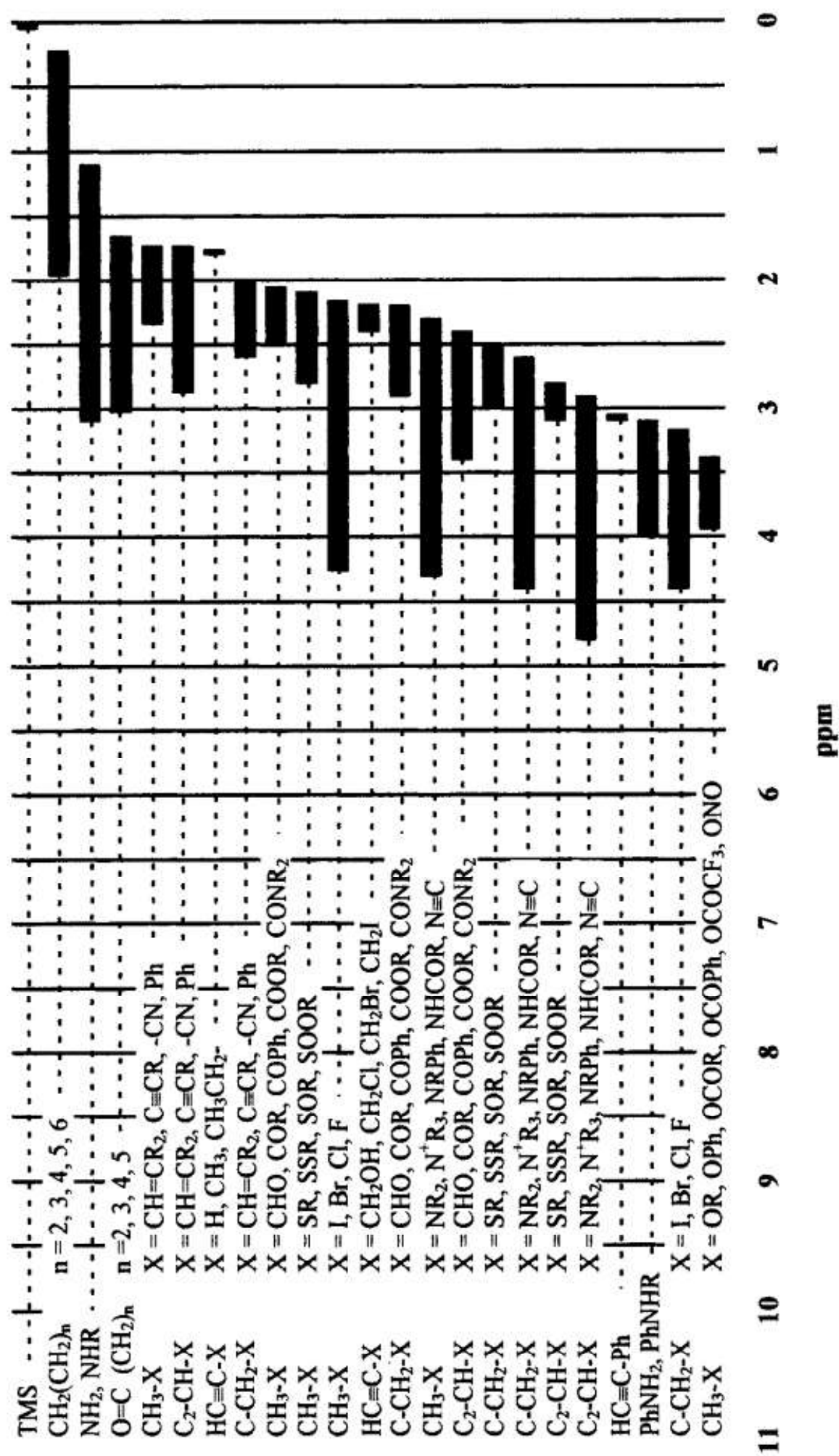


Table 4.33. Proton Chemical Shifts

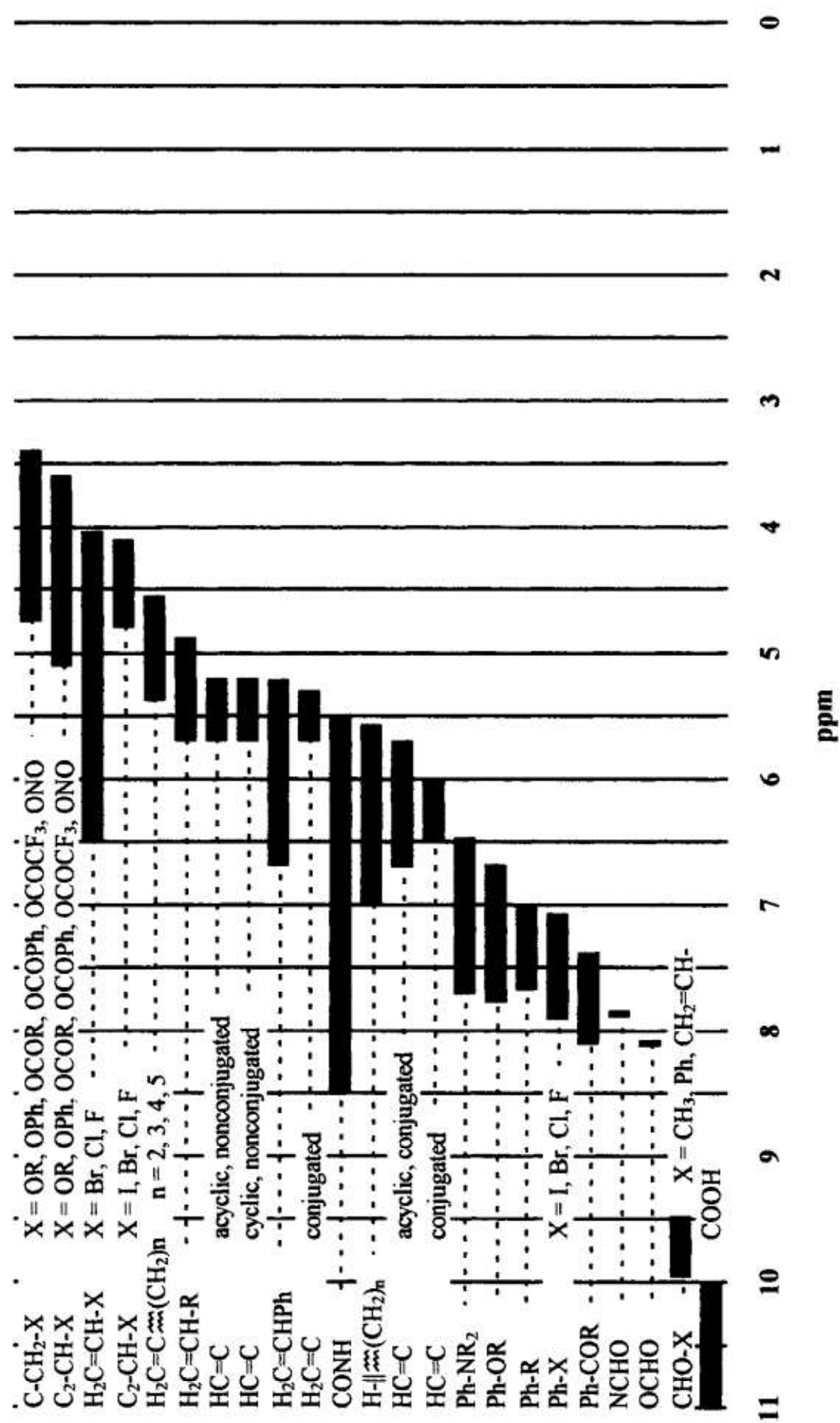


Table 4.33. (Continued)

## 4.4.4 NMR Chemical Shift Tables

The data in all of the tables are for the compound in dilute carbon tetrachloride or deuteriochloroform relative to internal TMS where such data were available. It is important to remember that solvent effects, especially in the case of aromatics, can cause significant variation in the observed chemical shifts. All chemical shifts listed are in ppm or  $\delta$ .

Table 4.34.  $^1\text{H}$  Chemical Shifts of Paraffinic Compounds with a Single Functional Groups

| Group X                        | $\text{CH}_3\text{-X}$ | $\text{C-CH}_2\text{-X}$ | $(\text{C})_2\text{-CH-X}$ | $\text{CH}_3\text{-C-X}$ | $\text{C-CH}_2\text{-C-X}$ | $(\text{C})_2\text{CH-C-X}$ |
|--------------------------------|------------------------|--------------------------|----------------------------|--------------------------|----------------------------|-----------------------------|
| -H                             | 0.233                  | 0.86                     | 1.33                       | 0.86                     | 1.33                       | 1.56                        |
| -CH=CR <sub>2</sub>            | 1.73                   | 2.00                     | 1.73                       | 1.55                     | 1.35                       | 1.00                        |
| -C=CR                          | 1.75                   | 2.15                     | 2.7                        | 1.15                     | 1.50                       | 1.80                        |
| -C=N                           | 1.98                   | 2.35                     | 2.8                        | 1.30                     | 1.6                        | 2.00                        |
| -Ph                            | 2.34                   | 2.60                     | 2.87                       | 1.18                     | 1.6                        | 1.8                         |
| -CHO                           | 2.17                   | 2.4                      | 2.4                        | 1.13                     | 1.65                       | ---                         |
| -COR                           | 2.10                   | 2.4                      | 2.55                       | 1.05                     | 1.5                        | 1.7                         |
| -COPh                          | 2.5                    | 2.9                      | 3.4                        | 1.18                     | 1.6                        | 2.0                         |
| -CO <sub>2</sub> R             | 2.1                    | 2.2                      | 2.5                        | 1.15                     | 1.7                        | 1.8                         |
| -CONR <sub>2</sub>             | 2.05                   | 2.23                     | 2.4                        | 1.1                      | 1.6                        | 1.8                         |
| -I                             | 2.16                   | 3.17                     | 4.25                       | 1.8                      | 1.8                        | 2.1                         |
| -Br                            | 2.68                   | 3.36                     | 4.2                        | 1.8                      | 1.9                        | 2.0                         |
| -Cl                            | 3.05                   | 3.44                     | 4.1                        | 1.5                      | 1.8                        | 2.0                         |
| -F                             | 4.26                   | 4.4                      | 4.8                        | 1.4                      | 1.8                        | 2.1                         |
| -OR                            | 3.38                   | 3.4                      | 3.6                        | 1.2                      | ---                        | ---                         |
| -OPh                           | 3.82                   | 3.95                     | 4.6                        | 1.3                      | 1.5                        | 1.7                         |
| -OCOR                          | 3.65                   | 4.1                      | 5.0                        | 1.25                     | 1.6                        | 1.8                         |
| -OCOPh                         | 3.82                   | 4.2                      | 5.1                        | 1.5                      | 1.7                        | 1.9                         |
| -OCOCF <sub>3</sub>            | 3.95                   | 4.3                      | ---                        | 1.4                      | 1.6                        | ---                         |
| -ONO                           | ---                    | 4.75                     | ---                        | 1.4                      | ---                        | ---                         |
| -NR <sub>2</sub>               | 2.3                    | 2.6                      | 2.9                        | 1.05                     | 1.45                       | 1.7                         |
| -N <sup>+</sup> R <sub>3</sub> | ~3.2                   | ~3.1                     | ~3.6                       | 1.4                      | 1.7                        | 2.0                         |
| -NRPh                          | ~2.7                   | ~3.1                     | ~3.6                       | 1.1                      | 1.5                        | 1.8                         |
| -NHCOR                         | 2.8                    | 3.3                      | 3.8                        | 1.1                      | 1.5                        | 1.9                         |
| -NO <sub>2</sub>               | 4.30                   | 4.4                      | 4.6                        | 1.6                      | 2.05                       | 2.5                         |
| -N=C                           | 2.85                   | ---                      | 4.8                        | 1.6                      | ---                        | ---                         |
| -SR                            | 2.09                   | 2.5                      | 3.0                        | 1.25                     | 1.6                        | 1.9                         |
| -SSR                           | 2.30                   | 2.7                      | ---                        | 1.3                      | 1.7                        | ---                         |
| -SOR                           | 2.5                    | 3.0                      | 2.8                        | 1.35                     | 1.7                        | ---                         |
| -SO <sub>2</sub> R             | 2.8                    | 2.9                      | 3.1                        | 1.35                     | 1.7                        | ---                         |

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Table 4.35.  $^1\text{H}$  Chemical Shifts of Paraffinic Compounds with Two Functional Groups

| YX              | CN     | CF <sub>3</sub> | Ph     | C≡C    | C=C  | CH <sub>3</sub> |
|-----------------|--------|-----------------|--------|--------|------|-----------------|
| CH <sub>3</sub> | 2.31   | (1.84)          | 2.63   | 2.14   | 1.97 | 1.34            |
| C=C             | 3.15   | (2.69)          | 3.30   | 3.39   | 2.73 |                 |
| C≡C             | (3.37) | (2.81)          | (3.52) | (3.11) |      |                 |
| Ph              | 3.68   | 3.50            | 3.92   |        |      |                 |
| CF <sub>3</sub> | (3.07) | (2.51)          |        |        |      |                 |
| CN              | 4.13   |                 |        |        |      |                 |

| YX                | COPh   | CONR <sub>2</sub> | COOR | COR  |
|-------------------|--------|-------------------|------|------|
| COR               | (3.77) | 3.52              | 3.32 | 3.62 |
| COOR              | (3.62) | (4.95)            | 4.22 |      |
| CONR <sub>2</sub> | (3.66) | 3.30              |      |      |
| COPh              | (3.91) |                   |      |      |

| YX   | OCOR   | OPh    | OR     | OH     |
|------|--------|--------|--------|--------|
| OH   | (5.92) | (6.02) | (5.15) | (5.35) |
| OR   | (5.72) | (5.82) | 4.49   |        |
| OPh  | (6.59) | (6.69) |        |        |
| OCOR | (6.49) |        |        |        |

| YX | I      | Br   | Cl   |
|----|--------|------|------|
| Cl | 4.99   | 5.16 | 5.28 |
| Br | (4.38) | 4.94 |      |
| I  | 3.89   |      |      |

| YX              | NHCOR  | N <sub>3</sub> | NR <sub>2</sub> |
|-----------------|--------|----------------|-----------------|
| NR <sub>2</sub> | (4.07) | (3.77)         | 3.10            |
| N <sub>3</sub>  | (4.47) | (4.17)         |                 |
| NHCOR           | (4.77) |                |                 |

Values in parentheses were calculated by the empirical method of Shoolery. All values refer to methylene ( $\text{CH}_2$ ) protons in  $\text{X-CH}_2\text{-Y}$ .

