CHAPTER 1

MASS SPECTROMETRY

1.1 INTRODUCTION

The concept of mass spectrometry is relatively simple: a compound is ionized (ionization method), the ions are separated on the basis of their mass/charge ratio (ion separation method), and the number of ions representing each mass/charge unit is recorded as a spectrum. There are many ionization methods and many methods for separating the resulting ions (see Section 1.2). For instance, in the commonly used electron impact (EI) mode, the mass spectrometer bombards molecules in the vapor phase with a high-energy electron beam and records the result as a spectrum of positive ions, which have been separated on the basis of mass/charge (m/z).*

To illustrate, the EI mass spectrum of benzamide is given in Figure 1.1 showing a plot of abundance (% of the base peak, the most intense peak in the spectrum) versus m/z. The positive ion peak at m/z 121 represents the intact molecule (M) less one electron, which was removed by the impacting electron beam; it is designated as the molecular ion, $M^{\cdot+}$. The energetic molecular ion produces a series of fragment ions, some of which are rationalized in Figure 1.1.

It is routine to couple a mass spectrometer to some form of chromatographic instrument, such as a gas chromatograph (GC-MS) or a liquid chromatograph (LC-MS). The mass spectrometer finds widespread use in the analysis of compounds whose mass spectrum is known and in the analysis of completely unknown compounds. In the case of known compounds, a computer search is conducted comparing the mass spectrum of the compound in question with a library of mass spectra. Electron impact mass spectrometry is particularly useful in this regard since EI mass spectrometry leads to considerable fragmentation. Congruence of mass spectra is convincing evidence for identification and is often even admissible in court. In the case of an unknown compound, the molecular ion, the fragmentation pattern, and evidence from other forms of spectrometry (e.g., IR and NMR) can lead to the identification of a new compound. Our focus and goal in this chapter is to develop skill in the latter use,

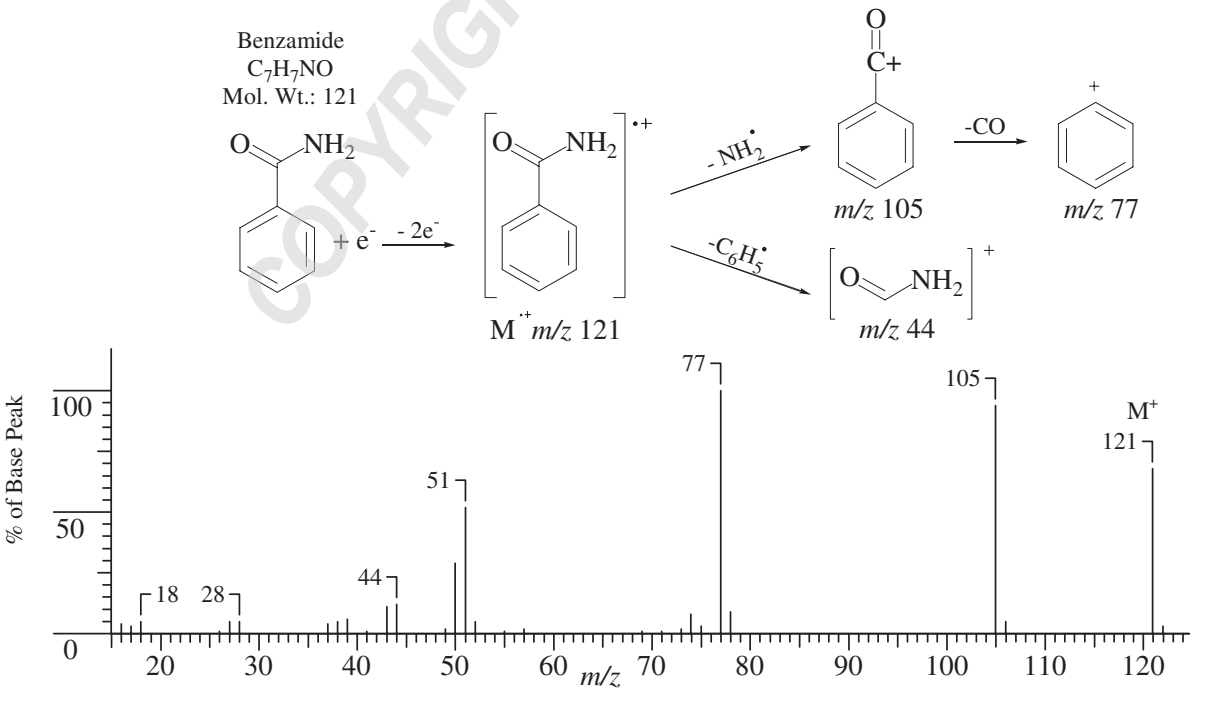


FIGURE 1.1 The EI mass spectrum of benzamide, above which is a fragmentation pathway to explain some of the important ions.

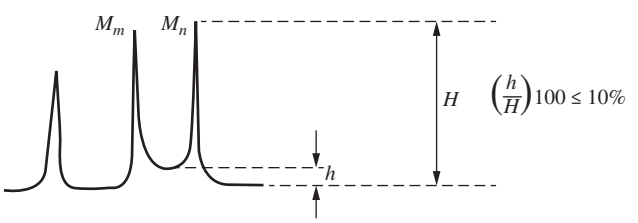
*The unit of mass is the Dalton (Da), defined as $\frac{1}{12}$ of the mass of an atom of the isotope ^{12}C, which is arbitrarily 12.0000 … mass units.

especially using the EI method. For other applications or for more detail, mass spectrometry texts and spectral compilations are listed online at www.wiley.com/college/silverstein.

1.2 INSTRUMENTATION

As with all modern analytical instrumentation, there has been recent, rapid growth and change in instrumentation for mass spectrometry. Instead of discussing individual instruments, the discussion will be broken down into (1) ionization methods and (2) ion separation methods. In general, the method of ionization is independent of the method of ion separation and vice versa, although there are exceptions. Some of the ionization methods depend on a specific chromatographic front end (e.g., LC-MS), while still others are precluded from using chromatography for introduction of the sample (e.g., FAB and MALDI). Before delving further into instrumentation, let us make a distinction between two types of mass spectrometers based on resolution.

The minimum requirement for the organic chemist is the ability to record the molecular weight of the compound under examination to the nearest whole number. Thus, the spectrum should show a peak at, say, m/z 400, which is distinguishable from a peak at m/z 399 or at m/z 401. In order to select possible molecular formulas by measuring isotope peak intensities (see Section 1.5.2.1), adjacent peaks must be cleanly separated. Arbitrarily, the valley between two such peaks should not be more than 10% of the height of the larger peak. This degree of resolution is qualitatively termed "unit" resolution and can be obtained up to a mass of approximately 3000 Da on readily available "unit resolution" instruments.



To determine the resolution* of an instrument, consider two adjacent peaks of approximately equal intensity. These peaks should be chosen so that the height of the valley between the peaks is less than 10% of the intensity of the peaks. The resolution (R) is $R = M_n/(M_n - M_m)$, where M_n is the higher mass number of the two adjacent peaks, and M_m is the lower mass number.

There are two important categories of mass spectrometers: low (unit) resolution and high resolution. Low-resolution instruments can be defined arbitrarily as the instruments that separate unit masses up to m/z 3000 [$R = 3000/(3000 - 2999) = 3000$]. A high-resolution instrument (e.g., $R = 20{,}000$) can distinguish between $C_{16}H_{26}O_2$ and $C_{15}H_{24}NO_2$ [$R = 250.1933/(250.1933 - 250.1807) = 19857$]. This important class of mass spectrometers, which can have R as large as 100,000, can measure the mass of an ion with sufficient accuracy to determine its atomic composition (molecular formula). As a practical matter, the term high-resolution mass spectrometry will be used to designate *accurate mass measurement*. The number of decimal places needed for an unambiguous determination of elemental composition is related to the mass of the ion. For instance, an accuracy of 0.0025 Da should be sufficient for ions with a mass of less than 500 Da.

All mass spectrometers share common features (see Figure 1.2). Introduction of the sample into the mass spectrometer is an important consideration, but it often depends on the type of ionization method (see below). All mass spectrometers have methods for ionizing the sample and for separating the ions on the basis of m/z. These methods are discussed in detail below. Once separated, the ions must be detected and quantified. A typical ion collector consists of collimating slits that direct only one set of ions at a time into the collector, where they are detected and amplified by an electron multiplier. Ion detectors are designed to balance sensitivity, accuracy, and response time. Generally speaking, fast response times and high accuracy are mutually exclusive. The method of ion detection is dependent to some extent on the method of ion separation.

*This definition is the most common way to calculate resolution, but not the only way.

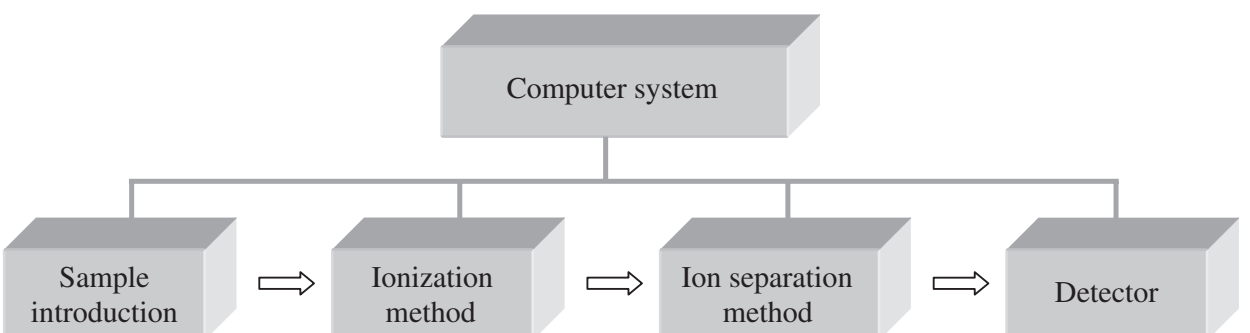


FIGURE 1.2 Block diagram of features of a typical mass spectrometer.

Nearly all mass spectrometers today are interfaced with a computer. Typically, the computer controls the operation of the instrument, which includes any chromatography, collects and stores the data, and provides either graphical output (essentially a bar graph) or tabular lists of the data.

1.3 IONIZATION METHODS

The large number of ionization methods, some of which are highly specialized, precludes complete coverage. The most common ones in the three general areas of gas-phase, desorption, and evaporative ionization are described below.

1.3.1 Gas-Phase Ionization Methods

Gas-phase methods for generating ions for mass spectrometry are the oldest and most popular methods for organic chemists. These methods are applicable to compounds that have a minimum vapor pressure of ca. 10^{-6} Torr at a temperature at which the compound is stable; this criterion applies to a large number of nonionic organic molecules with MW<1000 Da.

1.3.1.1 Electron Impact Ionization. Electron impact (EI) has historically been the most widely used method for generating ions for mass spectrometry. It is also the main focus in this chapter for interpreting mass spectra for structure determination. Vapor-phase sample molecules are bombarded with high-energy electrons (generally 70 eV), the purpose of which is to eject an electron from a sample molecule to produce a radical cation, known as the molecular ion. Because the ionization potential of typical organic compounds is generally less than 15 eV, the bombarding electrons impart 50 eV (or more) of excess energy to the newly created molecular ion, which is dissipated, in part, by the breaking of covalent bonds, which have strengths between 3 and 10 eV.

Bond breaking is usually extensive and critically, highly reproducible, and characteristic of the compound. Furthermore, this fragmentation process is also partly predictable and is the source of the powerful structure elucidation potential of mass spectrometry. Often, the excess energy imparted to the molecular ion is too great, which leads to a mass spectrum with no discernible molecular ion. Reduction of the ionization voltage is a commonly used strategy to obtain a molecular ion; the strategy is often successful because there is greatly reduced fragmentation. The disadvantage of this strategy is that the spectrum changes and cannot be compared to standard literature spectra.

To many organic chemists, mass spectrometry is synonymous with EI mass spectrometry. This view is understandable for two reasons. First, historically, EI was universally available before other ionization methods were developed. Much of the early work was EI mass spectrometry. Second, the major libraries and databases of mass spectral data, which are relied upon so heavily and cited so often, are of EI mass spectra. Some of the readily accessible databases contain EI mass spectra of over 390000 compounds and they are easily searched by efficient computer algorithms. The uniqueness of the EI mass spectrum for a given organic compound, even for diastereomers, is an almost certainty. This uniqueness, coupled with the great sensitivity of the method, is what makes GC-MS such a powerful and popular analytical tool. We will discuss EI mass spectra beginning in Section 1.5.

1.3.1.2 Chemical Ionization. Electron impact ionization often leads to such extensive fragmentation that no molecular ion is observed. One way to avoid this problem is to use an indirect ionization method; chemical ionization (CI) is popular and readily available on many commercial instruments. In CI, sample molecules (in the vapor phase) are not subjected to bombardment by high-energy electrons. Instead, a reagent gas (usually methane, isobutane, ammonia, but others are also used) is introduced into the ionization source and ionized. Sample molecules collide with ionized reagent gas molecules ($CH_5^+, C_4H_9^+$, etc.) in the relatively high-pressure CI source and undergo secondary ionization (i.e., chemical ionization) by proton transfer producing an $[M + 1]^+$ ion, by electrophilic addition producing $[M + 15]^+, [M + 29]^+, [M + 41]^+$, or $[M + 18]^+$ (with NH_4^+ ions), or by charge exchange (rare) producing a $[M]^+$ ion. Chemical ionization spectra sometimes have prominent $[M - 1]^+$ ion peaks because of hydride abstraction. The ions thus produced are even electron species. The excess energy transfered to the sample molecules during the ionization phase is small, generally less than 5 eV, so that much less fragmentation takes place. There are several important consequences, the most valuable of which are an abundance of quasimolecular ions and greater sensitivity because the total ion current is concentrated into a few ions. There is however, less information on structure. The quasimolecular ions are usually quite stable and they are readily detected. Oftentimes, there are only one or two fragment ions produced and sometimes there are none.

For example, the EI mass spectrum of 3, 4-dimethoxyacetophenone (Figure 1.3) shows, in addition to the molecular ion at m/z 180, numerous fragment peaks in the range of m/z 15 to 167; these include the base peak at m/z 165 and prominent peaks at m/z 137 and m/z 77. The CI mass spectrum (methane, CH_4, as reagent gas) shows the quasimolecular ion ($[M + 1]^+$, m/z 181) as the base peak (100%), and no fragment ion peaks. The only other peaks, each of just a few percent intensity, are the molecular ion peak, m/z 180, m/z 209 ($[M + 29]^+$ or $M + C_2H_5^+$), and m/z 221 ($[M + 41]^+$ or $M + C_3H_5^+$). These last two peaks are a result of electrophilic addition of carbocations and are very useful in identifying the molecular ion. The excess methane carrier gas is ionized by electron impact to the primary ions CH_4^+ and CH_3^+. These react with the excess methane to give secondary ions.

$$CH_3^+ + CH_4 \longrightarrow C_2H_5^+ \text{ and } H_2$$
$$CH_4 + C_2H_5^+ \longrightarrow C_3H_5^+ \text{ and } 2H_2$$

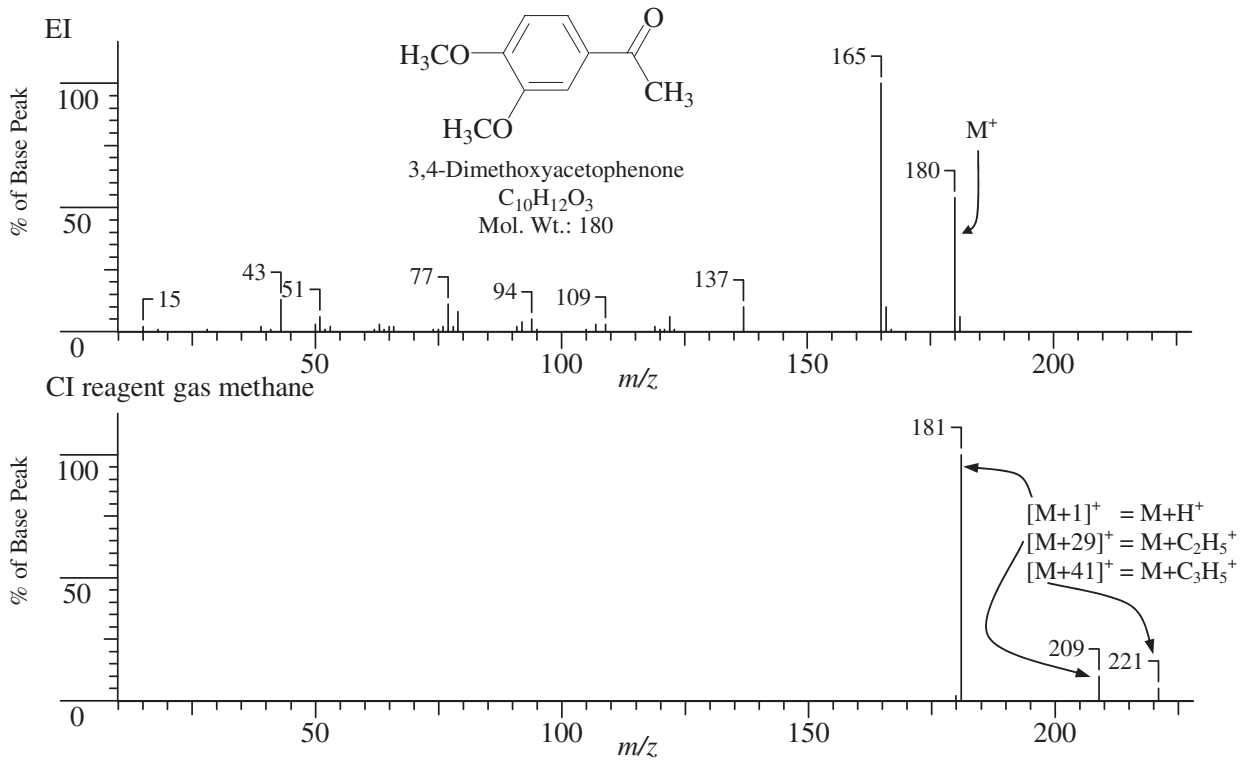


FIGURE 1.3 The EI and CI mass spectra of 3,4-dimethoxyacetophenone.

The energy content of the various secondary ions (from, respectively, methane, isobutane, and ammonia) decrease in the order: $C_3H_5^+ > t\text{-}C_4H_9^+ > NH_4^+$. Thus, by choice of reagent gas, we can control the tendency of the CI produced $[M + 1]^+$ ion to fragment. For example, when methane is the reagent gas, dioctyl phthalate shows its $[M + 1]^+$ peak (m/z 391) as the base peak; more importantly, the fragment peaks (e.g., m/z 113 and 149) are 30% to 60% of the intensity of the base beak. When isobutane is used, the $[M + 1]^+$ peak is still large, while the fragment peaks are only roughly 5% as intense as the $[M + 1]^+$ peak.

Chemical ionization mass spectrometry is neither useful for peak matching (either manually or by computer) nor is it particularly useful for structure elucidation; its main use is for the detection of molecular ions and hence molecular weights.

1.3.2 Desorption Ionization Methods

Desorption ionization methods are those techniques in which sample molecules are emitted directly from a condensed phase into the vapor phase as ions. The primary use of these methods is for large, nonvolatile, or ionic compounds. There can be significant disadvantages. Desorption methods generally do not use available sample efficiently. Often times, the information content is limited. For unknown compounds, the methods are used primarily to provide molecular weight, and in some cases to obtain an exact mass. However, even for this purpose, it should be used with caution because the molecular ion or the quasimolecular ion may not be evident. The resulting spectra are often complicated by abundant matrix ions.

1.3.2.1 Field Desorption Ionization. In the field desorption (FD) method, the sample is applied to a metal emitter on the surface of which is found carbon microneedles. The microneedles activate the surface, which is maintained at the accelerating voltage and functions as the anode. Very high voltage gradients at the tips of the needles remove an electron from the sample, and the resulting cation is repelled away from the emitter. The ions generated have little excess energy so there is minimal fragmentation, that is, the molecular ion is usually the only significant ion seen. For example, with cholest-5-ene-3,16,22,26-tetrol, the EI and CI mass spectra do not show a molecular ion peak. However, the FD mass spectrum (Figure 1.4) shows predominately the molecular ion with virtually no fragmentation.

1.3.2.2 Fast Atom Bombardment Ionization. Fast atom bombardment (FAB) uses high-energy xenon or argon atoms (6 keV to 10 keV) to bombard samples dissolved in a liquid of low vapor pressure (e.g., glycerol). The matrix protects the sample from excessive radiation damage. A related method, liquid secondary ionization mass spectrometry, LSIMS, is similar except that it uses somewhat more energetic cesium ions (10 keV to 30 keV).

In both methods, positive ions (by cation attachment ($[M + 1]^+$ or $[M + 23, Na]^+$) and negative ions (by

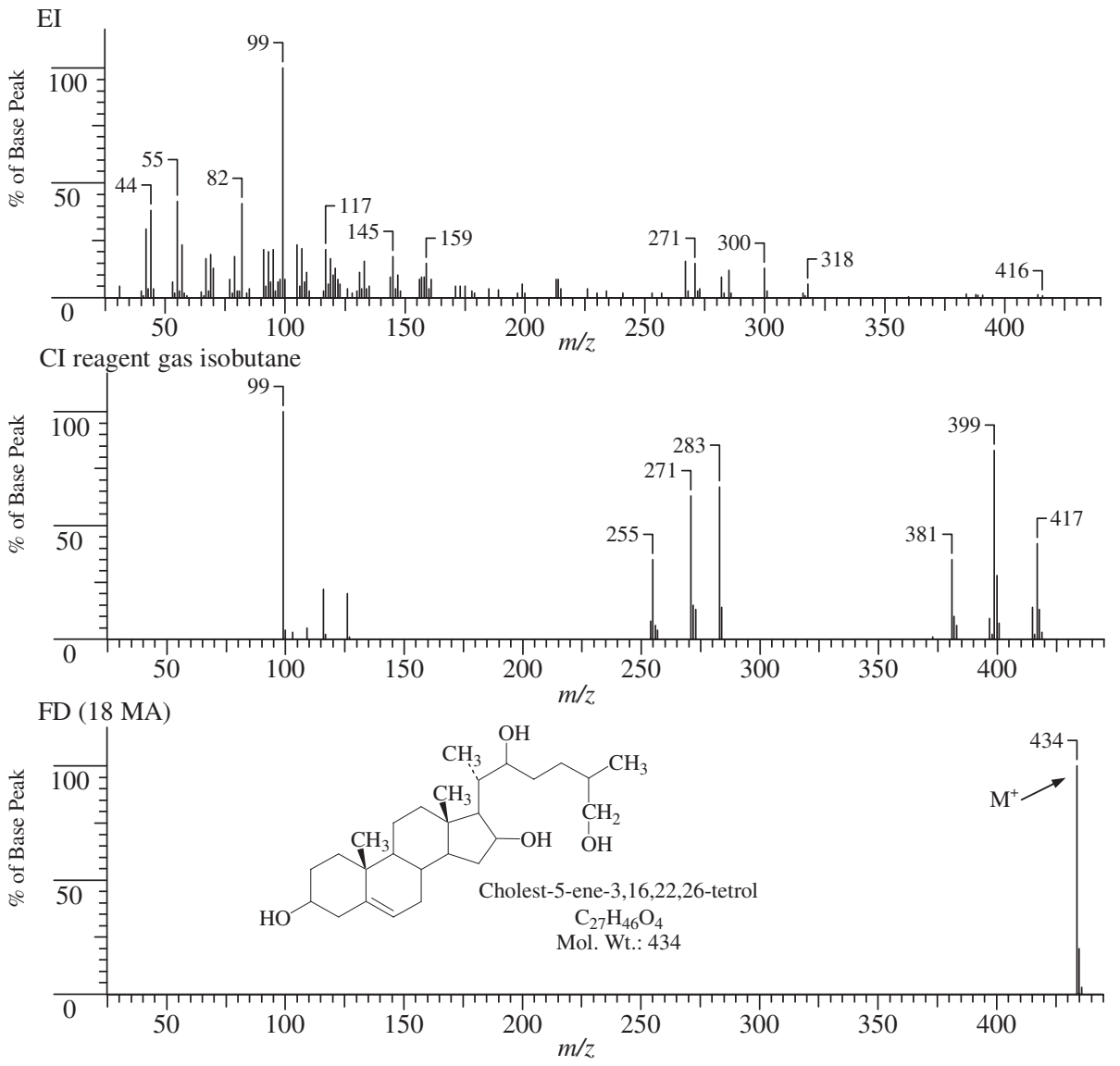


FIGURE 1.4 The electron impact (EI), chemical ionization (CI), and field desorption (FD) mass spectra of cholest-5-ene-3, 16, 22, 26-tetrol.

deprotonation $[M - 1]^-$) are formed; both types of ions are usually singly charged and, depending on the instrument, FAB can be used in high-resolution mode. FAB is used primarily with large nonvolatile molecules, particularly to determine molecular weight. For most classes of compounds, the rest of the spectrum is less useful, partially because the lower mass ranges may be composed of ions produced by the matrix itself. However, for certain classes of compounds that are composed of "building blocks," such as polysaccharides and peptides, some structural information may be obtained because fragmentation usually occurs at the glycosidic and peptide bonds, respectively, thereby affording a method of sequencing these classes of compounds.

The upper mass limit for FAB (and LSIMS) ionization is between 10 kDa and 20 kDa, and FAB is really most useful up to about 6 kDa. FAB is seen most often with double focusing magnetic sector instruments where it has a resolution of about 0.3 m/z over the entire mass range; FAB can, however, be used with most types of mass analyzers. The biggest drawback to using FAB is that the spectrum always shows a high level of matrix generated ions, which limit sensitivity and which may obscure important fragment ions.

1.3.2.3 Plasma Desorption Ionization. Plasma desorption ionization is a highly specialized technique used almost exclusively with a time-of-flight (TOF) mass analyzer (Section 1.4.4). The fission products from californium-252 (^{252}Cf), with energies in the range of 80 MeV to 100 MeV, are used to bombard and ionize the sample. Each time a ^{252}Cf splits, two particles are produced moving in opposite directions. One of the particles hits a triggering detector and signals a start time. The other particle strikes the sample matrix ejecting some sample ions into a time-of-flight mass spectrometer (TOF-MS). The sample ions

are most often released as singly, doubly, or triply protonated moieties. These ions are of fairly low energy so that structurally useful fragmentation is rarely observed and, for polysaccharides and polypeptides, sequencing information is not available. The mass accuracy of the method is limited by the TOF mass spectrometer. The technique is useful on compounds with molecular weights up to at least 45 kDa.

1.3.2.4 Laser Desorption Ionization. A pulsed laser beam can be used to ionize samples for mass spectrometry. Because this method of ionization is pulsed, it must be used with either a TOF or a Fourier transform mass spectrometer (Section 1.4.5). Two types of lasers have found widespread use: a CO_2 laser, which emits radiation in the far infrared region, and a frequency-quadrupled neodymium/yttrium-aluminum-garnet (Nd/YAG) laser, which emits radiation in the UV region at 266 nm. Without matrix assistance, the method is limited to low molecular weight molecules (<2 kDa).

The power of the method is greatly enhanced by using matrix assistance (matrix-assisted laser desorption ionization, or MALDI). Two matrix materials, 2,5-dihydroxybenzoic acid and sinapinic acid, which have absorption bands coinciding with the laser employed, have found widespread use and sample molecular weights of up to two to three hundred thousand Da have been successfully analyzed. A few picomoles of sample are mixed with the matrix compound followed by pulsed irradiation, which causes sample ions (usually singly charged monomers but occasionally multiply charged ions and dimers have been observed) to be ejected from the matrix into the mass spectrometer.

The ions have little excess energy and show little propensity to fragment. For this reason, the method is fairly useful for mixtures. MALDI is used most often with a TOF-MS or a Fourier transform mass spectrometer (FT-MS); both mass analyzers are capable of accurate mass measurement. As with other matrix-assisted methods, MALDI suffers from background interference from the matrix material, which is further exacerbated by matrix adduction. Thus, the assignment of a molecular ion of an unknown compound can be uncertain.

1.3.3 Evaporative Ionization Methods

There are two important methods in which ions or, less often, neutral compounds in solution (often containing formic acid) have their solvent molecules stripped by evaporation, with simultaneous ionization leaving behind the ions for mass analysis. Coupled with liquid chromatography instrumentation, these methods have become immensely popular.

1.3.3.1 Thermospray Mass Spectrometry. In the thermospray method, a solution of the sample is introduced into the mass spectrometer by means of a heated capillary tube. The tube nebulizes and partially vaporizes the solvent, forming a stream of fine droplets which enter the ion source. When the solvent completely evaporates, the sample ions can be mass analyzed. This method can handle high flow rates and buffers; it was an early solution to interfacing mass spectrometers with aqueous liquid chromatography. The method has largely been supplanted by electrospray.

1.3.3.2 Electrospray Mass Spectrometry. The electrospray (ES) ion source (Figure 1.5) is operated at or near atmospheric pressure and, thus is also called atmospheric pressure ionization or API. The sample in solution (usually a polar, volatile solvent) enters the ion source through a stainless steel capillary, which is surrounded by a co-axial flow of nitrogen, called the nebulizing gas. The tip of the capillary is maintained at a high potential with respect to a counter-electrode. The potential difference produces a field gradient of up to 5 kV/cm. As the solution exits the capillary, an aerosol of charged droplets forms. The flow of nebulizing gas directs the effluent toward the mass spectrometer.

Droplets in the aerosol shrink as the solvent evaporates, thereby concentrating the charged sample ions. When

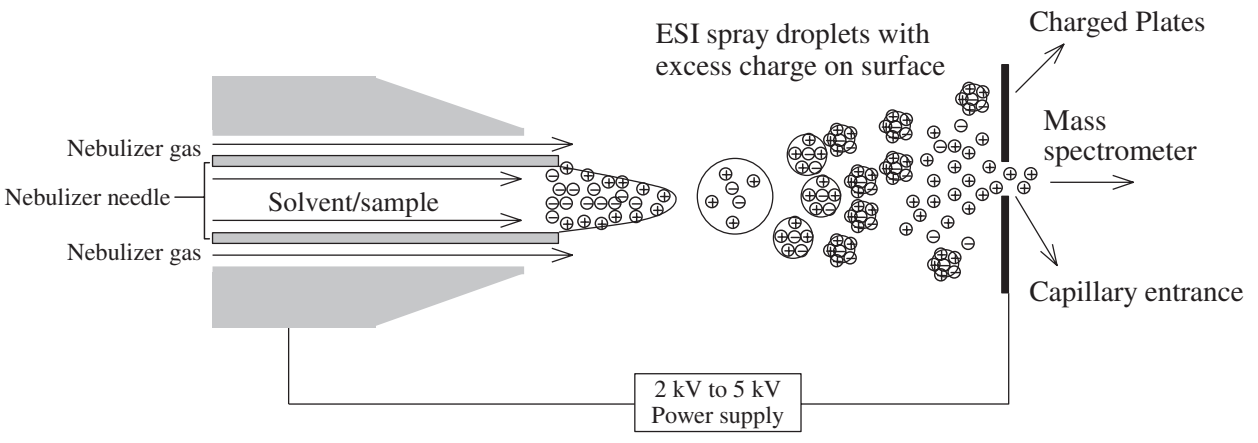


FIGURE 1.5 A diagram showing the evaporation of solvent leading to individual ions in an electrospray instrument.

the electrostatic repulsion among the charged sample ions reaches a critical point, the droplet undergoes a so-called Coulombic explosion, which releases the sample ions into the vapor phase. The vapor phase ions are focused with a number of sampling orifices into the mass analyzer.

Electrospray MS has undergone an explosion of activity since about 1990, mainly for compounds that have multiple charge-bearing sites. With proteins, for example, ions with multiple charges are formed. Since the mass spectrometer measures mass to charge ratio (m/z) rather than mass directly, these multiply charged ions are recorded at apparent mass values of $\frac{1}{2}, \frac{1}{3}, \ldots \frac{1}{n}$ of their actual masses, where n is the number of charges (z). Large proteins can have 40 or more charges so that molecules of up to 100 kDa can be detected in the range of conventional quadrupole, ion trap, or magnetic sector mass spectrometers. The appearance of the spectrum is a series of peaks increasing in mass, which correspond to pseudomolecular ions possessing sequentially one less proton and therefore one less charge.

Determination of the actual mass of the ion requires that the charge of the ion be known. If two peaks, which differ by a single charge, can be identified, the calculation is reduced to simple algebra. Recall that each ion of the sample molecule (M_s) has the general form $(M_s + zH)^{z+}$ where H is the mass of a proton (1.0079 Da). For two ions differing by one charge, $m_1 = [M_s + (z + 1)H]/(z + 1)$ and $m_2 = [(M_s + zH)/z]$. Solving the two simultaneous equations for the charge z, yields $z = (m_1 - H)/(m_2 - m_1)$. A simple computer program automates this calculation for every peak in the spectrum and calculates the mass directly.

Many manufacturers have introduced inexpensive mass spectrometers dedicated to electrospray for two reasons. First, the method has been very successful while remaining a fairly simple method to employ. Second, the analysis of proteins and smaller peptides has grown in importance, and they are probably analyzed best by the electrospray method.

Figure 1.6 compares the EI mass spectrum (lower portion of the figure) of lactose to its ES mass spectrum (upper portion of figure). Lactose is considered in more detail in Chapter 5. The EI mass spectrum is completely useless because lactose has low vapor pressure, it is thermally labile, and the spectrum shows no characteristic peaks. The ES mass spectrum shows a weak molecular ion peak at m/z 342 and a characteristic $[M + 23]^+$ peak, the molecular ion peak plus sodium. Because sodium ions are ubiquitous in aqueous solution, these sodium adducts are very common.

