**Chapter 12: Mass Spectrometry, Infrared Spectroscopy, and Ultraviolet/Visible Spectroscopy**

**Learning Objectives:**

1. Be able to predict the fragmentation patterns expected to arise in the mass spectrum of alkanes, alkyl halides, ethers, alcohols, and ketones.
2. Be able to describe what happens to a compound in a mass spectrometer
3. Be able to use the mass spectrum of a compound to find the molecular mass, and to help identify the structure of a compound.
4. Be able to describe what happens to a compound when it absorbs infrared radiation.
5. Be able to use of a chart of functional group IR absorptions, and to help identify the structure of a compound.
6. Be able to use result from elemental analysis to deduce the number of carbon, hydrogen, and nitrogen in the molecular formula.*

* Supplemental material, not included in the textbook

**Sections:**

12.1 Mass Spectrometry
12.2 The Mass Spectrum – Fragmentation
12.3 Isotope in Mass Spectrometry
12.4 High-Resolution Mass Spectrometry Can Reveal Molecular Formulas
12.5 Fragmentation Patterns of Functional Groups*
12.6 Spectroscopy and the Electromagnetic Spectrum#
12.7 Infrared Spectroscopy
12.8 Characteristic Infrared Absorption bands
12.9 The Intensity of Absorption bands#
12.10 The Position of Absorption bands
12.11 The Position of an Absorption band Is Affected by Electron Delocalization, Electron Donation and Withdrawal, and Hydrogen Bonding.
12.12 The Shape of Absorption Bands*
12.13 Absence of Absorption Bands#
12.14 Some Vibrations are Infrared Inactive
12.15 A Lesson in Interpreting Infrared Spectra
12.16 Ultraviolet and Visible Spectroscopy#
12.17 The Beer-Lambert Law#
12.18 The Effect of Conjugation on $\lambda_{max}$#
12.19 Visible Spectrum and Color#
12.20 Some Uses of UV/VIS Spectroscopy#

Additional material: Calculation of molecular formula using information from mass spectrometry and elemental analysis

* Sections that will be focused

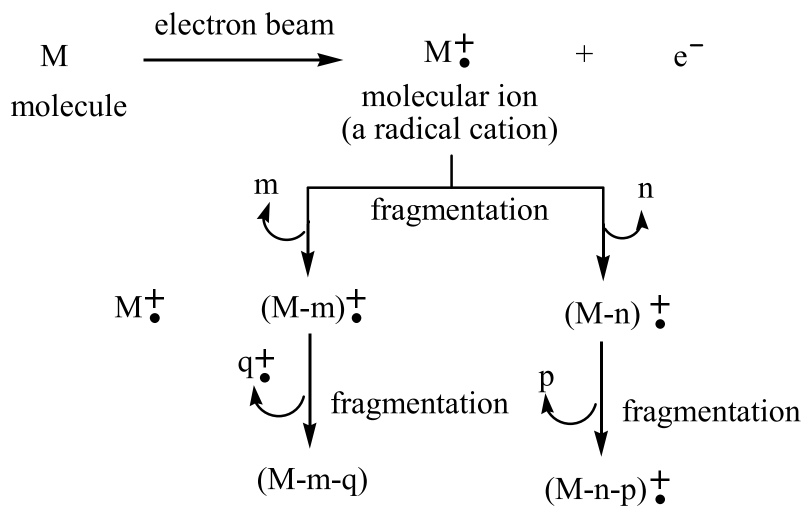
[#] Sections that will be skipped

**Recommended additional problems**

41, 43, 45, 54

**Class Note**

12.1 Mass Spectrometry and 12.2 The Mass Spectrum – Fragmentation




Cations detected by collector: $M^{+\bullet}$ $(M\text{-}m)^{+\bullet}$ $(M\text{-}n)^{+\bullet}$ $(M\text{-}n\text{-}p)^{+\bullet}$ $q^{+\bullet}$

A. Most of the instrument is designed to detect cations.

B. Relative abundance of fragmentation pattern depends on the energy of the electron beam.

## 12.3 Isotope in Mass Spectrometry

A. Relative abundance of carbon on molecular ion

$^{12}C$: 98.89% (0.989)    $^{13}C$: 1.11% (0.011)
(M)    (M+1)

Each carbon contributes 0.011 abundance to the abundance of M+1 peak =>

relative abundance of M+1 peak =
(number of carbon in the analyzed molecule) x relative abundance of M x 0.011

=> (number of carbon in the analyzed molecule) = relative abundance of M+1 peak ÷ (relative abundance of M x 0.011)