Table 4.36.  $^1\text{H}$  Chemical Shifts of Olefinic Compounds

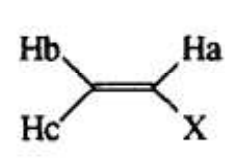
| Compound                                                                            | X=                            | a    | b    | c    |
|-------------------------------------------------------------------------------------|-------------------------------|------|------|------|
| $\text{H}_2\text{C=CH}_2$                                                           |                               | 5.33 |      |      |
|  | R                             | 5.70 | 4.88 | 4.96 |
|                                                                                     | F                             | 6.17 | 4.03 | 4.37 |
|                                                                                     | Cl                            | 6.30 | 5.44 | 5.52 |
|                                                                                     | Br                            | 6.49 | 5.88 | 6.03 |
|                                                                                     | C <sub>6</sub> H <sub>5</sub> | 6.69 | 5.21 | 5.71 |
|                                                                                     | CCl <sub>3</sub>              | 6.41 | 5.30 | 5.78 |
|                                                                                     | CN                            | 5.53 | 6.05 | 5.78 |
|                                                                                     | CH <sub>2</sub> OH            | 6.00 | 5.13 | 5.25 |
|                                                                                     | OCH <sub>3</sub>              | 6.43 | 3.90 | 4.04 |

Table 4.36. (Continued)

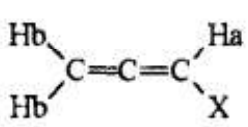
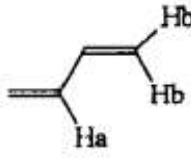
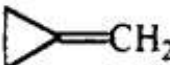
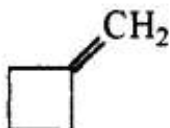
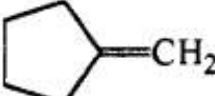
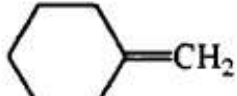
|                                                                                                                                          |               |                                      |                      |  |
|------------------------------------------------------------------------------------------------------------------------------------------|---------------|--------------------------------------|----------------------|--|
| $\text{H}_2\text{C}=\text{C}=\text{CH}_2$                                                                                                |               | 4.55                                 |                      |  |
|                                                         | Cl<br>Br<br>I | 5.76<br>5.85<br>5.62                 | 5.05<br>4.82<br>4.46 |  |
|                                                         |               | 5.20                                 | 5.11                 |  |
|                                                       |               | 5.38                                 |                      |  |
|                                                       |               | 4.70                                 |                      |  |
|                                                       |               | 4.82                                 |                      |  |
|                                                       |               | 4.55                                 |                      |  |
| $\text{CH}_3\text{-CHO}$<br>$\text{Ph-CHO}$<br>$\text{CH}_2=\text{CH-CHO}$<br>$(\text{CH}_3)_2\text{N-CHO}$<br>$\text{CH}_3\text{O-CHO}$ |               | 9.72<br>9.96<br>9.48<br>7.84<br>8.08 |                      |  |

Table 4.37.  $^1\text{H}$  Chemical Shifts of Acetylenic Compounds

| Compound                                                        | $\delta$ | Compound                                    | $\delta$ |
|-----------------------------------------------------------------|----------|---------------------------------------------|----------|
| $\text{H-C}\equiv\text{C-H}$                                    | 1.80     | $\text{OHC-C}\equiv\text{C-H}$              | 1.89     |
| $\text{CH}_3\text{-C}\equiv\text{C-H}$                          | 1.80     | $\text{HOCH}_2\text{-C}\equiv\text{C-H}$    | 2.33     |
| $\text{CH}_3\text{CH}_2\text{-C}\equiv\text{C-H}$               | 1.76     | $\text{Cl-CH}_2\text{-C}\equiv\text{C-H}$   | 2.40     |
| $\text{Ph-C}\equiv\text{C-H}$                                   | 3.05     | $\text{Br-CH}_2\text{-C}\equiv\text{C-H}$   | 2.33     |
| $\text{CH}_2=\text{CH-C}\equiv\text{C-H}$                       | 2.92     | $\text{I-CH}_2\text{-C}\equiv\text{C-H}$    | 2.19     |
| $\text{C}_2\text{H}_5\text{-C}\equiv\text{C-C}\equiv\text{C-H}$ | 1.95     | $\text{CH}_3\text{O-C}\equiv\text{C-H}$     | 1.33     |
| $\text{CH}_3(\text{C}\equiv\text{C})_2\text{C}\equiv\text{C-H}$ | 1.87     | $\text{CH}_2=\text{CH-O-C}\equiv\text{C-H}$ | 1.89     |

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Table 4.38.  $^1\text{H}$  Chemical Shifts of Cycloparaffinic Compounds

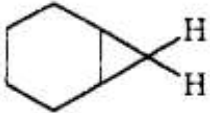
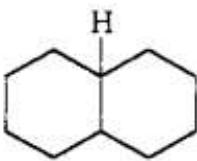
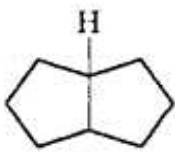
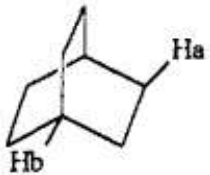
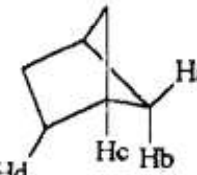
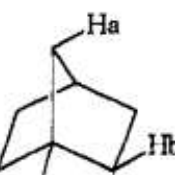
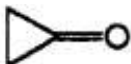
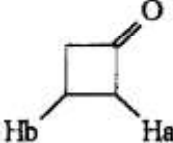
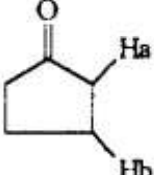
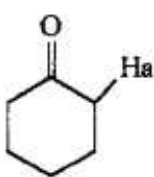
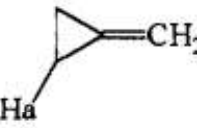
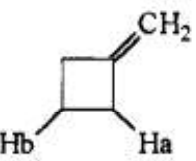
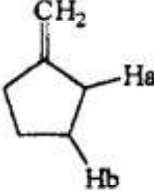
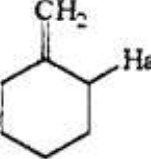
| Compound                                                                            | $\delta$               | Compound                                                                             | $\delta$                             | Compound                                                                              | $\delta$                             |
|-------------------------------------------------------------------------------------|------------------------|--------------------------------------------------------------------------------------|--------------------------------------|---------------------------------------------------------------------------------------|--------------------------------------|
| Cyclopropane                                                                        | 0.22                   | Cyclobutane                                                                          | 1.96                                 | Cyclopentane                                                                          | 1.51                                 |
| Cyclohexane                                                                         | 1.44                   | Cycloheptane                                                                         | 1.54                                 | Cyclooctane                                                                           | 1.54                                 |
| Adamantane                                                                          | 1.78                   |                                                                                      |                                      |                                                                                       |                                      |
|    | 0.02                   |    | $\sim 1.4$                           |    | 2.37                                 |
|   | a 1.51<br>b $\sim 2.1$ |   | a 1.56<br>b 0.87<br>c 2.49<br>d 1.58 |   | a 1.21<br>b 1.49<br>c 1.18<br>d 2.20 |
|  | 1.65                   |  | a 3.03<br>b 1.96                     |  | a 2.06<br>b 2.02                     |
|  | 2.25                   |  | 0.99                                 |  | a 2.70<br>b 1.92                     |
|  | a 2.70<br>b 1.92       |  | 1.5                                  |                                                                                       |                                      |

Table 4.39.  $^1\text{H}$  Chemical Shifts Of Cycloolefinic Compounds

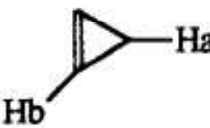
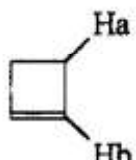
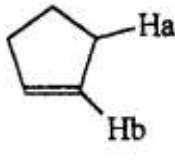
| Compound                                                                            | $\delta$         | Compound                                                                             | $\delta$         | Compound                                                                              | $\delta$         |
|-------------------------------------------------------------------------------------|------------------|--------------------------------------------------------------------------------------|------------------|---------------------------------------------------------------------------------------|------------------|
|  | a 0.92<br>b 7.01 |  | a 2.57<br>b 5.97 |  | a 2.28<br>b 5.60 |

Table 4.39. (Continued)

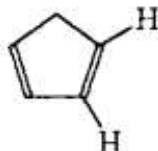
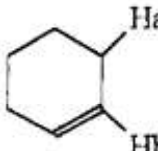
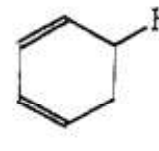
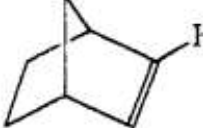
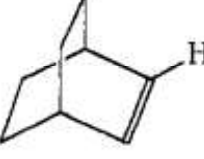
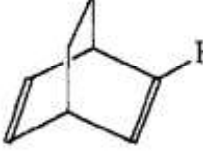
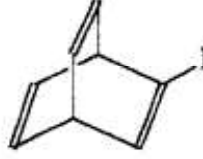
|                                                                                     |                  |                                                                                     |                  |                                                                                       |      |
|-------------------------------------------------------------------------------------|------------------|-------------------------------------------------------------------------------------|------------------|---------------------------------------------------------------------------------------|------|
|    | 6.42             |    | a 1.96<br>b 5.57 |    | 2.15 |
|    | a 1.95<br>b 3.53 |    | 5.95             |    | 6.66 |
|  | 6.25             |  | 6.27             |  | 6.70 |

Table 4.40. <sup>1</sup>H Chemical Shifts Of Monosubstituted Benzenes

| Substituent                      | Ortho | Meta | Para |
|----------------------------------|-------|------|------|
| H                                | 7.27  | 7.27 | 7.27 |
| CH <sub>3</sub>                  | 7.07  | 7.07 | 7.07 |
| CH <sub>2</sub> CH <sub>3</sub>  | 7.13  | 7.13 | 7.13 |
| CH <sub>2</sub> OH               | 7.28  | 7.28 | 7.28 |
| CH <sub>2</sub> Cl               | 7.32  | 7.32 | 7.32 |
| CHCl <sub>2</sub>                | 7.42  | 7.42 | 7.42 |
| CCl <sub>3</sub>                 | 7.91  | 7.40 | 7.37 |
| CH=CH <sub>2</sub>               | 7.5   | 7.5  | 7.5  |
| CHO                              | 7.83  | 7.49 | 7.56 |
| COCH <sub>3</sub>                | 7.89  | 7.41 | 7.56 |
| CO <sub>2</sub> H                | 8.12  | 7.43 | 7.51 |
| CO <sub>2</sub> CH <sub>3</sub>  | 7.98  | 7.38 | 7.48 |
| COCl                             | 8.11  | 7.49 | 7.63 |
| COBr                             | 8.07  | 7.48 | 7.64 |
| CONH <sub>2</sub>                | 7.8   | 7.5  | 7.5  |
| CN                               | 7.63  | 7.45 | 7.55 |
| F                                | 6.99  | 7.24 | 7.08 |
| Cl                               | 7.30  | 7.25 | 7.18 |
| Br                               | 7.45  | 7.19 | 7.23 |
| I                                | 7.67  | 7.06 | 7.27 |
| NH <sub>2</sub>                  | 6.52  | 7.02 | 6.62 |
| NHCH <sub>3</sub>                | 6.47  | 7.05 | 6.59 |
| N(CH <sub>3</sub> ) <sub>2</sub> | 6.61  | 7.09 | 6.60 |
| NHCOCH <sub>3</sub>              | 7.7   | 7.1  | 7.0  |

Table 4.40. (Continued)

|                                 |      |      |      |
|---------------------------------|------|------|------|
| NH <sub>3</sub> <sup>+</sup>    | 7.7  | 7.5  | 7.5  |
| NO                              | 7.81 | 7.55 | 7.61 |
| NO <sub>2</sub>                 | 8.22 | 7.53 | 7.65 |
| OH                              | 6.68 | 7.15 | 6.82 |
| OCH <sub>3</sub>                | 7.77 | 7.15 | 7.37 |
| OCOCH <sub>3</sub>              | 6.79 | 7.18 | 6.83 |
| SCH <sub>3</sub>                | 7.4  | 7.2  | 7.1  |
| SO <sub>2</sub> Cl              | 8.04 | 7.62 | 7.72 |
| SO <sub>3</sub> CH <sub>3</sub> | 7.87 | 7.53 | 7.60 |

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Table 4.41. <sup>1</sup>H Chemical Shifts Of Heteroaromatic Compounds