The ES mass spectrum of a tetra peptide comprised of valine, glycine, serine, and glutamic acid (VGSE) is given in Figure 1.7. VGSE is also an example compound in Chapter 5. The base beak is the $[M + 1]^+$ ion at m/z 391 and the sodium adduct, $[M + 23]^+$, is nearly 90% of the base peak. In addition, there is some useful fragmentation information characteristic of each of the amino acids. For small peptides, it is not uncommon to find some helpful fragmentation, but for proteins it is less likely.

Methods of ionization are summarized in Table 1.1.

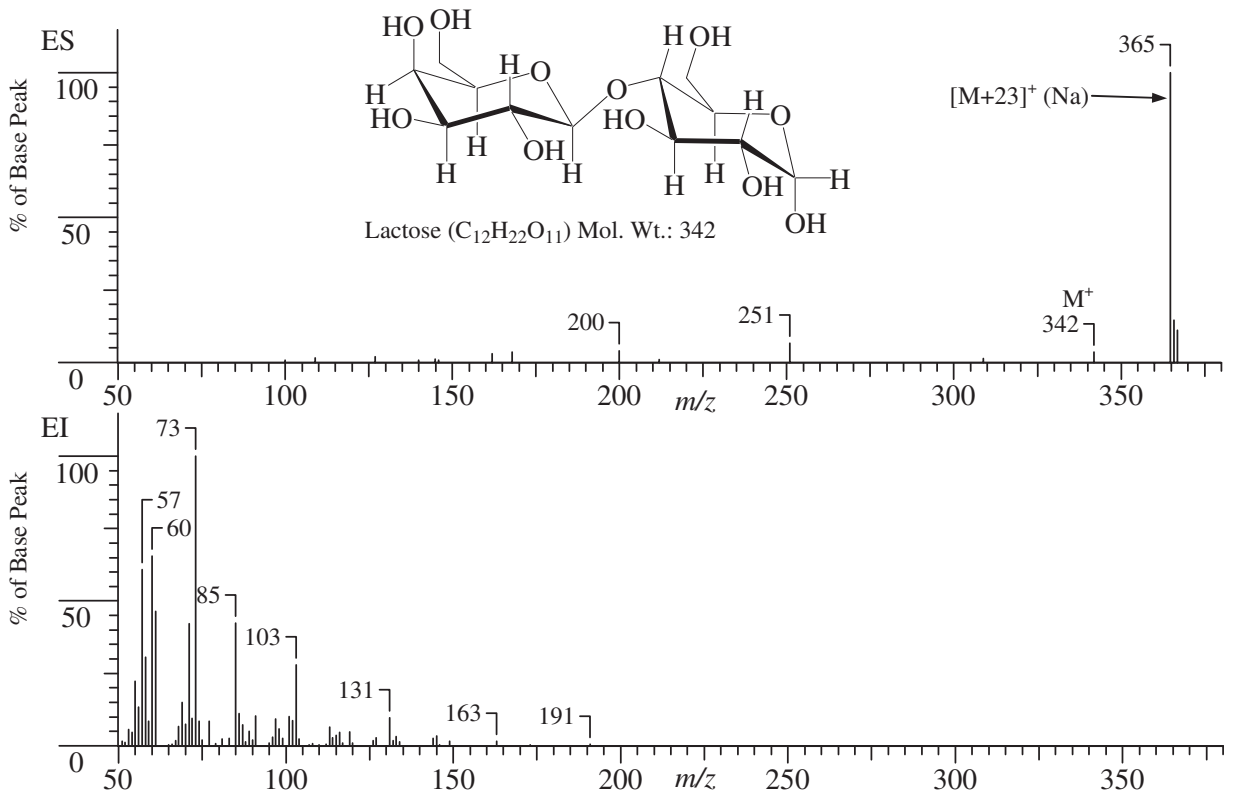


FIGURE 1.6 The EI and ES mass spectra of lactose.

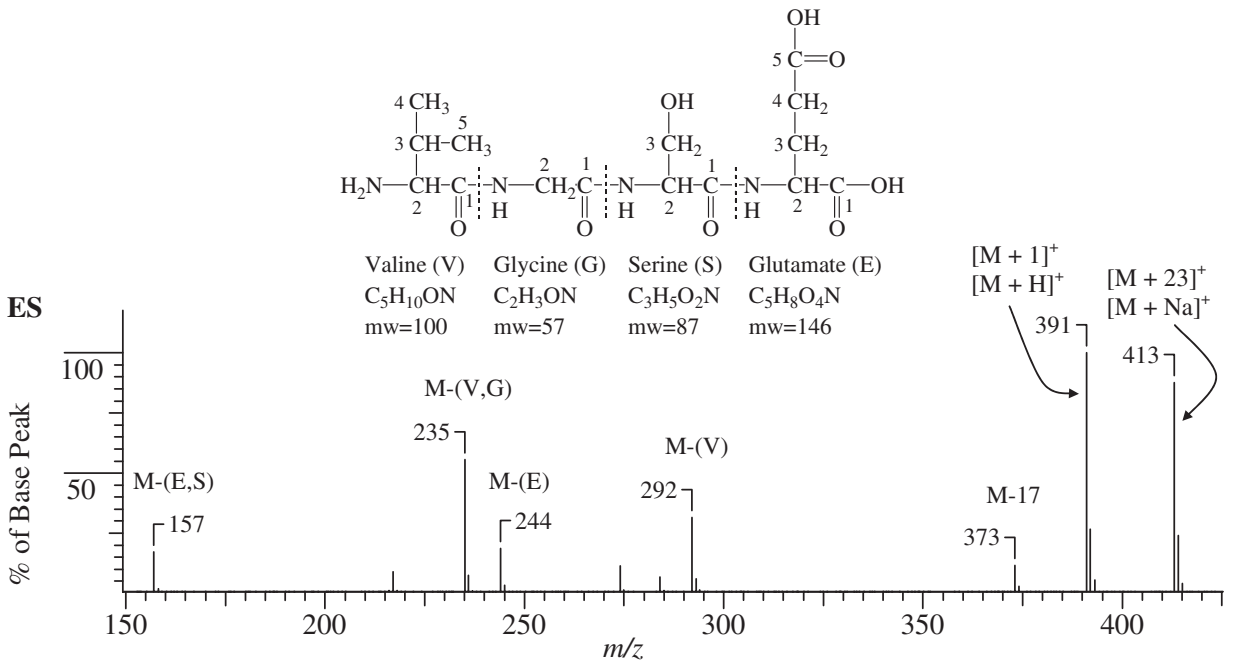


FIGURE 1.7 The electrospray (ES) mass spectrum for the tetra peptide whose structure is given in the figure. See text for explanation.

TABLE 1.1 Summary of Ionization Methods

Ionization Method	Ions Formed	Sensitivity	Advantage	Disadvantage
Electron impact	M^+	ng – pg	Data base searchable Structural information	M^+ occasionally absent
Chemical ionization	M + 1, M + 18, etc.	ng – pg	M^+ usually present	Little structural information
Field desorption	M^+	μg – ng	Nonvolatile compounds	Specialized equipment
Fast atom bombardment	M + 1, M + cation M + matrix	μg – ng	Nonvolatile compounds Sequencing information	Matrix interference Difficult to interpret
Plasma desorption	M+	μg – ng	Nonvolatile compounds	Matrix interference
Laser desorption	M + 1, M + matrix	μg – ng	Nonvolatile compounds Burst of ions	Matrix interference
Thermospray	M^+	μg – ng	Nonvolatile compounds	Outdated
Electrospray	M^+, M^{++}, M^{+++}, etc.	ng – pg	Nonvolatile compounds interfaces w/LC Forms multiply charged ions	Limited classes of compounds Little structural information

1.4 MASS ANALYZERS

The mass analyzer, which separates the mixture of ions that is generated during the ionization step by m/z in order to obtain a spectrum, is the heart of each mass spectrometer, and there are several different types with different characteristics. Each of the major types of mass analyzers is described below. This section concludes with a brief discussion of tandem MS and related processes.

1.4.1 Magnetic Sector Mass Spectrometers

Mass spectrometers were originally developed in the early twentieth century; the 1922 Nobel Prize in chemistry was awarded partly for the development of the mass spectrograph. All of the early instruments were of the magnetic sector type. The magnetic sector mass spectrometer uses a magnetic field to deflect moving ions around a curved path (see Figure 1.8). Even though magnetic sector mass spectrometers were the first commercially available instruments, they remain important today. Separation of ions occurs based on the mass/charge ratio, with lighter ions deflected to a greater extent than the heavier ions. Resolution depends on each ion entering the magnetic field (from the source) with the same kinetic energy, accomplished by accelerating the ions (which have a charge z) with a voltage V. Each ion acquires kinetic energy $E = zV = mv^2/2$. When an accelerated ion enters the magnetic field (B), it experiences a deflecting force (Bzv), which bends the path of the ion orthogonal to its original

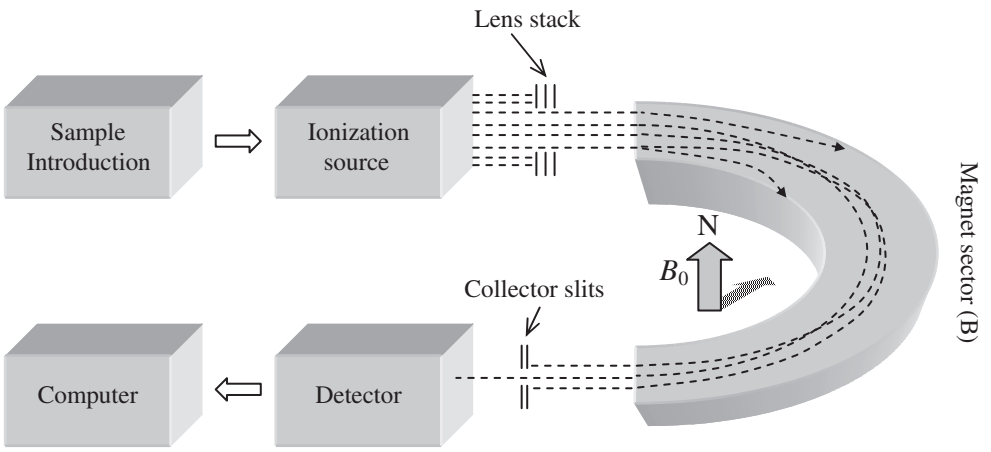


FIGURE 1.8 Schematic diagram of a single focusing, 180° sector mass analyzer. The magnetic field is perpendicular to the page. The radius of curvature varies from one instrument to another.

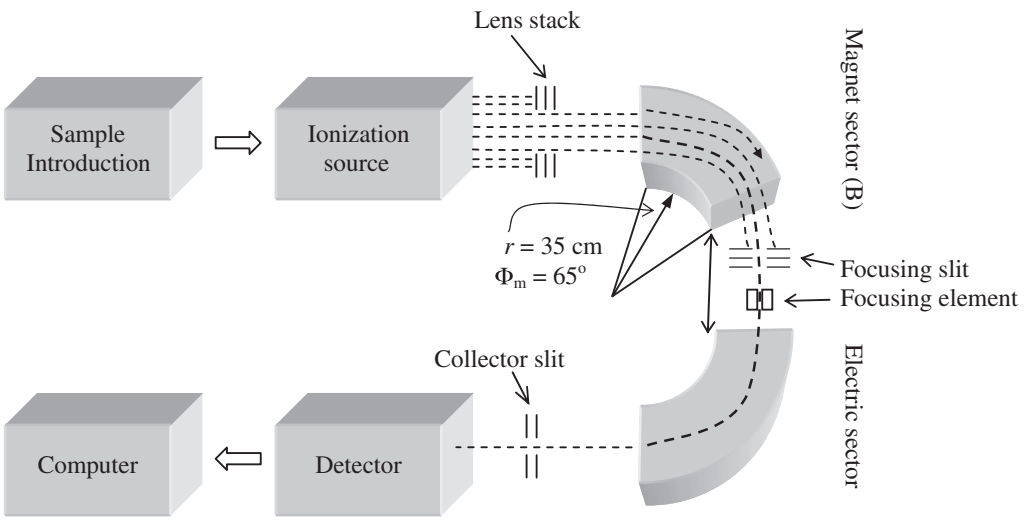


FIGURE 1.9 Schematic of double-focusing mass spectrometer.

direction. The ion is now traveling in a circular path of radius r, given by $Bzv = mv^2/r$. The two equations can be combined to give the familiar magnetic sector equation: $m/z = B^2r^2/2V$. Because the radius of the instrument is fixed, the magnetic field is scanned to bring the ions of different m/z sequentially into focus. As these equations show, a magnetic sector instrument separates ions on the basis of momentum, which is the product of mass and velocity, rather than mass alone; therefore, ions of the same mass but different energies will come into focus at different points.

An electrostatic analyzer (ESA) can greatly reduce the energy distribution of an ion beam by forcing ions of the same charge (z) and kinetic energy (regardless of mass) to follow the same path. A slit at the exit of the ESA further focuses the ion beam before it enters the detector. The combination of an ESA and a magnetic sector is known as double focusing because the two fields counteract the dispersive effects each has on direction and velocity.

The resolution of a double-focusing magnetic sector instrument (Figure 1.9) can be as high as 100000 through the use of extremely small slit widths. This very high resolution allows the measurement of "exact masses," which unequivocally provide molecular formulas and is enormously useful. By comparison, slits allowing an energy distribution for about 5000 resolution give at least 0.5 m/z accuracy across the entire mass range, that is, the "unit resolution" that is used in a standard mass spectrometer. The upper mass limit for commercial magnetic sector instruments is about m/z 15000. Raising this upper limit is theoretically possible but impractical.

1.4.2 Quadrupole Mass Spectrometers

The quadrupole mass analyzer (sometimes abbreviated QMF for quadrupole mass filter), also known as the transmission quadrupole, is much smaller and cheaper than a magnetic

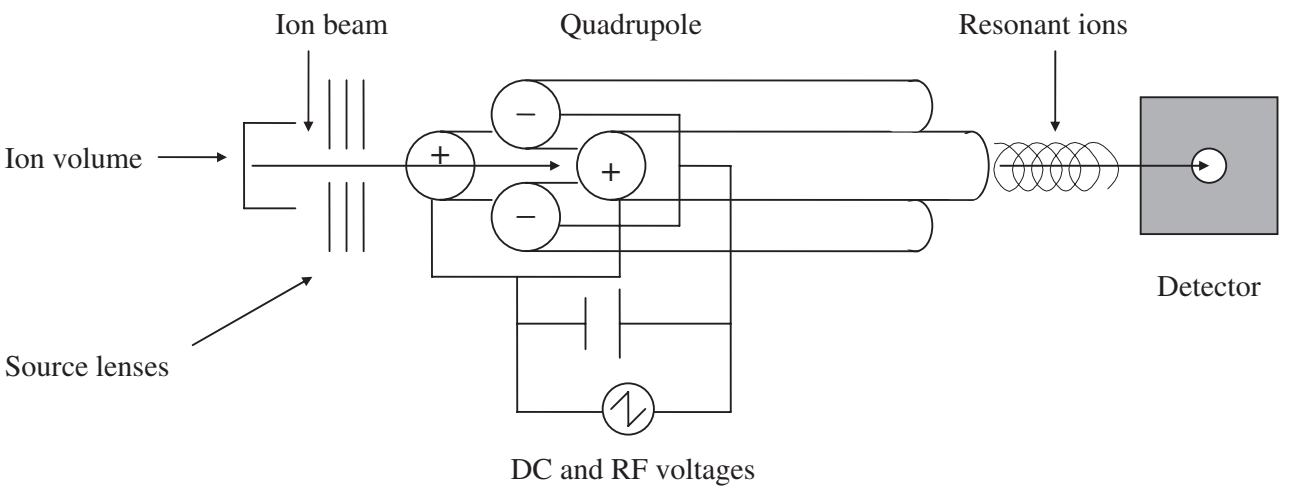


FIGURE 1.10 Schematic representation of a quadrupole "mass filter" or ion separator.

sector instrument. A quadrupole setup (seen schematically in Figure 1.10) consists of four cylindrical (or of hyperbolic cross-section) rods (100 mm to 200 mm long) mounted parallel to each other, at the corners of a square. A complete mathematical analysis of the quadrupole mass analyzer is complex, but we can discuss how it works in a simplified form. This nonmagnetic mass analyzer uses a constant DC voltage, which is modified by a radiofrequency voltage, applied to the rods. Ions are introduced to the "tunnel" formed by the four rods of the quadrupole in the center of the square at one end to the rods and travel down the axis.

For any given combination of DC voltage and modified voltage applied at the appropriate frequency (always at a constant ratio), only ions with a certain m/z value possess a stable trajectory and therefore are able to pass all the way to the end of the quadrupole to the detector. All ions with different m/z values travel unstable or erratic paths and collide with one of the rods or pass outside the quadrupole. An easy way to look at the quadrupole mass analyzer is as a tunable mass filter. In other words, as the ions enter at one end, only one m/z ion will pass through. In practice, the filtering can be carried out at a very fast rate so that the entire mass range can be scanned in considerably less than 1 second.

The development of the QMF forever changed mass spectrometry. Lower cost and ease-of-use led to "benchtop" instruments, which in turn led to everyday use by chemists and technicians. Also, the very fast scan times enabled the coupling of the quadrupole mass spectrometer with the gas chromatograph.

With respect to resolution and mass range, the quadrupole is generally inferior to the magnetic sector. For instance, the current upper mass range is generally less than 5000 m/z. On the other hand, sensitivity is generally high because there is no need for resolving slits, which would remove a portion of the ions. An important advantage of quadrupoles is that they operate most efficiently on ions of low velocity, which means that their ion sources can operate close to ground potential (i.e., low voltage). Since the entering ions generally have energies of less than 100 eV, the quadrupole mass spectrometer is ideal for interfacing to LC systems and for atmospheric pressure ionization (API) techniques such as electrospray (see Section 1.3.3.2). These techniques work best on ions of low energy so that fewer high-energy collisions will occur before they enter the quadrupole.

1.4.3 Ion Trap Mass Spectrometer

The ion trap, also known as the quadrupole ion trap, is sometimes considered as a variant of the quadrupole, since it resulted as a direct outgrowth of quadrupole research. However, the ion trap is much more versatile and clearly has greater potential for development. At one time the ion trap had a bad reputation because the earliest versions gave inferior results compared to quadrupoles. These problems have been overcome and the EI spectra obtained with an ion trap are now fully searchable with commercial databases. Furthermore, the ion trap is more sensitive than the quadrupole arrangement, and the ion trap is routinely configured to carry out tandem experiments with no extra hardware needed.

In one sense, an ion trap is aptly named because, unlike the quadrupole, which merely acts as a mass filter, the ion trap literally "traps" ions for relatively long periods of time, with important consequences. The simplest use of the trapped ions is to sequentially eject them to a detector, producing a conventional mass spectrum. Before other uses of trapped ions are briefly described, a closer look at the ion trap itself will be helpful.

The ion trap generally consists of three electrodes (hence, it is often called a 3D quadrupole ion trap or 3D QIT): one ring electrode with a hyperbolic inner surface, and two hyperbolic endcap electrodes at either end (a cross section of an ion trap is found in Figure 1.11). The ring electrode is operated with a sinusoidal radiofrequency field while the endcap electrodes are operated in one of three modes. The endcap may be operated at ground potential, or with either a DC or an AC voltage.

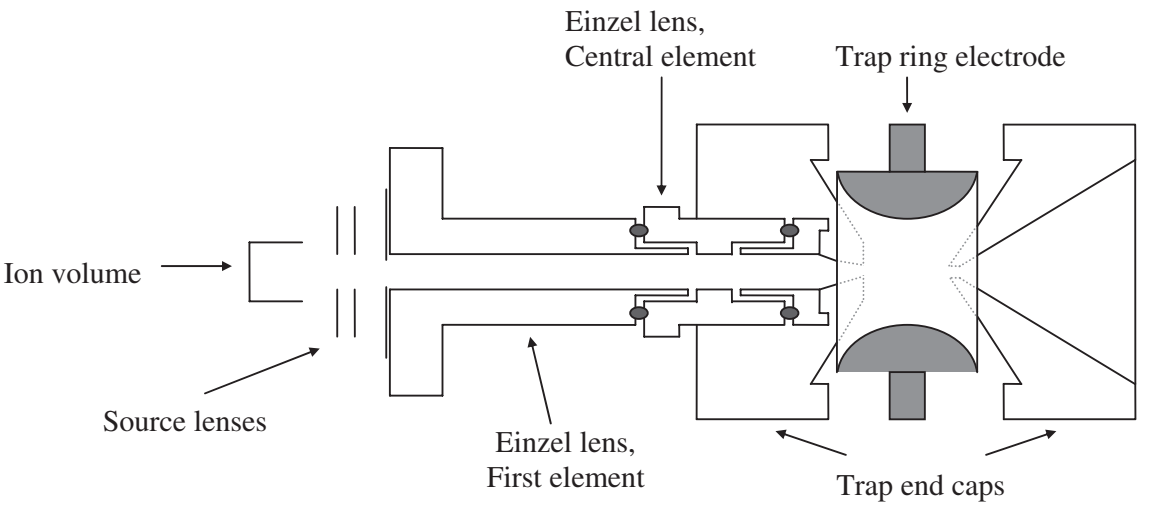


FIGURE 1.11 Cross-sectional view of an ion trap.

The mathematics that describes the motion of ions within the ion trap are given by the Mathieu equation. Details and discussions of three-dimensional ion stability diagrams can be found in either March and Hughes (1989) or Nourse and Cooks (1990). The beauty of the ion trap is that by controlling the three parameters of RF voltage, AC voltage, and DC voltage, a wide variety of experiments can be run quite easily (for details see March and Hughes, 1989).

There are three basic modes in which the ion trap can be operated. First, when the ion trap is operated with a fixed RF voltage and no DC bias between the endcap and ring electrodes, all ions above a certain cutoff m/z ratio will be trapped. As the RF voltage is raised, the cutoff m/z is increased in a controlled manner and the ions are sequentially ejected and detected. The result is the standard mass spectrum and this procedure is called the "mass-selective instability" mode of operation. The maximum RF potential that can be applied between the electrodes limits the upper mass range in this mode. Ions of mass contained beyond the upper limit are removed after the RF potential is brought back to zero.

The second mode of operation uses a DC potential across the endcaps; the general result is that there is now both a low- and high-end cutoff (m/z) of ions. The possibilities of experiments in this mode of operation are tremendous, and most operations with the ion trap use this mode. As few as one ion mass can be selected. Selective ion monitoring is an important use of this mode of operation. There is no practical limit on the number of ionic masses that can be selected.

The third mode of operation is similar to the second, with the addition of an auxiliary oscillatory field between the endcap electrodes, which results in adding kinetic energy selectively to a particular ion. With a small amplitude auxiliary field, selected ions gain kinetic energy slowly, during which time they usually undergo a fragmenting collision; the result can be a nearly 100% MS-MS efficiency. If the inherent sensitivity of the ion trap is considered along with the nearly 100% tandem efficiency, the use of the ion trap for the tandem MS experiment greatly outshines the so-called triple quad (see below).

Another way to use this kinetic energy addition mode is to selectively reject unwanted ions from the ion trap. These could be ions derived from solvent or from the matrix in FAB or LSIMS experiments. A constant frequency field at high voltage during the ionization period will selectively reject a single ion. Multiple ions can also be selected in this mode.

1.4.4 Time-of-Flight Mass Spectrometer

The concept of time-of-flight (TOF) mass spectrometers is simple. Ions are accelerated through a potential (V) and are then allowed to "drift" down a tube to a detector. If the assumption is made that all of the ions arriving at the beginning of the drift tube have the same energy given by $zeV = mv^2/2$, then ions of different mass will have different velocities: $v = (2zeV/m)^{\frac{1}{2}}$. If a spectrometer possesses a drift tube of length L, the time of flight for an ion is given by: $t = (L^2m/2zeV)^{\frac{1}{2}}$, from which the mass for a given ion can be easily calculated.

The critical aspect of this otherwise simple instrument is the need to produce the ions at an accurately known start time and position. These constraints generally limit TOF spectrometers to use pulsed ionization techniques, which include plasma and laser desorption (e.g., MALDI, matrix assisted laser desorption ionization).

The resolution of TOF instruments is usually less than 20000 because some variation in ion energy is unavoidable. Also, since the difference in arrival times at the detector can be less than 10^{-7} seconds, fast electronics are necessary for adequate resolution. On the positive side, the mass range of these instruments is unlimited, and, like quadrupoles, they have excellent sensitivity due to lack of resolving slits. Thus, the technique is most useful for large biomolecules.

1.4.5 Fourier Transform Mass Spectrometer

In a Fourier transform mass spectrometer (formerly called an ion cyclotron resonance mass spectrometer), ions are held in a cell with an electric trapping potential within a strong magnetic field. Within the cell, each ion orbits in a direction perpendicular to the magnetic field, with a frequency proportional to the ion's m/z value. A radiofrequency pulse applied to the cell brings all of the cycloidal frequencies into resonance simultaneously to yield an interferogram, conceptually similar to the free induction decay (FID) signal in NMR or the interferogram generated in FTIR experiments. The interferogram, which is a time domain spectrum, is Fourier transformed into a frequency domain spectrum, which then yields the conventional m/z spectrum. Pulsed Fourier transform methods applied to nuclear magnetic resonance spectroscopy are discussed in Chapters 3, 4, and 5.

Because the instrument is operated at fixed magnetic field strength, extremely high field superconducting magnets can be used. Also, because mass range is directly proportional to magnetic field strength, very high mass detection is possible. Finally, since all of the ions from a single ionization event can be trapped and analyzed, the method is very sensitive and works well with pulsed ionization methods. The most compelling aspect of the method is its high resolution, making FT mass spectrometers an attractive alternative to other mass analyzers. The FT mass spectrometer can be coupled to chromatographic instrumentation and various ionization methods, which means that it can be easily used with small molecules. Further information on FT mass spectrometers can be found in the book by Gross (1990).

1.4.6 Tandem Mass Spectrometry

Tandem mass spectrometry or MS-MS ("MS squared") is useful in studies with both known and unknown compounds; with certain ion traps, MS to the nth ($MS^{(n)}$) is possible where $n = 2$ to 9. In practice, n rarely exceeds 2 or 3. With MS-MS, a "parent" ion from the initial fragmentation (the initial fragmentation gives rise to the conventional mass spectrum) is selected and allowed or induced to fragment further thus giving rise to "daughter" ions. In complex mixtures, these daughter ions provide unequivocal evidence for the presence of a known compound. For unknown or new compounds, these daughter ions provide potential for further structural information.

One popular use of MS-MS involves ionizing a crude sample, selectively "fishing out" an ion characteristic for the compound under study and obtaining the diagnostic spectrum of the daughter ions produced from that ion. In this way, a compound can be unequivocally detected in a crude sample, with no prior chromatographic (or other separation steps) being required. Thus, MS-MS can be a very powerful screening tool. This type of analysis alleviates the need for complex separations of mixtures for many routine analyses. For instance, the analysis of urine samples from humans (or from other animals such as race horses) for the presence of drugs or drug metabolites can be carried out routinely on whole urine (i.e., no purification or separation) by MS-MS. For unknown compounds, these daughter ions can provide structural information as well.

One way to carry out MS-MS is to link two or more mass analyzers in series to produce an instrument capable of selecting a single ion, and examining how that ion (either a parent or daughter ion) fragments. For instance, three quadrupoles can be linked (a so-called triple quad) to produce a tandem mass spectrometer. In this arrangement, the first quadrupole selects a specific ion for further analysis, the second quadrupole functions as a collision cell (collision induced dissociation, CID) and is operated with radiofrequency only, and the third quadrupole separates the product ions to produce a spectrum of daughter ions. The field of tandem mass spectrometry is already rather mature with good books available (Benninghoven et al., 1987; Wilson et al., 1989).

In order for an instrument to carry out MS-MS, it must be able to do the three operations outlined above. As we have seen, however, ion-trap systems capable of MS-MS and $MS^{(n)}$ do not use a tandem arrangement of mass analyzers at all, but rather use a single ion trap for all three operations simultaneously. As has already been stated, these ion-trap tandem mass spectrometer experiments are very sensitive and are now user friendly. The ion trap brings the capability for carrying out MS-MS experiments to the benchtop at relatively low cost.

A summary of mass analyzers and ionization methods is displayed in Table 1.2.

1.5 INTERPRETATION OF EI MASS SPECTRA

Our discussion of interpreting mass spectra is limited to EI mass spectrometry. Fragmentation in EI mass spectra is rich with structural information; mastery of EI mass spectra is especially useful for the organic chemist.

EI mass spectra are routinely obtained at an electron beam energy of 70 eV. The desired and simplest event that occurs is the removal of a single electron from the molecule in the gas phase by an electron of the electron beam to form the molecular ion, which is a radical cation. For example, methanol forms a molecular ion in which the single dot represents the remaining odd electron as seen in Scheme 1.1. When the charge can be localized on one particular atom, the charge is shown on that atom:

$$CH_3\overset{\cdot}{\underset{\cdot\cdot}{\overset{+}{O}}}H$$

$$CH_3OH + e^- \rightarrow CH_3OH^{\cdot+}(m/z\ 32) + 2e^-$$

(Sch 1.1)

Many of these molecular ions rapidly disintegrate in 10^{-10} seconds to 10^{-3} seconds to give, in the simplest

TABLE 1.2 Summary of Mass Analyzers

Mass Analyzer	Mass Range	Resolution	Sensitivity	Advantage	Disadvantage
Magnetic sector	1 – 15000 m/z	0.0001	Low	High resolution	Low sensitivity Very expensive High technical expertise
Quadrupole	1 – 5000 m/z	Unit	High	Easy to use Inexpensive High sensitivity	Low resolution Low mass range
Ion trap	1 – 5000 m/z	Unit	High	Easy to use Inexpensive High sensitivity Tandem MS (MS^n)	Low resolution Low mass range
Time of flight	Unlimited	0.0001	High	High mass range Simple design	Very high resolution
Fourier transform	Up to 70 kDa	0.0001	High	Very high resolution and mass range	Very expensive High technical expertise

case, a positively charged fragment ion and a radical. Many fragment ions are thus formed, and each of these can cleave to yield smaller fragments; examples of possible cleavages for methanol are given in Scheme 1.2.

$$CH_3OH^{\cdot+} \longrightarrow CH_2OH^+ (m/z\ 31) + H^{\cdot}$$
$$CH_3OH^{\cdot+} \longrightarrow CH_3{}^+ (m/z\ 15) + {}^{\cdot}OH$$
$$CH_2OH^+ \longrightarrow CHO^+ (m/z\ 29) + H_2$$

(Sch 1.2)

If some of the molecular ions remain intact long enough to reach the detector, we see a molecular ion peak. It is important to recognize the molecular ion peak because this gives the molecular weight of the compound. With unit resolution, this weight is the molecular weight to the nearest whole number.

A mass spectrum is a presentation of the masses of the positively charged fragments (including the molecular ion) versus their relative abundances. The most intense peak in the spectrum, called the base peak, is assigned a value of 100%, and the intensities (height × sensitivity factor) of the other peaks, including the molecular ion peak, are reported as percentages of the base peak. Of course, the molecular ion peak may sometimes be the base peak. In Figure 1.1, the molecular ion peak is m/z 121, and the base peak is m/z 77.

A tabular or graphic presentation of a spectrum may be used. A graph has the advantage of presenting patterns that, with experience, can be quickly recognized. However, a graph must be drawn so that there is no difficulty in distinguishing mass units. Mistaking a peak at, say, m/z 79 for m/z 80 can result in total confusion. The molecular ion peak is usually the peak of highest mass number except for the isotope peaks.

1.5.1 Recognition of the Molecular Ion Peak

Quite often, under electron impact (EI), recognition of the molecular ion peak $(M)^+$ poses a problem. The peak may be very weak or it may not appear at all; how can we be sure that it is the molecular ion peak and not a fragment peak or an impurity? Often the best solution, if there is doubt, is to obtain a chemical ionization spectrum (see Section 1.3.1.2). The usual result is an intense peak at $[M + 1]^+$ and little fragmentation.

Many peaks can be ruled out as possible molecular ions simply on grounds of reasonable structure requirements. The nitrogen rule is often helpful. It states that a molecule of even-numbered molecular weight must contain either no nitrogen atoms or an even number of nitrogen atoms; an odd-numbered molecular weight requires an odd number of nitrogen atoms.* This rule holds for all compounds containing carbon, hydrogen, oxygen, nitrogen, sulfur, and the halogens, as well as many of the less usual atoms such as phosphorus, boron, silicon, arsenic, and the alkaline earths.

A useful corollary of the nitrogen rule states that fragmentation at a single bond gives an odd-numbered ion fragment from an even-numbered molecular ion, and an even-numbered ion fragment from an odd-numbered molecular ion. For this corollary to hold, the ion fragment must contain all of the nitrogen (if any) of the molecular ion.

Consideration of the breakdown pattern coupled with other information will also assist in identifying molecular ions. It should be kept in mind that Appendix A contains fragment formulas as well as molecular formulas. Some of the formulas may be discarded as trivial in attempts to solve a particular problem.

The intensity of the molecular ion peak depends on the stability of the molecular ion. The most stable molecular ions are those of purely aromatic systems. If substituents that have favorable modes of cleavage are present, the molecular ion peak will be less intense, and the fragment peaks relatively more intense. In general, the following group of compounds will, in order of decreasing ability, give prominent molecular ion peaks: aromatic compounds > conjugated alkenes >

*For the nitrogen rule to hold, only unit atomic masses (i.e., integers) are used in calculating the formula masses.

cyclic compounds > organic sulfides > short, normal alkanes > mercaptans. Recognizable molecular ions are usually produced for these compounds in order of decreasing ability: ketones > amines > esters > ethers > carboxylic acids ~ aldehydes ~ amides ~ halides. The molecular ion is frequently not detectable in aliphatic alcohols, nitrites, nitrates, nitro compounds, nitriles, and in highly branched compounds.