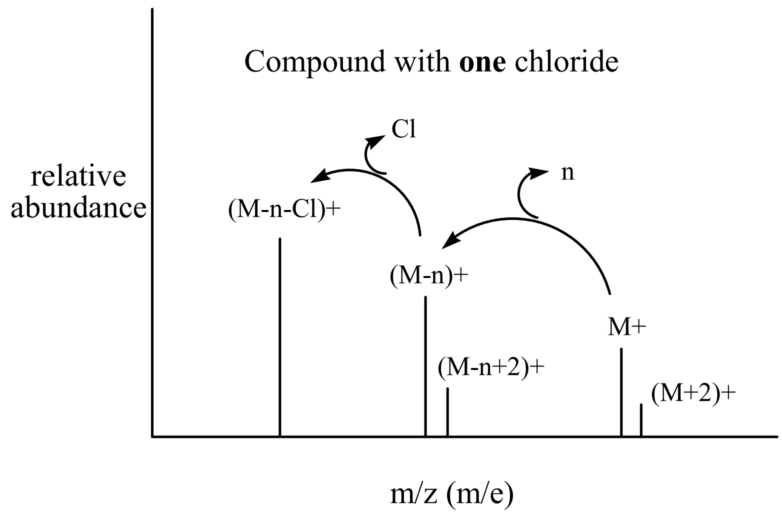
* Not very accurate for compound with high molecular weight

Example: M (150): 16.28 and (M+1) (151): 1.66

B. Relative abundance of Cl on molecular ion

$^{35}Cl$: 75.77% (0.76) (M) $^{37}Cl$: 24.23% (0.24) (M+2)

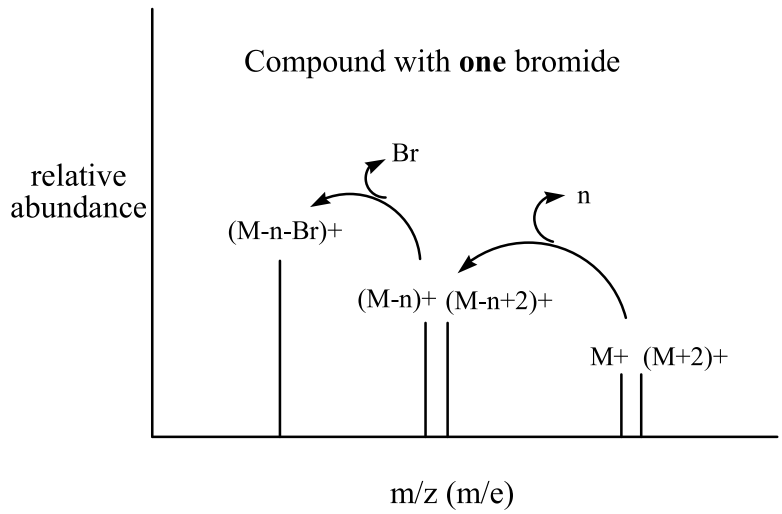
For compound with one Cl: M/(M+2) $\approx$ 3/1



C. Relative abundance of Br on molecular ion

$^{79}$Br: 50.69% (0.51) (M) $^{81}$Br: 49.31% (0.49) (M+2)

For compound with one Br: M/(M+2) $\approx$ 1/1



## 12.4 High-Resolution Mass Spectrometry Can Reveal Molecular Formulas

Use Table 12.3

## 12.5 Fragmentation Patterns of Functional Groups*

A. Alkyl halides ($CH_3CH_2CH_2Br$ and $(CH_3)_2CHCl$)

B. Ethers ($CH_3CH_2CH(CH_3)OCH(CH_3)_2$)

C. Alcohols ($CH_3CH_2CH_2CH_2CH(OH)CH_3$)

D. Ketones ($CH_3CH_2CH_2COCH_3$)

12.6 Spectroscopy and the Electromagnetic Spectrum#

Figure 12.11

12.7 Infrared Spectroscopy

Figure 12.12 (stretching and bending)

12.8 Characteristic Infrared Absorption bands

Table 12.4 (OH, NH, and C=O)

12.10 The Position of Absorption bands and 12.11 The Position of an Absorption band Is Affected by Electron Delocalization, Electron Donation and Withdrawal, and Hydrogen Bonding.

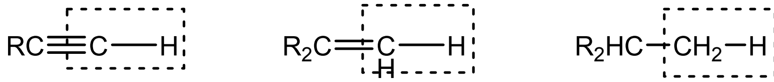
A. Effect of mass

B. Effect of bond order

D. Effect of resonance and inductive effect

acyl halide > ester > aldehyde > ketone > amide

E. C-H Absorption Bands



* NMR provides more reliable characterization.

12.12 The Shape of Absorption Bands*

NH, $NH_2$, OH, and $CO_2H$

## 12.14 Some Vibrations are Infrared Inactive

## 12.15 A Lesson in Interpreting Infrared Spectra

C=O and H-bond

**Additional material: Calculation of molecular formula using information from mass spectrometry and elemental analysis**

A. Example 1

From Mass Spec $M^+$: 99
From elemental analysis: C: 60.5%; H: 9.1%; N: 14.1%

B. Example 2

From Mass Spec $M^+$: 142, relative intensity: $(M^+/(M+2)^+ = 100/35$
From elemental analysis: C: 58.9%; H: 4.9%