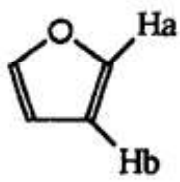
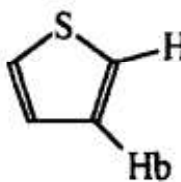
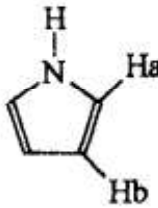
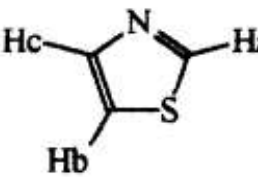
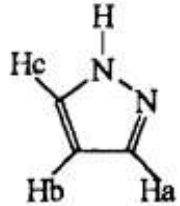
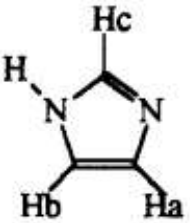
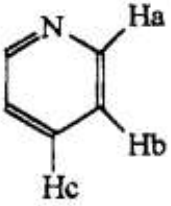
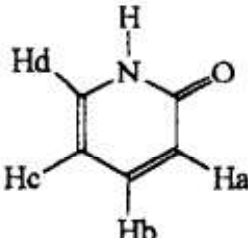
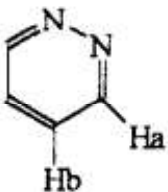
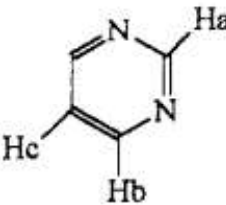
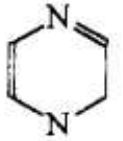
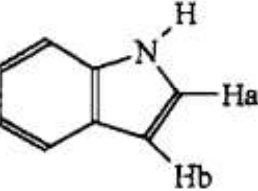
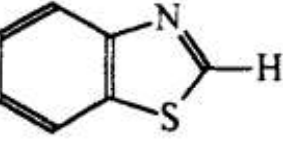
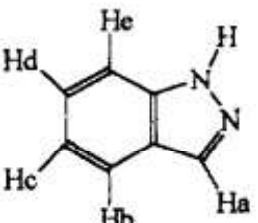
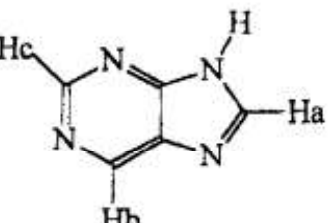
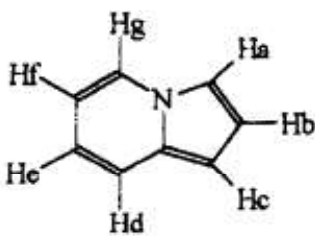
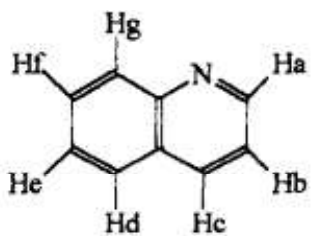
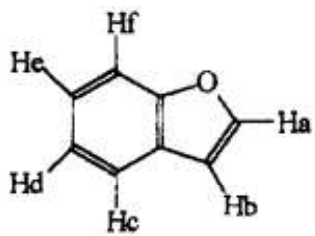
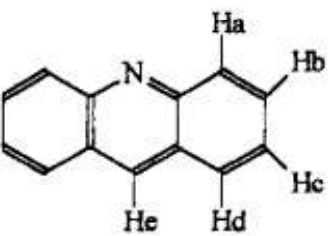
| Compound                                                                            | δ                          | Compound                                                                              | δ                                    |
|-------------------------------------------------------------------------------------|----------------------------|---------------------------------------------------------------------------------------|--------------------------------------|
|  | a 7.38<br>b 6.30           |  | a 7.19<br>b 7.04                     |
|  | 8.19                       |  | 8.58                                 |
|  | a 6.62<br>b 6.05           |  | a 8.88<br>b 7.41<br>c 7.98           |
|  | a 7.55<br>b 6.25<br>c 7.55 |  | a 7.14<br>b 7.14<br>c 7.70           |
|  | a 8.50<br>b 7.06<br>c 7.46 |  | a 6.57<br>b 7.26<br>c 6.15<br>d 7.13 |

Table 4.41. (Continued)

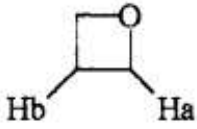
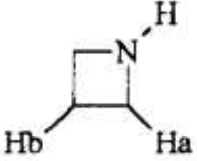
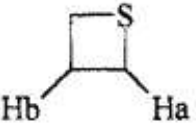
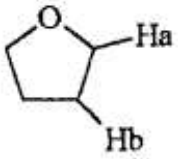
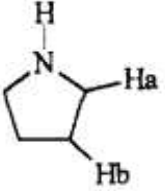
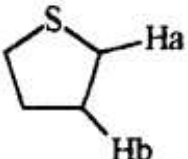
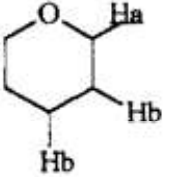
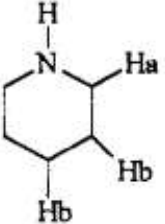
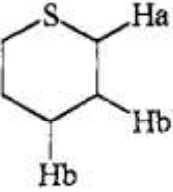
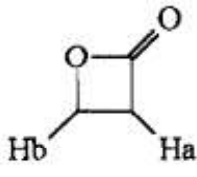
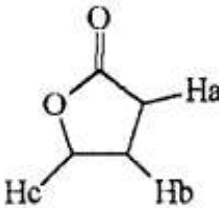
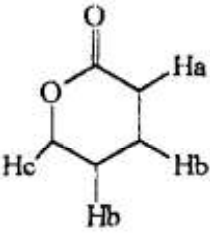
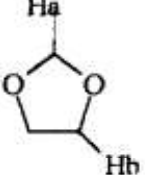
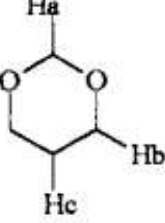
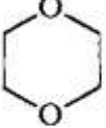
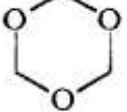
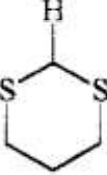
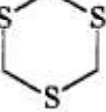
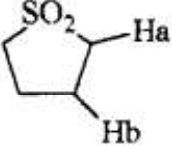
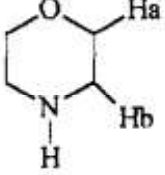
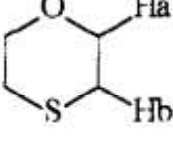
|                                                                                     |                                                                    |                                                                                       |                                                                    |
|-------------------------------------------------------------------------------------|--------------------------------------------------------------------|---------------------------------------------------------------------------------------|--------------------------------------------------------------------|
|    | a 9.17<br>b 7.68                                                   |    | a 9.15<br>b 8.60<br>c 7.09                                         |
|    | 8.5                                                                |    | 9.18                                                               |
|  | a 6.54<br>b 6.34                                                   |  | 8.95                                                               |
|  | a 8.03<br>b 7.77<br>c 7.12<br>d 7.34<br>e 7.58                     |  | a 8.63<br>b 9.16<br>c 8.95                                         |
|  | a 7.14<br>b 6.64<br>c 6.28<br>d 7.25<br>e 6.50<br>f 6.35<br>g 7.76 |  | a 8.81<br>b 7.26<br>c 8.00<br>d 7.68<br>e 7.43<br>f 7.61<br>g 8.05 |
|  | a 7.52<br>b 6.66<br>c 7.49<br>d 7.13<br>e 7.19<br>f 7.42           |  | a 8.20<br>b 7.69<br>c 7.39<br>d 7.80<br>e 8.53                     |

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Table 4.42.  $^1\text{H}$  Chemical Shifts Of Heterocyclic Compounds

| Compound                                                                            | $\delta$ | Compound                                                                            | $\delta$ | Compound                                                                              | $\delta$ |
|-------------------------------------------------------------------------------------|----------|-------------------------------------------------------------------------------------|----------|---------------------------------------------------------------------------------------|----------|
|  | 2.54     |  | 1.48     |  | 2.27     |

Table 4.42. (Continued)

|                                                                                     |                  |                                                                                      |                            |                                                                                       |                            |
|-------------------------------------------------------------------------------------|------------------|--------------------------------------------------------------------------------------|----------------------------|---------------------------------------------------------------------------------------|----------------------------|
|    | a 4.73<br>b 2.72 |    | a 3.54<br>b 2.23           |    | a 2.82<br>b 1.93           |
|    | a 3.63<br>b 1.79 |    | a 2.74<br>b 1.62           |    | a 2.82<br>b 1.93           |
|  | a 3.56<br>b 1.58 |  | a 2.69<br>b 1.49           |  | a 2.57<br>b 1.60           |
|  | a 3.48<br>b 4.22 |  | a 2.31<br>b 2.08<br>c 4.28 |  | a 2.27<br>b 1.62<br>c 4.06 |
|  | a 4.77<br>b 3.77 |  | a 4.82<br>b 3.80<br>c 1.68 |  | 3.59                       |
|  | 5.00             |  | 3.69                       |  | 4.18                       |
|  | a 2.92<br>b 2.16 |  | a 3.57<br>b 2.83           |  | a 3.88<br>b 2.57           |

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Table 4.43.  $^1\text{H}$  Chemical Shifts of Hydrogen Bonded To Oxygen, Nitrogen, Sulfur

| Compound                      | $\delta$ | Compound                                 | $\delta$ |
|-------------------------------|----------|------------------------------------------|----------|
| ROH (monomeric) <sup>a</sup>  | 0.5      | Oximes                                   | 7-11     |
| ROH (hydrogen bonded)         | 0.5-5.0  | RNH <sub>2</sub>                         | 1.1-1.8  |
| ArOH (monomeric) <sup>a</sup> | 4.5      | R <sub>2</sub> NH                        | 1.2-2.1  |
| ArOH (hydrogen bonded)        | 4.5-9    | ArNH <sub>2</sub>                        | 3.3-4.0  |
| Enols (intramolecular bonded) | 15-19    | ArNHR                                    | 3.1-3.8  |
| Carboxylic acids              | 10-13    | RCONH <sub>2</sub> , ArCONH <sub>2</sub> | 5-6.5    |
| Sulfonic acids                | 11-12    | RCONHR, ArCONHR                          | 6-8.2    |
| RSH                           | 1-2      | RCONHAr, ArCONHAr                        | 7.8-9.4  |
| ArSH                          | 3-4      | R <sub>3</sub> N <sup>+</sup> H          | 7.1-7.7  |

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## 4.5 Mass Spectroscopy

### 4.5.1 Common Molecular Ions Table

Table 4.44. Common Elemental Compositions of Molecular Ions<sup>1</sup>

| m/z | Composition                                                                                                                            |
|-----|----------------------------------------------------------------------------------------------------------------------------------------|
| 16  | CH <sub>4</sub>                                                                                                                        |
| 17  | NH <sub>3</sub>                                                                                                                        |
| 18  | H <sub>2</sub> O                                                                                                                       |
| 26  | C <sub>2</sub> H <sub>2</sub>                                                                                                          |
| 27  | CHN                                                                                                                                    |
| 28  | C <sub>2</sub> H <sub>4</sub> , CO, N <sub>2</sub>                                                                                     |
| 30  | C <sub>2</sub> H <sub>6</sub> , CH <sub>2</sub> O, NO                                                                                  |
| 31  | CH <sub>5</sub> N                                                                                                                      |
| 32  | CH <sub>4</sub> O, N <sub>2</sub> H <sub>4</sub> , SiH <sub>4</sub> , O <sub>2</sub>                                                   |
| 34  | CH <sub>3</sub> F, PH <sub>3</sub> , H <sub>2</sub> S                                                                                  |
| 36  | HCl                                                                                                                                    |
| 40  | C <sub>3</sub> H <sub>4</sub>                                                                                                          |
| 41  | C <sub>2</sub> H <sub>3</sub> N                                                                                                        |
| 42  | C <sub>3</sub> H <sub>6</sub> , C <sub>2</sub> H <sub>2</sub> O, CH <sub>2</sub> N <sub>2</sub>                                        |
| 43  | C <sub>2</sub> H <sub>5</sub> N, N <sub>3</sub> H                                                                                      |
| 44  | C <sub>2</sub> H <sub>4</sub> O, C <sub>3</sub> H <sub>8</sub> , C <sub>2</sub> HF, CO <sub>2</sub> , N <sub>2</sub> O                 |
| 45  | C <sub>2</sub> H <sub>7</sub> N, CH <sub>3</sub> NO                                                                                    |
| 46  | C <sub>2</sub> H <sub>6</sub> O, C <sub>2</sub> H <sub>3</sub> F, CH <sub>6</sub> Si, CH <sub>2</sub> O <sub>2</sub> , NO <sub>2</sub> |
| 48  | C <sub>2</sub> H <sub>5</sub> F, CH <sub>4</sub> S, CH <sub>3</sub> P                                                                  |
| 50  | C <sub>4</sub> H <sub>2</sub> , CH <sub>3</sub> Cl                                                                                     |
| 52  | C <sub>4</sub> H <sub>4</sub> , CH <sub>2</sub> F <sub>2</sub>                                                                         |
| 53  | C <sub>3</sub> H <sub>3</sub> N, HF <sub>2</sub> N                                                                                     |
| 54  | C <sub>4</sub> H <sub>6</sub> , F <sub>2</sub> O                                                                                       |
| 55  | C <sub>3</sub> H <sub>5</sub> N                                                                                                        |
| 56  | C <sub>4</sub> H <sub>8</sub> , C <sub>3</sub> H <sub>4</sub> O, C <sub>2</sub> H <sub>4</sub> N <sub>2</sub>                          |
| 57  | C <sub>3</sub> H <sub>7</sub> N, C <sub>2</sub> H <sub>3</sub> NO                                                                      |