The presence of an M − 15 peak (loss of CH_3), or an M − 18 peak (loss of H_2O), or an M − 31 peak (loss of OCH_3 from methyl esters), and so on, is taken as confirmation of a molecular ion peak. An M − 1 peak is common, and occasionally an M − 2 peak (loss of H_2 by either fragmentation or thermolysis), or even a rare M − 3 peak (from alcohols) is reasonable. Peaks in the range of M − 3 to M − 14, however, indicate that contaminants may be present or that the presumed molecular ion peak is actually a fragment ion peak. Losses of fragments of masses of 19 to 25 are also unlikely (except for loss of F = 19 or HF = 20 from fluorinated compounds). Loss of 16 (O), 17 (OH), or 18 (H_2O) are likely only if an oxygen atom is in the molecule.

1.5.2 Determination of a Molecular Formula

1.5.2.1 Unit-Mass Molecular Ion and Isotope Peaks. So far, we have discussed the mass spectrum in terms of unit resolutions: The unit mass of the molecular ion of C_7H_7NO (Figure 1.1) is m/z 121—that is, the sum of the unit masses of the most abundant isotopes: $(7 \times 12$ [for $^{12}C]) + (7 \times 1$ [for $^{1}H]) + (1 \times 14$ [for $^{14}N] + (1 \times 16$ [for $^{16}O]) = 121$.

In addition, molecular species exist that contain the less abundant isotopes, and these give rise to the "isotope peaks" at M + 1, M + 2, etc. In Figure 1.1, the M + 1 peak is approximately 8% of the intensity of the molecular ion peak, which for this purpose, is assigned an intensity of 100%. Contributing to the M + 1 peak are the isotopes, ^{13}C, ^{2}H, ^{15}N, and ^{17}O. Table 1.3 gives the abundances of these isotopes relative to those of the most abundant isotopes. The only contributor to the M + 2 peak of C_7H_7NO is ^{18}O, whose relative abundance is very low (or a combination of two of the isotopes that contribute to the M + 1, for example, one ^{13}C and one ^{2}H); thus the M + 2 peak is undetected. If only C, H, N, O, F, P, and I are present, the approximate expected percentage (M + 1) and percentage (M + 2) intensities can be calculated by use of the following equations for a compound of formula $C_nH_mN_xO_y$ (note: F, P, and I are monoisotopic and do not contribute and can be ignored for the calculation):

$$\%\,(M+1) \approx (1.1 \cdot n) + (0.36 \cdot x) \text{ and } \%\,(M+2) \approx (1.1 \cdot n)^2/200 + (0.2 \cdot y)$$

If these isotope peaks are intense enough to be measured accurately, the above calculations may be useful in determining the molecular formula.*

If sulfur or silicon is present, the M + 2 peak will be more intense. In the case of a single sulfur atom, ^{34}S contributes approximately 4.40% to the M + 2 peak; for a single silicon in the molecule, ^{30}Si contributes about 3.35% to the M + 2 peak (see Section 1.6.15). A single chlorine atom results in a contribution of 32.50% to the M + 2 peak, while a single bromine atom contributes 98.00% to the M + 2 isotope peak. The effect of several bromine and chlorine atoms is described in Section 1.6.16. Note the appearance of additional isotope peaks in the case of multiple bromine and chlorine atoms. Obviously the mass spectrum should be routinely scanned for the relative intensities of the M + 2, M + 4, and higher isotope peaks, and the relative intensities should be carefully measured. Since F, P, and I are monoisotopic, they can be difficult to spot.

For most of the Problems in this text, the unit-resolution molecular ion, used in conjunction with IR and NMR, will suffice for determining the molecular formula by browsing

*There are limitations beyond the difficulty of measuring small peaks: The $^{13}C/^{12}C$ ratio differs with the source of the compound—synthetic compared with a natural source. A natural product from different organisms or regions may show differences. Furthermore, isotope peaks may be more intense than the calculated value because of ion – molecule interactions that vary with the sample concentration or with the class of compound involved.

TABLE 1.3 Relative Isotopic Abundances of Common Elements

Element	Isotope	Relative Abundance	Isotope	Relative Abundance	Isotope	Relative Abundance
Carbon	^{12}C	100	^{13}C	1.11		
Hydrogen	^{1}H	100	^{2}H	0.016		
Nitrogen	^{14}N	100	^{15}N	0.38		
Oxygen	^{16}O	100	^{17}O	0.04	^{18}O	0.2
Fluorine	^{19}F	100				
Silicon	^{28}Si	100	^{29}Si	5.1	^{30}Si	3.35
Phosphorus	^{31}P	100				
Sulfur	^{32}S	100	^{33}S	0.78	^{34}S	4.4
Chlorine	^{35}Cl	100			^{37}Cl	32.5
Bromine	^{79}Br	100			^{81}Br	98
Iodine	^{127}I	100				

Appendix A. For several more difficult Problems, the high-resolution formula masses—for use with Appendix A (see Section 1.5.2.2)—have been supplied.

Table 1.3 lists the principal stable isotopes of the common elements and their relative abundance calculated on the basis of 100 molecules containing the most common isotope. Note that this presentation differs from many isotopic abundance tables, in which the sum of all the isotopes of an element adds up to 100%.

1.5.2.2 High-Resolution Molecular Ion. A unique molecular formula (or fragment formula) can often be derived from a sufficiently accurate mass measurement alone (high-resolution mass spectrometry). This is possible because the nuclide masses are not integers (see Table 1.4). For example, we can distinguish at a unit mass of 28 among CO, N_2, CH_2N, and C_2H_4. The exact mass of CO is: 12.0000 (for ^{12}C) + 15.9949 (for ^{16}O) = 27.9949; the exact mass of N_2 is: 2×14.0031 (for ^{14}N) = 28.0062. Similar calculations give an exact mass of 28.0187 for CH_2N and 28.0312 for C_2H_4.

Thus, the mass observed for the molecular ion of CO, for example, is the sum of the exact formula masses of the most abundant isotope of carbon and of oxygen. This differs from a molecular weight of CO based on atomic weights that are the average of weights of all natural isotopes of an element (e.g., C = 12.01, O = 15.999).

Table 1.4 gives the masses to four or five decimal places for the common naturally occurring isotopes; it also gives the familiar atomic weights (average weights for the elements).

TABLE 1.4 Exact Masses of Isotopes

Element	Atomic Weight	Nuclide	Mass
Hydrogen	1.00794	^{1}H	1.00783
		D(^{2}H)	2.01410
Carbon	12.01115	^{12}C	12.00000 (std)
		^{13}C	13.00336
Nitrogen	14.0067	^{14}N	14.0031
		^{15}N	15.0001
Oxygen	15.9994	^{16}O	15.9949
		^{17}O	16.9991
		^{18}O	17.9992
Fluorine	18.9984	^{19}F	18.9984
Silicon	28.0855	^{28}Si	27.9769
		^{29}Si	28.9765
		^{30}Si	29.9738
Phosphorus	30.9738	^{31}P	30.9738
Sulfur	32.0660	^{32}S	31.9721
		^{33}S	32.9715
		^{34}S	33.9679
Chlorine	35.4527	^{35}Cl	34.9689
		^{37}Cl	36.9659
Bromine	79.9094	^{79}Br	78.9183
		^{81}Br	80.9163
Iodine	126.9045	^{127}I	126.9045

Appendix A lists molecular and fragment formulas in order of the unit masses. Under each unit mass, the formulas are listed in order of the standard *Chemical Abstract* system. The calculated formula mass (FM) to four decimal places is given for each formula. Appendix A is designed for browsing, on the assumption that the student has a unit molecular mass from a unit-resolution mass spectrometer and clues from other spectra. Note that the table includes only C, H, N, and O.

1.5.3 Use of the Molecular Formula. Index of Hydrogen Deficiency

If organic chemists had to choose a single item of information above all others that are usually available from spectra or from chemical manipulations, they would certainly choose the molecular formula.

In addition to the kinds and numbers of atoms, the molecular formula gives the index of hydrogen deficiency. The index of hydrogen deficiency is the number of *pairs* of hydrogen atoms that must be removed from the corresponding "saturated" formula to produce the molecular formula of the compound of interest. The index of hydrogen deficiency is also called the number of "sites (or degrees) of unsaturation"; this description is incomplete since hydrogen deficiency can result from cyclic structures as well as from multiple bonds. The index is thus the sum of the number of rings, the number of double bonds, and twice the number of triple bonds.

The index of hydrogen deficiency can be calculated for compounds containing carbon, hydrogen, nitrogen, halogen, oxygen, and sulfur having the generalized molecular formula, $C_nH_mX_xN_yO_z$, from the equation

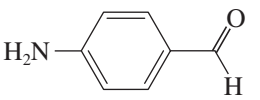
$$\text{Index} = (n) - (m/2) - (x/2) + (y/2) + 1$$

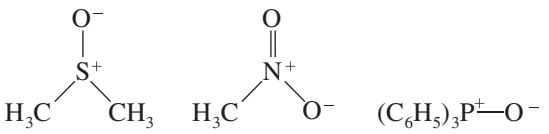
Thus, the compound C_7H_7NO has an index of $7 - 3.5 + 0.5 + 1 = 5$. Note that divalent atoms (oxygen and sulfur) are not counted in the formula.

For the generalized molecular formula $\alpha_I\beta_{II}\gamma_{III}\delta_{IV}$, the index is given by (IV) − (I/2) + (III/2) + 1, where α is H, D, or halogen (i.e., any monovalent atom), β is O, S, or any other bivalent atom, γ is N, P, or any other trivalent atom, and δ is C, Si, or any other tetravalent atom. The numerals I – IV designate the numbers of the mono-, di-, tri-, and tetravalent atoms, respectively.

For simple molecular formulas, we can arrive at the index by comparison of the formula of interest with the molecular formula of the corresponding saturated compound. Compare C_6H_6 and C_6H_{14}; the index is 4 for the former and 0 for the latter.

The index for C_7H_7NO is 5, and a possible structure is benzamide (see Figure 1.1). Of course, other isomers (i.e., compounds with the same molecular formula) are possible, such as





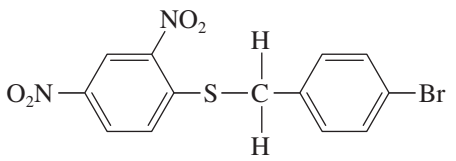
Dimethyl sulfoxide | Nitromethane | Triphenylphosphine oxide

FIGURE 1.12 "Polar" Lewis structures of dimethyl sulfoxide, nitromethane, and triphenylphosphine oxide that correctly account for the index of hydrogen deficiency.

Note that the benzene ring itself accounts for four sites of unsaturation: three for the double bonds and one for the ring.

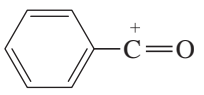
"Polar" structures must be used for compounds containing an atom in a higher valence state, such as sulfur or phosphorus. Thus, if we treat sulfur in dimethyl sulfoxide (DMSO) formally as a divalent atom, the calculated index, 0, is compatible with the structure in Figure 1.12. We must use only formulas with filled valence shells; that is, the Lewis octet rule must be obeyed.

Similarly, if we treat the nitrogen in nitromethane as a trivalent atom, the index is 1, which is compatible with Figure 1.12. If we treat phosphorus in triphenylphosphine oxide as trivalent, the index is 12, which fits the Lewis structure in Figure 1.12. As an example, let us consider the molecular formula $C_{13}H_9N_2O_4BrS$. The index of hydrogen deficiency would be $13 - \frac{10}{2} + \frac{2}{2} + 1 = 10$ and a consistent structure would be



(Index of hydrogen deficiency = 4 per benzene ring and 1 per NO_2 group.)

The formula above for the index can be applied to fragment ions as well as to the molecular ion. When it is applied to even-electron (all electrons paired) ions, the result is always an odd multiple of 0.5. As an example, consider $C_7H_5O^+$ with an index of 5.5. A reasonable structure is



since 5.5 pairs of hydrogen atoms would be necessary to obtain the corresponding saturated formula $C_7H_{16}O$ ($C_nH_{2n+2}O$). Odd-electron fragment ions will always give integer values of the index.

Such simple considerations give the chemist very ready information about structure. As another example, a compound containing a single oxygen atom might quickly be determined to be an ether or a carbonyl compound simply by the degree of hydrogen deficiency. Much of the potential structural information is readily confirmed with information from IR and NMR spectra (See Chapters 2, 3, and 4).

1.5.4 Fragmentation

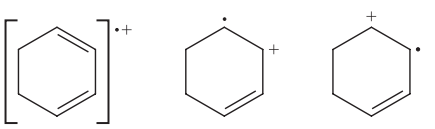
As a first impression, fragmenting a molecule with a huge excess of energy would seem a brute-force approach to molecular structure. The rationalizations used to correlate spectral patterns with structure, however, can only be described as elegant, though sometimes arbitrary. The insight of such pioneers as McLafferty, Beynon, Stenhagen, Ryhage, and Meyerson led to a number of rational mechanisms for fragmentation. These were masterfully summarized and elaborated by Biemann (1962), Budzikiewicz et al. (1967), and others.

Generally, the tendency is to represent the molecular ion with a localized charge. The approach of Budzikiewicz et al. (1967) is to localize the positive charge on either a π bond (except in conjugated systems), or on a heteroatom. Whether or not this concept is totally rigorous, it is, at the least, a pedagogic *tour de force.* We shall use such locally charged molecular ions in this book.

Structures **A**, **B**, and **C** in Figure 1.13, for example, represent the molecular ion of cyclohexadiene. Compound **A** is a delocalized structure with one less electron than the original uncharged diene; both the electron and the positive charge are delocalized over the π system. Since the electron removed to form the molecular ion is a π electron, other structures, such as **B** or **C** (resonance structures) can be used. Structures such as **B** and **C** localize the electron and the positive charge and thus are useful for describing fragmentation processes.

Fragmentation is initiated by electron impact. Only a small part of the driving force for fragmentation is energy transferred as the result of the impact. The major driving force is the cation-radical character that is imposed upon the structure.

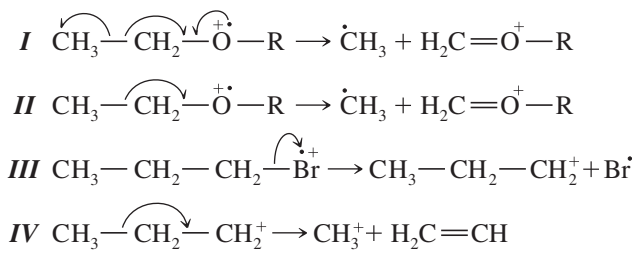
Fragmentation of the odd-electron molecular ion (radical-cation, $M^{+\cdot}$) may occur by homolytic or heterolytic cleavage of a single bond. In homolytic cleavage (Scheme 1.3, ***I***) each electron moves independently as shown by a (single-barbed) fishhook: the fragments are an even-electron cation and a free radical (odd electron). To prevent clutter, only one of each pair of fishhooks need to be shown (Scheme 1.3, ***II***). In heterolytic cleavage, a pair of electrons move together



A **B** **C**

FIGURE 1.13 Different representations of the radical cation of cyclohexadiene.

toward the charged site as shown by the conventional curved arrow; the fragments are again an even-electron cation and a radical, but here the final charge site is on the alkyl product (Scheme 1.3, ***III***).



(Sch 1.3)

In the absence of rings (whose fragmentation requires cleavage of two or more bonds), most of the prominent fragments in a mass spectrum are even-electron cations formed as above by a single cleavage. Further fragmentation of an even-electron cation usually results in another even-electron cation and an even-electron neutral molecule or fragment (Scheme 1.3, ***IV***).

Simultaneous or consecutive cleavage of several bonds may occur when energy benefits accrue from formation of a highly stabilized cation and/or a stable radical, or a neutral molecule, often through a well-defined low-energy pathway. These are treated in Section 1.5.5 (rearrangements) and in Section 1.6 under individual chemical classes.

The probability of cleavage of a particular bond is related to the bond strength, to the possibility of low energy transitions, and to the stability of the fragments, both charged and uncharged, formed in the fragmentation process. Our knowledge of pyrolytic cleavages can be used, to some extent, to predict likely modes of cleavage of the molecular ion. Because of the extremely low pressure in the mass spectrometer, there are very few fragment collisions; we are dealing largely with unimolecular decompositions. This assumption, backed by a large collection of reference spectra, is the basis for the vast amount of information available from the fragmentation pattern of a molecule. Whereas conventional organic chemistry deals with reactions initiated by chemical reagents, by thermal energy, or by light, mass spectrometry is concerned with the consequences suffered by an organic molecule at a vapor pressure of about 10^{-6} mm Hg struck by an ionizing electron beam.

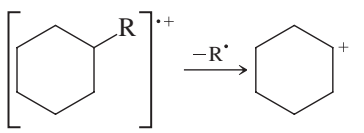
A number of general guidelines for predicting prominent peaks in EI spectra can be written and rationalized by using standard concepts of physical organic chemistry:

1. The relative intensity of the molecular ion peak is greatest for the straight-chain compound and decreases as the degree of branching increases (see rule 3).
2. The relative intensity of the molecular ion peak usually decreases with increasing molecular weight in a homologous series. Fatty esters appear to be an exception.
3. Cleavage is favored at alkyl-substituted carbon atoms: the more substituted, the more likely is cleavage. This is a consequence of the increased stability of a tertiary carbocation over a secondary, which in turn is more stable than a primary. Generally, the largest substituent at a branch is eliminated most readily as a radical, presumably because a long-chain radical can achieve some stability by delocalization of the lone electron.

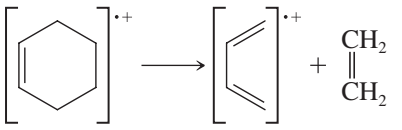
   Cation stability order:

   $$CH_3^+ < R_2CH_2^+ < R_3CH^+ < R_3C^+$$

4. Double bonds, cyclic structures, and especially aromatic (or heteroaromatic) rings stabilize the molecular ion and thus increase the probability of its appearance.
5. Double bonds favor allylic cleavage and give the resonance-stabilized allylic carbocation. This rule does not hold for simple alkenes because of the ready migration of the double bond, but it does hold for cycloalkenes.
6. Saturated rings tend to lose alkyl side chains at the α bond. This is merely a special case of branching (rule 3). The positive charge tends to stay with the ring fragment. See Scheme 1.4. Unsaturated rings can undergo a retro-Diels-Alder reaction (see Scheme 1.5).

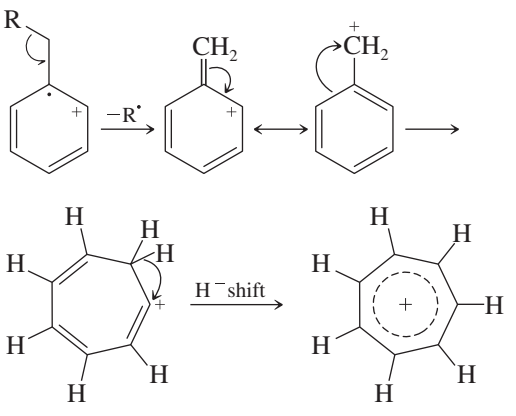


(Sch 1.4)



(Sch 1.5)

7. In alkyl-substituted aromatic compounds, cleavage is very probable at the bond β to the ring, giving the resonance-stabilized benzyl ion or, more likely, the tropylium ion (see Scheme 1.6).



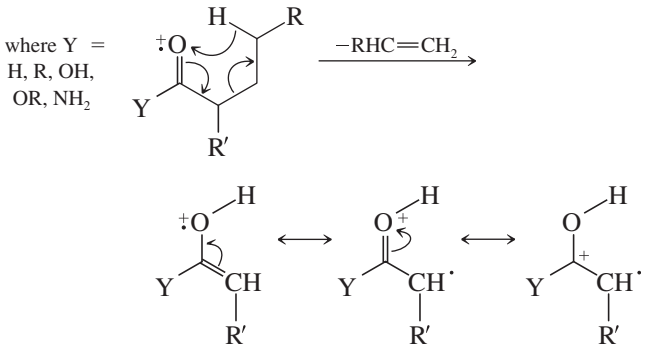
(Sch 1.6)

8. The C—C bonds next to a heteroatom are frequently cleaved, leaving the charge on the fragment containing the heteroatom whose nonbonding electrons provide resonance stabilization.
9. Cleavage is often associated with elimination of small, stable, neutral molecules, such as carbon monoxide, alkenes, water, ammonia, hydrogen sulfide, hydrogen cyanide, mercaptans, ketenes, or alcohols, often with rearrangement (Section 1.5.5).

It should be kept in mind that the fragmentation guidelines above apply to EI mass spectrometry. Since other ionizing techniques (CI, etc.) often produce molecular ions with much lower energy or quasimolecular ions with very different fragmentation patterns, different rules govern the fragmentation of these molecular ions.

1.5.5 Rearrangements

Rearrangement ions are fragments whose origin cannot be described by simple cleavage of bonds in the molecular ion but are a result of intramolecular atomic rearrangement during fragmentation. Rearrangements involving migration of hydrogen atoms in molecules that contain a heteroatom are especially common. One important example is the so-called McLafferty rearrangement; it is illustrated in Scheme 1.7 for the general case.



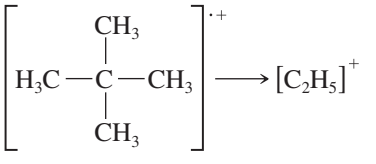
(Sch 1.7)

To undergo a McLafferty rearrangement, a molecule must possess an appropriately located heteroatom (e.g., O), a π system (usually a double bond), and an abstractable hydrogen atom γ to the C═O system.

Such rearrangements often account for prominent characteristic peaks and are consequently very useful for our purpose. They can frequently be rationalized on the basis of low-energy transitions and increased stability of the products. Rearrangements resulting in elimination of a stable neutral molecule are common (e.g., the alkene product in the McLafferty rearrangement) and will be encountered in the discussion of mass spectra of chemical classes.

Rearrangement peaks, with loss of a neutral molecule, can be recognized by considering the unit mass number (m/z) for fragment ions and for their corresponding molecular ions. A simple (no rearrangement) cleavage of an even-numbered molecular ion gives an odd-numbered fragment ion and simple cleavage of an odd-numbered molecular ion gives an even-numbered fragment. Observation of a fragment ion mass different by 1 unit from that expected for a fragment resulting from simple cleavage (e.g., an even-numbered fragment mass from an even-numbered molecular ion mass) indicates rearrangement of a hydrogen atom has accompanied fragmentation. Rearrangement peaks may be recognized by considering the corollary to the "nitrogen rule" (Section 1.5.1). Thus, an even-numbered peak derived from an even-numbered molecular ion is a result of two cleavages, which may involve a rearrangement.

Seemingly random rearrangements of hydrocarbons were noted by the early mass spectrometrists in the petroleum industry. For example, the rearrangement of the *neo*-pentyl radical-cation to the ethyl cation, shown in Scheme 1.8, defies a straightforward explanation.



(Sch 1.8)

1.6 MASS SPECTRA OF SOME CHEMICAL CLASSES

Mass spectra of a number of chemical classes are briefly described in this section in terms of the most useful generalizations for identification. For more details, the references cited should be consulted (in particular, the thorough treatment by Budzikiewicz et al., 1967). Databases are available both from publishers and as part of instrument capabilities. The references are selective rather than comprehensive. A table of frequently encountered fragment ions is given in Appendix B. A table of fragments (uncharged) that are commonly eliminated and some structural inferences are presented in Appendix C. More exhaustive listings of common fragment ions have been compiled (see References).

1.6.1 Hydrocarbons

1.6.1.1 Saturated Hydrocarbons. Most of the early work in mass spectrometry was done on hydrocarbons of interest to the petroleum industry. Guidelines 1 – 3, (Section 1.5.4) apply quite generally; rearrangement peaks, though common, are not usually intense (random rearrangements), and numerous reference spectra are available.

The molecular ion peak of a straight-chain, saturated hydrocarbon is always present, though of low intensity for

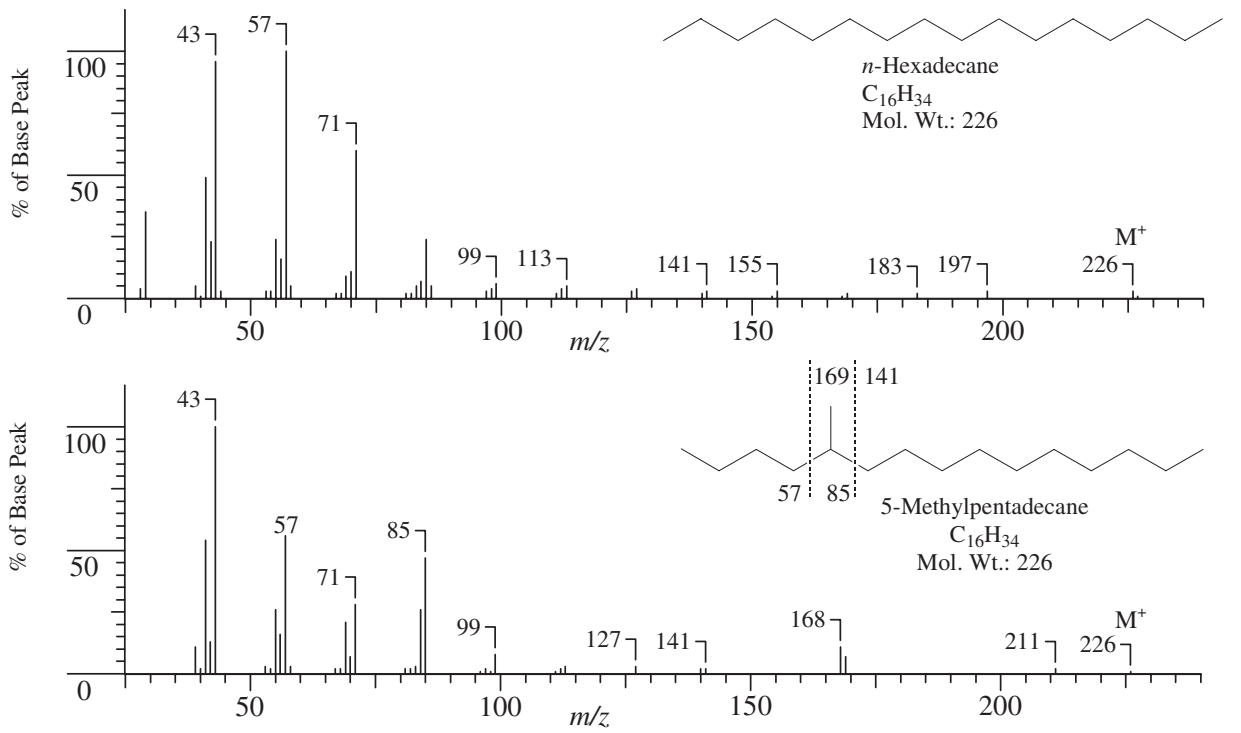


FIGURE 1.14 EI mass spectra of isomeric C_{16} hydrocarbons.

long-chain compounds. The fragmentation pattern is characterized by clusters of peaks, and the corresponding peaks of each cluster are 14 mass units (—CH_2—) apart. The largest peak in each cluster represents a C_nH_{2n+1} fragment and thus occurs at $m/z = 14n + 1$; this peak is accompanied by C_nH_{2n} and C_nH_{2n-1} fragments. The most abundant fragments are at C_3 and C_4, and the fragment abundances logarithmically decrease down to $[M - C_2H_5]^+$; the $[M - CH_3]^+$ peak is characteristically very weak or missing. Compounds containing more than eight carbon atoms show fairly similar spectra; identification then depends on the molecular ion peak.

Spectra of branched saturated hydrocarbons are grossly similar to those of straight-chain compounds, but the smooth curve of decreasing intensities is broken by preferred fragmentation at each branch. The smooth curve for the *n*-alkane in Figure 1.14 (top) is in contrast to the discontinuity at C_{12} for the branched alkane (Figure 1.14, bottom). This discontinuity indicates that the longest branch of 5-methylpentadecane has 10 carbon atoms.

In the bottom spectrum of Figure 1.14, the peaks at m/z 169 and 85 represent cleavage on either side of the branch with charge retention on the substituted carbon atom. Subtraction of the molecular weight from the sum of these fragments accounts for the fragment —CH—CH_3. Again, we appreciate the absence of a C_{11} unit, which cannot form by a single cleavage. Finally, the presence of a distinct M − 15 peak also indicates a methyl branch. The fragment resulting from cleavage at a branch tends to lose a single hydrogen atom so that the resulting C_nH_{2n} peak is prominent and sometimes more intense than the corresponding C_nH_{2n+1} peak.

A saturated ring in a hydrocarbon increases the relative intensity of the molecular ion peak and favors cleavage at the bond connecting the ring to the rest of the molecule (guideline 6, Section 1.5.4). Fragmentation of the ring is usually characterized by the loss of two carbon atoms as C_2H_4 (28) and C_2H_5 (29). This tendency to lose even-numbered fragments gives a spectrum that contains a greater proportion of even-numbered mass ions than the spectrum of an acyclic hydrocarbon. As in branched hydrocarbons, C—C cleavage is accompanied by the loss of a hydrogen atom. The characteristic peaks are therefore in the C_nH_{2n-1} and C_nH_{2n-2} series.

The mass spectrum of cyclohexane (Figure 1.15) shows a much more intense molecular ion than those of acyclic compounds, since fragmentation requires the cleavage of two carbon-carbon bonds. This spectrum has its base peak at m/z 56 (because of a loss of C_2H_4) and a large peak at m/z 41, which is a fragment in the C_nH_{2n-1} series with $n = 3$.

1.6.1.2 Alkenes (Olefins). The molecular ion peak of alkenes, especially polyalkenes, is usually distinct. Location of the double bond in acyclic alkenes is sometimes difficult because of its facile migration in the fragments. In cyclic (especially polycyclic) alkenes, location of the double bond is frequently evident as a result of a strong tendency for allylic cleavage without much double-bond migration (guideline 5, Section 1.5.4). Conjugation with a carbonyl group also fixes the position of the double bond. As with

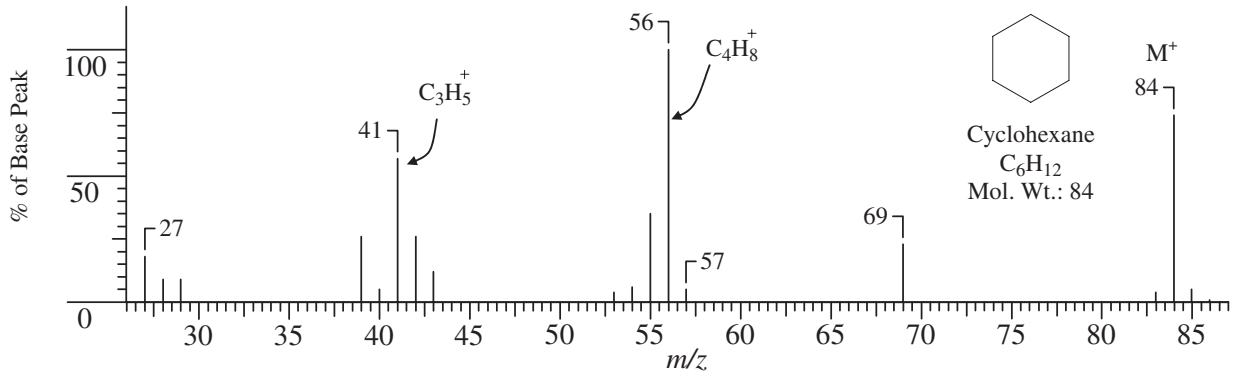
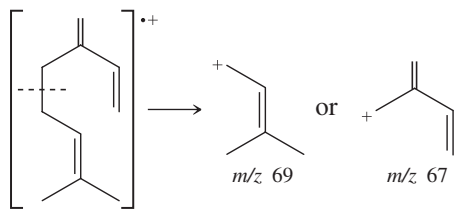


FIGURE 1.15 EI mass spectrum of cyclohexane.

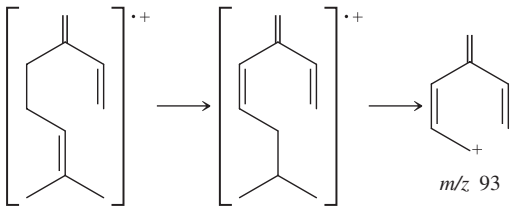
saturated hydrocarbons, acyclic alkenes are characterized by clusters of peaks at intervals of 14 units. In these clusters the C_nH_{2n-1} and C_nH_{2n} peaks are more intense than the C_nH_{2n+1} peaks.

The mass spectrum of β-myrcene, a monoterpene, is shown in Figure 1.16. The peaks at m/z 41, 55, and 69 correspond to the formula C_nH_{2n-1} with $n = 3$, 4, and 5, respectively. Formation of the m/z 41 peak must involve isomerization. The peaks at m/z 67 and 69 are the fragments from cleavage of a bi-allylic bond, which is shown in Scheme 1.9.



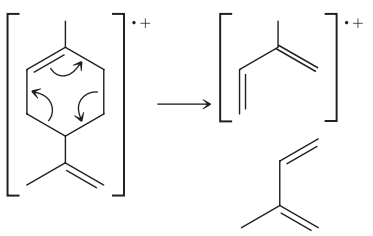
(Sch 1.9)

The peak at m/z 93 is rationalized in Scheme 1.10 as a structure of formula $C_7H_9^+$ formed by double bond isomerization (resulting in increased conjugation), followed by allylic cleavage. The ion at m/z 93 has at least two important resonance forms that contribute to its stability. As an exercise, the student is encouraged to draw them.



(Sch 1.10)

Cyclic alkenes usually show a distinct molecular ion peak. A unique mode of cleavage is the *retro*-Diels-Alder reaction. This reaction is illustrated with limonene in Scheme 1.11 (see Figure 1.17). A retro-Diels-Alder reaction in this example gives two isoprene molecules. Since the reaction is an example of a rearrangement, one of the isoprene moieties is a neutral molecule.