Table 4.44. (Continued)

|    |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
|----|----------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 58 | C <sub>3</sub> H <sub>6</sub> O, C <sub>4</sub> H <sub>10</sub> , C <sub>2</sub> H <sub>2</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> N <sub>2</sub>                                                                                                                                                                                                                                                                                                                                            |
| 59 | C <sub>3</sub> H <sub>9</sub> N, C <sub>2</sub> H <sub>5</sub> NO, CH <sub>5</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                        |
| 60 | C <sub>3</sub> H <sub>8</sub> O, C <sub>3</sub> H <sub>5</sub> F, C <sub>2</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>8</sub> Si, C <sub>2</sub> H <sub>4</sub> S, C <sub>2</sub> HCl, CH <sub>4</sub> N <sub>2</sub> O, COS                                                                                                                                                                                                             |
| 61 | C <sub>2</sub> H <sub>7</sub> NO, CH <sub>3</sub> NO <sub>2</sub> , CCIN                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| 62 | C <sub>3</sub> H <sub>7</sub> F, C <sub>2</sub> H <sub>7</sub> P, C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> S, C <sub>2</sub> H <sub>3</sub> Cl                                                                                                                                                                                                                                                                                                                       |
| 64 | C <sub>2</sub> H <sub>2</sub> F <sub>2</sub> , C <sub>2</sub> H <sub>5</sub> FO, C <sub>2</sub> H <sub>5</sub> Cl, SO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                       |
| 66 | C <sub>5</sub> H <sub>6</sub> , C <sub>2</sub> H <sub>4</sub> F <sub>2</sub> , CF <sub>2</sub> O, F <sub>2</sub> N <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                          |
| 67 | C <sub>4</sub> H <sub>5</sub> N, CH <sub>3</sub> F <sub>2</sub> N, ClO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 68 | C <sub>5</sub> H <sub>8</sub> , C <sub>4</sub> H <sub>4</sub> O, C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>3</sub> O <sub>2</sub> , CH <sub>2</sub> ClF                                                                                                                                                                                                                                                                                                                                      |
| 69 | C <sub>4</sub> H <sub>7</sub> N, C <sub>3</sub> H <sub>3</sub> NO, C <sub>2</sub> H <sub>3</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                          |
| 70 | C <sub>5</sub> H <sub>10</sub> , C <sub>4</sub> H <sub>6</sub> O, C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> , CH <sub>2</sub> N <sub>4</sub> , CHF <sub>3</sub>                                                                                                                                                                                                                                                                                                                                       |
| 71 | C <sub>4</sub> H <sub>9</sub> N, C <sub>3</sub> H <sub>5</sub> NO, F <sub>3</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 72 | C <sub>4</sub> H <sub>8</sub> O, C <sub>5</sub> H <sub>12</sub> , C <sub>3</sub> H <sub>4</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>5</sub> F                                                                                                                                                                                                                                                                                                                                                         |
| 73 | C <sub>4</sub> H <sub>11</sub> N, C <sub>3</sub> H <sub>7</sub> NO, C <sub>2</sub> H <sub>3</sub> NS, C <sub>2</sub> H <sub>7</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                       |
| 74 | C <sub>4</sub> H <sub>10</sub> O, C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>10</sub> N <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> S, C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>3</sub> H <sub>10</sub> Si, C <sub>3</sub> H <sub>3</sub> Cl, CH <sub>6</sub> N <sub>4</sub> ,<br>C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>2</sub> H <sub>2</sub> O <sub>3</sub> ,                                                                                |
| 75 | C <sub>3</sub> H <sub>9</sub> NO, C <sub>2</sub> H <sub>5</sub> NO <sub>2</sub> , C <sub>2</sub> H <sub>2</sub> ClN                                                                                                                                                                                                                                                                                                                                                                                      |
| 76 | C <sub>3</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>8</sub> S, C <sub>3</sub> H <sub>5</sub> Cl, C <sub>4</sub> H <sub>9</sub> F, C <sub>4</sub> N <sub>2</sub> , C <sub>3</sub> H <sub>9</sub> P, C <sub>3</sub> H <sub>5</sub> FO, C <sub>2</sub> H <sub>4</sub> O <sub>3</sub> ,<br>C <sub>2</sub> H <sub>4</sub> OS, CH <sub>8</sub> Si <sub>2</sub> , CH <sub>4</sub> N <sub>2</sub> S, CS <sub>2</sub>                                                                            |
| 77 | CH <sub>3</sub> NO <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| 78 | C <sub>6</sub> H <sub>6</sub> , C <sub>3</sub> H <sub>7</sub> Cl, C <sub>4</sub> HSN <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> OS, C <sub>2</sub> H <sub>3</sub> ClO, C <sub>2</sub> H <sub>3</sub> FO <sub>2</sub> , CF <sub>2</sub> N <sub>2</sub> , CH <sub>6</sub> N <sub>2</sub> O <sub>2</sub>                                                                                                                                                                                                  |
| 79 | C <sub>5</sub> H <sub>5</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| 80 | C <sub>6</sub> H <sub>8</sub> , C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> F <sub>2</sub> , C <sub>2</sub> H <sub>5</sub> ClO, C <sub>2</sub> H <sub>2</sub> ClF, CH <sub>4</sub> O <sub>2</sub> S, HBr                                                                                                                                                                                                                                                                |
| 81 | C <sub>5</sub> H <sub>7</sub> N, C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> F <sub>2</sub> N                                                                                                                                                                                                                                                                                                                                                                           |
| 82 | C <sub>6</sub> H <sub>10</sub> , C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> O, C <sub>2</sub> H <sub>4</sub> ClF, C <sub>2</sub> H <sub>2</sub> N <sub>4</sub> , C <sub>2</sub> HF <sub>3</sub> , CCIFO                                                                                                                                                                                                                                                                |
| 83 | C <sub>5</sub> H <sub>9</sub> N, C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> , C <sub>4</sub> H <sub>5</sub> NO                                                                                                                                                                                                                                                                                                                                                                                         |
| 84 | C <sub>6</sub> H <sub>12</sub> , C <sub>5</sub> H <sub>8</sub> O, C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>4</sub> H <sub>4</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>4</sub> N <sub>4</sub> , C <sub>4</sub> H <sub>4</sub> S, C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> , CH <sub>2</sub> Cl <sub>2</sub>                                                                                                                                                                           |
| 85 | C <sub>5</sub> H <sub>11</sub> N, C <sub>4</sub> H <sub>7</sub> NO, C <sub>3</sub> H <sub>3</sub> NS, CH <sub>3</sub> N <sub>5</sub>                                                                                                                                                                                                                                                                                                                                                                     |
| 86 | C <sub>5</sub> H <sub>10</sub> O, C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>14</sub> , C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> S, C <sub>4</sub> H <sub>3</sub> Cl, C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>2</sub> H <sub>2</sub> N <sub>2</sub> S,<br>CHClF <sub>2</sub> , HF <sub>2</sub> O, Cl <sub>2</sub> O, F <sub>2</sub> OS                                                                                     |
| 87 | C <sub>5</sub> H <sub>13</sub> N, C <sub>4</sub> H <sub>9</sub> NO, C <sub>3</sub> H <sub>9</sub> N <sub>3</sub> , C <sub>3</sub> H <sub>5</sub> NS, C <sub>3</sub> H <sub>2</sub> ClN, ClF <sub>2</sub> N, F <sub>3</sub> NO                                                                                                                                                                                                                                                                            |
| 88 | C <sub>5</sub> H <sub>12</sub> O, C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>4</sub> H <sub>8</sub> S, C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> O, C <sub>3</sub> H <sub>4</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>12</sub> Si, C <sub>4</sub> H <sub>5</sub> Cl,<br>CF <sub>4</sub>                                                                                                                                                 |
| 89 | C <sub>4</sub> H <sub>11</sub> NO, C <sub>3</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>3</sub> H <sub>4</sub> ClN                                                                                                                                                                                                                                                                                                                                                                                     |
| 90 | C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>10</sub> S, C <sub>4</sub> H <sub>7</sub> Cl, C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>3</sub> H <sub>10</sub> OSi, C <sub>3</sub> H <sub>6</sub> OS, C <sub>3</sub> H <sub>3</sub> ClO,<br>C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> S, C <sub>2</sub> H <sub>2</sub> O <sub>4</sub> , C <sub>4</sub> H <sub>11</sub> P                             |
| 91 | C <sub>2</sub> H <sub>5</sub> NO <sub>3</sub> , CH <sub>5</sub> N <sub>3</sub> S, C <sub>3</sub> H <sub>6</sub> ClN                                                                                                                                                                                                                                                                                                                                                                                      |
| 92 | C <sub>7</sub> H <sub>8</sub> , C <sub>4</sub> H <sub>9</sub> Cl, C <sub>3</sub> H <sub>5</sub> ClO, C <sub>2</sub> H <sub>4</sub> O <sub>2</sub> S, C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>3</sub> H <sub>9</sub> FSi, C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> O                                                                                                                                                                                    |
| 93 | C <sub>6</sub> H <sub>7</sub> N, C <sub>5</sub> H <sub>3</sub> NO, C <sub>4</sub> H <sub>3</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                          |
| 94 | C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>10</sub> , C <sub>6</sub> H <sub>6</sub> O, C <sub>3</sub> H <sub>7</sub> ClO, C <sub>2</sub> H <sub>2</sub> S <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> O <sub>2</sub> SC <sub>3</sub> HF <sub>3</sub> , C <sub>2</sub> H <sub>3</sub> ClO <sub>2</sub> ,<br>C <sub>2</sub> Cl <sub>2</sub> , CH <sub>3</sub> Br                                                                                                                |
| 95 | C <sub>5</sub> H <sub>5</sub> NO, C <sub>6</sub> H <sub>9</sub> N, C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> , C <sub>2</sub> F <sub>3</sub> N                                                                                                                                                                                                                                                                                                                                                        |
| 96 | C <sub>7</sub> H <sub>12</sub> , C <sub>6</sub> H <sub>8</sub> O, C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>5</sub> H <sub>4</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O, C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> , C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> , C <sub>2</sub> H <sub>6</sub> F <sub>2</sub> Si                                                                                                                                           |
| 97 | C <sub>5</sub> H <sub>7</sub> NO, C <sub>6</sub> H <sub>11</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 98 | C <sub>7</sub> H <sub>14</sub> , C <sub>6</sub> H <sub>10</sub> O, C <sub>5</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>3</sub> H <sub>6</sub> N <sub>4</sub> , C <sub>5</sub> H <sub>16</sub> N <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> S,<br>C <sub>4</sub> H <sub>2</sub> O <sub>3</sub> , C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> , C <sub>2</sub> HClF <sub>2</sub> , CCl <sub>2</sub> O |
| 99 | C <sub>6</sub> H <sub>13</sub> N, C <sub>5</sub> H <sub>9</sub> NO, C <sub>4</sub> H <sub>5</sub> NS, C <sub>4</sub> H <sub>5</sub> NO <sub>2</sub> , CH <sub>3</sub> F <sub>2</sub> NS                                                                                                                                                                                                                                                                                                                  |

Table 4.44. (Continued)