(Sch 1.11)

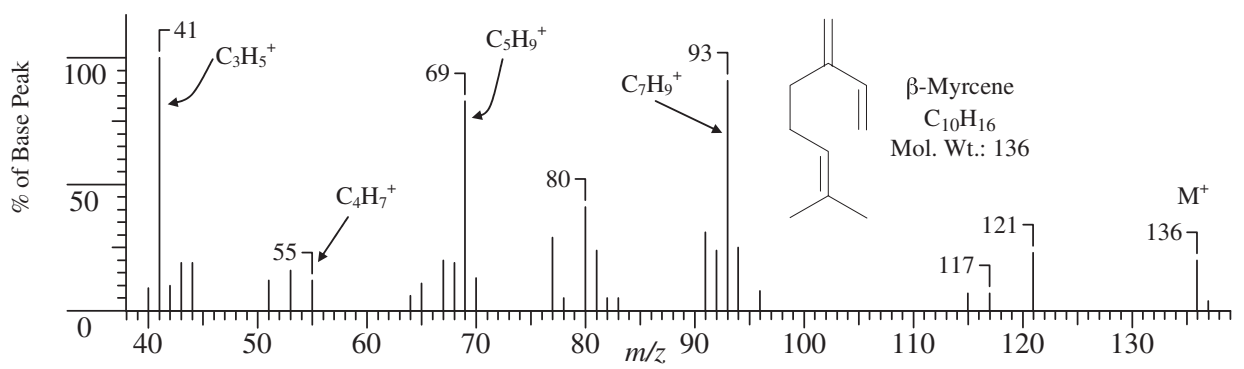


FIGURE 1.16 EI mass spectrum of β-myrcene.

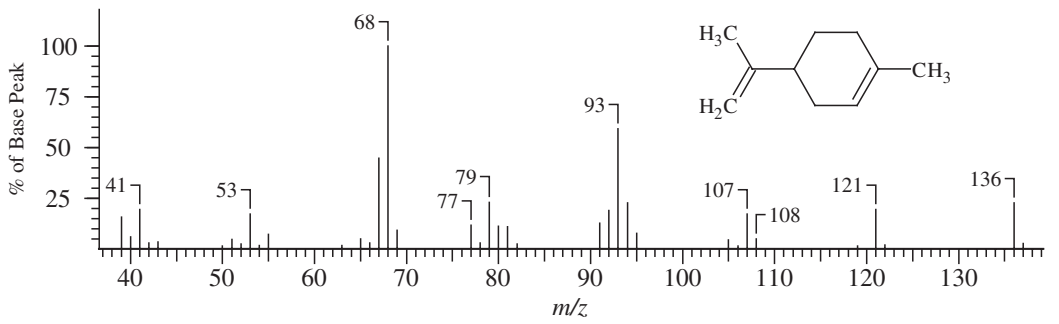


FIGURE 1.17 EI mass spectrum of limonene.

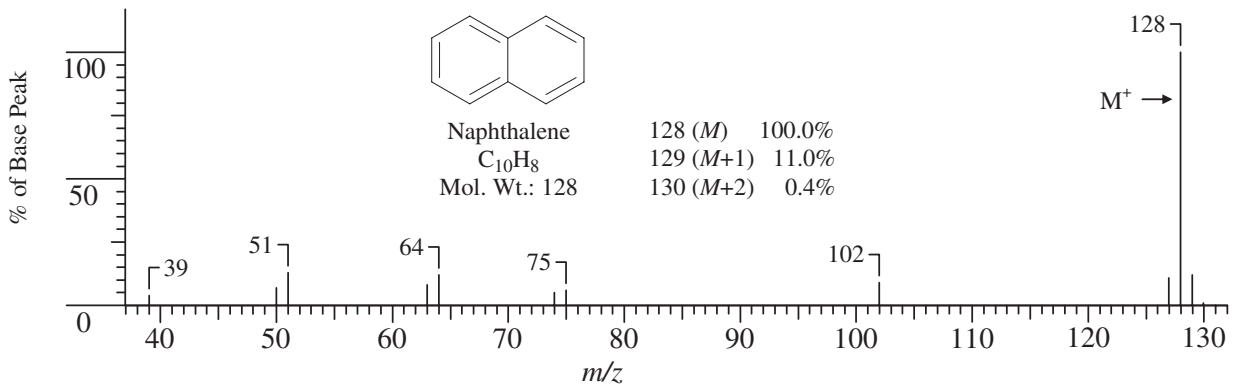


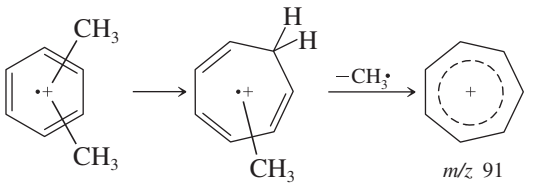
FIGURE 1.18 EI mass spectrum of naphthalene.

1.6.1.3 Aromatic and Aralkyl Hydrocarbons. An aromatic ring in a molecule stabilizes the molecular ion peak (guideline 4, Section 1.5.4), which is usually sufficiently large that accurate intensity measurements can be made on the M + 1 and M + 2 peaks.

Shown in Figure 1.18 is the mass spectrum of naphthalene. The molecular ion peak is also the base peak, and the largest fragment peak, m/z 51, is only 12.5% as intense as the molecular ion peak.

An alkyl-substituted benzene ring frequently gives a prominent peak (often the base peak) at m/z 91 ($C_6H_5CH_2^+$). Branching at the α-carbon leads to masses higher than 91, by increments of 14, the largest substituent being eliminated most readily (guideline 3, Section 1.5.4). The mere presence of a peak at mass 91, however, does not preclude branching at the α-carbon because this highly stabilized fragment may result from rearrangements. A distinct and sometimes prominent M − 1 peak results from similar benzylic cleavage of a C—H bond.

It has been proposed that, in most cases, the ion of mass 91 is a tropylium rather than a benzylic cation. This explains the ready loss of a methyl group, which seems to violate guideline 7, from xylenes (Scheme 1.12, see Figure 1.19). By comparison, toluene does not easily lose a methyl group. The incipient molecular radical ion of xylene rearranges to the methylcycloheptatriene radical ion, which then cleaves to the tropylium ion ($C_7H_7^+$). The frequently observed peak at m/z 65 results from the elimination of a neutral acetylene molecule from the tropylium ion.



(Sch 1.12)

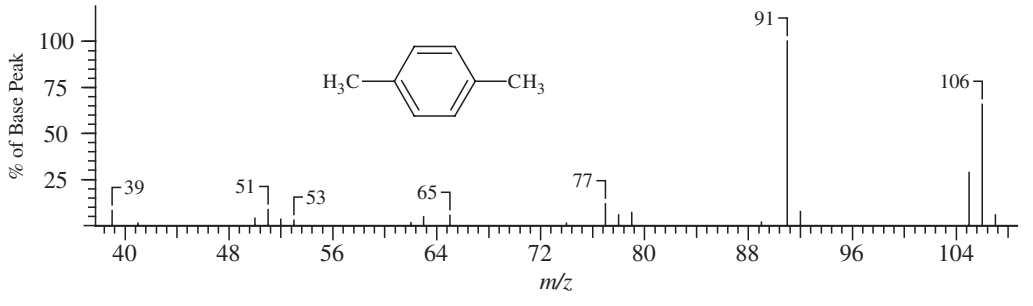
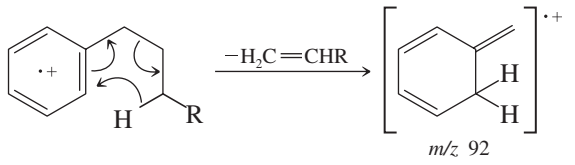


FIGURE 1.19 EI mass spectrum of *p*-xylene.

Hydrogen migration with elimination of a neutral alkene molecule accounts for the peak at m/z 92 observed when the alkyl group is longer than C_2. Scheme 1.13 illustrates with a general example. Note again that this is an example of a rearrangement.



(Sch 1.13)

A characteristic cluster of ions resulting from an α cleavage and hydrogen migration in monoalkylbenzenes appears at m/z 77 ($C_6H_5^+$), 78 ($C_6H_6^+$), and 79 ($C_6H_7^+$).

Alkylated polyphenyls and alkylated polycyclic aromatic hydrocarbons exhibit the same β cleavage as alkylbenzene compounds.

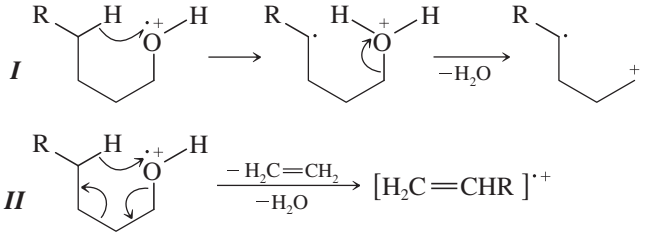
1.6.2 Hydroxy Compounds

1.6.2.1 Alcohols. The molecular ion peak of a primary or secondary alcohol is usually quite small and for a tertiary alcohol is often undetectable. The molecular ion of 1-pentanol is extremely weak compared with its near homologs. Expedients such as CI, or derivatization, may be used to obtain the molecular weight.

Cleavage of the C—C bond next to the oxygen atom is of general occurrence (guideline 8, Section 1.5.4). Thus, primary alcohols show a prominent peak resulting from $^+CH_2$—OH (m/z 31). Secondary and tertiary alcohols cleave analogously to give a prominent peak resulting from $^+$CHR—OH (m/z 45, 59, 73, etc.) and $^+$CRR′—OH (m/z 59, 73, 87, etc.), respectively. The largest substituent is expelled most readily (guideline 3). It is not unusual that the C—H bond next to the oxygen atom is cleaved; this less (or least) favored pathway gives rise to an M − 1 peak.

Primary alcohols, in addition to the principal C—C cleavage next to the oxygen atom, show a homologous series of peaks of progressively decreasing intensity resulting from cleavage at C—C bonds successively removed from the oxygen atom. In long-chain (>C_6) alcohols, the fragmentation becomes dominated by the hydrocarbon pattern; in fact, the spectrum resembles that of the corresponding alkene. The spectrum in the vicinity of a very weak or missing molecular ion peak of a primary alcohol is sometimes complicated by weak M − 2 and M − 3 peaks.

A distinct and sometimes prominent peak can usually be found at M − 18 from loss of water. This peak is most noticeable in spectra of primary alcohols. This elimination by electron impact has been rationalized and a mechanism in which a δ-hydrogen is lost is shown in Scheme 1.14, ***I***. A similar mechanism can be drawn in which a γ-hydrogen is lost. The M − 18 peak is frequently exaggerated by thermal decomposition of higher alcohols on hot inlet surfaces. Elimination of water, together with elimination of an alkene from primary alcohols (see Scheme 1.14, ***II***), accounts for the presence of a peak at M − (alkene + H_2O), that is, a peak at M − 46, M − 74, M − 102, …



(Sch 1.14)

Alcohols containing branched methyl groups (e.g., terpene alcohols) frequently show a fairly strong peak at M − 33 resulting from loss of CH_3 and H_2O.

Cyclic alcohols undergo fragmentation by complicated pathways; for example, cyclohexanol (Figure 1.20) (M = m/z 100) forms $C_6H_{11}O^+$ by simple loss of the α-hydrogen, loses H_2O to form $C_6H_{10}^+$ (which appears to have more than one possible bridged bicyclic structure), and forms $C_3H_5O^+$ (m/z 57) by a complex ring cleavage pathway.

A peak at m/z 31 (see above) is quite diagnostic for a primary alcohol provided it is more intense than peaks at m/z 45, 59, 73 …. However, the first-formed ion of a secondary alcohol can decompose further to give a moderately intense m/z 31 peak.

Figure 1.21 gives the characteristic spectra of isomeric primary, secondary, and tertiary C_5 alcohols.

Benzyl alcohols and their substituted homologs and analogs constitute a distinct class. Generally, the parent peak is strong. A moderate benzylic peak (M − OH) may be present as expected from cleavage β to the ring.

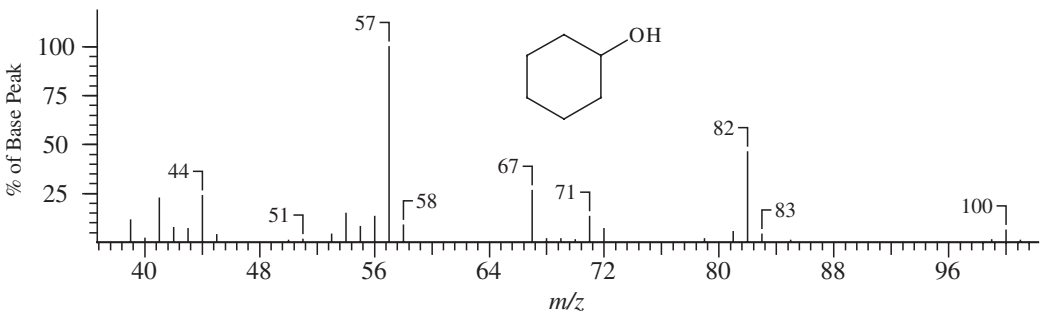


FIGURE 1.20 EI mass spectrum of cyclohexanol.

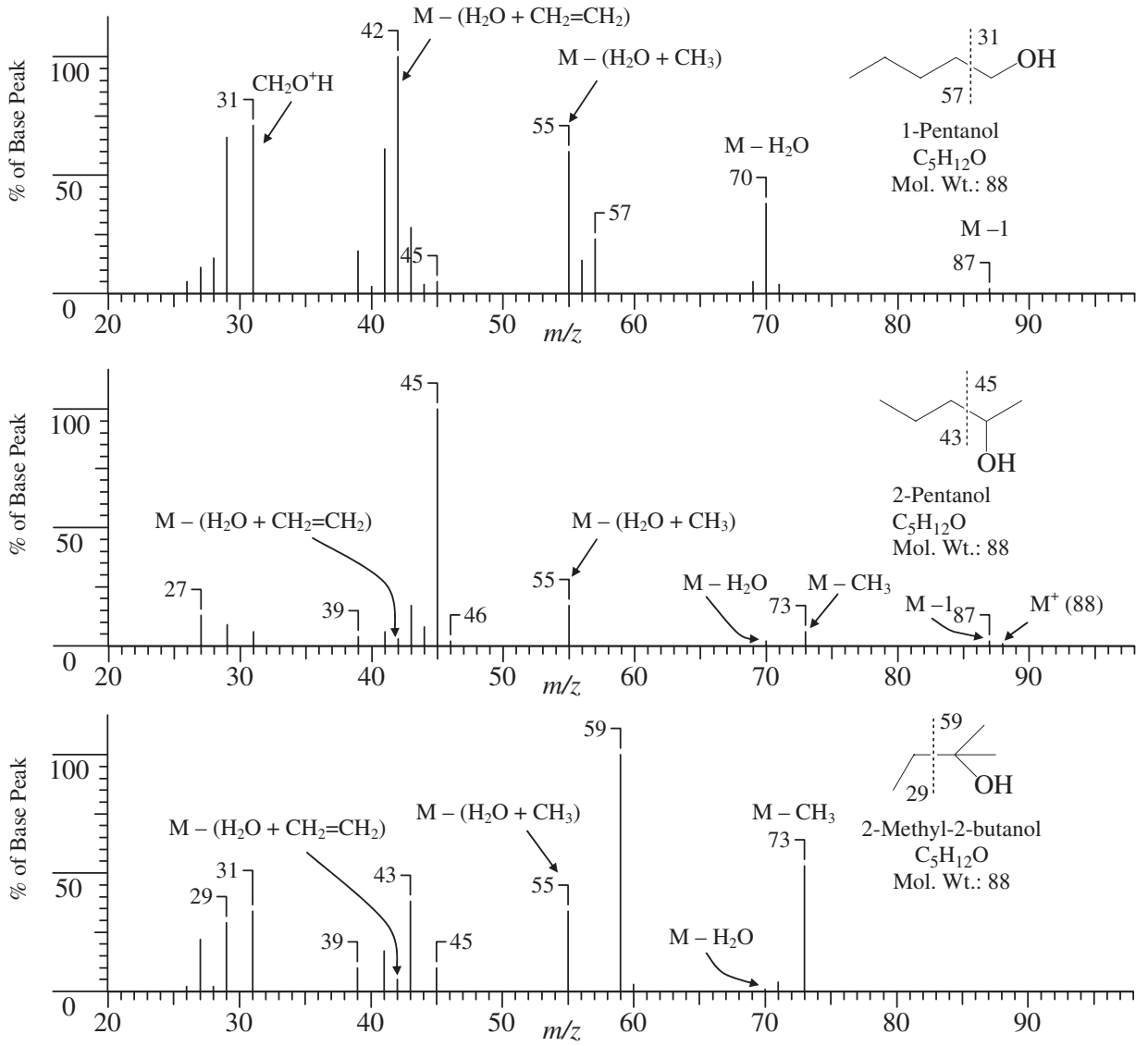
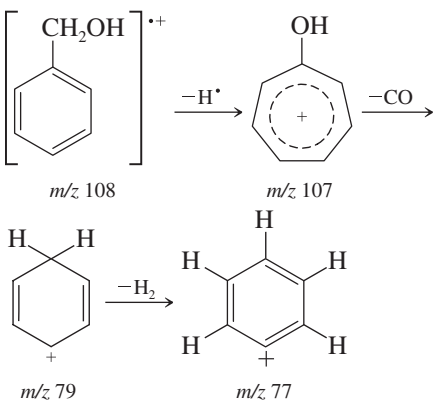


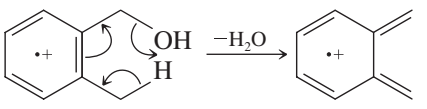
FIGURE 1.21 EI mass spectra of isomeric pentanols.

A complicated sequence leads to prominent M – 1, M – 2, and M – 3 peaks. Benzyl alcohol itself (Figure 1.22) fragments to give sequentially the M – 1 ion, the $C_6H_7^+$ ion by loss of CO, and the $C_6H_5^+$ ion by loss of H_2 (see Scheme 1.15).



(Sch 1.15)

Loss of H_2O to give a distinct M – 18 peak is a common feature, especially pronounced and mechanistically straightforward in some *ortho*-substituted benzyl alcohols (see Figure 1.23). The loss of water shown in Scheme 1.16 works equally well with an oxygen atom at the *ortho*-position (a phenol). The aromatic cluster at m/z 77, 78, and 79 resulting from complex degradation is prominent here also.



(Sch 1.16)

1.6.2.2 Phenols. A conspicuous molecular ion peak facilitates identification of phenols. In phenol itself, the molecular ion peak is the base peak, and the M – 1 peak is small. In cresols, the M – 1 peak is larger than that of the molecular ion as a result of a facile benzylic C—H cleavage.

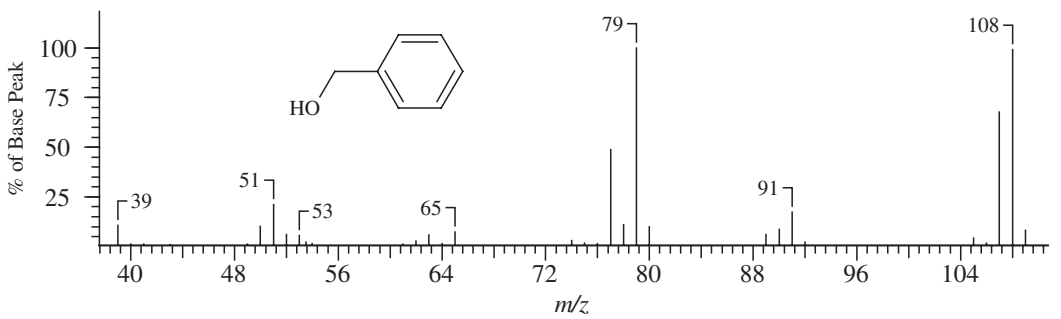


FIGURE 1.22 EI mass spectrum of benzyl alcohol.

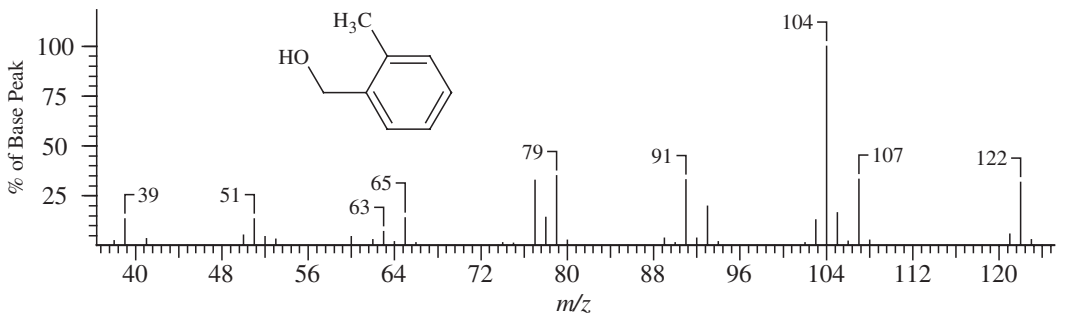


FIGURE 1.23 EI mass spectrum of *o*-methylbenzyl alcohol.

A rearrangement peak at m/z 77 and peaks resulting from the loss of CO (M − 28) and CHO (M − 29) are usually found in the mass spectra of phenols.

The mass spectrum of *o*-ethylphenol, a typical phenol, is shown in Figure 1.24. This spectrum shows that a methyl group is lost much more readily than an α-hydrogen.

1.6.3 Ethers

1.6.3.1 Aliphatic Ethers (and Acetals). The molecular ion peak (two mass units larger than that of an analogous hydrocarbon) is small, but larger sample size usually will make the molecular ion peak or the M + 1 peak obvious ($H^{\cdot}$ transfer during ion-molecule collision).

The presence of an oxygen atom can be deduced from strong peaks at m/z $31, 45, 59, 73, \ldots$ These peaks represent the RO^+ and $ROCH_2{}^+$ fragments. A typical aliphatic ether is shown in Figure 1.25. Fragmentation occurs in two principal ways:

1. Cleavage of the C—C bond next to the oxygen atom (α, β bond, guideline 8, Section 1.5.4). One or the other of these oxygen-containing ions may account for the base peak. In the case shown in Figure 1.25, the first cleavage (i.e., at the branch position leading to loss of the larger fragment) is preferred. However, the first-formed fragment decomposes further by loss of ethylene to give the base peak; this decomposition is important when the α-carbon is substituted (see McLafferty rearrangement, Section 1.5.5)

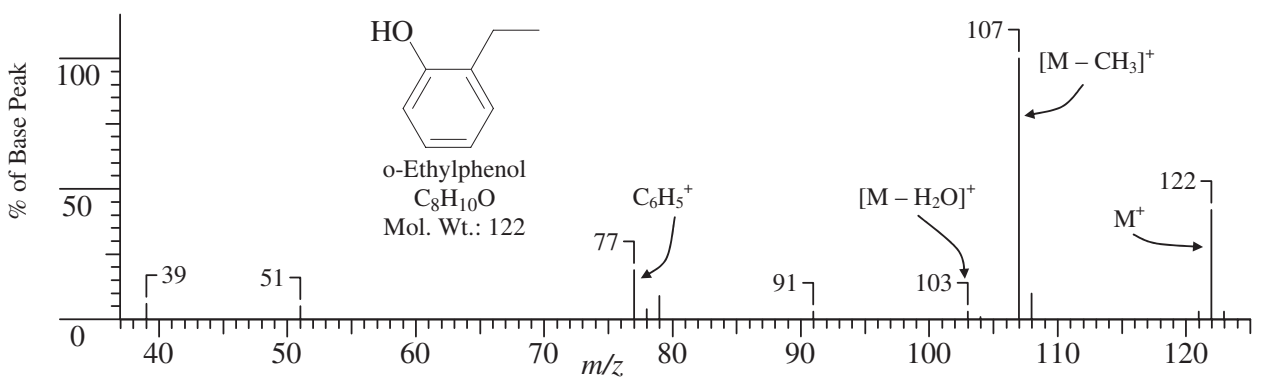


FIGURE 1.24 EI mass spectrum of *o*-ethylphenol.

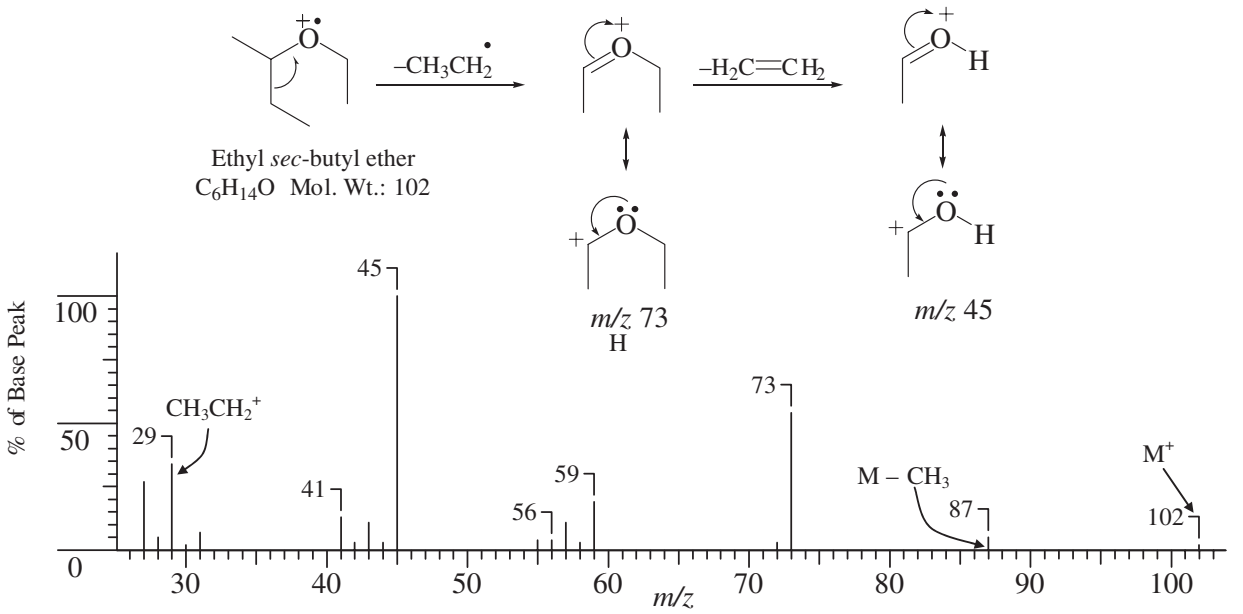
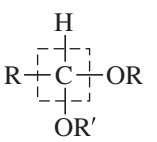


FIGURE 1.25 EI mass spectrum of ethyl *sec*-butyl ether.

2. C—O bond cleavage with the charge remaining on the alkyl fragment. The spectrum of long-chain ethers becomes dominated by the hydrocarbon pattern.

Acetals are a special class of ethers. Their mass spectra are characterized by an extremely weak molecular ion peak, by the prominent peaks at M – R and M – OR (and/or M – OR′), and a weak peak at M – H. Each of these cleavages is mediated by an oxygen atom and thus facile. As usual, elimination of the largest group is preferred. As with aliphatic ethers, the first-formed oxygen-containing fragments can decompose further with hydrogen migration and alkene elimination. Ketals behave similarly.



1.6.3.2 Aromatic Ethers. The molecular ion peak of aromatic ethers is prominent. Primary cleavage occurs at the bond β to the ring, and the first-formed ion can decompose further. Thus, anisole (Figure 1.26, MW 108) gives ions of m/z 93 and 65. The characteristic aromatic peaks at m/z 78 and 77 may arise from anisole.

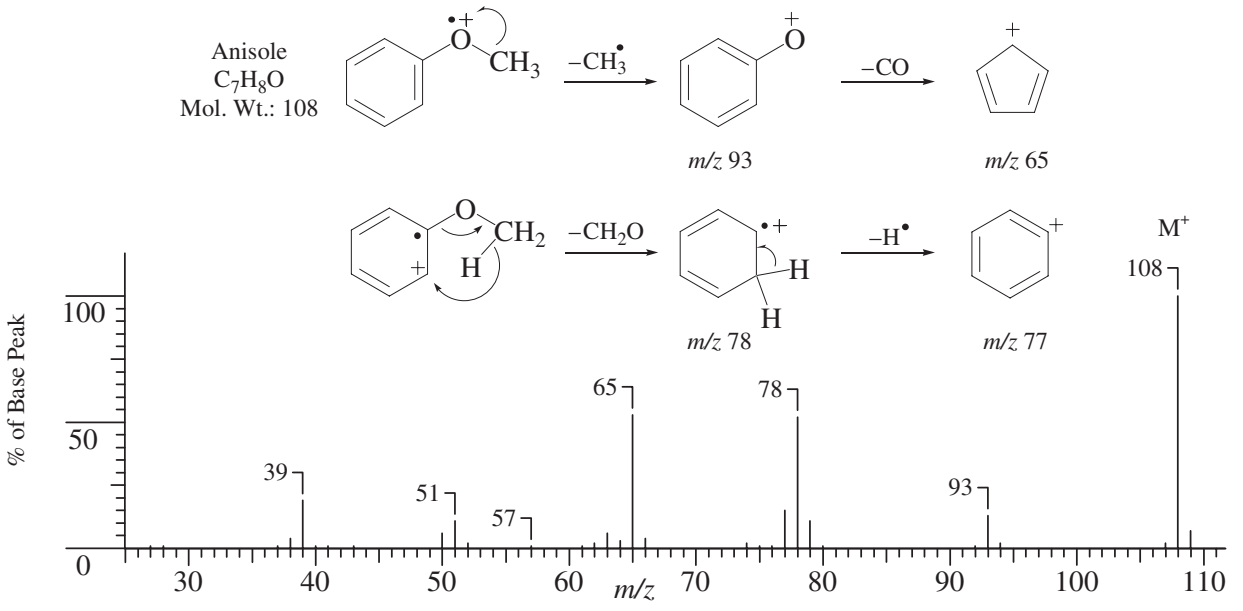


FIGURE 1.26 EI mass spectrum of anisole.

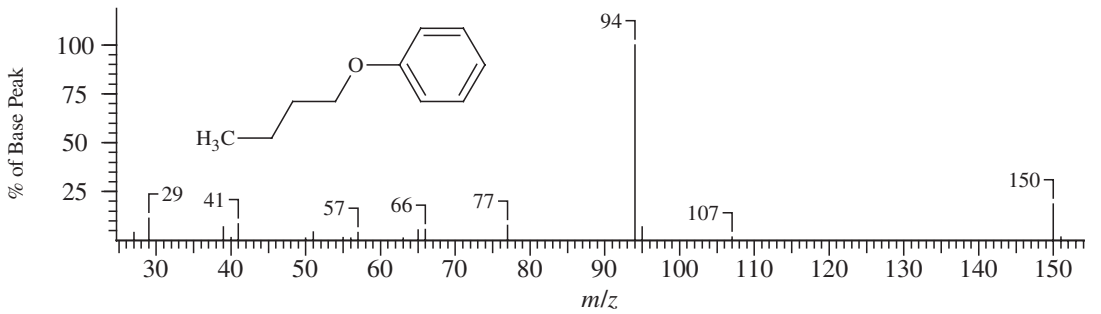
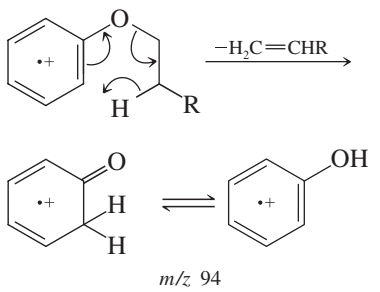


FIGURE 1.27 EI mass spectrum of butyl phenyl ether.

When the alkyl portion of an aromatic alkyl ether is C_2 or larger, cleavage β to the ring is accompanied by hydrogen migration (Scheme 1.17) as noted above for alkylbenzenes. Clearly, cleavage is mediated by the ring rather than by the oxygen atom; C—C cleavage next to the oxygen atom is insignificant. An example of this type is illustrated in the spectrum of butyl phenyl ether, Figure 1.27.

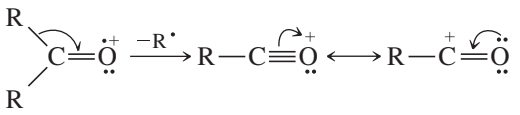


(Sch 1.17)

Diphenyl ethers show peaks at M − H, M − CO, and M − CHO by complex rearrangements.

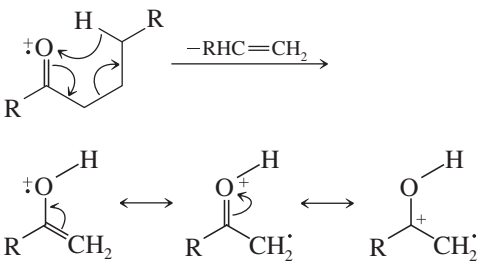
1.6.4 Ketones

1.6.4.1 Aliphatic Ketones. The molecular ion peak of ketones is usually quite pronounced. Major fragmentation peaks of aliphatic ketones result from cleavage at one of the C—C bonds adjacent to the oxygen atom, the charge remaining with the resonance-stabilized acylium ion (Scheme 1.18). Thus, as with alcohols and ethers, cleavage is mediated by the oxygen atom. This cleavage gives rise to a peak at m/z 43 or 57 or 71…. The base peak very often results from loss of the larger alkyl group.



(Sch 1.18)

When one of the alkyl chains attached to the C═O group is C_3 or longer, cleavage of the C—C bond once removed (α,β-bond) from the C═O group occurs with hydrogen migration to give a major peak (McLafferty rearrangement, Scheme 1.19). Simple cleavage of the α,β-bond, which does not occur to any extent, would give an ion of low stability because it would have two adjacent positive centers.



(Sch 1.19)

Note that in long-chain ketones the hydrocarbon peaks are indistinguishable (without the aid of high-resolution techniques) from the acyl peaks, since the mass of the C═O unit (28) is the same as two methylene units. The multiple cleavage modes in ketones sometimes make difficult the determination of the carbon chain configuration. Reduction of the carbonyl group to a methylene group yields the corresponding hydrocarbon whose fragmentation pattern leads to the carbon skeleton.

1.6.4.2 Cyclic Ketones. The molecular ion peak in cyclic ketones is prominent. As with acyclic ketones, the primary cleavage of cyclic ketones is adjacent to the C═O group, but the ion thus formed must undergo further cleavage in order to produce a fragment. The base peak in the spectrum of cyclopentanone and of cyclohexanone (Figure 1.28) is m/z 55. The mechanisms are similar in both cases: hydrogen shift to convert a primary radical to a conjugated secondary radical followed by formation of the resonance-stabilized ion, m/z 55. The other distinctive peaks at m/z 83 and 42 in the spectrum of cyclohexanone have been rationalized as depicted in Figure 1.28.

1.6.4.3 Aromatic Ketones. The molecular ion peak of an aromatic ketone is prominent. Cleavage of aryl alkyl ketones occurs at the bond β to the ring, leaving a characteristic $ArC{\equiv}O^+$ fragment (m/z 105 when Ar = phenyl), which usually accounts for the base peak. Loss of CO from this fragment gives the "aryl" ion (m/z 77 in the case of acetophenone). Cleavage of the bond adjacent to the ring to form a $RC{\equiv}O^+$ fragment (R = alkyl) is less important though somewhat enhanced by electron-withdrawing groups

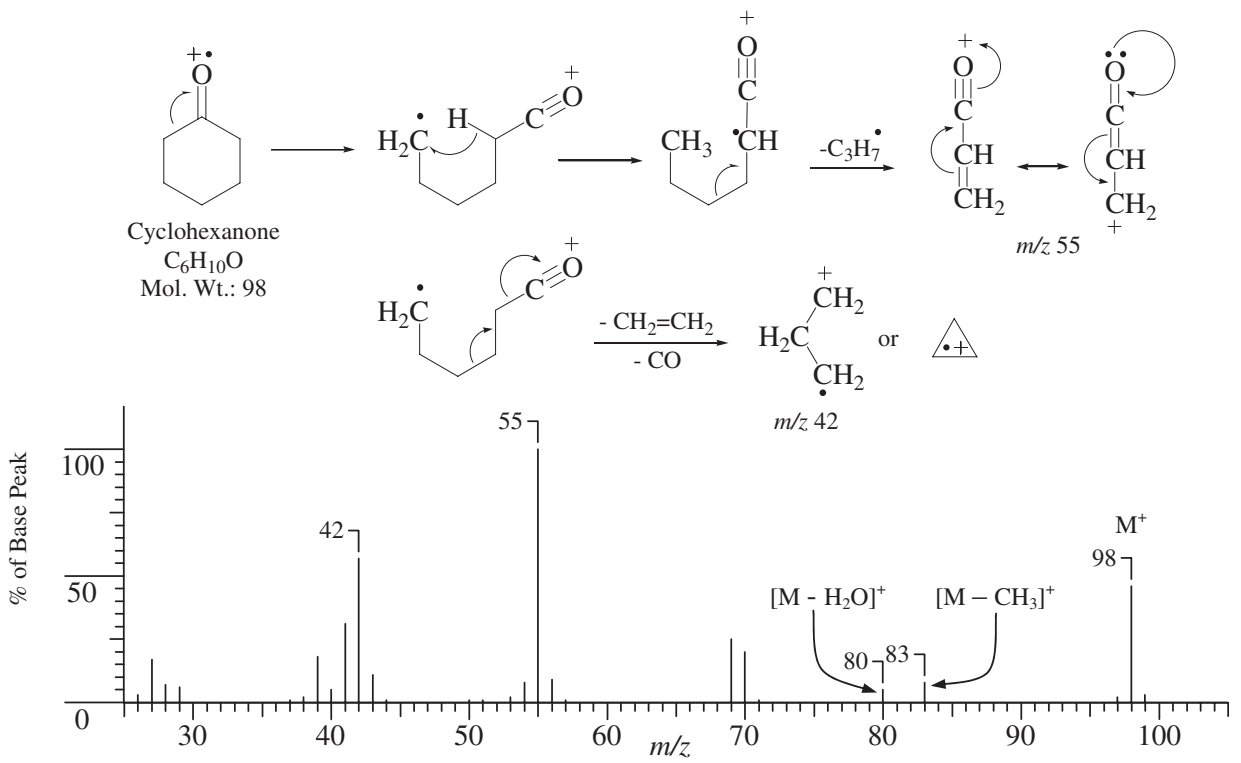


FIGURE 1.28 EI mass spectrum of cyclohexanone.

(and diminished by electron-donating groups) in the *para*-position of the Ar group.

When the alkyl chain is C_3 or longer, cleavage of the C—C bond once removed from the C═O group occurs with hydrogen migration. This is the same cleavage noted for aliphatic ketones that proceeds through a cyclic transition state and results in elimination of an alkene and formation of a stable ion.

The mass spectrum of an unsymmetrical diaryl ketone, *p*-chlorobenzophenone, is displayed in Figure 1.29. The molecular ion peak (m/z 216) is prominent and the intensity of the M + 2 peak (33.99%, relative to the molecular ion peak) demonstrates that chlorine is in the structure (see the discussion of Table 1.5 and Figure 1.35 in Section 1.6.16).

Since the intensity of the m/z 141 peak is about $\frac{1}{3}$ the intensity of the m/z 139 peak, these peaks, which are

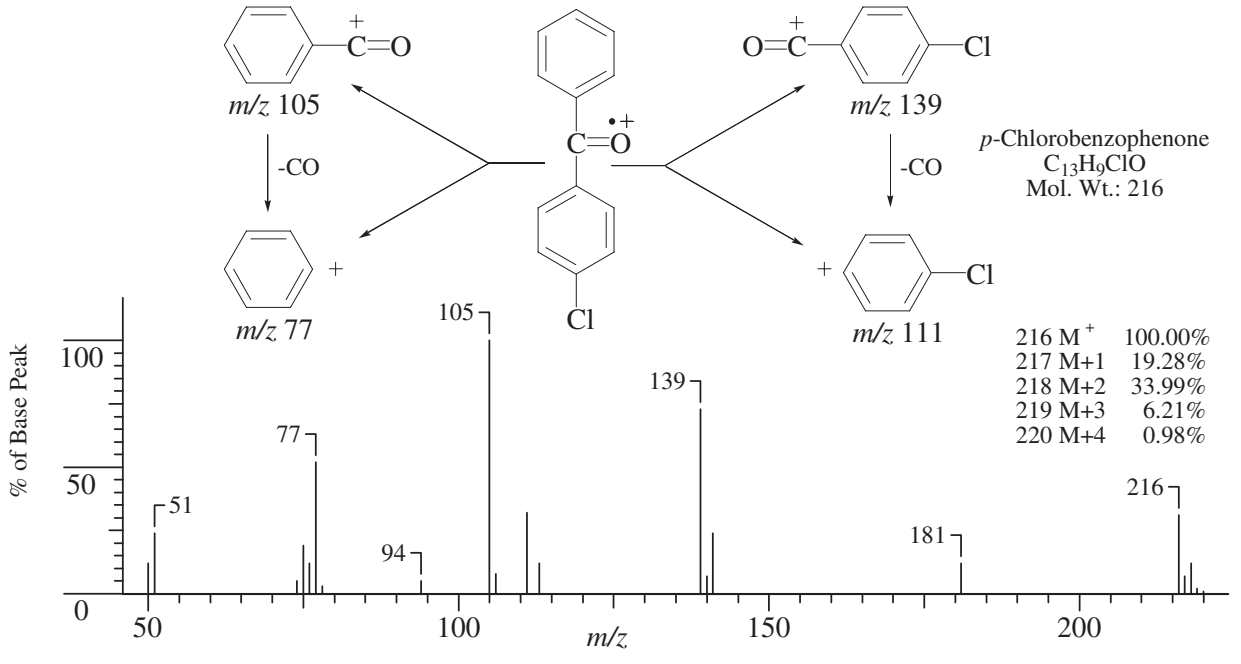


FIGURE 1.29 EI mass spectrum of *p*-chlorobenzophenone.

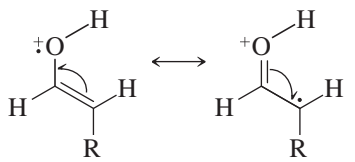
due to fragments which contain chlorine, correspond to the same fragment. The same can be said about the fragments producing the m/z 111 and 113 peaks.

The fragmentation leading to the major peaks is sketched in Figure 1.29. The Cl—ArC≡O^+ peak is larger than the Cl—Ar^+ peak, and the ArC≡O^+ peak is larger than the Ar^+ peak (β cleavage favored). If the [fragment + 2] peaks for the Cl-substituted moieties are taken into account however, there is little difference in abundance between Cl—$ArCO^+$ and $ArCO^+$, or between Cl—Ar^+ and Ar^+; the inductive (electron withdrawing) and resonance (electron releasing) effects of the *para*-substituted Cl are roughly balanced out as they are in electrophilic aromatic substitution reactions.

1.6.5 Aldehydes

1.6.5.1 Aliphatic Aldehydes. The molecular ion peak of aliphatic aldehydes is usually discernible. Cleavage of the C—H and C—C bonds next to the oxygen atom results in an M − 1 peak and in an M − R peak (m/z 29, CHO^+). The M − 1 peak is a good diagnostic peak even for long-chain aldehydes, but the m/z 29 peak present in C_4 and higher aldehydes results from the hydrocarbon $C_2H_5{}^+$ ion.

In the C_4 and higher aldehydes, McLafferty cleavage of the α,β C—C bond occurs to give a major peak at m/z 44, 58, or 72, …, depending on the α substituents. This is the resonance-stabilized ion (Scheme 1.20) formed through the cyclic transition state as shown in Scheme 1.7, where Y═H.



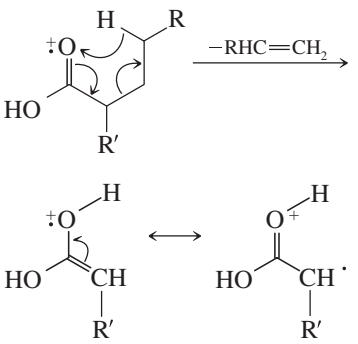
(Sch 1.20)

In straight-chain aldehydes, other unique, diagnostic peaks are at M − 18 (loss of water), M − 28 (loss of ethylene), M − 43 (loss of CH_2═CH—O·), and M − 44 (loss of CH_2═CH—OH). The rearrangements leading to these peaks have been rationalized (see Budzikiewicz et al., 1967). As the chain lengthens, the hydrocarbon pattern (m/z 29, 43, 57, 71, …) becomes dominant. These features are evident in the spectrum of nonanal (Figure 1.30).

1.6.5.2 Aromatic Aldehydes. Aromatic aldehydes are characterized by a large molecular ion peak and by an M − 1 peak (Ar—C═O^+) that is always large and may be larger than the molecular ion peak. The M − 1 ion, C_6H_5—CO^+ when Ar = phenyl, eliminates CO to give the phenyl ion (m/z 77), which in turn eliminates acetylene to give the $C_4H_3{}^+$ ion (m/z 51).

1.6.6 Carboxylic Acids

1.6.6.1 Aliphatic Acids. The molecular ion peak of a straight-chain monocarboxylic acid is weak but usually discernible. The most characteristic (sometimes the base) peak is m/z 60 resulting from the McLafferty rearrangement (Scheme 1.21). Branching at the α-carbon enhances this cleavage.



(Sch 1.21)

In short-chain acids, peaks at M − OH and M − CO_2H are prominent: these represent cleavage of bonds next to C═O. In long-chain acids, the spectrum consists of two series of peaks resulting from cleavage at each C—C bond with retention of charge either on the oxygen-containing fragment (m/z 45, 59, 73, 87, …) or on the alkyl fragment (m/z 29, 43, 57, 71, 85, …). As previously discussed, the hydrocarbon pattern also shows peaks at m/z 27, 28; 41, 42;

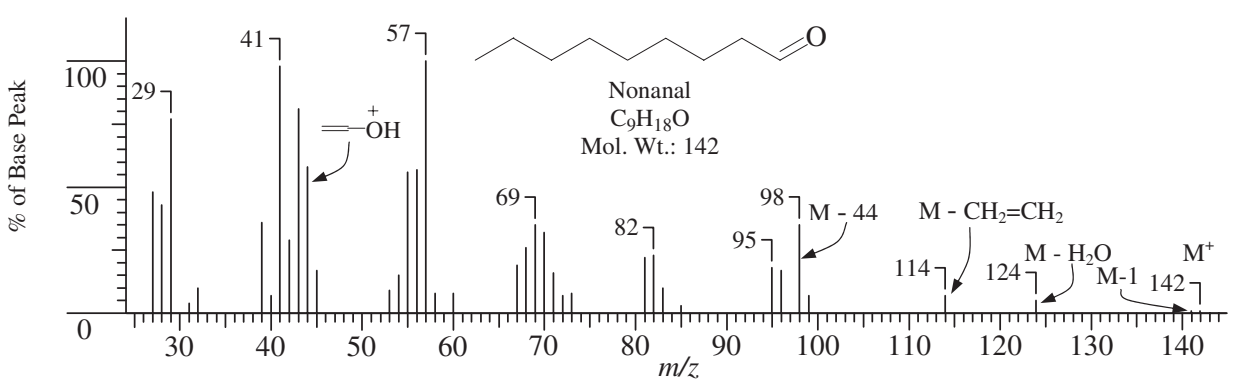


FIGURE 1.30 EI mass spectrum of nonanal.

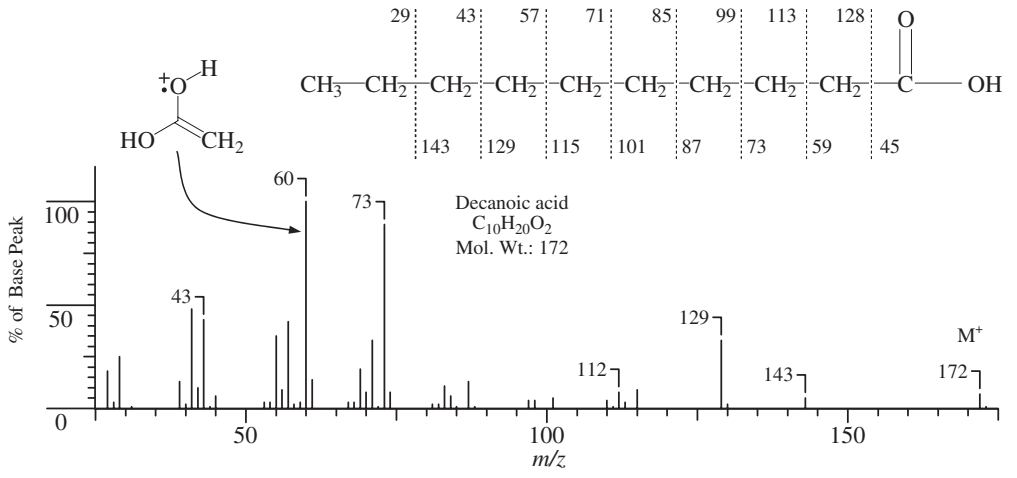
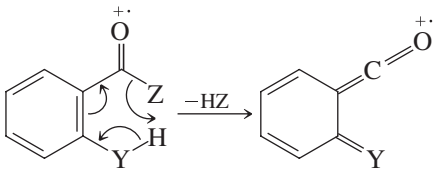


FIGURE 1.31 EI mass spectrum of decanoic acid.

55, 56; 69, 70; …. In summary, besides the McLafferty rearrangement peak, the spectrum of a long-chain acid resembles the series of hydrocarbon clusters at intervals of 14 mass units. In each cluster, however, is a prominent peak at $C_nH_{2n-1}O_2$. Decanoic acid, (Figure 1.31), nicely illustrates many of the points discussed above.

Dibasic acids usually have low volatility and hence are converted to esters to increase vapor pressure. Trimethylsilyl esters are often successful.

1.6.6.2 Aromatic Acids. The molecular ion peak of aromatic acids is large. The other prominent peaks are formed by loss of OH (M − 17) and of CO_2H (M − 45). Loss of H_2O (M − 18) is prominent if a hydrogen-bearing *ortho* group is available as outlined in Scheme 1.22. This is one example of the general "*ortho* effect" noted when the substituents can be in a six-membered transition state to facilitate loss of a neutral molecule of H_2O, ROH, or NH_3.

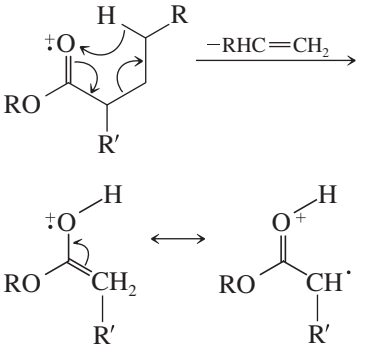


Z = OH, OR, NH_2; Y = CH_2, O, NH

(Sch 1.22)

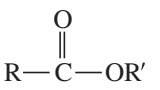
1.6.7 Carboxylic Esters

1.6.7.1 Aliphatic Esters. The molecular ion peak of a methyl ester of a straight-chain aliphatic acid is usually distinct. Even waxes usually show a discernible molecular ion peak. The molecular ion peak is weak in the range m/z 130 to ~200, but becomes somewhat more intense beyond this range. The most characteristic peak results from the familiar McLafferty rearrangement (Scheme 1.23 gives the rearrangement for an ester) and cleavage one bond removed from the C═O group. Thus, a methyl ester of an aliphatic acid unbranched at the α-carbon gives a strong peak at m/z 74, which in fact, is the base peak in straight-chain methyl esters from C_6 to C_{26}. The alcohol moiety and/or the α substituent can often be deduced by the location of the peak resulting from this cleavage.



(Sch 1.23)

For the general ester, four ions can result from bond cleavage next to C═O.



The ion R^+ is prominent for the short-chain esters but diminishes rapidly with increasing chain length and is barely perceptible in methyl hexanoate. The ion $R—C{\equiv}O^+$ gives an easily recognizable peak for esters. In methyl esters, it occurs at M − 31. It is the base peak in methyl acetate and is still 4% of the base peak in the C_{26} methyl ester. The ions $[OR']^+$ and $[C(═O)OR']^+$ are usually of little importance. The latter is discernible when $R'═CH_3$ (see m/z 59 peak of Figure 1.32).

First, consider esters in which the acid portion is the predominant portion of the molecule. The fragmentation pattern for methyl esters of straight-chain acids can be described in the same terms used for the pattern of the free acid. Cleavage at each C—C bond gives an alkyl ion (m/z 29, 43, 57, …) and an oxygen-containing ion, $C_nH_{2n-1}O_2^+$ (m/z 59, 73, 87, …). Thus, there are hydrocarbon clusters at intervals of 14 mass units; in each cluster is a

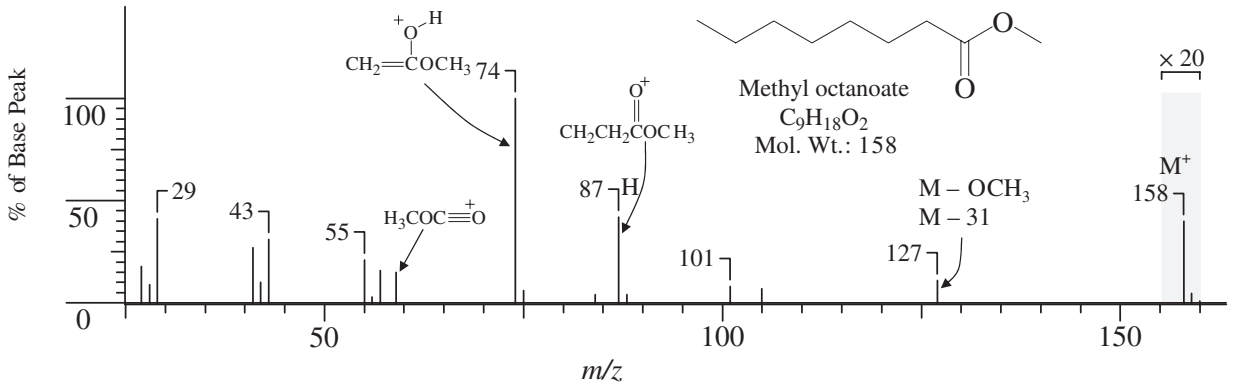


FIGURE 1.32 EI mass spectrum of methyl octanoate.

prominent peak at $C_nH_{2n-1}O_2^+$. The peak (m/z 87) formally represented by the ion $[CH_2CH_2COOCH_3]^+$ is always more intense than its homologs, but the reason is not immediately obvious. However, it seems clear that the $C_nH_{2n-1}O_2^+$ ions do not at all arise from simple cleavage.

The spectrum of methyl octanoate is presented as Figure 1.32. This spectrum illustrates one difficulty in using the M + 1 peak to arrive at a molecular formula (previously mentioned, Section 1.5.2.1). The measured value for the M + 1 peak is 12%. The calculated value is 10.0%. The measured value is high because of an ion-molecule reaction induced by the relatively large sample that was used to see the weak molecular ion peak.

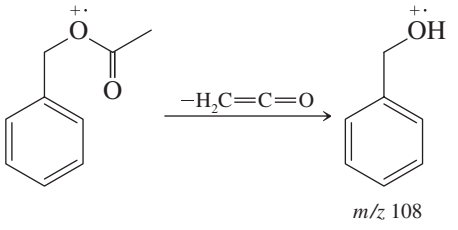
Now let us consider esters in which the alcohol portion is the predominant portion of the molecule. Esters of fatty alcohols (except methyl esters) eliminate a molecule of acid in the same manner that alcohols eliminate water. A scheme similar to that described earlier for alcohols, involving a single hydrogen transfer to the alcohol oxygen of the ester, can be written. An alternative mechanism involves a hydride transfer to the carbonyl oxygen (McLafferty rearrangement).

The loss of acetic acid by the mechanism described above is so facile in steroidal acetates that they frequently show no detectable molecular ion peak. Steroidal systems also seem unusual in that they often display significant molecular ions as alcohols, even when the corresponding acetates do not.

Esters of long-chain alcohols show a diagnostic peak at m/z 61, 75, or 89 … from elimination of the alkyl moiety as an alkene and transfer of *two* hydrogen atoms to the fragment containing the oxygen atoms, which in essence is the protonated carboxylic acid.

Esters of dibasic acids $ROOC(CH_2)_nCOOR$, in general, give recognizable molecular ion peaks. Intense peaks are found at $[ROOC(CH_2)_nC{=}O]^+$ and at $[ROOC(CH_2)_n]^+$.

1.6.7.2 Benzyl and Phenyl Esters. Benzyl acetate (also furfuryl acetate and other similar acetates) and phenyl acetate eliminate the neutral molecule ketene (Scheme 1.24); frequently this gives rise to the base peak.



(Sch 1.24)

Of course, the m/z 43 peak $(CH_3C{=}O)^+$ and m/z 91 $(C_7H_7)^+$ peaks are prominent for benzyl acetate.

1.6.7.3 Esters of Aromatic Acids. The molecular ion peak of methyl esters of aromatic acids is prominent ($ArCOOR, R{=}CH_3$). As the size of the alcohol moiety increases, the intensity of the molecular ion peak decreases rapidly to practically zero at C_5. The base peak results from elimination of $\cdot OR$, and elimination of $\cdot COOR$ accounts for another prominent peak. In methyl esters, these peaks are at M − 31 and M − 59, respectively.

As the alkyl moiety increases in length, three modes of cleavage become important: (1) McLafferty rearrangement, (2) rearrangement of two hydrogen atoms with elimination of an allylic radical, and (3) retention of the positive charge by the alkyl group.

The familiar McLafferty rearrangement pathway gives rise to a peak for the aromatic acid, $(ArCOOH)^+$. The second, similar pathway gives the protonated aromatic acid, $(ArCOOH_2)^+$. The third mode of cleavage gives the alkyl cation, R^+.

Appropriately, *ortho*-substituted benzoates eliminate ROH through the general *"ortho"* effect described above under aromatic acids. Thus, the base peak in the spectrum of methyl salicylate is m/z 120; this ion eliminates carbon monoxide to give a strong peak at m/z 92.

A strong characteristic peak at mass 149 is found in the spectra of all esters of phthalic acid, starting with the diethyl

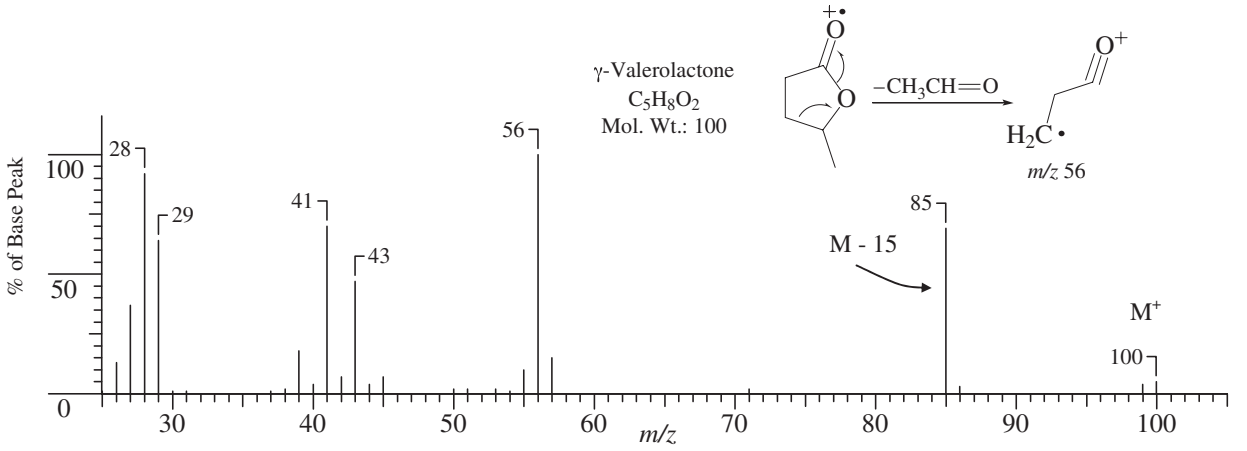


FIGURE 1.33 EI mass spectrum of γ-valerolactone.

ester. This peak is not significant in the dimethyl or methyl ethyl ester of phthalic acid, nor in esters of isophthalic or terephthalic acids, all of which give the expected peaks at $M-R, M-2R, M-CO_2R$, and $M-2CO_2R$. Since long-chain phthalate esters are widely used as plasticizers, a strong peak at m/z 149 may indicate contamination. The m/z 149 fragment (essentially a protonated phthalic anhydride) is probably formed by two ester cleavages involving the shift of two hydrogen atoms and then another hydrogen atom, followed by elimination of H_2O.

1.6.8 Lactones

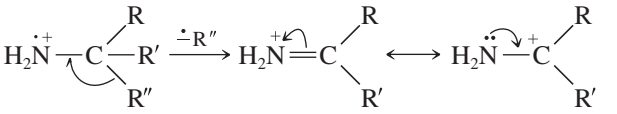
The molecular ion peak of five-membered ring lactones is distinct but is weaker when an alkyl substituent is present at C_4. Facile cleavage of the side chain at C_4 (guidelines 3 and 8, Section 1.5.4) gives a strong peak at M − alkyl.

The base peak (m/z 56) of γ-valerolactone (Figure 1.33) and the same strong peak of butyrolactone are rationalized, which shows the elimination of acetaldehyde.

Labeling experiments indicate that some of the m/z 56 peak in γ-valerolactone arises from the $C_4H_8^+$ ion. The other intense peaks in γ-valerolactone are at m/z 27 ($C_2H_3^+$), 28 ($C_2H_4^+$), 29 ($C_2H_5^+$), 41 ($C_3H_5^+$), and 43 ($C_3H_7^+$), and 85 ($C_4H_5O_2^+$, loss of the methyl group). In butyrolactone, there are strong peaks at m/z 27, 28, 29, 41, and 42 ($C_3H_6^+$).

1.6.9 Amines

1.6.9.1 Aliphatic Amines. The molecular ion peak of an aliphatic monoamine is an odd number, but it is usually quite weak and, in long-chain or highly branched amines, undetectable. The base peak frequently results from C—C cleavage next to the nitrogen atom (α, β guideline 8, Section 1.5.4); for primary amines unbranched at the α-carbon, this is m/z 30 ($CH_2NH_2^+$) shown in Scheme 1.25. This cleavage accounts for the base peak in all primary amines and secondary and tertiary amines that are not branched at the α-carbon. Loss of the largest branch ($\cdot R''$ in Scheme 1.25) from the α-C atom is preferred.

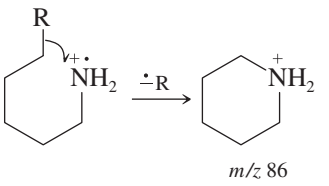


(Sch 1.25)

When branching at the α-carbon is absent, an M − 1 peak is usually visible. This is the same type of cleavage noted above for alcohols. The effect is more pronounced in amines because of the better resonance stabilization of the ion fragment by the less electronegative N atom compared with the O atom.

Primary straight-chain amines show a homologous series of peaks of progressively decreasing intensity (the cleavage at the ϵ-bond is slightly more important than at the neighboring bonds) at m/z 30, 44, 58,…resulting from cleavage at C—C bonds successively removed from the nitrogen atom with retention of the charge on the *N*-containing fragment. These peaks are accompanied by the hydrocarbon pattern of C_nH_{2n+1}, C_nH_{2n}, and C_nH_{2n-1} ions. Thus, we note characteristic clusters at intervals of 14 mass units, each cluster containing a peak resulting from a $C_nH_{2n+2}N$ ion. Because of the very facile cleavage to form the base peak, the fragmentation pattern in the high mass region becomes extremely weak.

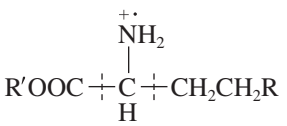
Cyclic fragments apparently occur during the fragmentation of longer chain amines. The fragment shown in Scheme 1.26 gives a six-membered ring; five-membered rings are also commonly formed.



(Sch 1.26)

A peak at m/z 30 is good though not conclusive evidence for a straight-chain primary amine. Further decomposition of the first-formed ion from a secondary or tertiary amine leads to a peak at m/z 30, 44, 58, 72, …. This is a process similar to that described for aliphatic alcohols and ethers above and, similarly, is enhanced by branching at one of the α-carbon atoms.

Cleavage of amino acid esters occurs at both C—C bonds (dashed lines below) next to the nitrogen atom; loss of the carbalkoxy group (—COOR′) is preferred. The aliphatic amine fragment ($^+NH_2{=}CHCH_2CH_2R$) decomposes further to give a peak at m/z 30.

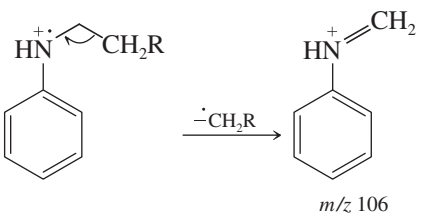


1.6.9.2 Cyclic Amines. In contrast to acyclic amines, the molecular ion peaks of cyclic amines are usually intense unless there is substitution at the α position; for example, the molecular ion peak of pyrrolidine is strong. Primary cleavage at the bonds next to the N atom leads either to loss of an α-hydrogen atom to give a strong M − 1 peak or to opening of the ring; the latter event is followed by elimination of ethylene to give $\cdot CH_2{-}{}^+NH{=}CH_2$ (m/z 43, base peak), hence by loss of a hydrogen atom to give $CH_2{=}N^+{=}CH_2$ (m/z 42). *N*-methyl pyrrolidine also gives a $C_2H_4N^+$ (m/z 42) peak, apparently by more than one pathway.

Piperidine likewise shows a strong molecular ion and M − 1 (base) peak. Ring opening followed by several available sequences leads to characteristic peaks at m/z 70, 57, 56, 44, 43, 42, 30, 29, and 28. Substituents are cleaved from the ring (guideline 6, Section 1.5.4).

1.6.9.3 Aromatic Amines (Anilines). The molecular ion peak (odd number) of an aromatic monoamine is intense. Loss of one of the amino H atoms of aniline gives a moderately intense M − 1 peak; loss of a neutral molecule of HCN followed by loss of a hydrogen atom gives prominent peaks at m/z 66 and 65, respectively.

It was noted above that cleavage of alkyl aryl ethers occurs with rearrangement involving cleavage of the ArO—R bond: that is, cleavage was controlled by the ring rather than by the oxygen atom. In the case of alkyl aryl amines, cleavage of the C—C bond next to the nitrogen atom is dominant (Scheme 1.27): that is, the heteroatom controls cleavage.



m/z 106

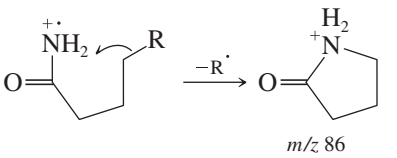
(Sch 1.27)

1.6.10 Amides

1.6.10.1 Aliphatic Amides. The molecular ion peak of straight-chain monoamides is usually discernible. The dominant modes of cleavage depend on the length of the acyl moiety and on the lengths and number of the alkyl groups attached to the nitrogen atom.

The base peak (m/z 59, $H_2NC(=OH^+)CH_2\cdot$) in all straight-chain primary amides higher than propionamide results from the familiar McLafferty rearrangement. Branching at the α-carbon (CH_3, etc.) gives a homologous peak at m/z 73 or 87, ….