|     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                        |
|-----|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 100 | C <sub>6</sub> H <sub>12</sub> O, C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>16</sub> , C <sub>4</sub> H <sub>4</sub> O <sub>3</sub> , C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S, C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>9</sub> F, C <sub>5</sub> H <sub>12</sub> Si, C <sub>4</sub> H <sub>4</sub> OS, C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>2</sub> H <sub>3</sub> F <sub>3</sub> O, C <sub>2</sub> F <sub>4</sub>                                                                                                                                                                                                                                                                                     |
| 101 | C <sub>6</sub> H <sub>15</sub> N, C <sub>5</sub> H <sub>11</sub> NO, C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>4</sub> H <sub>7</sub> NS, C <sub>2</sub> H <sub>3</sub> N <sub>3</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 102 | C <sub>6</sub> H <sub>14</sub> O, C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>10</sub> S, C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O, C <sub>4</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>2</sub> H <sub>2</sub> F <sub>4</sub> , C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> S, C <sub>8</sub> H <sub>6</sub> , CHCl <sub>2</sub> F, CHF <sub>3</sub> S, HF <sub>2</sub> PS, Cl <sub>2</sub> S                                                                                                                                                                                                                                                                                                                                                                      |
| 103 | C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> , C <sub>7</sub> H <sub>5</sub> N, C <sub>5</sub> H <sub>13</sub> NO, C <sub>4</sub> H <sub>13</sub> N <sub>3</sub> , C <sub>4</sub> H <sub>6</sub> CIN, C <sub>2</sub> H <sub>2</sub> CIN <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 104 | C <sub>5</sub> H <sub>12</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>12</sub> S, C <sub>5</sub> H <sub>9</sub> Cl, C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> OS, C <sub>8</sub> H <sub>8</sub> , C <sub>6</sub> H <sub>13</sub> F, C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>4</sub> H <sub>12</sub> N <sub>2</sub> O, C <sub>4</sub> H <sub>12</sub> OSi, C <sub>4</sub> H <sub>5</sub> ClO, C <sub>3</sub> H <sub>8</sub> N <sub>2</sub> S, CClF <sub>3</sub> , SiF <sub>4</sub>                                                                                                                                                                                                                      |
| 105 | C <sub>7</sub> H <sub>7</sub> N, C <sub>3</sub> H <sub>7</sub> NO <sub>3</sub> , C <sub>4</sub> H <sub>11</sub> NO <sub>2</sub> , C <sub>4</sub> H <sub>8</sub> CIN, CBrN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 106 | C <sub>8</sub> H <sub>10</sub> , C <sub>5</sub> H <sub>11</sub> Cl, C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>6</sub> O, C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>7</sub> ClO, C <sub>4</sub> H <sub>10</sub> OS, C <sub>3</sub> H <sub>6</sub> O <sub>2</sub> S, C <sub>2</sub> H <sub>3</sub> Br                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 107 | C <sub>7</sub> H <sub>9</sub> N, C <sub>6</sub> H <sub>5</sub> NO, C <sub>2</sub> H <sub>5</sub> NO <sub>4</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 108 | C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>8</sub> H <sub>12</sub> , C <sub>7</sub> H <sub>8</sub> O, C <sub>4</sub> H <sub>9</sub> ClO, C <sub>3</sub> H <sub>9</sub> ClSi, C <sub>3</sub> H <sub>3</sub> ClO <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>8</sub> S <sub>2</sub> , C <sub>2</sub> H <sub>5</sub> Br, C <sub>2</sub> H <sub>4</sub> O <sub>3</sub> S, SF <sub>4</sub>                                                                                                                                                                                                                                                                                                                                                               |
| 109 | C <sub>6</sub> H <sub>7</sub> NO, C <sub>7</sub> H <sub>11</sub> N, C <sub>2</sub> H <sub>4</sub> CINO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 110 | C <sub>8</sub> H <sub>14</sub> , C <sub>7</sub> H <sub>10</sub> O, C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> , C <sub>7</sub> H <sub>7</sub> F, C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> , C <sub>2</sub> H <sub>6</sub> O <sub>3</sub> S, C <sub>2</sub> H <sub>7</sub> O <sub>3</sub> P, C <sub>3</sub> H <sub>7</sub> ClO <sub>2</sub> , C <sub>6</sub> H <sub>10</sub> N <sub>2</sub>                                                                                                                                                                                                                                                                                                       |
| 111 | C <sub>7</sub> H <sub>13</sub> N, C <sub>6</sub> H <sub>9</sub> NO, C <sub>5</sub> H <sub>5</sub> NO <sub>2</sub> , C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> O, C <sub>2</sub> ClF <sub>2</sub> N, C <sub>6</sub> H <sub>6</sub> FN, C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> , C <sub>5</sub> H <sub>5</sub> NS                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| 112 | C <sub>8</sub> H <sub>16</sub> , C <sub>7</sub> H <sub>12</sub> O, C <sub>6</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>8</sub> S, C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O, C <sub>5</sub> H <sub>4</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> FO, C <sub>6</sub> H <sub>5</sub> Cl, C <sub>5</sub> H <sub>4</sub> OS, C <sub>3</sub> F <sub>4</sub> , C <sub>3</sub> H <sub>3</sub> F <sub>3</sub> O, CH <sub>2</sub> BrF                                                                                                                              |
| 113 | C <sub>7</sub> H <sub>15</sub> N, C <sub>6</sub> H <sub>11</sub> NO, C <sub>5</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>5</sub> H <sub>7</sub> NS, C <sub>5</sub> H <sub>4</sub> CIN, C <sub>3</sub> H <sub>3</sub> NO <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> F <sub>2</sub> NP                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 114 | C <sub>7</sub> H <sub>14</sub> O, C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>18</sub> , C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> OS, C <sub>6</sub> H <sub>4</sub> F <sub>2</sub> , C <sub>5</sub> H <sub>2</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>7</sub> Cl, C <sub>4</sub> H <sub>6</sub> N <sub>2</sub> S, C <sub>2</sub> H <sub>4</sub> Cl <sub>2</sub> O, C <sub>2</sub> HCl <sub>2</sub> F, C <sub>2</sub> HCIF <sub>2</sub> O, C <sub>2</sub> HF <sub>3</sub> O <sub>2</sub>                                                                                                                 |
| 115 | C <sub>6</sub> H <sub>13</sub> NO, C <sub>7</sub> H <sub>17</sub> N, C <sub>5</sub> H <sub>9</sub> NO <sub>2</sub> , C <sub>5</sub> H <sub>9</sub> NS, C <sub>4</sub> H <sub>5</sub> NOS, C <sub>3</sub> H <sub>5</sub> N <sub>3</sub> S, C <sub>5</sub> H <sub>13</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 116 | C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>16</sub> O, C <sub>6</sub> H <sub>12</sub> S, C <sub>9</sub> H <sub>8</sub> , C <sub>6</sub> H <sub>16</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>16</sub> Si, C <sub>6</sub> H <sub>9</sub> Cl, C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O, C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>4</sub> O <sub>4</sub> , C <sub>4</sub> H <sub>8</sub> N <sub>2</sub> S, C <sub>4</sub> H <sub>4</sub> S <sub>2</sub> , C <sub>2</sub> H <sub>3</sub> Cl <sub>2</sub> F, C <sub>2</sub> ClF                                                                                                                                               |
| 117 | C <sub>8</sub> H <sub>7</sub> N, C <sub>6</sub> H <sub>15</sub> NO, C <sub>5</sub> H <sub>11</sub> NO <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> CIN, C <sub>4</sub> H <sub>7</sub> NO <sub>3</sub> , C <sub>3</sub> H <sub>4</sub> CIN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 118 | C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>14</sub> S, C <sub>5</sub> H <sub>10</sub> O <sub>3</sub> , C <sub>9</sub> H <sub>10</sub> , C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> , C <sub>5</sub> H <sub>10</sub> OS, C <sub>6</sub> H <sub>15</sub> P, C <sub>7</sub> H <sub>15</sub> F, C <sub>6</sub> H <sub>11</sub> Cl, C <sub>5</sub> H <sub>14</sub> OSi, C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> O <sub>4</sub> , C <sub>4</sub> H <sub>3</sub> ClS, C <sub>4</sub> H <sub>10</sub> N <sub>2</sub> S, C <sub>4</sub> H <sub>14</sub> Si <sub>2</sub> , C <sub>3</sub> H <sub>3</sub> Br, C <sub>2</sub> H <sub>2</sub> ClF <sub>3</sub> , CHCl <sub>3</sub>                                               |
| 119 | C <sub>7</sub> H <sub>5</sub> NO, C <sub>6</sub> H <sub>4</sub> N <sub>3</sub> , C <sub>8</sub> H <sub>9</sub> N, C <sub>4</sub> H <sub>9</sub> NO <sub>3</sub> , C <sub>4</sub> H <sub>9</sub> NOS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 120 | C <sub>9</sub> H <sub>12</sub> , C <sub>8</sub> H <sub>8</sub> O, C <sub>4</sub> H <sub>8</sub> O <sub>2</sub> S, C <sub>4</sub> H <sub>8</sub> S <sub>2</sub> , C <sub>7</sub> H <sub>8</sub> S <sub>2</sub> , C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>13</sub> Cl, C <sub>5</sub> H <sub>12</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O, C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> , C <sub>4</sub> H <sub>8</sub> O <sub>4</sub> , C <sub>5</sub> H <sub>9</sub> OCl, C <sub>4</sub> H <sub>12</sub> O <sub>2</sub> Si, C <sub>3</sub> H <sub>5</sub> Br, CCl <sub>2</sub> F <sub>2</sub>                                                                                                                                                 |
| 121 | C <sub>8</sub> H <sub>11</sub> N, C <sub>7</sub> H <sub>7</sub> NO, C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> , C <sub>4</sub> H <sub>3</sub> N <sub>5</sub> , C <sub>7</sub> H <sub>3</sub> FN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 122 | C <sub>8</sub> H <sub>10</sub> O, C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>7</sub> ClO <sub>2</sub> , C <sub>4</sub> H <sub>10</sub> S <sub>2</sub> , C <sub>9</sub> H <sub>14</sub> , C <sub>3</sub> H <sub>7</sub> Br, C <sub>8</sub> H <sub>7</sub> F, C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>4</sub> H <sub>10</sub> O <sub>2</sub> S, C <sub>4</sub> H <sub>4</sub> Cl <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> O <sub>3</sub> S, C <sub>2</sub> H <sub>6</sub> N <sub>2</sub> S <sub>2</sub> , C <sub>2</sub> H <sub>3</sub> BrO                                                                                                                                                                 |
| 123 | C <sub>7</sub> H <sub>9</sub> NO, C <sub>6</sub> H <sub>5</sub> NO <sub>2</sub> , C <sub>8</sub> H <sub>13</sub> N, C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> , C <sub>4</sub> H <sub>4</sub> F <sub>3</sub> N, C <sub>3</sub> H <sub>9</sub> NO <sub>2</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 124 | C <sub>3</sub> H <sub>8</sub> O <sub>3</sub> S, C <sub>8</sub> H <sub>9</sub> F, C <sub>7</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>5</sub> FO, C <sub>5</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> F <sub>2</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>5</sub> ClO <sub>3</sub> , C <sub>2</sub> H <sub>5</sub> BrO, C <sub>2</sub> H <sub>4</sub> S <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                        |
| 125 | C <sub>8</sub> H <sub>15</sub> N, C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> , C <sub>6</sub> H <sub>7</sub> NS, C <sub>7</sub> H <sub>11</sub> NO, C <sub>6</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>2</sub> H <sub>8</sub> NO <sub>3</sub> P, C <sub>2</sub> H <sub>4</sub> CINO <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 126 | C <sub>9</sub> H <sub>18</sub> , C <sub>8</sub> H <sub>14</sub> O, C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> , C <sub>7</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>7</sub> Cl, C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O, C <sub>6</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>7</sub> H <sub>10</sub> S, C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> , C <sub>2</sub> H <sub>6</sub> S <sub>3</sub> , C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>7</sub> FO, C <sub>6</sub> H <sub>6</sub> OS, C <sub>4</sub> H <sub>6</sub> N <sub>4</sub> O, C <sub>4</sub> H <sub>5</sub> F <sub>3</sub> O, C <sub>3</sub> H <sub>2</sub> N <sub>6</sub> , C <sub>2</sub> ClO <sub>2</sub> |
| 127 | C <sub>7</sub> H <sub>13</sub> NO, C <sub>8</sub> H <sub>17</sub> N, C <sub>6</sub> H <sub>2</sub> CIN, C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> O, C <sub>5</sub> H <sub>5</sub> NO <sub>3</sub> , C <sub>6</sub> H <sub>9</sub> NO <sub>2</sub> , C <sub>4</sub> H <sub>5</sub> N <sub>3</sub> S, C <sub>2</sub> Cl <sub>2</sub> FN                                                                                                                                                                                                                                                                                                                                                                                                                                                              |

Table 4.44. (Continued)