Primary amides give a strong peak at m/z 44 from cleavage of the R—$CONH_2$ bond: ($O{=}C{=}{}^+NH_2$); this is the base peak in C_1—C_3 primary amides and in isobutyramide. A moderate peak at m/z 86 results from γ,δ C—C cleavage, possibly accompanied by cyclization (Scheme 1.28).



m/z 86

(Sch 1.28)

Secondary and tertiary amides with an available hydrogen on the γ-carbon of the acyl moiety and methyl groups on the N atom show the dominant peak resulting from the McLafferty rearrangement. When the *N*-alkyl groups are C_2 or longer and the acyl moiety is shorter than C_3, another mode of cleavage predominates. This is cleavage of the *N*-alkyl group β to the nitrogen atom, and cleavage of the carbonyl C—N bond with migration of an α-hydrogen atom of the acyl moiety (expelling a neutral ketene molecule) and leaving $^+NH_2{=}CH_2$ (m/z 30).

1.6.10.2 Aromatic Amides. Benzamide (Figure 1.1) is a typical example. Loss of NH_2 from the molecular ion yields a resonance-stabilized benzoyl cation that in turn undergoes cleavage to a phenyl cation. A separate fragmentation pathway gives rise to a modest m/z 44 peak.

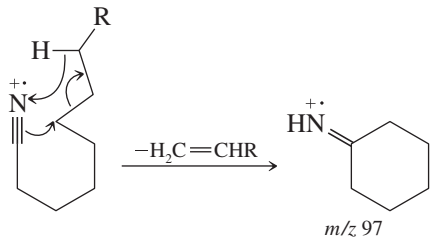
1.6.11 Aliphatic Nitriles

The molecular ion peaks of aliphatic nitriles (except for acetonitrile and propionitrile) are weak or absent, but the M + 1 peak can usually be located by its behavior on increasing the sample size (Section 1.5.2.1). A weak but diagnostically useful M − 1 peak is formed by loss of an α-hydrogen to form the stable ion: $RCH{=}C{=}N^+$.

The base peak of straight-chain nitriles between C4 and C9 is m/z 41. This peak corresponds to the ion resulting from hydrogen rearrangement in a six-membered transition state, similar to a McLafferty rearrangement giving a peak at m/z 41 $CH_2{=}C{=}N^+{-}H$. However, this peak lacks diagnostic value because of the presence of $C_3H_5^+$ (m/z 41) for all molecules containing a hydrocarbon chain.

A peak at m/z 97 is characteristic and intense (sometimes the base peak) in straight-chain nitriles C_8 and higher.

The mechanism depicted in Scheme 1.29 has been proposed to account for this ion.



(Sch 1.29)

Simple cleavage at each C—C bond (except the one next to the N atom) gives a characteristic series of homologous peaks of even mass number down the entire length of the chain (m/z 40, 54, 68, 82, …) resulting from the $(CH_2)_nC{\equiv}N^+$ ions. Accompanying these peaks are the usual peaks of the hydrocarbon pattern.

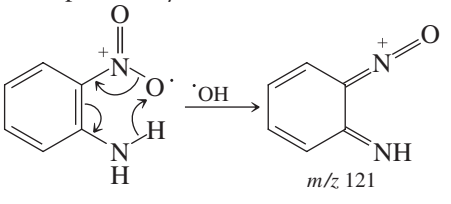
1.6.12 Nitro Compounds

1.6.12.1 Aliphatic Nitro Compounds. The molecular ion peak (odd number) of an aliphatic mononitro compound is weak or absent (except in the lower homologs). The main peaks are attributable to the hydrocarbon fragments up to M − NO_2. Presence of a nitro group is indicated by an appreciable peak at m/z 30 (NO^+) and a smaller peak at mass 46 ($NO_2{}^+$).

1.6.12.2 Aromatic Nitro Compounds. The molecular ion peak of aromatic nitro compounds (odd number for one N atom) is strong. Prominent peaks result from elimination of an NO_2 radical (M − 46, the base peak in nitrobenzene), and of a neutral NO molecule with rearrangement to form the phenoxy cation (M − 30); both are good diagnostic peaks. Loss of acetylene from the M − 46 ion accounts for a strong peak at M − 72; loss of CO from the M − 30 ion gives a peak at M − 58. A diagnostic peak at m/z 30 results from the NO^+ ion.

The isomeric *o*-, *m*-, and *p*-nitroanilines each give a strong molecular ion (even number). They all give prominent peaks resulting from two sequences. The first pathway entails a loss of an NO_2 group (M − 46) to give an m/z 92; this ion loses HCN to give an m/z 65. The second sequence records a loss of NO (M − 30) to give m/z 108, which loses CO to give m/z 80.

Aside from differences in intensities, the three isomers give very similar spectra. The *meta* and *para* compounds give a small peak at m/z 122 from loss of an O atom, whereas the *ortho* compound eliminates OH as depicted in Scheme 1.30 to give a small peak at m/z 121.



(Sch 1.30)

1.6.13 Aliphatic Nitrites

The molecular ion peak (odd number) of aliphatic nitrites (one N present) is weak or absent. The peak at m/z 30 (NO^+) is always large and is often the base peak. There is a large peak at m/z 60 ($CH_2{=}{=}{}^+ONO$) in all nitrites unbranched at the α-carbon; this represents cleavage of the C—C bond next to the ONO group. An α branch can be identified by a peak at m/z 74, 88, or 102 …. Absence of a large peak at m/z 46 permits differentiation from nitro compounds. Hydrocarbon peaks are prominent, and their distribution and intensities describe the arrangement of the carbon chain.

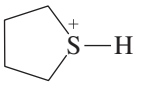
1.6.14 Aliphatic Nitrates

The molecular ion peak (odd number) of aliphatic nitrates (one nitrogen present) is weak or absent. A prominent (frequently the base) peak is formed by cleavage of the C—C bond next to the ONO_2 group with loss of the heaviest alkyl group attached to the α-carbon. The $NO_2{}^+$ peak at m/z 46 is also prominent. As in the case of aliphatic nitrites, the hydrocarbon fragment ions are distinct.

1.6.15 Sulfur Compounds

The contribution (4.4%, see Table 1.3 and Figure 1.34) of the ^{34}S isotope to the M + 2 peak, and often to a (fragment + 2) peak, affords ready recognition of sulfur-containing compounds. A homologous series of sulfur containing fragments is four mass units higher than the hydrocarbon fragment series. The number of sulfur atoms can be determined from the size of the contribution of the ^{34}S isotope to the M + 2 peak. The mass of the sulfur atom(s) present is subtracted from the molecular weight. In diisopentyl disulfide, for example, the molecular weight is 206, and the molecule contains two sulfur atoms. The formula for the rest of the molecule is therefore found under mass 142, that is, 206 − (2 × 32).

1.6.15.1 Aliphatic Mercaptans (Thiols). The molecular ion peak of aliphatic mercaptans, except for higher tertiary mercaptans, is usually strong enough so that the M + 2 peak can be accurately measured. In general, the cleavage modes resemble those of alcohols. Cleavage of the C—C bond (α,β-bond) next to the SH group gives the characteristic ion $CH_2{=}{=}SH^+$ (m/z 47). Sulfur is poorer than nitrogen, but better than oxygen, at stabilizing such a fragment. Cleavage at the β,γ bond gives a peak at m/z 61 of about one-half the intensity of the m/z 47 peak. Cleavage at the γ,δ-bond gives a small peak at m/z 75, and cleavage at the δ,ϵ-bond gives a peak at m/z 89 that is more intense than the peak at m/z 73; presumably the m/z 89 ion is stabilized by cyclization:



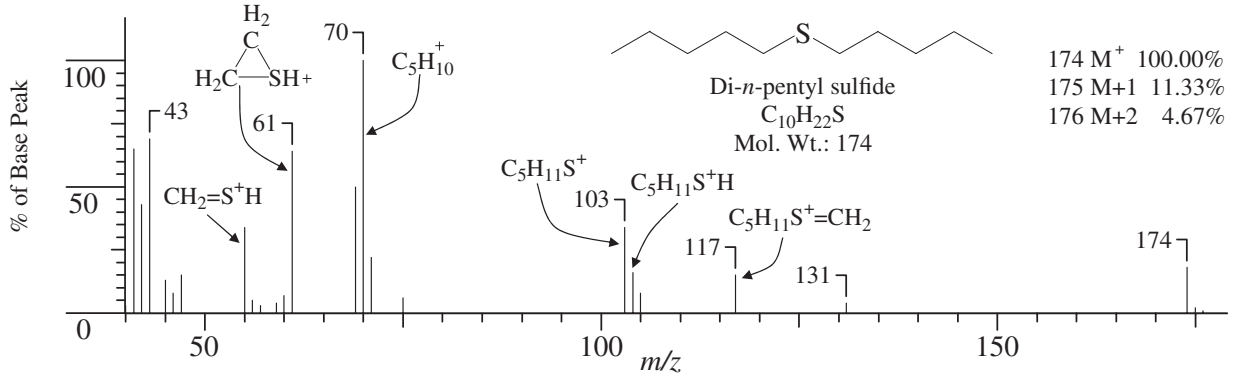


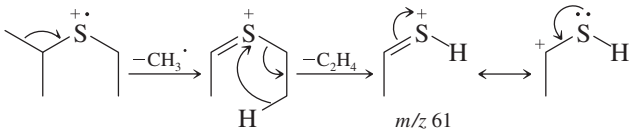
FIGURE 1.34 EI mass spectrum of di-*n*-pentyl sulfide.

Again analogous to alcohols, primary mercaptans fragment to give H_2S and a strong M − 34 peak, the resulting ion then eliminating ethylene: thus the homologous series $M - H_2S - (CH_2{=}CH_2)_n$ arises.

Secondary and tertiary mercaptans cleave at the α-carbon atom with loss of the largest group to give a prominent peak $M - CH_3, M - C_2H_5, M - C_3H_7, \ldots$. However, a peak at m/z 47 may also appear as a rearrangement peak of secondary and tertiary mercaptans. A peak at M − 33 (loss of HS) is usually present for secondary mercaptans.

In long-chain mercaptans, the hydrocarbon pattern is superimposed on the mercaptan pattern. As for alcohols, the alkenyl peaks (i.e., m/z 41, 55, 69, …) are as intense or even more so than the alkyl peaks (m/z 43, 57, 71, …).

1.6.15.2 Aliphatic Sulfides. The molecular ion peak of aliphatic sulfides is usually intense enough so that the M + 2 peak can be accurately measured. The cleavage modes generally resemble those of ethers. Cleavage of one or the other of the α, β C—C bonds occurs, with loss of the largest group being favored. These first-formed ions decompose further with hydrogen transfer and elimination of an alkene. The steps for aliphatic ethers also occur for sulfides (Scheme 1.31); the end result is the ion $RCH{=}SH^+$ (see Figure 1.34 for an example.)

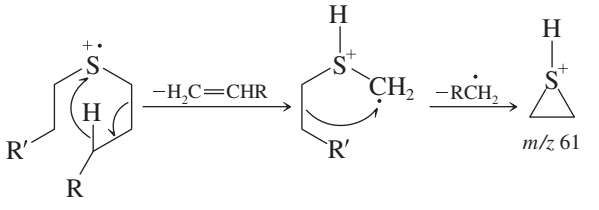


(Sch 1.31)

For a sulfide unbranched at either δ-carbon atom, this ion is $CH_2{=}SH^+$ (m/z 47), and its intensity may lead to confusion with the same ion derived from a mercaptan. However, the absence of $M - H_2S$ or M − SH peaks in sulfide spectra makes the distinction.

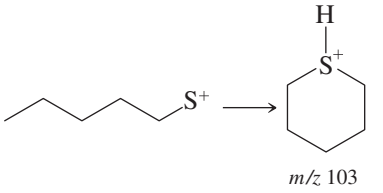
A moderate to strong peak at m/z 61 is present (see alkyl sulfide cleavage, Figure 1.34) in the spectrum of all except tertiary sulfides. When an α-methyl substituent is present, m/z 61 is the ion $CH_3CH{=}SH^+$, resulting from the double cleavage. Methyl primary sulfides cleave at the α, β-bond to give the m/z 61 ion, $CH_3{-}S^+{=}CH_2$.

However, a strong m/z 61 peak in the spectrum of a straight-chain sulfide calls for a different explanation. Scheme 1.32 offers a plausible explanation.



(Sch 1.32)

Sulfides give a characteristic ion by cleavage of the C—S bond with retention of charge on sulfur. The resulting RS^+ ion gives a peak at m/z $32 + CH_3, 32 + C_2H_5, 32 + C_3H_7, \ldots$. The ion of m/z 103 seems especially favored possibly because of formation of a rearranged cyclic ion (Scheme 1.33). These features are illustrated by the spectrum of di-*n*-pentyl sulfide (Figure 1.34).



(Sch 1.33)

As with long-chain ethers, the hydrocarbon pattern may dominate the spectrum of long-chain sulfides; the C_nH_{2n} peaks seem especially prominent. In branched chain sulfides, cleavage at the branch may reduce the relative intensity of the characteristic sulfide peaks.

1.6.15.3 Aliphatic Disulfides. The molecular ion peak for at least up to C_{10} disulfides is strong. A major peak found in these spectra results from cleavage of one of the C—S bonds with retention of the charge on the alkyl fragment. Another major peak results from the same cleavage along

with a shift of a hydrogen atom to form the RSSH fragment, which retains the charge. Other peaks apparently result from cleavage between the sulfur atoms without rearrangement, and with migration of one or two hydrogen atoms to give, respectively, RS^+, $RS^+ - 1$, and $RS^+ - 2$.

1.6.16 Halogen Compounds

A compound that contains one chlorine atom will have an M + 2 peak approximately one-third the intensity of the molecular ion peak because of the presence of a molecular ion containing the ^{37}Cl isotope (see Table 1.4). A compound that contains one bromine atom will have an M + 2 peak almost equal in intensity to the molecular ion because of the presence of a molecular ion containing the ^{81}Br isotope. A compound that contains two chlorines, or two bromines, or one chlorine and one bromine will show a distinct M + 4 peak, in addition to the M + 2 peak, because of the presence of a molecular ion containing two atoms of the heavy isotope. In general, the number of chlorine and/or bromine atoms in a molecule can be ascertained by the number of alternate peaks beyond the molecular ion peak. Thus, three chlorine atoms in a molecule will give peaks at M + 2, M + 4, and M + 6; in polychloro compounds, the peak of highest mass may be so weak as to escape notice.

The relative abundances of the peaks (molecular ion, M + 2, M + 4, and so on) have been calculated by Beynon et al. (1968) for compounds containing chlorine and bromine (atoms other than chlorine and bromine were ignored). A portion of these results is presented here, somewhat modified, as Table 1.5. We can now tell what combination of chlorine and bromine atoms is present. It should be noted that Table 1.5 presents the isotope contributions in terms of percent of the molecular ion peak. Figure 1.35 provides the corresponding bar graphs.

As required by Table 1.5, the M + 2 peak in the spectrum of *p*-chlorobenzophenone (Figure 1.29) is about one-third the intensity of the molecular ion peak (m/z 218). As mentioned earlier, the chlorine containing fragments (m/z 141 and 113) show [fragment + 2] peaks of the proper intensity.

Unfortunately, the application of isotope contributions, though generally useful for aromatic halogen compounds, is limited by the weak molecular ion peak of many aliphatic halogen compounds of more than about six carbon atoms for a straight chain, or fewer for a branched chain. However, the halogen-containing fragments are recognizable by the ratio of the (fragment + 2) peaks to fragment peaks in monochlorides or monobromides. In polychloro or polybromo compounds, these (fragment + isotope) peaks form a distinctive series of multiplets (Figure 1.36). Coincidence of a fragment ion with one of the isotope fragments, with another disruption of the characteristic ratios, must always be kept in mind.

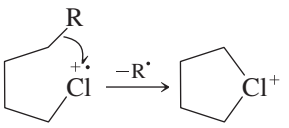
TABLE 1.5 Intensities of Isotope Peaks (Relative to the Molecular Ion) for Combinations of Chlorine and Bromine

Halogen Present	% M + 2	% M + 4	% M + 6	% M + 8	% M + 10	% M + 12
Cl	32.6					
Cl_2	65.3	10.6				
Cl_3	97.8	31.9	3.5			
Cl_4	131.0	63.9	14.0	1.2		
Cl_5	163.0	106.0	34.7	5.7	0.4	
Cl_6	196.0	161.0	69.4	17.0	2.2	0.1
Br	97.9					
Br_2	195.0	95.5				
Br_3	293.0	286.0	93.4			
BrCl	130.0	31.9				
$BrCl_2$	163.0	74.4	10.4			
Br_2Cl	228.0	159.0	31.2			

1.6.16.1 Aliphatic Chlorides. The molecular ion peak is detectable only in the lower monochlorides. Fragmentation of the molecular ion is mediated by the chlorine atom but to a much lesser degree than is the case in oxygen-, nitrogen-, or sulfur-containing compounds. Thus, cleavage of a straight-chain monochloride at the C—C bond adjacent to the chlorine atom accounts for a small peak at m/z 49, $CH_2{=}Cl^+$ (and, of course, the isotope peak at m/z 51).

Cleavage of the C—Cl bond leads to a small Cl^+ peak and to a R^+ peak, which is prominent in the lower chlorides but quite small when the chain is longer than about C_5.

Straight-chain chlorides longer than C_6 give $C_3H_6Cl^+$, $C_4H_8Cl^+$, and $C_5H_{10}Cl^+$ ions. Of these, the $C_4H_8Cl^+$ ion forms the most intense (sometimes the base) peak; a five-membered cyclic structure (Scheme 1.34) may explain its stability.



(Sch 1.34)

Loss of HCl occurs, possibly by 1,3 elimination, to give a peak (weak or moderate) at M − 36.

In general, the spectrum of an aliphatic monochloride is dominated by the hydrocarbon pattern to a greater extent than that of a corresponding alcohol, amine, or mercaptan.

1.6.16.2 Aliphatic Bromides. The remarks under aliphatic chlorides apply quite generally to the corresponding bromides.

1.6.16.3 Aliphatic Iodides. Aliphatic iodides give the strongest molecular ion peak of the aliphatic halides. Since iodine is monoisotopic, there is no distinctive isotope peak. The presence of an iodine atom can sometimes be deduced from isotope peaks that are suspiciously low in relation to the molecular ion peaks, and from several distinctive peaks; in polyiodo compounds, the large interval between major peaks is characteristic.

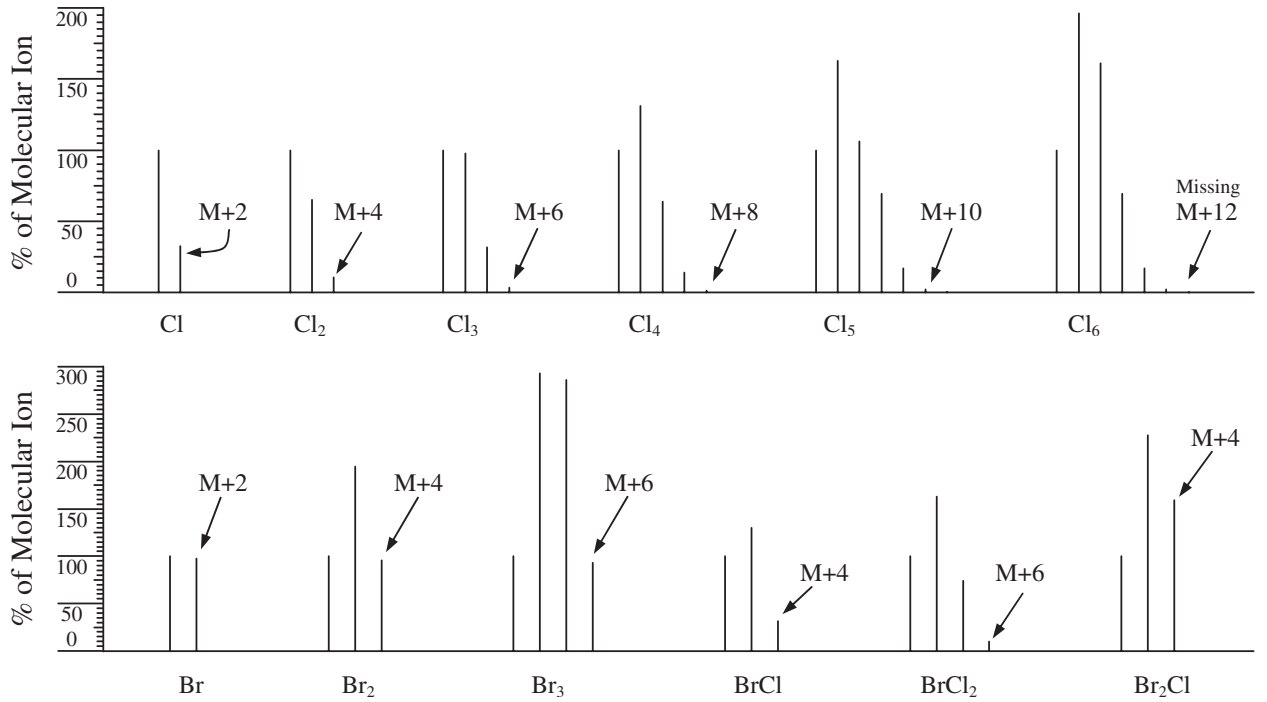


FIGURE 1.35 Predicted patterns of M, M + 2, M + 4, … for compounds with various combinations of chlorine and bromine.

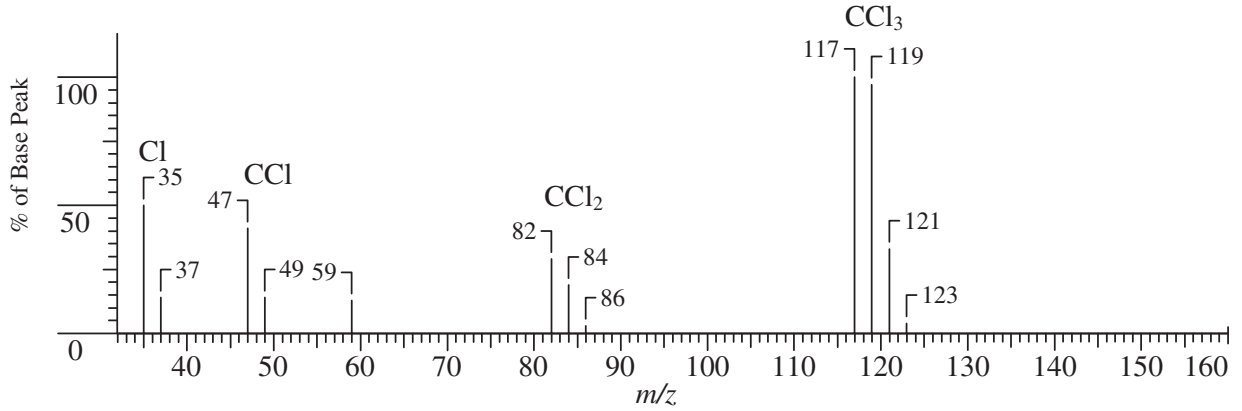
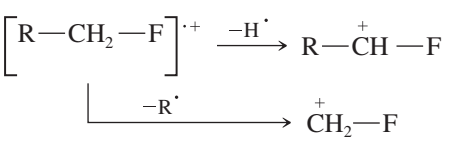


FIGURE 1.36 EI mass spectrum of carbon tetrachloride (CCl_4).

Iodides cleave much as do chlorides and bromides, but the $C_4H_8I^+$ ion is not as evident as the corresponding chloride and bromide ions.

1.6.16.4 Aliphatic Fluorides. Aliphatic fluorides give the weakest molecular ion peak of the aliphatic halides. Fluorine is monoisotopic, and its detection in polyfluoro compounds depends on suspiciously small isotopic peaks relative to the molecular ion, on the intervals between peaks, and on characteristic peaks. Of these, the most characteristic is m/z 69 resulting from the ion CF_3^+, which is the base peak in all perfluorocarbons. Prominent peaks are noted at m/z 119, 169, 219…; these are increments of CF_2. The stable ions $C_3F_5^+$ and $C_4F_7^+$ give large peaks at m/z 131 and 181. The M − F peak is frequently visible in perfluorinated compounds. In monofluorides, cleavage of the α,β C—C bond is less important than in the other monohalides, but cleavage of a C—H bond on the α-carbon atom is more important. This reversal is a consequence of the high electronegativity of the F atom and is rationalized by placing the positive charge on the α-carbon atom. The secondary carbonium ion thus depicted in Scheme 1.35 by a loss of a hydrogen atom is more stable than the primary carbonium ion resulting from loss of an alkyl radical.



(Sch 1.35)

1.6.16.5 Benzyl Halides. The molecular ion peak of benzyl halides is usually detectable. The benzyl (or tropylium) ion from loss of the halide (guideline 8, Section 1.5.4) is favored even over β-bond cleavage of an alkyl substituent. A substituted phenyl ion (α-bond cleavage) is prominent when the ring is polysubstituted.

1.6.16.6 Aromatic Halides. The molecular ion peak of an aryl halide is readily apparent. The M – X peak is large for all compounds in which X is attached directly to the ring.

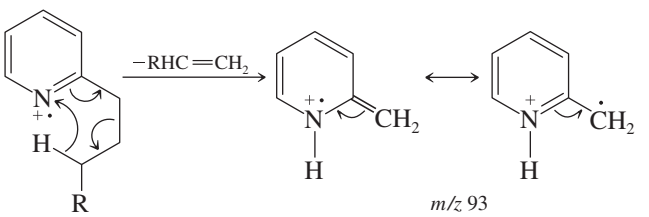
1.6.17 Heteroaromatic Compounds

The molecular ion peak of heteroaromatics and alkylated heteroaromatics is intense. Cleavage of the bond β to the ring, as in alkylbenzenes, is the general rule; in pyridine, the position of substitution determines the ease of cleavage of the β-bond (see below).

Localizing the charge of the molecular ion on the heteroatom, rather than in the ring π structure, provides a satisfactory rationale for the observed mode of cleavage. The present treatment follows that used by Djerassi (Budzikiewicz et al., 1967).

The five-membered ring heteroaromatics (furan, thiophene, and pyrrole) show very similar ring cleavage patterns. The first step in each case is cleavage of the carbon-heteroatom bond, followed by loss of either a neutral acetylene molecule or by loss of radical fragments. Thus, furan exhibits two principal peaks: $C_3H_3^+$(m/z 39) and $HC{\equiv}O^+$ (m/z 29). For thiophene, there are three peaks, $C_3H_3^+$(m/z 39), $HC{\equiv}S^+$ (m/z 45), and $C_2H_2S^+$ (m/z 58). For pyrrole, there are three peaks: $C_3H_3^+$(m/z 39), $HC{=}NH^+$ (m/z 28) and $C_2H_2\ NH^+$ (m/z 41). Pyrrole also eliminates a neutral molecule of HCN to give an intense peak at m/z 40. The base peak of 2,5-dimethylfuran is m/z 43 ($CH_3C{\equiv}O^+$).

Cleavage of the β C—C bond in alkylpyridines (Scheme 1.36) depends on the position of the ring substitution, being more pronounced when the alkyl group is in the 3 position. An alkyl group of more than three carbon atoms in the 2 position can undergo migration of a hydrogen atom to the ring nitrogen.



(Sch 1.36)

A similar cleavage is found in pyrazines since all ring substituents are necessarily ortho to one of the nitrogen atoms.

REFERENCES

For a list of Chapter References, please visit: www.wiley.com/college/silverstein.

STUDENT EXERCISES

1.1 Using Table 1.4, calculate the exact mass for the compounds below (**a** – **o**).

1.2 Determine the index of hydrogen deficiency for the compounds below.

1.3 Write the structure for the molecular ion for each compound (**a** – **o**) showing, when possible, the location of the radical cation.

1.4 Predict three major fragmentation/rearrangement pathways for the compounds below. For each pathway, cite the guideline from Section 1.5.4 that supports your prediction.

1.5 For each fragmentation/rearrangement pathway from exercise 1.4, show a detailed mechanism using either single barbed or double barbed arrows as appropriate.

1.6 Match each of the exact masses to the mass spectra shown on the following pages (labelled **A – W**). Note that two compounds have the same exact mass, and you will need to consider the CI mass spectrum when given. The masses are: (a) 56.0264, (b) 73.0896, (c) 74.0363, (d) 89.0479, (e) 94.0535, (f) 96.0572, (g) 98.0736, (h) 100.0893, (i) 102.0678, (j) 113.0845, (k) 114.1043, (l) 116.0841, (m) 116.1206, (n) 122.0733, (o) 122.0733, (p) 126.1041, (q) 138.0687, (r) 150.0041, (s) 152.0476, (t) 156.9934, (u) 161.9637, (v) 169.9735, (w) 208.0094.

1.7 For each of the mass spectra (**A**–**W**), determine if there are any of the following heteroatoms in the compound: S, Cl, Br.

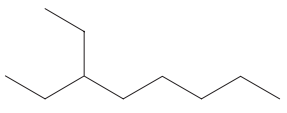
1.8 For each exact mass corresponding to mass spectra **A**–**W**, determine the molecular formula. Remember to look at the heteroatoms that were determined in exercise 1.7.

1.9 Determine the index of hydrogen deficiency for each of the formulas in exercise 1.6.

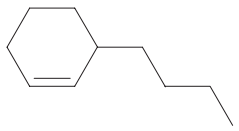
1.10 List the base peak and molecular ion peak for each of the EI mass spectra (**A** – **W**).

1.11 Choose three ions (besides the molecular ion) from each EI mass spectrum (**A** – **W**, except for H), determine the molecular formula for each fragment ion, and give the molecular formula for the portion that is lost from the molecular ion. Indicate which ions result from a rearrangement.

Exercise 1.1



a



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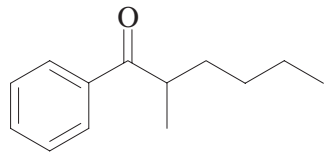

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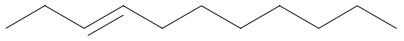

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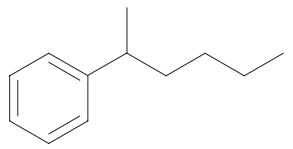

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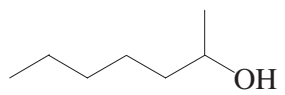

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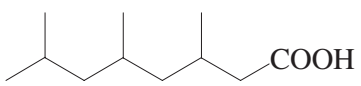

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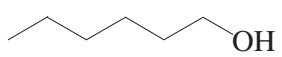

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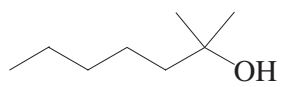

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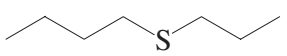

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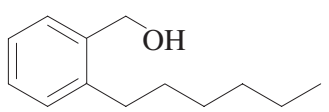

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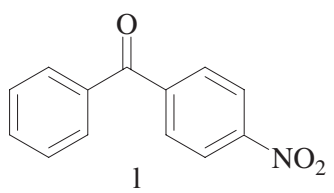

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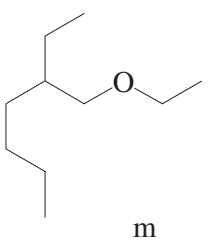

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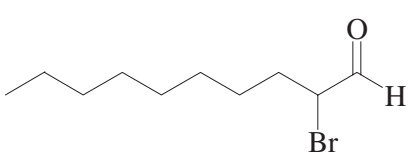

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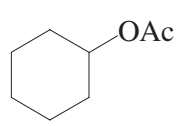

o

Exercise 1.6 (A – C)

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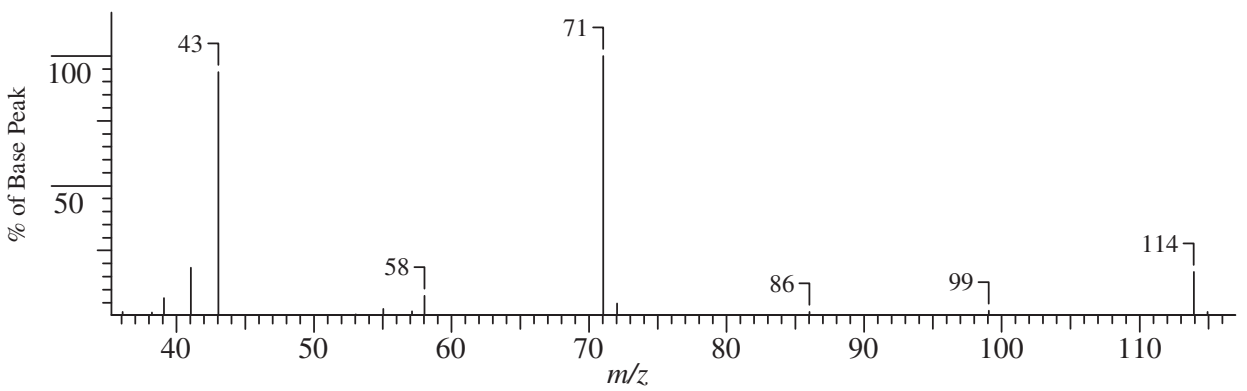

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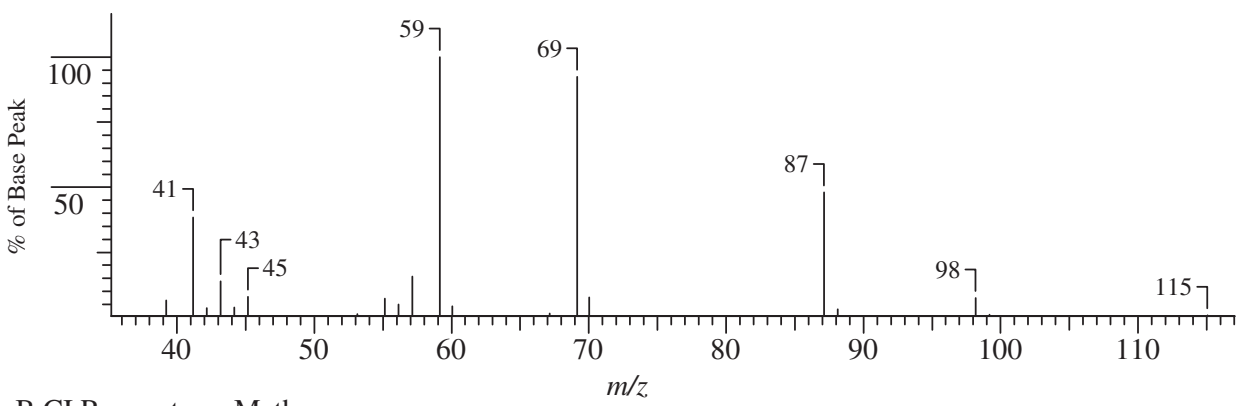
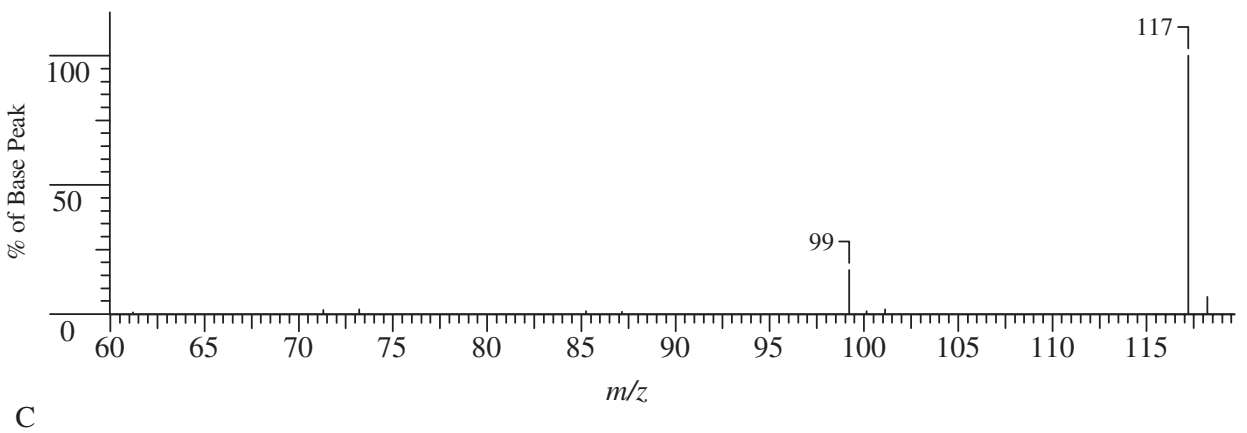


B CI Reagent gas Methane



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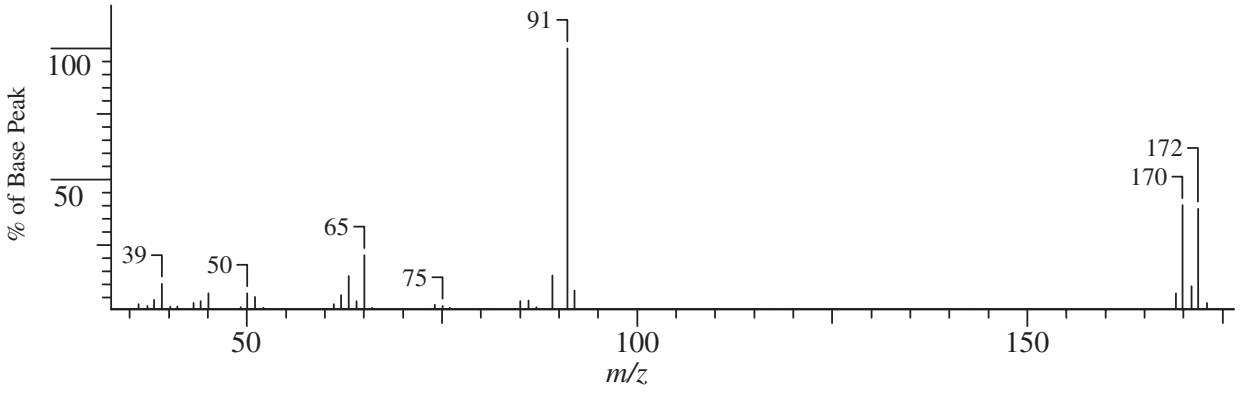

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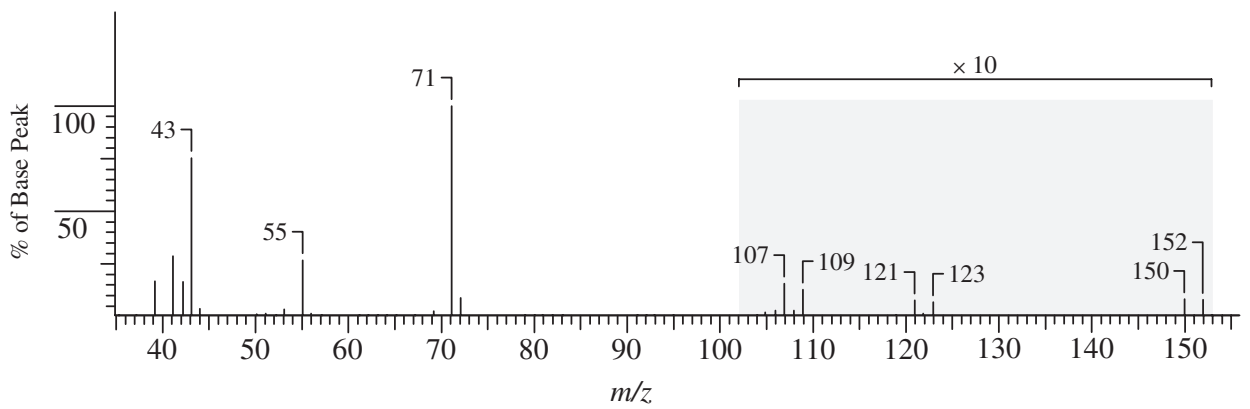

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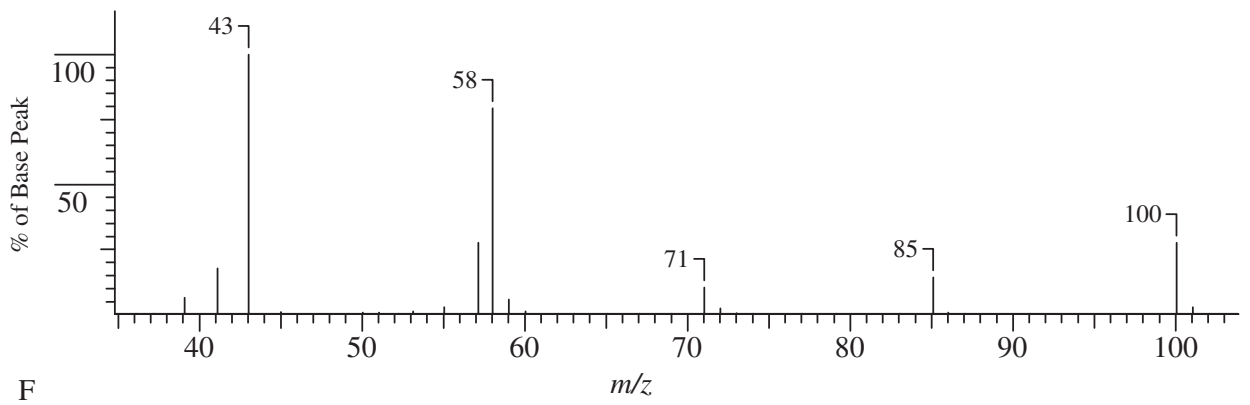

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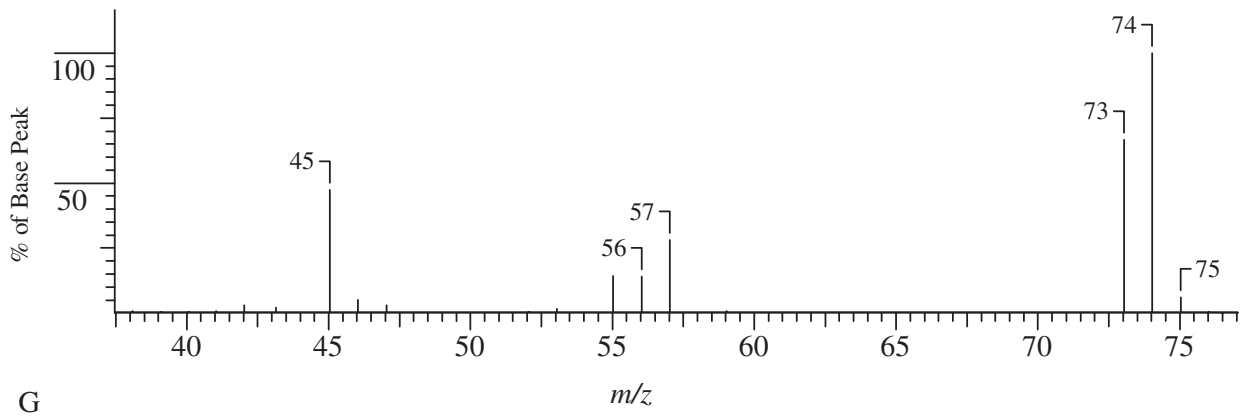

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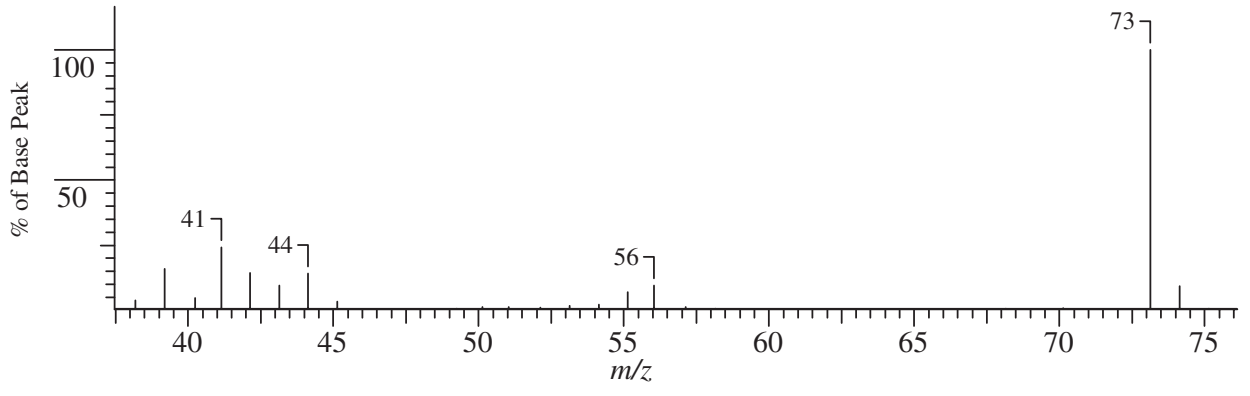

Exercise 1.6 (H – I)

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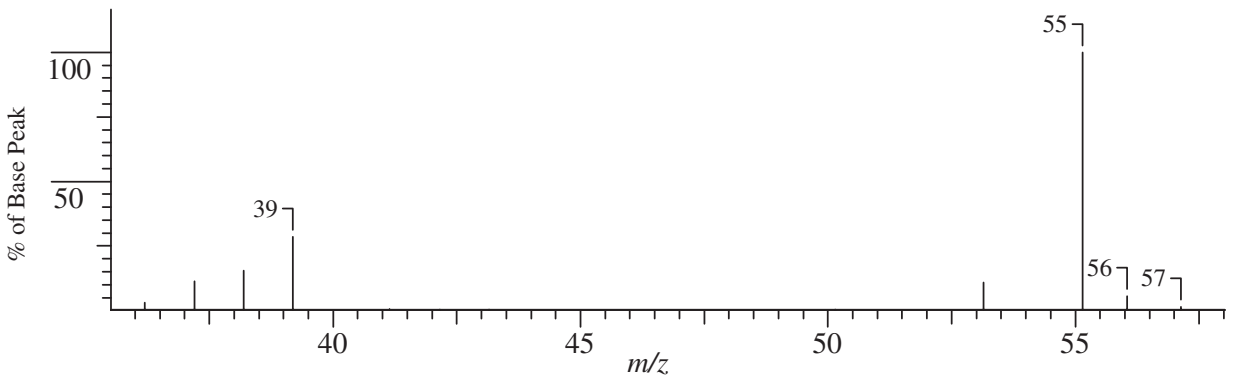
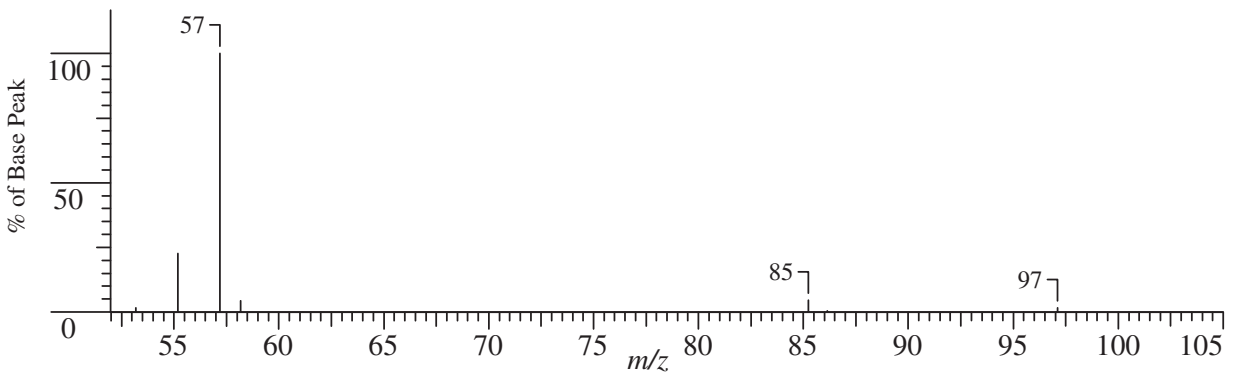


H CI Reagent gas Methane



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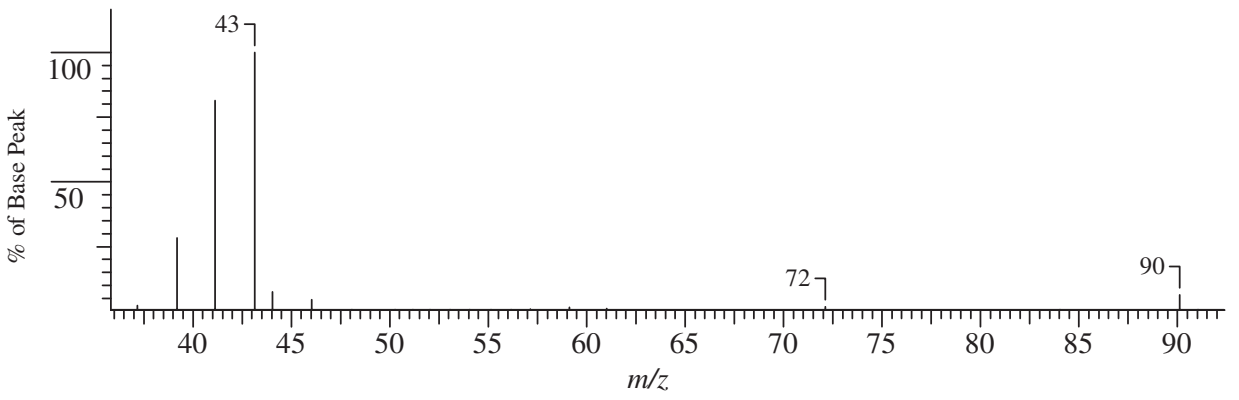
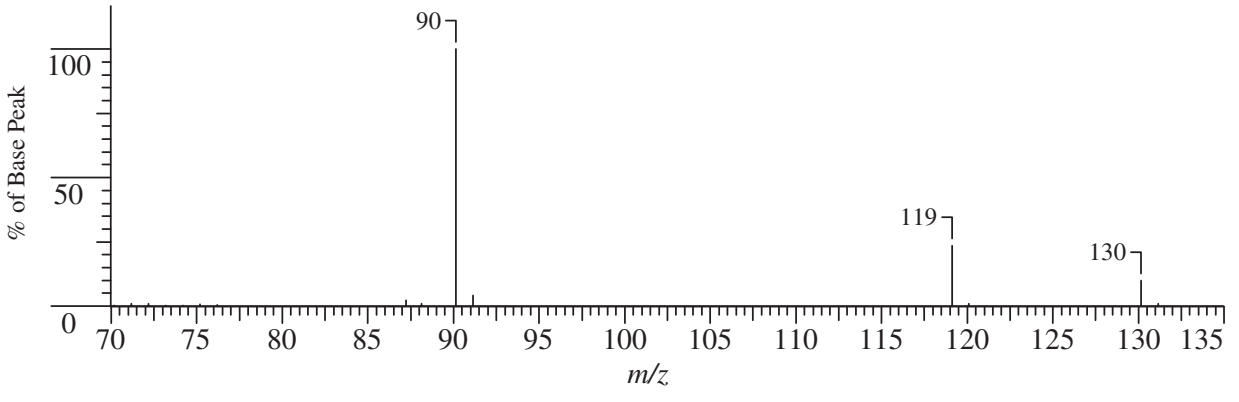


I CI Reagent gas Methane



Exercise 1.6 (J – M)

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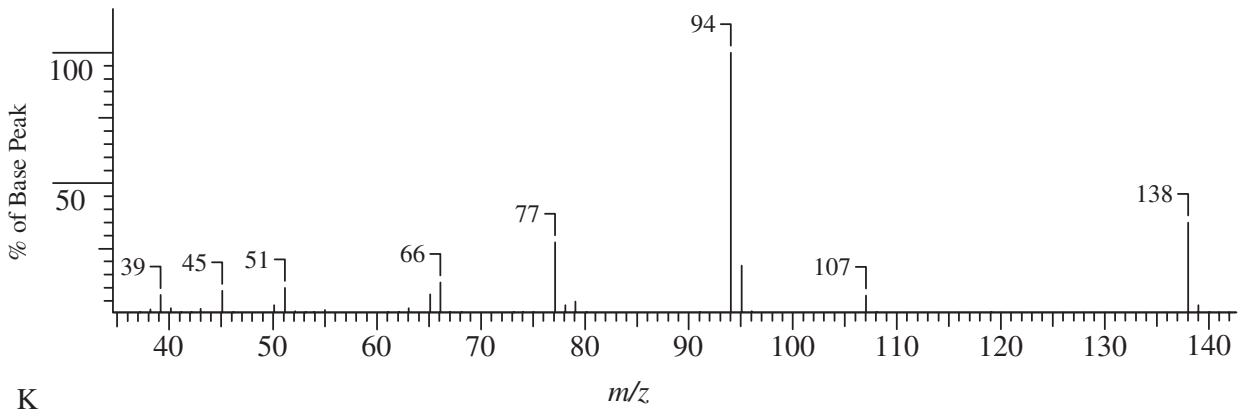

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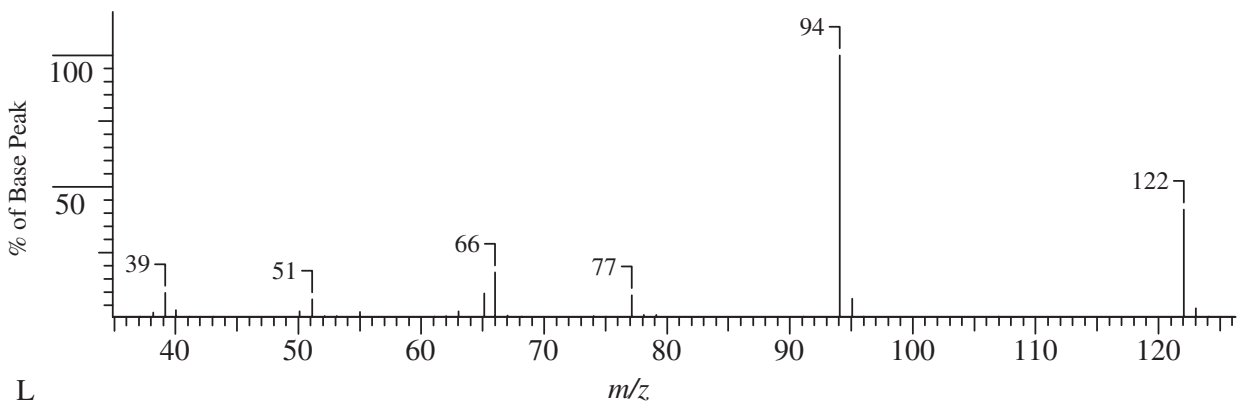

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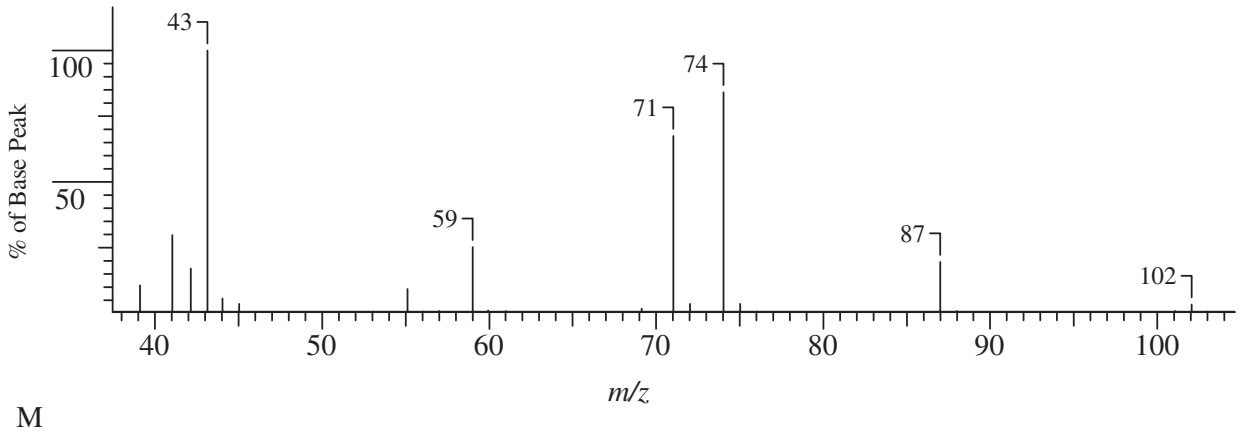

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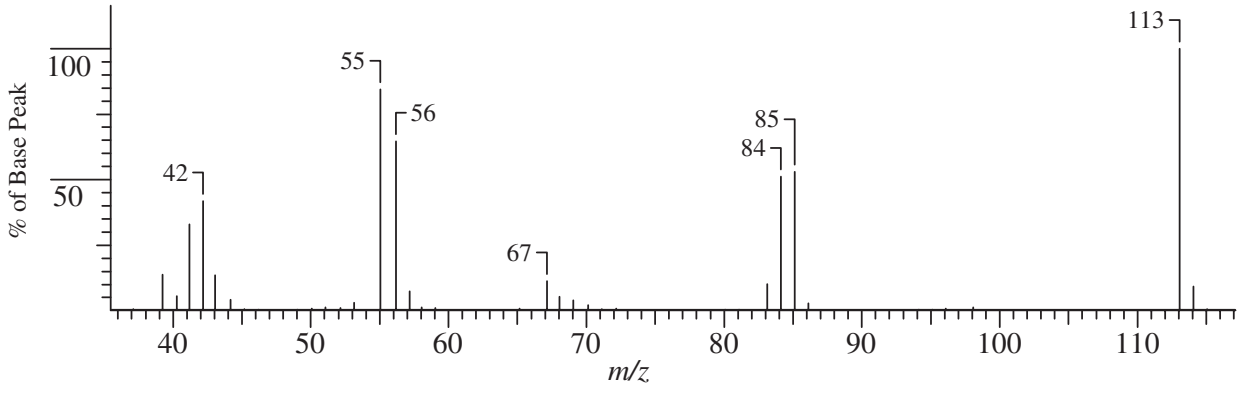

Exercise 1.6 (N – Q)

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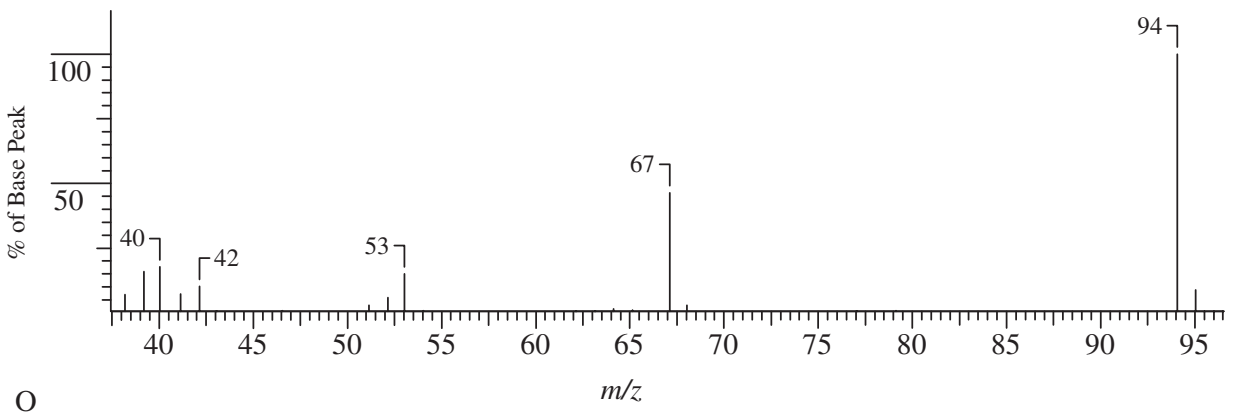

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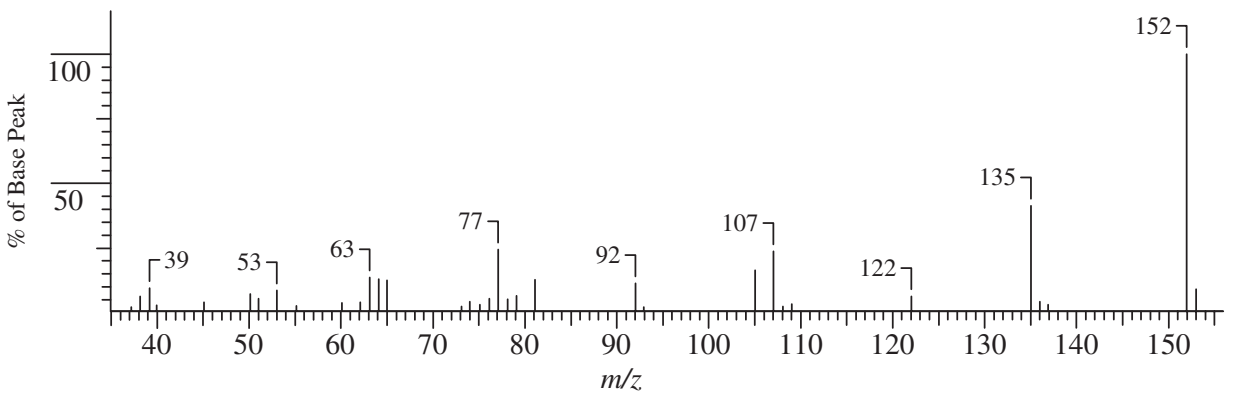

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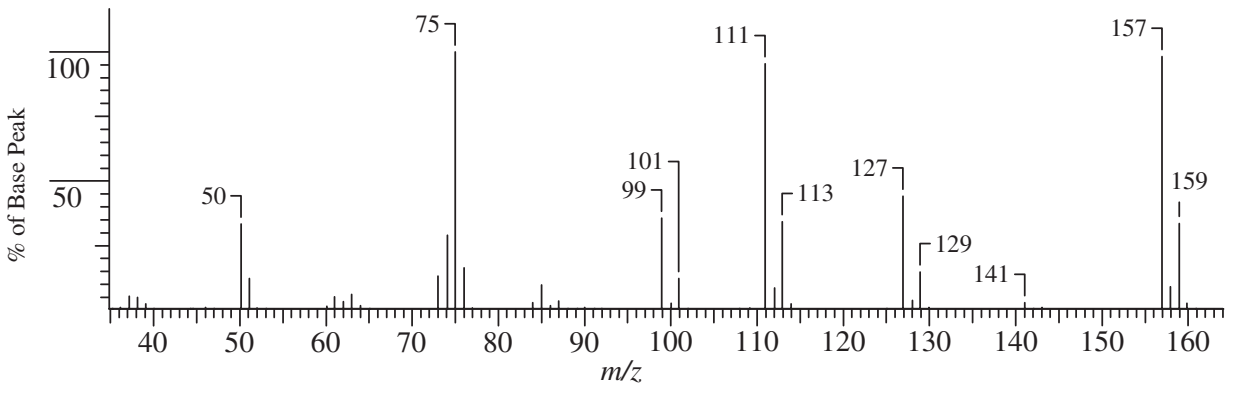

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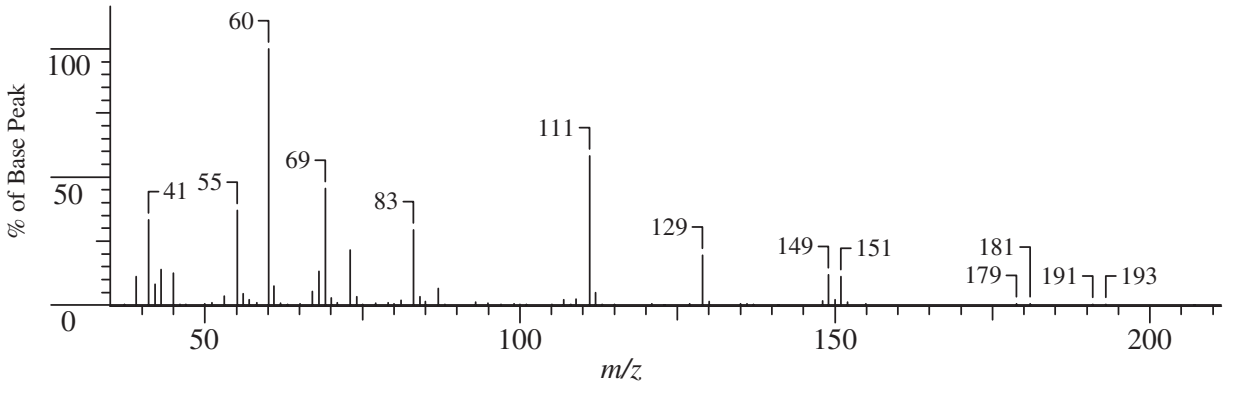

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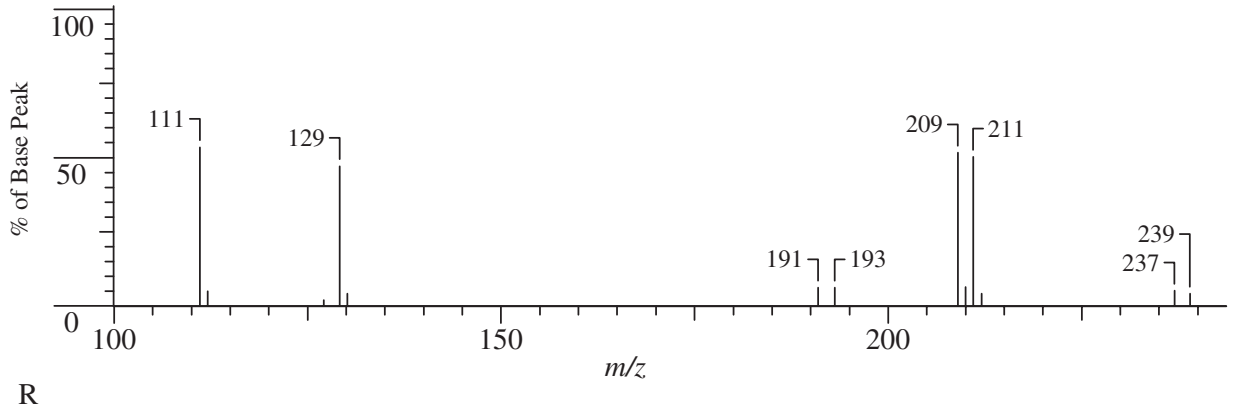

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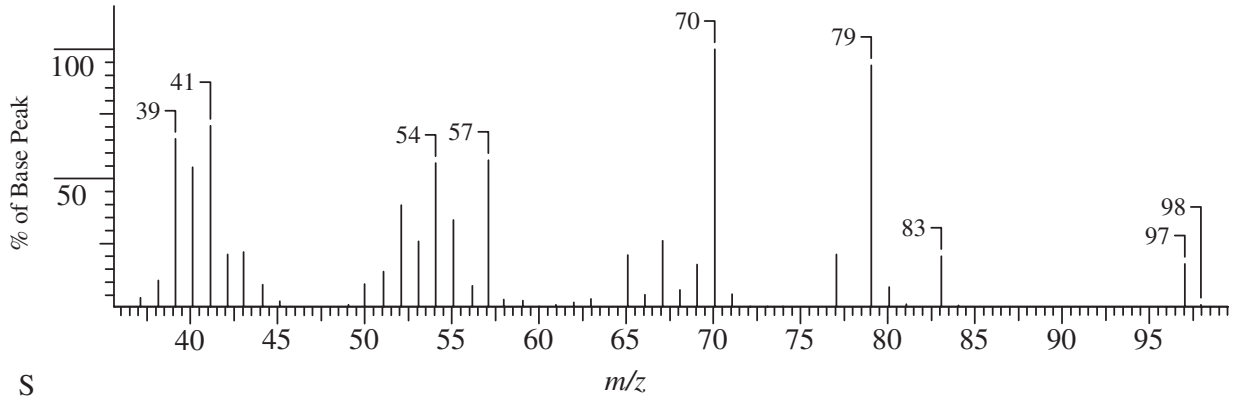