|     |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                           |
|-----|-------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 128 | C <sub>8</sub> H <sub>16</sub> O, C <sub>9</sub> H <sub>20</sub> , C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>12</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>12</sub> S, C <sub>8</sub> H <sub>4</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>6</sub> OS, C <sub>6</sub> H <sub>5</sub> ClO, C <sub>4</sub> H <sub>4</sub> N <sub>2</sub> OS, C <sub>3</sub> H <sub>6</sub> Cl <sub>2</sub> O, C <sub>10</sub> H <sub>8</sub> , C <sub>2</sub> H <sub>6</sub> Cl <sub>2</sub> Si, C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> O <sub>2</sub> , CH <sub>2</sub> BrCl, C <sub>2</sub> H <sub>5</sub> ClO <sub>2</sub> S, C <sub>8</sub> H <sub>13</sub> F, HI                                                                                                                                                                                                  |
| 129 | C <sub>8</sub> H <sub>19</sub> N, C <sub>7</sub> H <sub>15</sub> NO, C <sub>6</sub> H <sub>11</sub> NO <sub>2</sub> , C <sub>9</sub> H <sub>7</sub> N, C <sub>7</sub> H <sub>3</sub> N <sub>3</sub> , C <sub>6</sub> H <sub>15</sub> N <sub>3</sub> , C <sub>5</sub> H <sub>7</sub> NO <sub>3</sub> , C <sub>5</sub> H <sub>7</sub> NOS, C <sub>4</sub> H <sub>7</sub> N <sub>3</sub> S, C <sub>4</sub> H <sub>4</sub> CIN <sub>3</sub> , C <sub>4</sub> H <sub>3</sub> NO <sub>2</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| 130 | C <sub>7</sub> H <sub>14</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>18</sub> O, C <sub>6</sub> H <sub>10</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> , C <sub>10</sub> H <sub>10</sub> , C <sub>9</sub> H <sub>6</sub> O, C <sub>7</sub> H <sub>14</sub> S, C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O, C <sub>6</sub> H <sub>4</sub> ClF, C <sub>5</sub> H <sub>6</sub> O <sub>4</sub> , C <sub>5</sub> H <sub>6</sub> S <sub>2</sub> , C <sub>3</sub> H <sub>5</sub> Cl <sub>2</sub> F, C <sub>5</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> N <sub>4</sub> S, C <sub>3</sub> H <sub>2</sub> ClF <sub>3</sub> , C <sub>3</sub> H <sub>2</sub> N <sub>2</sub> O <sub>2</sub> S, C <sub>2</sub> HCl <sub>3</sub> , CHBrF <sub>2</sub>                                                                                                                              |
| 131 | C <sub>9</sub> H <sub>9</sub> N, C <sub>7</sub> H <sub>17</sub> NO, C <sub>5</sub> H <sub>9</sub> NO <sub>3</sub> , C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> , C <sub>6</sub> H <sub>17</sub> N <sub>3</sub> , C <sub>6</sub> H <sub>13</sub> NO <sub>2</sub> , C <sub>4</sub> H <sub>9</sub> N <sub>3</sub> S, CF <sub>3</sub> NOS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 132 | C <sub>7</sub> H <sub>16</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>12</sub> O <sub>3</sub> , C <sub>10</sub> H <sub>12</sub> , C <sub>9</sub> H <sub>8</sub> O, C <sub>7</sub> H <sub>16</sub> S, C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>16</sub> OSi, C <sub>5</sub> H <sub>8</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>12</sub> OS, C <sub>6</sub> H <sub>9</sub> ClO, C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>12</sub> N <sub>2</sub> S, C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> S, C <sub>5</sub> H <sub>5</sub> ClO <sub>2</sub> , C <sub>4</sub> H <sub>4</sub> OS <sub>2</sub> , C <sub>3</sub> H <sub>12</sub> Si <sub>3</sub> , C <sub>3</sub> H <sub>4</sub> N <sub>2</sub> S <sub>2</sub> , C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> , C <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub> , C <sub>2</sub> F <sub>4</sub> O <sub>2</sub> |
| 133 | C <sub>9</sub> H <sub>11</sub> N, C <sub>8</sub> H <sub>7</sub> NO, C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> , C <sub>5</sub> H <sub>11</sub> NO <sub>3</sub> , C <sub>4</sub> H <sub>7</sub> NO <sub>2</sub> S, C <sub>3</sub> H <sub>4</sub> BrN, C <sub>2</sub> H <sub>3</sub> ClF <sub>3</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 134 | C <sub>9</sub> H <sub>10</sub> O, C <sub>10</sub> H <sub>14</sub> , C <sub>6</sub> H <sub>14</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> , C <sub>5</sub> H <sub>10</sub> O <sub>2</sub> S, C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> , C <sub>8</sub> H <sub>6</sub> S, C <sub>7</sub> H <sub>15</sub> Cl, C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>6</sub> H <sub>14</sub> OS, C <sub>6</sub> H <sub>11</sub> ClO, C <sub>5</sub> H <sub>11</sub> ClSi, C <sub>5</sub> H <sub>10</sub> S <sub>2</sub> , C <sub>5</sub> H <sub>7</sub> ClO <sub>2</sub> , C <sub>3</sub> H <sub>3</sub> F <sub>5</sub> , C <sub>3</sub> Cl <sub>2</sub> N <sub>2</sub> , C <sub>2</sub> H <sub>2</sub> Cl <sub>2</sub> F <sub>2</sub>                                                                            |
| 135 | C <sub>9</sub> H <sub>13</sub> N, C <sub>8</sub> H <sub>9</sub> NO, C <sub>7</sub> H <sub>5</sub> NS, C <sub>5</sub> H <sub>5</sub> N <sub>5</sub> , C <sub>7</sub> H <sub>5</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> N <sub>3</sub> O, C <sub>4</sub> H <sub>9</sub> NO <sub>2</sub> S, C <sub>3</sub> H <sub>6</sub> BrN, C <sub>3</sub> F <sub>3</sub> N <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                     |
| 136 | C <sub>9</sub> H <sub>12</sub> O, C <sub>10</sub> H <sub>16</sub> , C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>4</sub> H <sub>9</sub> Br, C <sub>8</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>8</sub> H <sub>12</sub> Si, C <sub>8</sub> H <sub>8</sub> S, C <sub>8</sub> H <sub>5</sub> Cl, C <sub>7</sub> H <sub>8</sub> N <sub>2</sub> O, C <sub>7</sub> H <sub>4</sub> O <sub>3</sub> , C <sub>5</sub> H <sub>12</sub> S <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> S, C <sub>5</sub> H <sub>12</sub> O <sub>4</sub> , C <sub>5</sub> H <sub>12</sub> OS, C <sub>5</sub> H <sub>9</sub> ClO <sub>2</sub> , C <sub>5</sub> H <sub>4</sub> N <sub>4</sub> O, C <sub>2</sub> HClF <sub>4</sub> , CCl <sub>3</sub> F                                                           |
| 137 | C <sub>8</sub> H <sub>11</sub> NO, C <sub>9</sub> H <sub>15</sub> N, C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> , C <sub>7</sub> H <sub>7</sub> NS, C <sub>7</sub> H <sub>4</sub> CIN, C <sub>6</sub> H <sub>7</sub> N <sub>3</sub> O, C <sub>5</sub> H <sub>6</sub> F <sub>3</sub> N, C <sub>5</sub> H <sub>3</sub> N <sub>3</sub> S, C <sub>3</sub> H <sub>7</sub> NO <sub>5</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                   |
| 138 | C <sub>10</sub> H <sub>18</sub> , C <sub>9</sub> H <sub>14</sub> O, C <sub>8</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>10</sub> S, C <sub>7</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>7</sub> Cl, C <sub>7</sub> H <sub>10</sub> N <sub>2</sub> O, C <sub>7</sub> H <sub>6</sub> OS, C <sub>6</sub> H <sub>10</sub> N <sub>4</sub> , C <sub>5</sub> H <sub>6</sub> N <sub>4</sub> O, C <sub>4</sub> H <sub>11</sub> O <sub>3</sub> P, C <sub>4</sub> H <sub>10</sub> O <sub>3</sub> S, C <sub>3</sub> H <sub>7</sub> BrO, C <sub>3</sub> H <sub>6</sub> S <sub>3</sub> , C <sub>2</sub> H <sub>3</sub> BrO <sub>2</sub> , C <sub>2</sub> F <sub>6</sub>                                                                                                                                                                                |
| 139 | C <sub>7</sub> H <sub>9</sub> NS, C <sub>9</sub> H <sub>17</sub> N, C <sub>7</sub> H <sub>13</sub> N <sub>3</sub> , C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> NO <sub>3</sub> , C <sub>5</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> NOS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 140 | C <sub>9</sub> H <sub>16</sub> O, C <sub>10</sub> H <sub>20</sub> , C <sub>8</sub> H <sub>9</sub> Cl, C <sub>8</sub> H <sub>12</sub> O <sub>2</sub> , C <sub>8</sub> H <sub>12</sub> S, C <sub>7</sub> H <sub>8</sub> O <sub>3</sub> , C <sub>5</sub> H <sub>10</sub> Cl <sub>2</sub> , C <sub>7</sub> H <sub>8</sub> OS, C <sub>8</sub> H <sub>9</sub> FO, C <sub>8</sub> H <sub>16</sub> N <sub>2</sub> , C <sub>8</sub> H <sub>6</sub> F <sub>2</sub> , C <sub>7</sub> H <sub>5</sub> ClO, C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> S, C <sub>6</sub> H <sub>4</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>4</sub> S <sub>2</sub> , C <sub>4</sub> H <sub>6</sub> Cl <sub>2</sub> O, C <sub>2</sub> H <sub>2</sub> BrCl                                                                                                                                             |
| 141 | C <sub>8</sub> H <sub>15</sub> NO, C <sub>7</sub> H <sub>11</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>11</sub> N <sub>3</sub> O, C <sub>6</sub> H <sub>7</sub> NO <sub>3</sub> , C <sub>9</sub> H <sub>19</sub> N, C <sub>7</sub> H <sub>15</sub> N <sub>3</sub> , C <sub>5</sub> H <sub>7</sub> N <sub>3</sub> S, C <sub>4</sub> H <sub>6</sub> F <sub>3</sub> NO, C <sub>4</sub> H <sub>3</sub> F <sub>4</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 142 | C <sub>8</sub> H <sub>14</sub> O <sub>2</sub> , C <sub>9</sub> H <sub>18</sub> O, C <sub>10</sub> H <sub>22</sub> , C <sub>6</sub> H <sub>6</sub> O <sub>4</sub> , C <sub>8</sub> H <sub>14</sub> S, C <sub>3</sub> H <sub>4</sub> Cl <sub>2</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>7</sub> ClO, C <sub>11</sub> H <sub>10</sub> , C <sub>9</sub> H <sub>15</sub> F, C <sub>8</sub> H <sub>18</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>14</sub> N <sub>2</sub> O, C <sub>7</sub> H <sub>10</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>10</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> O <sub>2</sub> S, C <sub>5</sub> H <sub>6</sub> N <sub>2</sub> OS, C <sub>4</sub> H <sub>8</sub> Cl <sub>2</sub> O, C <sub>4</sub> H <sub>5</sub> ClF <sub>2</sub> O, C <sub>2</sub> H <sub>4</sub> BrCl, C <sub>2</sub> HBrF <sub>2</sub> , CH <sub>3</sub> I                                                   |
| 143 | C <sub>10</sub> H <sub>9</sub> N, C <sub>8</sub> H <sub>17</sub> NO, C <sub>7</sub> H <sub>13</sub> NO <sub>2</sub> , C <sub>9</sub> H <sub>21</sub> N, C <sub>7</sub> H <sub>10</sub> CIN, C <sub>6</sub> H <sub>13</sub> N <sub>3</sub> O, C <sub>6</sub> H <sub>9</sub> NO <sub>3</sub> , C <sub>4</sub> H <sub>9</sub> NOS, C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> S, C <sub>2</sub> Cl <sub>3</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                          |
| 144 | C <sub>8</sub> H <sub>16</sub> O <sub>2</sub> , C <sub>9</sub> H <sub>20</sub> O, C <sub>9</sub> H <sub>8</sub> N <sub>2</sub> , C <sub>7</sub> H <sub>12</sub> O <sub>3</sub> , C <sub>6</sub> H <sub>8</sub> O <sub>4</sub> , C <sub>10</sub> H <sub>8</sub> O, C <sub>11</sub> H <sub>12</sub> , C <sub>8</sub> H <sub>16</sub> S, C <sub>8</sub> H <sub>13</sub> Cl, C <sub>7</sub> H <sub>16</sub> N <sub>2</sub> O, C <sub>7</sub> H <sub>12</sub> OS, C <sub>6</sub> H <sub>9</sub> CIN <sub>2</sub> , C <sub>5</sub> H <sub>8</sub> N <sub>2</sub> O <sub>3</sub> , C <sub>3</sub> H <sub>3</sub> Cl <sub>3</sub>                                                                                                                                                                                                                                                                                                                 |
| 145 | C <sub>10</sub> H <sub>11</sub> N, C <sub>9</sub> H <sub>7</sub> NO, C <sub>8</sub> H <sub>7</sub> N <sub>3</sub> , C <sub>7</sub> H <sub>15</sub> NO <sub>2</sub> , C <sub>6</sub> H <sub>11</sub> NO <sub>3</sub> , C <sub>5</sub> H <sub>11</sub> N <sub>3</sub> S, C <sub>3</sub> H <sub>3</sub> N <sub>3</sub> O <sub>2</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 146 | C <sub>8</sub> H <sub>18</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>14</sub> O <sub>3</sub> , C <sub>8</sub> H <sub>18</sub> S, C <sub>6</sub> H <sub>10</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>10</sub> O <sub>2</sub> S, C <sub>11</sub> H <sub>14</sub> , C <sub>10</sub> H <sub>10</sub> O, C <sub>9</sub> H <sub>10</sub> N <sub>2</sub> , C <sub>10</sub> H <sub>7</sub> F, C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> O, C <sub>7</sub> H <sub>18</sub> OSi, C <sub>7</sub> H <sub>14</sub> OS, C <sub>7</sub> H <sub>6</sub> N <sub>4</sub> , C <sub>6</sub> H <sub>14</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> OS <sub>2</sub> , C <sub>3</sub> H <sub>5</sub> Cl <sub>3</sub> , C <sub>3</sub> H <sub>3</sub> BrN <sub>2</sub> , C <sub>2</sub> HCl <sub>3</sub> O, CHBrClF                                                                |
| 147 | C <sub>10</sub> H <sub>13</sub> N, C <sub>9</sub> H <sub>9</sub> NO, C <sub>8</sub> H <sub>9</sub> N <sub>3</sub> , C <sub>8</sub> H <sub>5</sub> NO <sub>2</sub> , C <sub>7</sub> H <sub>5</sub> N <sub>3</sub> O, C <sub>6</sub> H <sub>13</sub> NO <sub>3</sub> , C <sub>5</sub> H <sub>9</sub> NO <sub>4</sub> , C <sub>2</sub> H <sub>2</sub> BrN <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |

Table 4.44. (Continued)

|                  |                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
|------------------|--------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------------|
| 148              | C <sub>11</sub> H <sub>16</sub> , C <sub>10</sub> H <sub>12</sub> O, C <sub>9</sub> H <sub>8</sub> O <sub>2</sub> , C <sub>7</sub> H <sub>8</sub> N <sub>4</sub> , C <sub>9</sub> H <sub>12</sub> N <sub>2</sub> , C <sub>6</sub> H <sub>12</sub> O <sub>2</sub> S, C <sub>8</sub> H <sub>17</sub> Cl, C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O, C <sub>8</sub> H <sub>4</sub> O <sub>3</sub> , C <sub>9</sub> H <sub>8</sub> S, C <sub>7</sub> H <sub>16</sub> O <sub>3</sub> , C <sub>7</sub> H <sub>16</sub> OS, C <sub>7</sub> H <sub>4</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>12</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O, C <sub>5</sub> H <sub>8</sub> O <sub>3</sub> S, C <sub>3</sub> HF <sub>5</sub> O, C <sub>2</sub> H <sub>3</sub> Cl <sub>3</sub> O, C <sub>2</sub> Cl <sub>3</sub> F, CBrF <sub>3</sub> |
| 149              | C <sub>10</sub> H <sub>15</sub> N, C <sub>9</sub> H <sub>11</sub> NO, C <sub>7</sub> H <sub>7</sub> N <sub>3</sub> O, C <sub>8</sub> H <sub>11</sub> N <sub>3</sub> , C <sub>8</sub> H <sub>7</sub> NO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| 150              | C <sub>10</sub> H <sub>14</sub> O, C <sub>9</sub> H <sub>10</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>14</sub> S <sub>2</sub> , C <sub>8</sub> H <sub>10</sub> N <sub>2</sub> O, C <sub>6</sub> H <sub>11</sub> ClO <sub>2</sub> , C <sub>5</sub> H <sub>11</sub> Br, C <sub>11</sub> H <sub>18</sub> , C <sub>8</sub> H <sub>14</sub> N <sub>2</sub> , C <sub>9</sub> H <sub>10</sub> S, C <sub>8</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>7</sub> H <sub>6</sub> N <sub>2</sub> S, C <sub>6</sub> H <sub>14</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>14</sub> O <sub>2</sub> S, C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O, C <sub>6</sub> H <sub>2</sub> F <sub>4</sub> , C <sub>3</sub> F <sub>6</sub> , C <sub>2</sub> H <sub>2</sub> Cl <sub>3</sub> F                                                                                                    |
| 151 <sup>2</sup> | (see m/z 137) C <sub>7</sub> H <sub>5</sub> NO <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                    |
| 152              | (see m/z 138) C <sub>8</sub> H <sub>5</sub> ClO, C <sub>6</sub> H <sub>10</sub> Cl <sub>2</sub> , CCl <sub>4</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 153              | (see m/z 139) C <sub>9</sub> H <sub>15</sub> NO, C <sub>7</sub> H <sub>5</sub> CINO                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                            |
| 154              | (see m/z 140; C <sub>10</sub> H <sub>8</sub> O has highest occurrence of data base) C <sub>8</sub> H <sub>7</sub> ClO, C <sub>2</sub> ClO, C <sub>2</sub> ClF <sub>5</sub> , C <sub>8</sub> H <sub>10</sub> OS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| 155              | (see m/z 141) C <sub>8</sub> H <sub>13</sub> NS                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 156              | (see m/z 142) C <sub>7</sub> H <sub>5</sub> ClO <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> Br, C <sub>6</sub> H <sub>4</sub> O <sub>5</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 157              | (see m/z 143) C <sub>5</sub> H <sub>4</sub> BrN                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 158              | (see m/z 144) CF <sub>6</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 159              | (see m/z 145) C <sub>6</sub> H <sub>9</sub> NS <sub>2</sub> , C <sub>5</sub> H <sub>6</sub> CIN <sub>3</sub> O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                 |
| 160              | (see m/z 146) C <sub>7</sub> H <sub>20</sub> Si <sub>2</sub> , C <sub>6</sub> H <sub>9</sub> Br, C <sub>5</sub> H <sub>16</sub> Si <sub>3</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |
| 161              | (see m/z 147) C <sub>6</sub> H <sub>5</sub> Cl <sub>2</sub> N                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 162              | (see m/z 148) C <sub>10</sub> H <sub>7</sub> Cl, C <sub>8</sub> H <sub>6</sub> N <sub>2</sub> S, C <sub>6</sub> H <sub>11</sub> Br, C <sub>4</sub> F <sub>6</sub> , C <sub>6</sub> H <sub>4</sub> Cl <sub>2</sub> O, CHBrCl <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                       |
| 163              | (see m/z 149) C <sub>7</sub> H <sub>9</sub> N <sub>5</sub> , C <sub>3</sub> H <sub>2</sub> BrNS, CCl <sub>3</sub> NO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 164              | (see m/z 150) C <sub>9</sub> H <sub>8</sub> OS, C <sub>8</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>5</sub> CIN <sub>2</sub> , C <sub>7</sub> H <sub>16</sub> O <sub>4</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>4</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>9</sub> BrO, C <sub>5</sub> H <sub>8</sub> O <sub>2</sub> S <sub>2</sub> , C <sub>2</sub> Cl <sub>4</sub> , CBrClF <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 165              | (see m/z 137, 151) C <sub>6</sub> H <sub>7</sub> N <sub>5</sub> O                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                              |
| 166              | (see m/z 138, 152) C <sub>13</sub> H <sub>10</sub> , C <sub>8</sub> H <sub>6</sub> O <sub>4</sub> , C <sub>8</sub> H <sub>6</sub> O <sub>2</sub> S, C <sub>8</sub> H <sub>6</sub> S <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>6</sub> N <sub>4</sub> S, C <sub>3</sub> H <sub>6</sub> N <sub>2</sub> O <sub>6</sub> , C <sub>3</sub> ClF <sub>5</sub> , C <sub>3</sub> F <sub>6</sub> O                                                                                                                                                                                                                                                                                                                                                                                                                               |
| 167              | (see m/z 139, 153) C <sub>7</sub> H <sub>13</sub> N <sub>5</sub> , C <sub>7</sub> H <sub>5</sub> NO <sub>4</sub> , C <sub>7</sub> H <sub>5</sub> NS <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                               |
| 168              | (see m/z 140, 154) C <sub>13</sub> H <sub>12</sub> , C <sub>9</sub> H <sub>16</sub> N <sub>2</sub> O, C <sub>8</sub> H <sub>8</sub> O <sub>4</sub> , C <sub>8</sub> H <sub>8</sub> O <sub>2</sub> S, C <sub>8</sub> H <sub>8</sub> S <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> N <sub>2</sub> O <sub>4</sub> , C <sub>6</sub> HF <sub>5</sub> , C <sub>3</sub> H <sub>5</sub> I, C <sub>2</sub> HCl <sub>3</sub> F <sub>2</sub> , Cl <sub>4</sub> Si                                                                                                                                                                                                                                                                                                                                                                                                                        |
| 169              | (see m/z 141, 155) C <sub>8</sub> H <sub>8</sub> CINO, C <sub>7</sub> H <sub>7</sub> NO <sub>2</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                         |
| 170              | (see m/z 142, 156) C <sub>9</sub> H <sub>16</sub> NO <sub>2</sub> , C <sub>8</sub> H <sub>10</sub> S <sub>2</sub> , C <sub>3</sub> H <sub>6</sub> S <sub>4</sub> , C <sub>2</sub> Cl <sub>2</sub> F <sub>4</sub> , C <sub>2</sub> F <sub>6</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 171              | (see m/z 143, 157) C <sub>7</sub> H <sub>9</sub> NO <sub>2</sub> S, C <sub>6</sub> H <sub>9</sub> N <sub>3</sub> O <sub>3</sub> , C <sub>5</sub> H <sub>2</sub> CIN <sub>3</sub> S                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                             |
| 172              | (see m/z 144, 158) C <sub>12</sub> H <sub>9</sub> F, C <sub>8</sub> H <sub>6</sub> Cl <sub>2</sub> , C <sub>8</sub> H <sub>9</sub> ClO <sub>2</sub> , C <sub>7</sub> H <sub>8</sub> O <sub>3</sub> S, C <sub>6</sub> H <sub>8</sub> N <sub>2</sub> O <sub>2</sub> S, C <sub>6</sub> H <sub>5</sub> BrO, C <sub>6</sub> H <sub>4</sub> O <sub>6</sub> , CH <sub>2</sub> Br <sub>2</sub><br>(see m/z 145, 159) C <sub>6</sub> H <sub>4</sub> CINOS, C <sub>5</sub> H <sub>8</sub> CIN <sub>5</sub>                                                                                                                                                                                                                                                                                                                                                                               |
| 173              | (see m/z 146, 160) C <sub>11</sub> H <sub>10</sub> S, C <sub>10</sub> H <sub>6</sub> O <sub>3</sub> , C <sub>10</sub> H <sub>6</sub> OS, C <sub>9</sub> H <sub>6</sub> N <sub>2</sub> O <sub>2</sub> , C <sub>6</sub> H <sub>4</sub> BrF,                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                      |
| 174              | C <sub>5</sub> F <sub>6</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                  |
| 175              | (see m/z 147, 161) C <sub>8</sub> H <sub>5</sub> N <sub>3</sub> O <sub>2</sub> , C <sub>5</sub> H <sub>9</sub> N <sub>3</sub> S <sub>2</sub> , C <sub>7</sub> H <sub>10</sub> CINO <sub>2</sub>                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                                |

1. Compositions are listed by m/z value, ranked in decreasing order of Occurrence probability for compounds in the *Registry of Mass Spectral Data* (Stenhagen *et al.* 1974). Only the more probable combinations of the elements H, C, N, O, F, Si, P, S, Cl, Br and I are included. Note that these are odd-electron ion compositions; many common even-electron fragment ions have compositions differing by  $\pm 1$  hydrogen atom, and can therefore be found  $\pm 1$  mass unit from those listed. The above table can also be used to suggest possible elemental compositions of fragment ions
2. For masses above 150 the only compositions included are those for which a corresponding composition differing by a CH<sub>2</sub> less unit.

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## Chapter 5

### Units and Measurements

#### 5.1 Fundamental Physical Constants

#### 5.2 Units

#### 5.3 Prefixes

#### 5.4 Conversion Factors

### 5.1 Fundamental Physical Constants

Table 5.1. Physical Constants

| Symbol | Name                       | Value                       | Units                     |
|--------|----------------------------|-----------------------------|---------------------------|
| amu    | Atomic Mass Unit           | $1.6605655 \times 10^{-24}$ | g                         |
| $N_0$  | Avogadro's Number          | $6.022045 \times 10^{23}$   | units/mole                |
| K      | Boltzman's Constant        | $1.380663 \times 10^{-16}$  | erg/ $^{\circ}$ K         |
| e      | Electron Charge            | $1.6021892 \times 10^{-19}$ | coulomb                   |
| $m_e$  | Electron Rest Mass         | $9.109534 \times 10^{-28}$  | g                         |
|        |                            | $5.485803 \times 10^{-4}$   | amu                       |
| eV     | Electron Volt              | $1.60 \times 10^{-19}$      | joule                     |
| F      | Faraday's Constant         | $9.648456 \times 10^4$      | coulombs/equiv            |
|        |                            | $2.8925342 \times 10$       | cal/volt                  |
| R      | Gas Constant               | $8.2056 \times 10^{-2}$     | l atm/ $^{\circ}$ K-mole  |
|        |                            | 8.3144                      | joules/ $^{\circ}$ K-mole |
|        |                            | $8.3144 \times 10^7$        | erg/ $^{\circ}$ K-mole    |
|        |                            | 1.9872                      | cal/ $^{\circ}$ K-mole    |
| $m_n$  | Neutron Rest Mass          | $1.6749543 \times 10^{-24}$ | g                         |
|        |                            | 1.0086650                   | amu                       |
| h      | Planck's Constant          | $6.626176 \times 10^{-27}$  | erg/sec                   |
| $m_p$  | Proton Rest Mass           | $1.6726485 \times 10^{-24}$ | g                         |
|        |                            | 1.0072674                   | amu                       |
| $R^*$  | Rydberg Constant           | $1.0973718 \times 10^5$     | cm                        |
| c      | Speed of Light (in vacuum) | $2.9979246 \times 10^{10}$  | cm/sec                    |
| atm    | Standard Pressure          | 101.3                       | kPa                       |
|        |                            | 760                         | mmHg                      |

## 5.2 Units

### 5.2.1 Base SI Units

Table 5.2. Base SI Units

| Symbol | Physical Quantity         | Name of Base Unit |
|--------|---------------------------|-------------------|
| m      | Length                    | Meter             |
| kg     | Mass                      | Kilogram          |
| s      | Time                      | Second            |
| A      | Electric Current          | Ampere            |
| K      | Thermodynamic Temperature | Kelvin            |
| mol    | Amount of Substance       | Mole              |
| cd     | Luminous Intensity        | Candela           |

### 5.2.2 Derived SI Units

Table 5.3. Common Derived SI Units

| Symbol | Physical Quantity | Name of Unit | Definition of Unit                    |
|--------|-------------------|--------------|---------------------------------------|
| Å      | length            | Angstrom     | $10^{-10}\text{m}$                    |
| μ      | length            | Micron       | $10^{-6}\text{m}$                     |
| dyn    | force             | Dyne         | $10^{-5}\text{N}$                     |
| bar    | pressure          | Bar          | $10^{-5}\text{N} \cdot \text{m}^{-2}$ |
| erg    | energy            | Erg          | $10^{-7}\text{J}$                     |

Table 5.4. Derived SI Units with Special Names

| Symbol | Physical Quantity     | Name of Unit | Definition of Unit                    |
|--------|-----------------------|--------------|---------------------------------------|
| Hz     | frequency             | Hertz        | $1/\text{s}$                          |
| J      | energy                | Joule        | $\text{N} \cdot \text{m}$             |
| N      | force                 | Newton       | $\text{kg} \cdot \text{m}/\text{s}^2$ |
| W      | power                 | Watt         | $\text{J}/\text{s}$                   |
| Pa     | pressure              | Pascal       | $\text{N}/\text{m}^2$                 |
| C      | electric charge       | Coulomb      | $\text{A} \cdot \text{s}$             |
| V      | difference            | Volt         | $\text{W}/\text{A}$                   |
| Ohm    | electrical resistance | Ohm          | $\text{V}/\text{A}$                   |

### 5.2.3 Non SI Units

Table 5.5. Non SI Units

| Symbol            | Physical Quantity | Name of Unit           | Definition of Unit                          |
|-------------------|-------------------|------------------------|---------------------------------------------|
| in                | length            | inch                   | $2.54 \cdot 10^{-2} \text{m}$               |
| lb                | mass              | pound                  | $0.45359237 \text{kg}$                      |
| kgf               | force             | kilogram-force         | $9.80665 \text{N}$                          |
| atm               | pressure          | atmosphere             | $101.325 \text{N} \cdot \text{m}^{-2}$      |
| torr              | pressure          | torr                   | $(101.325/760)\text{N} \cdot \text{m}^{-2}$ |
| BTU               | energy            | British Thermal Unit   | $1055.056 \text{J}$                         |
| kW                | energy            | kilowatt-hour          | $3.6 \times 10^6 \text{J}$                  |
| cal <sub>th</sub> | energy            | thermochemical calorie | $4.184 \text{J}$                            |

Table 5.5. (Continued)

|     |                        |                  |                                                                 |
|-----|------------------------|------------------|-----------------------------------------------------------------|
| eV  | energy                 | electron Volt    | $1.60219 \cdot 10^{-19} \text{ J}$                              |
| amu | mass                   | atomic mass unit | $1.6605655 \cdot 10^{-27} \text{ kg}$                           |
| D   | electric dipole moment | Debye            | $3.3356 \cdot 10^{-30} \text{ A} \cdot \text{m} \cdot \text{s}$ |
| F   | charge per molecule    | Faraday          | $9.648456 \cdot 10^4 \text{ C mol}^{-1}$                        |

## 5.3 Prefixes

### 5.3.1 SI Prefixes

Table 5.6. SI Prefixes

| Factor     | Prefix | Symbol |
|------------|--------|--------|
| $10^{15}$  | penta  | P      |
| $10^{12}$  | tera   | T      |
| $10^9$     | giga   | G      |
| $10^6$     | mega   | M      |
| $10^3$     | kilo   | k      |
| $10^2$     | hecto  | h      |
| $10^1$     | deka   | da     |
| $10^{-1}$  | deci   | d      |
| $10^{-2}$  | centi  | c      |
| $10^{-3}$  | milli  | m      |
| $10^{-6}$  | micro  | $\mu$  |
| $10^{-9}$  | nano   | n      |
| $10^{-12}$ | pico   | p      |
| $10^{-15}$ | femto  | f      |

### 5.3.2 Greek Prefixes

Table 5.7. Greek Prefixes

| Value | Prefix |
|-------|--------|
| 1     | mono   |
| 2     | di     |
| 3     | tri    |
| 4     | tetra  |
| 5     | penta  |
| 6     | hexa   |
| 7     | hepta  |
| 8     | octa   |
| 9     | ennea  |
| 10    | deca   |

## 5.4 Conversion Factors

### 5.4.1 Linear Conversion

1 inch = 2.5400 centimeters  
 1 foot = 0.3048 meter  
 1 yard = 0.9144 meter  
 1 mile = 1.6093 kilometers

1 centimeter = 0.3937 inch  
 1 meter = 3.281 feet  
 1 meter = 1.0936 yards  
 1 kilometer = 0.62137 miles

### 5.4.2 Area Conversion

1 sq. inch = 6.4516 sq. centimeters  
 1 sq. foot = 0.0929 sq. meter  
 1 sq. yard = 0.8361 sq. meter  
 1 sq. mile = 2.59 sq kilometers

1 sq. centimeter = 0.155 sq. inch  
 1 sq. meter = 10.764 sq. feet  
 1 sq. meter = 1.196 sq. yards  
 1 sq. kilometers = 0.3861 sq. mile

### 5.4.3 Cubic Conversion

1 cu. inch = 16.3872 cu. centimeters  
 1 cu. foot = 28.3 17 cu. centimeters  
 1 cu. yard = 0.7645 cu. meter

1 cu. centimeter = 0.0610 cu. inch  
 1 cu. decimeter = 0.0353 cu. foot  
 1 cu. meter = 1.3079 cu. yards

### 5.4.4 Capacity Conversion

1 fluid ounce = 29.5730 milliliters  
 1 liquid pint = 0.4732 liter  
 1 liquid quart = 0.9463 liter  
 1 gallon = 3.7853 liters  
 1 dry quart = 1.1012 liters

1 milliliter = 0.0338 fluid ounce  
 1 liter = 2.1134 fluid pints  
 1 liter = 1.0567 liquid quarts  
 1 liter = 0.2642 gallon  
 1 liter = 0.908 1 dry quart

### 5.4.5 Weight Conversion

1 ounce = 28.350 grams  
 1 pound = 0.4536 kilograms

1 gram = 0.0353 ounce  
 1 kilogram = 2.2046 pounds

### 5.4.6 Temperature Conversion

| Temperature<br>given in | To Convert to                  |                                 |                            |
|-------------------------|--------------------------------|---------------------------------|----------------------------|
|                         | $^{\circ}\text{C}$             | K                               | $^{\circ}\text{F}$         |
|                         | $^{\circ}\text{C}$             | $^{\circ}\text{C} + 273.15$     | $1.8^{\circ}\text{C} + 32$ |
|                         | $\text{K} - 273.15$            | K                               | $1.8\text{K} - 459.4$      |
| $^{\circ}\text{F}$      | $0.556^{\circ}\text{F} - 17.8$ | $0.556^{\circ}\text{F} + 255.3$ | $^{\circ}\text{F}$         |

## Chapter 6

### Mathematical Concepts

#### 6.1 Algebraic Formulas

#### 6.2 Plane Figure Formulas

#### 6.3 Solid Figure Formulas

### 6.1 Algebraic Formulas

#### 6.1.1 Laws of Exponents

$$x^m \cdot x^n = x^{m+n}$$

$$x^m \div x^n = x^{m-n}$$

$$(x^m)^n = x^{m \cdot n}$$

$$(x \cdot y)^m = x^m \cdot y^m$$

$$(x/y)^m = x^m/y^m$$

$$x^0 = 1$$

$$x^{1/n} = \sqrt[n]{x}$$

$$x^{-m} = 1/x^m$$

#### 6.1.2 Laws of Logarithms

$$\log (A \cdot B) = \log A + \log B$$

$$\log \frac{A}{B} = \log A - \log B$$

$$\log A^b = b \log A$$

$$\log \sqrt[b]{A} = \frac{\log A}{b} = \frac{1}{b} \log A$$

#### 6.1.3 Quadratic Equation

$$ax^2 + bx + c = 0 \text{ (Where } a \neq 0 \text{ and } a, b, \text{ and } c \text{ are real numbers)}$$

If the roots of  $ax^2 + bx + c = 0$  are represented by  $r_1$  and  $r_2$ , then:

$$1. r_1 = \frac{-b + \sqrt{b^2 - 4ac}}{2a} \quad \text{and} \quad r_2 = \frac{-b - \sqrt{b^2 - 4ac}}{2a}$$

$$2. r_1 + r_2 = -b/a$$

$$3. r_1 r_2 = c/a$$

$$4. x^2 - (r_1 + r_2)x + r_1 r_2 = 0$$

Using the discriminant to determine the nature of the roots of  $ax^2 + bx + c = 0$ :

5. If  $b^2 - 4ac$  is zero or positive, the roots are real.

6. If  $b^2 - 4ac$  is negative, the roots are imaginary.

7. If  $b^2 - 4ac$  is zero, the roots are equal.

8. If  $b^2 - 4ac$  is not zero, the roots are unequal.

9. If  $b^2 - 4ac$  is a perfect square, the roots are rational numbers.

10. If  $b^2 - 4ac$  is positive and not a perfect square, the roots are irrational numbers.

#### 6.1.4 Graphs ( $a, b, c, m$ , and $r$ are real numbers)

1. The slope of a line that passes through two points  $P_1(x_1, y_1)$  and  $P_2(x_2, y_2)$ ,  $x_1 \neq x_2$ :

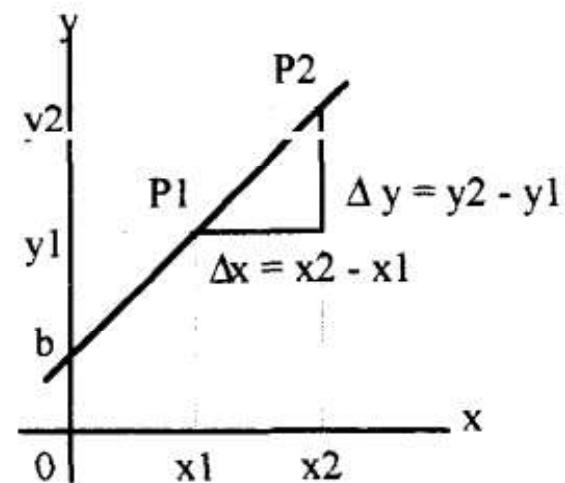
$$m = \text{slope of } P_1P_2 = \frac{y_2 - y_1}{x_2 - x_1} = \frac{\Delta y}{\Delta x}$$

2. Equation of a straight line:  $y = mx + b$   
where  $m$  = slope of the line and  $b$  =  $y$  intercept.

3. Equation of a parabola:  $y = ax^2 + bx + c$  or  $x = ay^2 + by + c$ ,  $a \neq 0$ .

4. Equation of a circle:  $(x-h)^2 + (y-k)^2 = r^2$  where the center is  $(h, k)$  and the radius is  $r$ ,  $r > 0$ .

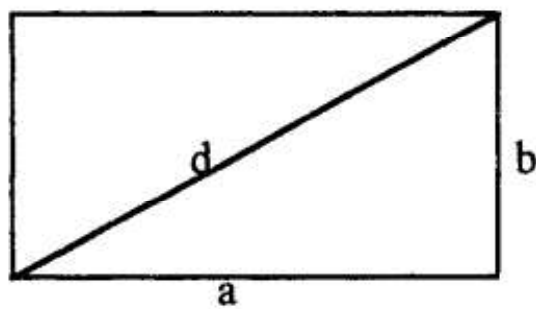
5. Equation of a circle:  $x^2 + y^2 = r^2$  where the center is at the origin and the radius is  $r$ ,  $r > 0$ .



6. Equation of an ellipse:  $ax^2 + by^2 = c$  where the center is at the origin;  $a$ ,  $b$ , and  $c$  are positive;  $c \neq 0$ .
7. Equation of a hyperbola:  $ax^2 - by^2 = c$ ,  $ay^2 - bx^2 = c$  where the center is at the origin;  $a$  and  $b$  are positive. Also  $xy = k$ ,  $k$  is a constant.
8. At the turning point of the parabola  $y = ax^2 + bx + c$ ,  $x = -b/2a$
9. The graph of the parabola  $y = ax^2 + bx + c$  opens upward and has a minimum turning point when  $a$  is positive,  $a > 0$ .
10. The graph of the parabola  $y = ax^2 + bx + c$  opens downward and has a maximum turning point when  $a$  is negative,  $a < 0$ .

## 6.2 Plane Figure Formulas

### 6.2.1 Rectangle



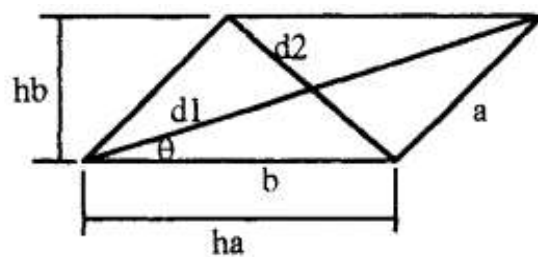
Area  $A = ab$

Perimeter  $P = 2(a + b)$

Diagonal  $d = \sqrt{a^2 + b^2}$

If  $a = b$  then it is a square

### 6.2.2 Parallelogram



Area  $A = ah_a = bh_b = ab \sin \theta$

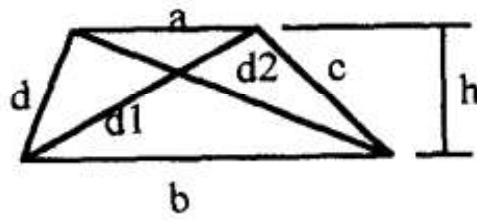
Perimeter  $P = 2(a + b)$

Diagonal:

$$d1 = \sqrt{a^2 + b^2 - 2ab \cos \theta}$$

$$d2 = \sqrt{a^2 + b^2 + 2ab \cos \theta}$$

### 6.2.3 Trapezoid



$$\text{Area } A = \frac{(a+b)h}{2}$$

$$\text{Perimeter } P = a + b + c + d$$

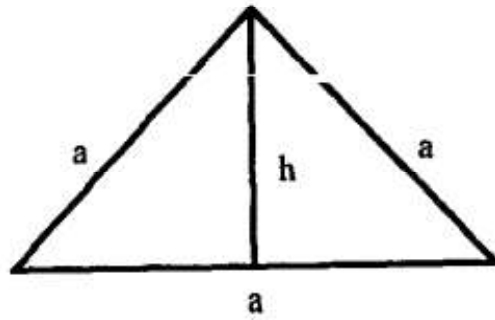
$$\text{Diagonal } = d_1 = \sqrt{ab + \frac{ac^2 - bd^2}{a-b}}$$

$$d_2 = \sqrt{ab + \frac{ad^2 - bc^2}{a-b}}$$

$$\text{Height } = h = \frac{2}{a-b} \cdot \sqrt{s(s-a+b)(s-c)(s-d)}$$

$$\text{where } s = \frac{1}{2}(a+b+c+d)$$

### 6.2.4 Equilateral Triangle



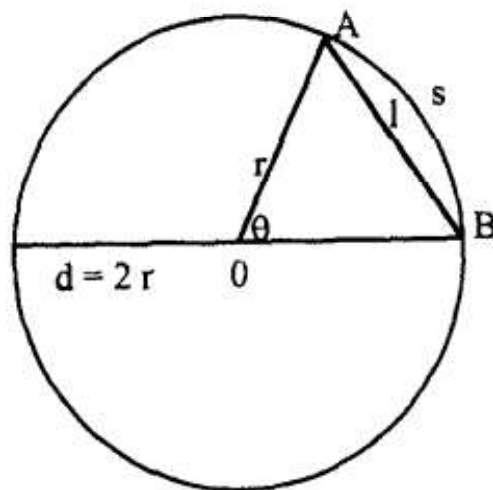
$a$  = all sides equal

$$\text{Area } A = a^2 \frac{\sqrt{3}}{4} = 0.433 a^2$$

$$\text{Perimeter } P = 3 a$$

$$h = \frac{\sqrt{3}}{2} a = 0.866 a$$

### 6.2.5 Circle



$$\text{Area of circle } A = \pi r^2 = 3.14159 r^2$$

$$= \pi \frac{d^2}{4} = 0.78539 d^2$$

$$\text{Area of sector AsBOA} = \frac{\pi \theta r^2}{360}$$

$$\text{Area of segment AsBlA} = \frac{\pi r^2 \theta}{360} - \frac{r^2 \sin \theta}{2}$$

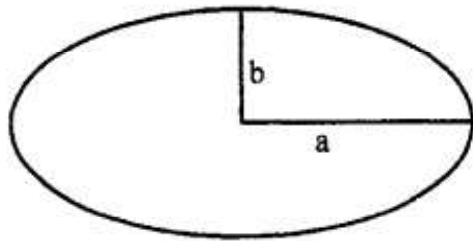
$$\text{Circumference} = 2 \pi r = 6.28318 r$$

$$= \pi d = 3.14159 d$$

$$\text{Length of chord AlB} = 2 r \sin \frac{\theta}{2}$$

$$\text{Length of arc AsB} = \frac{\pi r \theta}{180}$$

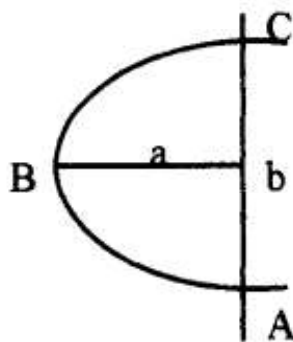
### 6.2.6 Ellipse



$$\text{Area } A = \pi ab = 3.14159 ab$$

$$\text{Circumference} \approx 2\pi \sqrt{\frac{a^2 + b^2}{2}}$$

### 6.2.7 Parabola

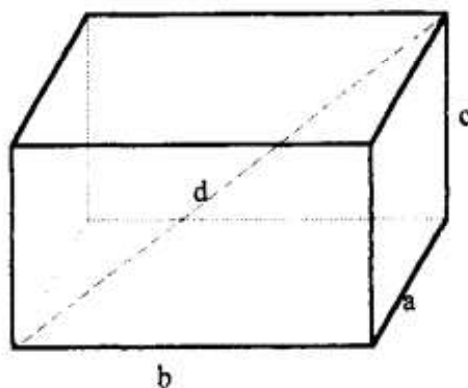


$$\text{Area } ABCA = \frac{2}{3} ab$$

$$\text{Length of arc } ABC = b \left\{ \frac{1}{2} (1 + 16 (a/b)^2)^{1/2} + \frac{1}{8 (a/b)} \ln [4n + (1 + 16 (a/b)^2)^{1/2}] \right\}$$

## 6.3 Solid Figure Formulas

### 6.3.1 Parallelepiped



$$\text{Surface area } A = 2(ab + bc + ca)$$

$$\text{Volume } V = abc$$

$$\text{Diagonal } d = \sqrt{a^2 + b^2 + c^2}$$

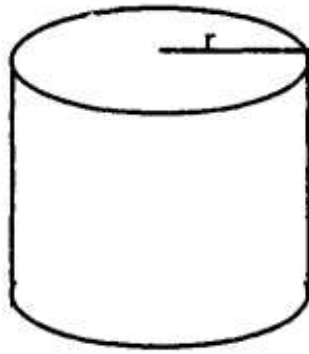
In the case of a cube,  $a = b = c$  then;

$$\text{Surface} = 6a^2$$

$$\text{Volume } V = a^3$$

$$\text{Diagonal } d = a\sqrt{3}$$

### 6.3.2 Right Cylinder

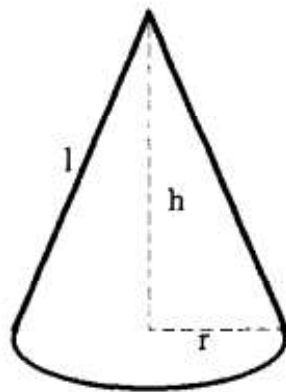


$$\begin{aligned}\text{Surface area of convex surface } A_c &= 2 \pi r h \\ &= 6.283 r h\end{aligned}$$

$$\text{Total surface area } A = 2 \pi r (r + h)$$

$$\text{Volume } V = \pi r^2 h$$

### 6.3.3 Right Cone

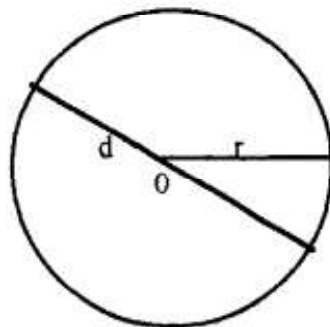


$$\text{Surface area of convex surface } A_c = \pi r l$$

$$(l = \text{slant height} = \sqrt{r^2 + h^2})$$

$$\text{Total surface area } A = \pi r (r + l)$$

$$\text{Volume } V = 1/3 \pi r^2 h$$



### 6.3.4 Sphere

$$\text{Surface area } A = 4 \pi r^2 = \pi d^2$$

$$\text{Volume } V = 4/3 \pi r^3 = 1/6 \pi d^3$$

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