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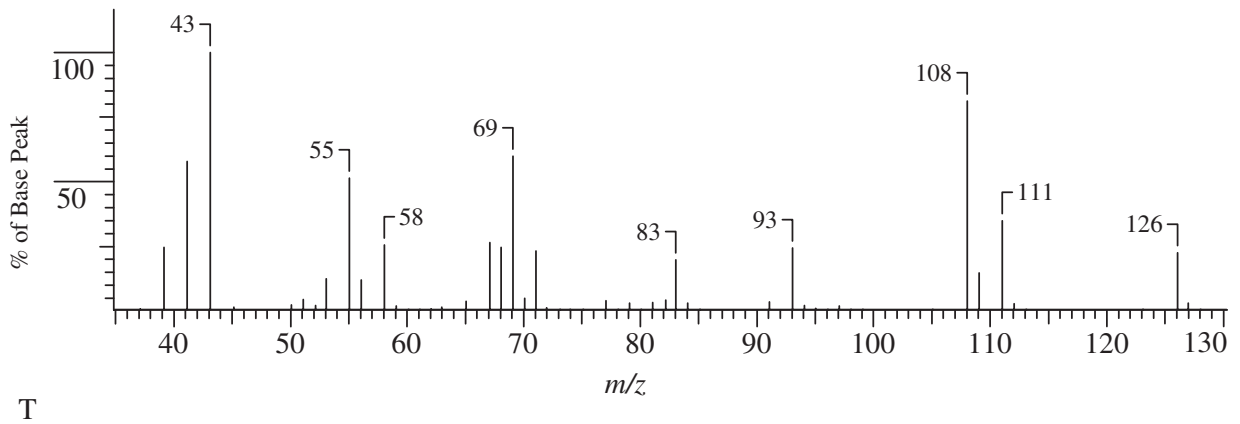

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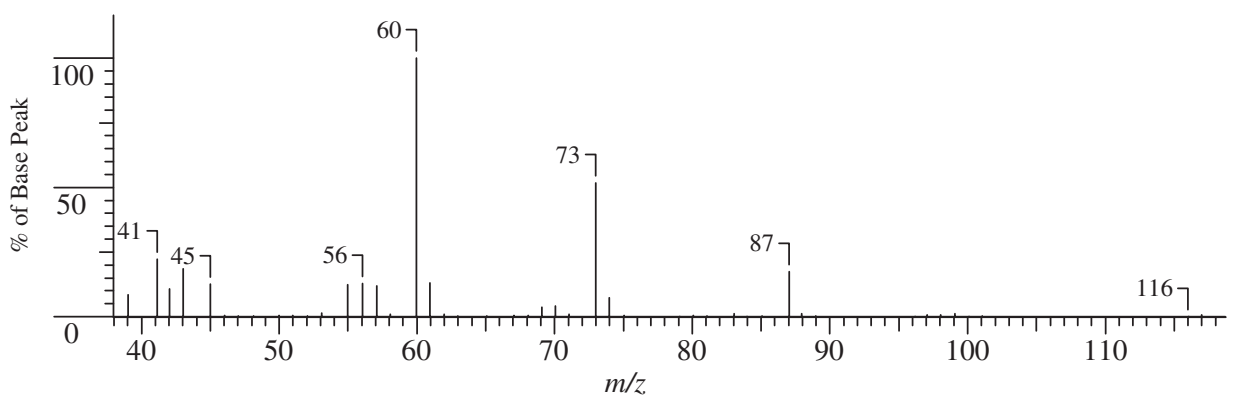

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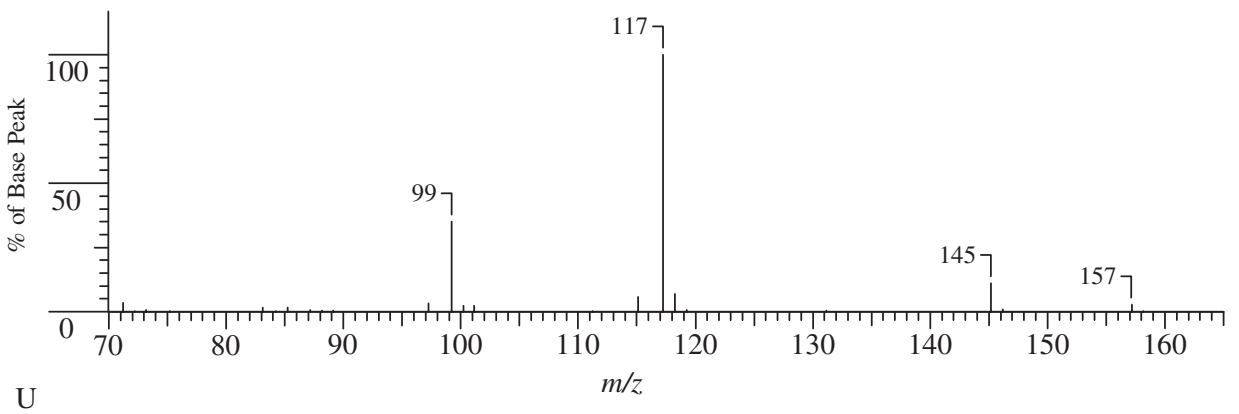

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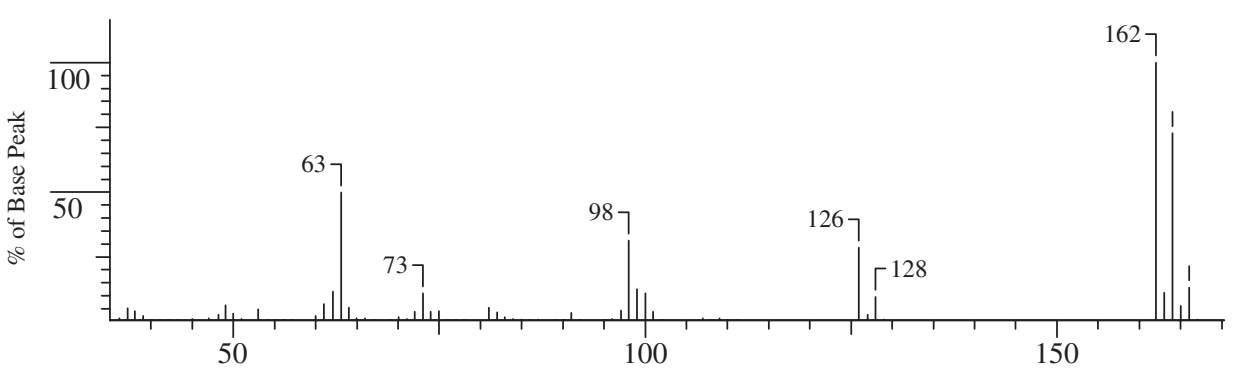

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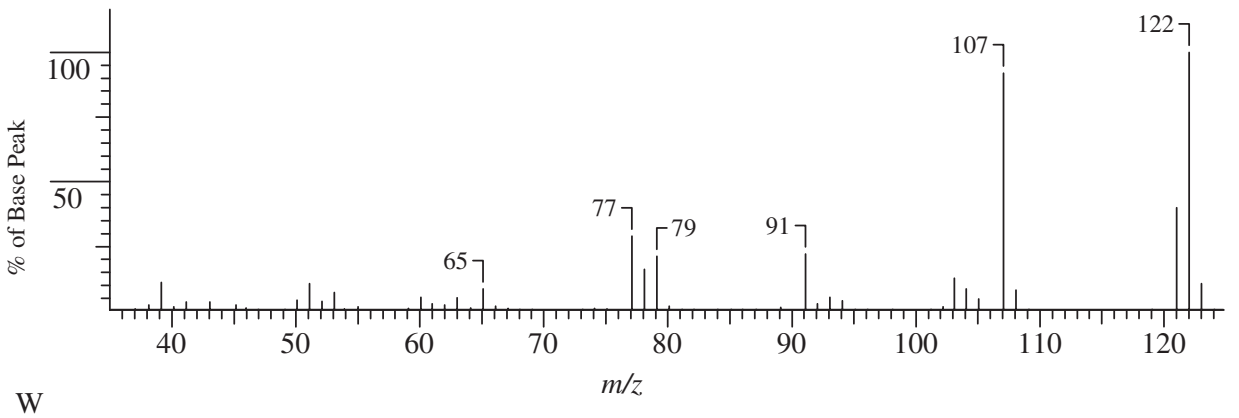

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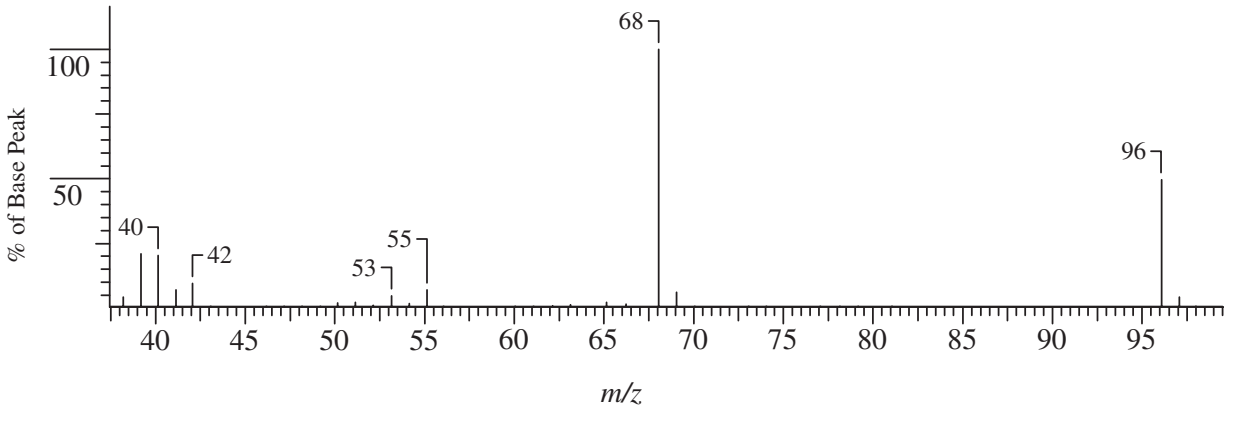


APPENDIX A FORMULA MASSES (FM) FOR VARIOUS COMBINATIONS OF CARBON, HYDROGEN, NITROGEN, AND OXYGEN[a]

	FM		FM		FM		FM
12		H_4N_2	32.0375	C_2H_6O	46.0419	CH_3N_2O	59.0246
C	12.0000	CH_4O	32.0262	**47**		CH_5N_3	59.0484
13		**33**		HNO_2	47.0007	$C_2H_3O_2$	59.0133
CH	13.0078	HO_2	32.9976	CH_3O_2	47.0133	C_2H_5NO	59.0371
14		H_3NO	33.0215	CH_5NO	47.0371	$C_2H_7N_2$	59.0610
N	14.0031	**34**		**48**		C_3H_7O	59.0497
CH_2	14.0157	H_2O_2	34.0054	O_3	47.9847	C_3H_9N	59.0736
15		**38**		H_2NO_2	48.0085	**60**	
HN	15.0109	C_3H_2	38.0157	H_4N_2O	48.0324	CH_2NO_2	60.0085
CH_3	15.0235	**39**		CH_4O_2	48.0211	CH_4N_2O	60.0324
16		C_2HN	39.0109	**49**		CH_6N_3	60.0563
O	15.9949	C_3H_3	39.0235	H_3NO_2	49.0164	$C_2H_4O_2$	60.0211
H_2N	16.0187	**40**		**52**		C_2H_6NO	60.0450
CH_4	16.0313	C_2H_2N	40.0187	C_4H_4	52.0313	$C_2H_8N_2$	60.0688
17		C_3H_4	40.0313	**53**		C_3H_8O	60.0575
HO	17.0027	**41**		C_3H_3N	53.0266	C_5	60.0000
H_3N	17.0266	CHN_2	41.0140	C_4H_5	53.0391	**61**	
18		C_2H_3N	41.0266	**54**		CH_3NO_2	61.0164
H_2O	18.0106	C_3H_5	41.0391	$C_2H_2N_2$	54.0218	CH_5N_2O	61.0402
24		**42**		C_3H_2O	54.0106	CH_7N_3	61.0641
C_2	24.0000	N_3	42.0093	C_3H_4N	54.0344	$C_2H_5O_2$	61.0289
26		CNO	41.9980	C_4H_6	54.0470	C_2H_7NO	61.0528
CN	26.0031	CH_2N_2	42.0218	**55**		**62**	
C_2H_2	26.0157	C_2H_2O	42.0106	$C_2H_3N_2$	55.0297	CH_2O_3	62.0003
27		C_2H_4N	42.0344	C_3H_3O	55.0184	CH_4NO_2	62.0242
CHN	27.0109	C_3H_6	42.0470	C_3H_5N	55.0422	CH_6N_2O	62.0480
C_2H_3	27.0235	**43**		C_4H_7	55.0548	$C_2H_6O_2$	62.0368
28		HN_3	43.0170	**56**		**63**	
N_2	28.0062	CHNO	43.0058	C_2O_2	55.9898	HNO_3	62.9956
CO	27.9949	CH_3N_2	43.0297	C_2H_2NO	56.0136	CH_5NO_2	63.0320
CH_2N	28.0187	C_2H_3O	43.0184	$C_2H_4N_2$	56.0375	**64**	
C_2H_4	28.0313	C_2H_5N	43.0422	C_3H_4O	56.0262	C_5H_4	64.0313
29		C_3H_7	43.0548	C_3H_6N	56.0501	**65**	
HN_2	29.0140	**44**		C_4H_8	56.0626	C_4H_3N	65.0266
CHO	29.0027	N_2O	44.0011	**57**		C_5H_5	65.0391
CH_3N	29.0266	CO_2	43.9898	C_2H_3NO	57.0215	**66**	
C_2H_5	29.0391	CH_2NO	44.0136	$C_2H_5N_2$	57.0453	C_4H_4N	66.0344
30		CH_4N_2	44.0375	C_3H_5O	57.0340	C_5H_6	66.0470
NO	29.9980	C_2H_4O	44.0262	C_3H_7N	57.0579	**67**	
H_2N_2	30.0218	C_2H_6N	44.0501	C_4H_9	57.0705	$C_3H_3N_2$	67.0297
CH_2O	30.0106	C_3H_8	44.0626	**58**		C_4H_3O	67.0184
CH_4N	30.0344	**45**		CH_2N_2O	58.0167	C_4H_5N	67.0422
C_2H_6	30.0470	CH_3NO	45.0215	CH_4N_3	58.0406	C_5H_7	67.0548
31		CH_5N_2	45.0453	$C_2H_2O_2$	58.0054	**68**	
HNO	31.0058	C_2H_5O	45.0340	C_2H_4NO	58.0293	$C_3H_4N_2$	68.0375
H_3N_2	31.0297	C_2H_7N	45.0579	$C_2H_6N_2$	58.0532	C_4H_4O	68.0262
CH_3O	31.0184	**46**		C_3H_6O	58.0419	C_4H_6N	68.0501
CH_5N	31.0422	NO_2	45.9929	C_3H_8N	58.0657	C_5H_8	68.0626
32		CH_2O_2	46.0054	C_4H_{10}	58.0783	**69**	
O_2	31.9898	CH_4NO	46.0293	**59**		C_3H_3NO	69.0215
H_2NO	32.0136	CH_6N_2	46.0532	$CHNO_2$	59.0007	$C_3H_5N_2$	69.0453

[a]With permission from J.H. Beynon, *Mass Spectrometry and its Application to Organic Chemistry*, Amsterdam, 1960. The columns headed FM contain the *formula masses* based on the exact mass of the most abundant isotope of each element; these masses are based on the most abundant isotope of carbon having a mass of 12.0000. Note that the table includes only C, H, N, and O.

APPENDIX A (*Continued*)

	FM		FM		FM		FM
C_4H_5O	69.0340	$C_2H_6NO_2$	76.0399	$C_4H_9N_2$	85.0767	$C_3H_8NO_2$	90.0555
C_4H_7N	69.0579	$C_2H_8N_2O$	76.0637	C_5H_9O	85.0653	$C_3H_{10}N_2O$	90.0794
C_5H_9	69.0705	$C_3H_8O_2$	76.0524	$C_5H_{11}N$	85.0892	$C_4H_{10}O_2$	90.0681
70		C_5H_2N	76.0187	C_6H_{13}	85.1018	C_7H_6	90.0470
$C_2H_4N_3$	70.0406	C_6H_4	76.0313	**86**		**91**	
$C_3H_2O_2$	70.0054	**77**		$C_2H_2N_2O_2$	86.0116	$C_2H_3O_4$	91.0031
C_3H_4NO	70.0293	CH_3NO_3	77.0113	$C_2H_4N_3O$	86.0355	$C_2H_5NO_3$	91.0269
$C_3H_6N_2$	70.0532	$C_2H_5O_3$	77.0238	$C_2H_6N_4$	86.0594	$C_2H_7N_2O_2$	91.0508
C_4H_6O	70.0419	$C_2H_7NO_2$	77.0477	$C_3H_4NO_2$	86.0242	$C_2H_9N_3O$	91.0746
C_4H_8N	70.0657	C_6H_5	77.0391	$C_3H_6N_2O$	86.0480	$C_3H_7O_3$	91.0395
C_5H_{10}	70.0783	**78**		$C_3H_8N_3$	86.0719	$C_3H_9NO_2$	91.0634
71		$C_2H_6O_3$	78.0317	$C_4H_6O_2$	86.0368	C_6H_5N	91.0422
$C_2H_3N_2O$	71.0246	C_5H_4N	78.0344	C_4H_8NO	86.0606	C_7H_7	91.0548
$C_2H_5N_3$	71.0484	C_6H_6	78.0470	$C_4H_{10}N_2$	86.0845	**92**	
$C_3H_3O_2$	71.0133	**79**		$C_5H_{10}O$	86.0732	$C_2H_4O_4$	92.0109
C_3H_5NO	71.0371	C_5H_5N	79.0422	$C_5H_{12}N$	86.0970	$C_2H_6NO_3$	92.0348
$C_3H_7N_2$	71.0610	C_6H_7	79.0548	C_6H_{14}	86.1096	$C_2H_8N_2O_2$	92.0586
C_4H_7O	71.0497	**80**		**87**		$C_3H_8O_3$	92.0473
C_4H_9N	71.0736	$C_3H_2N_3$	80.0249	$C_2H_7N_4$	87.0672	C_6H_4O	92.0262
C_5H_{11}	71.0861	$C_4H_4N_2$	80.0375	$C_3H_3O_3$	87.0082	C_6H_6N	92.0501
72		C_5H_4O	80.0262	$C_3H_5NO_2$	87.0320	C_7H_8	92.0626
$C_2H_2NO_2$	72.0085	C_5H_6N	80.0501	$C_3H_7N_2O$	87.0559	**93**	
$C_2H_4N_2O$	72.0324	C_6H_8	80.0626	$C_3H_9N_3$	87.0798	$C_2H_5O_4$	93.0187
$C_2H_6N_3$	72.0563	**81**		$C_4H_7O_2$	87.0446	$C_2H_7NO_3$	92.0426
$C_3H_4O_2$	72.0211	$C_3H_3N_3$	81.0328	C_4H_9NO	87.0684	$C_5H_5N_2$	93.0453
C_3H_6NO	72.0449	$C_4H_5N_2$	81.0453	$C_4H_{11}N_2$	87.0923	C_6H_5O	93.0340
$C_3H_8N_2$	72.0688	C_5H_5O	81.0340	$C_5H_{11}O$	87.0810	C_6H_7N	93.0579
C_4H_8O	72.0575	C_5H_7N	81.0579	$C_5H_{13}N$	87.1049	C_7H_9	93.0705
$C_4H_{10}N$	72.0814	C_6H_9	81.0705	**88**		**94**	
C_5H_{12}	72.0939	**82**		$C_2H_4N_2O_2$	88.0273	$C_2H_6O_4$	94.0266
73		$C_3H_4N_3$	82.0406	$C_2H_6N_3O$	88.0511	$C_4H_4N_3$	94.0406
$C_2H_3NO_2$	73.0164	C_4H_4NO	82.0293	$C_2H_8N_4$	88.0750	C_5H_4NO	94.0293
$C_2H_5N_2O$	73.0402	$C_4H_6N_2$	82.0532	$C_3H_4O_3$	88.0160	$C_5H_6N_2$	94.0532
$C_2H_7N_3$	73.0641	C_5H_6O	82.0419	$C_3H_6NO_2$	88.0399	C_6H_6O	94.0419
$C_3H_5O_2$	73.0289	C_5H_8N	82.0657	$C_3H_8N_2O$	88.0637	C_6H_8N	94.0657
C_3H_7NO	73.0528	C_6H_{10}	82.0783	$C_3H_{10}N_3$	88.0876	C_7H_{10}	94.0783
$C_3H_9N_2$	73.0767	**83**		$C_4H_8O_2$	88.0524	**95**	
C_4H_9O	73.0653	$C_3H_5N_3$	83.0484	$C_4H_{10}NO$	88.0763	$C_4H_5N_3$	95.0484
$C_4H_{11}N$	73.0892	$C_4H_3O_2$	83.0133	$C_4H_{12}N_2$	88.1001	C_5H_5NO	95.0371
74		C_4H_5NO	83.0371	$C_5H_{12}O$	88.0888	$C_5H_7N_2$	95.0610
$C_2H_2O_3$	74.0003	$C_4H_7N_2$	83.0610	**89**		C_6H_7O	95.0497
$C_2H_4NO_2$	74.0242	C_5H_7O	83.0497	$C_2H_5N_2O_2$	89.0351	C_6H_9N	95.0736
$C_2H_6N_2O$	74.0480	C_5H_9N	83.0736	$C_2H_7N_3O$	89.0590	C_7H_{11}	95.0861
$C_2H_8N_3$	74.0719	C_6H_{11}	83.0861	$C_2H_9N_4$	89.0829	**96**	
$C_3H_6O_2$	74.0368	**84**		$C_3H_5O_3$	89.0238	$C_4H_6N_3$	96.0563
C_3H_8NO	74.0606	$C_3H_6N_3$	84.0563	$C_3H_7NO_2$	89.0477	$C_5H_4O_2$	96.0211
$C_3H_{10}N_2$	74.0845	$C_4H_4O_2$	84.0211	$C_3H_9N_2O$	89.0715	C_5H_6NO	96.0449
$C_4H_{10}O$	74.0732	C_4H_6NO	84.0449	$C_3H_{11}N_3$	89.0954	$C_5H_8N_2$	96.0688
75		$C_4H_8N_2$	84.0688	$C_4H_9O_2$	89.0603	C_6H_8O	96.0575
$C_2H_3O_3$	75.0082	C_5H_8O	84.0575	$C_4H_{11}NO$	89.0841	$C_6H_{10}N$	96.0814
$C_2H_5NO_2$	75.0320	$C_5H_{10}N$	84.0814	C_7H_5	89.0391	C_7H_{12}	96.0939
$C_2H_7N_2O$	75.0559	C_6H_{12}	84.0939	**90**		**97**	
$C_2H_9N_3$	75.0798	**85**		$C_2H_4NO_3$	90.0191	$C_3H_5N_4$	97.0515
$C_3H_7O_2$	75.0446	$C_3H_5N_2O$	85.0402	$C_2H_6N_2O_2$	90.0429	$C_4H_5N_2O$	97.0402
C_3H_9NO	75.0684	$C_3H_7N_3$	85.0641	$C_2H_8N_3O$	90.0668	$C_5H_5O_2$	97.0289
76		$C_4H_5O_2$	85.0289	$C_2H_{10}N_4$	90.0907	C_5H_7NO	97.0528
$C_2H_4O_3$	76.0160	C_4H_7NO	85.0528	$C_3H_6O_3$	90.0317	$C_5H_9N_2$	97.0767

APPENDIX A (*Continued*)

FM		FM		FM		FM	
C_6H_9O	97.0653	**102**		$C_4H_{11}NO_2$	105.0790	$C_4H_6N_4$	110.0594
$C_6H_{11}N$	97.0892	$C_2H_6N_4O$	102.0542	$C_6H_5N_2$	105.0453	$C_5H_6N_2O$	110.0480
C_7H_{13}	97.1018	$C_3H_4NO_3$	102.0191	C_7H_5O	105.0340	$C_5H_8N_3$	110.0719
98		$C_3H_6N_2O_2$	102.0429	C_7H_7N	105.0579	$C_6H_6O_2$	110.0368
$C_3H_4N_3O$	98.0355	$C_3H_8N_3O$	102.0668	C_8H_9	105.0705	C_6H_8NO	110.0606
$C_3H_6N_4$	98.0594	$C_3H_{10}N_4$	102.0907	**106**		$C_6H_{10}N_2$	110.0845
$C_4H_4NO_2$	98.0242	$C_4H_6O_3$	102.0317	$C_2H_4NO_4$	106.0140	$C_7H_{10}O$	110.0732
$C_4H_6N_2O$	98.0480	$C_4H_8NO_2$	102.0555	$C_2H_6N_2O_3$	106.0379	$C_7H_{12}N$	110.0970
$C_4H_8N_3$	98.0719	$C_4H_{10}N_2O$	102.0794	$C_2H_8N_3O_2$	106.0617	C_8H_{14}	110.1096
$C_5H_6O_2$	98.0368	$C_4H_{12}N_3$	102.1032	$C_2H_{10}N_4O$	106.0856	**111**	
C_5H_8NO	98.0606	$C_5H_{10}O_2$	102.0681	$C_3H_6O_4$	106.0266	$C_4H_5N_3O$	111.0433
$C_5H_{10}N_2$	98.0845	$C_5H_{12}NO$	102.0919	$C_3H_8NO_3$	106.0504	$C_4H_7N_4$	111.0672
$C_6H_{10}O$	98.0732	$C_5H_{14}N_2$	102.1158	$C_3H_{10}N_2O_2$	106.0743	$C_5H_5NO_2$	111.0320
$C_6H_{12}N$	98.0970	$C_6H_{14}O$	102.1045	$C_4H_{10}O_3$	106.0630	$C_5H_7N_2O$	111.0559
C_7H_{14}	98.1096	C_8H_6	102.0470	C_6H_4NO	106.0293	$C_5H_9N_3$	111.0789
99		**103**		$C_6H_6N_2$	106.0532	$C_6H_7O_2$	111.0446
$C_3H_5N_3O$	99.0433	$C_2H_5N_3O_2$	103.0382	C_7H_6O	106.0419	C_6H_9NO	111.0684
$C_3H_7N_4$	99.0672	$C_2H_7N_4O$	103.0621	C_7H_8N	106.0657	$C_6H_{11}N_2$	111.0923
$C_4H_3O_3$	99.0082	$C_3H_3O_4$	103.0031	C_8H_{10}	106.0783	$C_7H_{11}O$	111.0810
$C_4H_5NO_2$	99.0320	$C_3H_5NO_3$	103.0269	**107**		$C_7H_{13}N$	111.1049
$C_4H_7N_2O$	99.0559	$C_3H_7N_2O_2$	103.0508	$C_2H_5NO_4$	107.0218	C_8H_{15}	111.1174
$C_4H_9N_3$	99.0798	$C_3H_9N_3O$	103.0746	$C_2H_7N_2O_3$	107.0457	**112**	
$C_5H_7O_2$	99.0446	$C_3H_{11}N_4$	103.0985	$C_2H_9N_3O_2$	107.0695	$C_3H_4N_4O$	112.0386
C_5H_9NO	99.0685	$C_4H_7O_3$	103.0395	$C_3H_7O_4$	107.0344	$C_4H_4N_2O_2$	112.0273
$C_5H_{11}N_2$	99.0923	$C_4H_9NO_2$	103.0634	$C_3H_9NO_3$	107.0583	$C_4H_6N_3O$	112.0511
$C_6H_{11}O$	99.0810	$C_4H_{11}N_2O$	103.0872	$C_5H_5N_3$	107.0484	$C_4H_8N_4$	112.0750
$C_6H_{13}N$	99.1049	$C_4H_{13}N_3$	103.1111	C_6H_5NO	107.0371	$C_5H_4O_3$	112.0160
C_7H_{15}	99.1174	$C_5H_{11}O_2$	103.0759	$C_6H_7N_2$	107.0610	$C_5H_6NO_2$	112.0399
100		$C_5H_{13}NO$	103.0998	C_7H_7O	107.0497	$C_5H_8N_2O$	112.0637
$C_2H_4N_4O$	100.0386	C_7H_5N	103.0422	C_7H_9N	107.0736	$C_5H_{10}N_3$	112.0876
$C_3H_4N_2O_2$	100.0273	C_8H_7	103.0548	C_8H_{11}	107.0861	$C_6H_8O_2$	112.0524
$C_3H_6N_3O$	100.0511	**104**		**108**		$C_6H_{10}NO$	112.0763
$C_3H_8N_4$	100.0750	$C_2H_4N_2O_3$	104.0222	$C_2H_6NO_4$	108.0297	$C_6H_{12}N_2$	112.1001
$C_4H_4O_3$	100.0160	$C_2H_6N_3O_2$	104.0460	$C_2H_8N_2O_3$	108.0535	$C_7H_{12}O$	112.0888
$C_4H_6NO_2$	100.0399	$C_2H_8N_4O$	104.0699	$C_3H_8O_4$	108.0422	$C_7H_{14}N$	112.1127
$C_4H_8N_2O$	100.0637	$C_3H_4O_4$	104.0109	$C_4H_4N_4$	108.0437	C_8H_{16}	112.1253
$C_4H_{10}N_3$	100.0876	$C_3H_6NO_3$	104.0348	$C_5H_4N_2O$	108.0324	**113**	
$C_5H_8O_2$	100.0524	$C_3H_8N_2O_2$	104.0586	$C_5H_6N_3$	108.0563	$C_3H_5N_4O$	113.0464
$C_5H_{10}NO$	100.0763	$C_3H_{10}N_3O$	104.0825	$C_6H_4O_2$	108.0211	$C_4H_5N_2O_2$	113.0351
$C_5H_{12}N_2$	100.1001	$C_3H_{12}N_4$	104.1063	C_6H_6NO	108.0449	$C_4H_7N_3O$	113.0590
$C_6H_{12}O$	100.0888	$C_4H_8O_3$	104.0473	$C_6H_8N_2$	108.0688	$C_4H_9N_4$	113.0829
$C_6H_{14}N$	100.1127	$C_4H_{10}NO_2$	104.0712	C_7H_8O	108.0575	$C_5H_5O_3$	113.0238
C_7H_{16}	100.1253	$C_4H_{12}N_2O$	104.0950	$C_7H_{10}N$	108.0814	$C_5H_7NO_2$	113.0477
101		$C_5H_{12}O_2$	104.0837	C_8H_{12}	108.0939	$C_5H_9N_2O$	113.0715
$C_3H_3NO_3$	101.0113	$C_6H_4N_2$	104.0375	**109**		$C_5H_{11}N_3$	113.0954
$C_3H_5N_2O_2$	101.0351	C_7H_4O	104.0262	$C_2H_7NO_4$	109.0375	$C_6H_9O_2$	113.0603
$C_3H_7N_3O$	101.0590	C_7H_6N	104.0501	$C_4H_5N_4$	109.0515	$C_6H_{11}NO$	113.0841
$C_3H_9N_4$	101.0829	C_8H_8	104.0626	$C_5H_5N_2O$	109.0402	$C_6H_{13}N_2$	113.1080
$C_4H_5O_3$	101.0238	**105**		$C_5H_7N_3$	109.0641	$C_7H_{13}O$	113.0967
$C_4H_7NO_2$	101.0477	$C_2H_5N_2O_3$	105.0300	$C_6H_5O_2$	109.0289	$C_7H_{15}N$	113.1205
$C_4H_9N_2O$	101.0715	$C_2H_7N_3O_2$	105.0539	C_6H_7NO	109.0528	C_8H_{17}	113.1331
$C_4H_{11}N_3$	101.0954	$C_2H_9N_4O$	105.0777	$C_6H_9N_2$	109.0767	**114**	
$C_5H_9O_2$	101.0603	$C_3H_5O_4$	105.0187	C_7H_9O	109.0653	$C_3H_6N_4O$	114.0542
$C_5H_{11}NO$	101.0841	$C_3H_7NO_3$	105.0426	$C_7H_{11}N$	109.0892	$C_4H_4NO_3$	114.0191
$C_5H_{13}N_2$	101.1080	$C_3H_9N_2O_2$	105.0664	C_8H_{13}	109.1018	$C_4H_6N_2O_2$	114.0429
$C_6H_{13}O$	101.0967	$C_3H_{11}N_3O$	105.0903	**110**		$C_4H_8N_3O$	114.0668
$C_6H_{15}N$	101.1205	$C_4H_9O_3$	105.0552	$C_4H_4N_3O$	110.0355	$C_4H_{10}N_4$	114.0907

APPENDIX A (*Continued*)

	FM		FM		FM		FM
$C_5H_6O_3$	114.0317	$C_4H_9N_2O_2$	117.0664	$C_4H_8O_4$	120.0422	C_7H_9NO	123.0684
$C_5H_8NO_2$	114.0555	$C_4H_{11}N_3O$	117.0903	$C_4H_{10}NO_3$	120.0661	$C_7H_{11}N_2$	123.0923
$C_5H_{10}N_2O$	114.0794	$C_4H_{13}N_4$	117.1142	$C_4H_{12}N_2O_2$	120.0899	$C_8H_{11}O$	123.0810
$C_5H_{12}N_3$	114.1032	$C_5H_9O_3$	117.0552	$C_5H_4N_4$	120.0437	$C_8H_{13}N$	123.1049
$C_6H_{10}O_2$	114.0681	$C_5H_{11}NO_2$	117.0790	$C_5H_{12}O_3$	120.0786	C_9H_{15}	123.1174
$C_6H_{12}NO$	114.0919	$C_5H_{13}N_2O$	117.1029	$C_6H_4N_2O$	120.0324	**124**	
$C_6H_{14}N_2$	114.1158	$C_5H_{15}N_3$	117.1267	$C_6H_6N_3$	120.0563	$C_2H_8N_2O_4$	124.0484
$C_7H_{14}O$	114.1045	$C_6H_{13}O_2$	117.0916	C_7H_6NO	120.0449	$C_4H_4N_4O$	124.0386
$C_7H_{16}N$	114.1284	$C_6H_{15}NO$	117.1154	$C_7H_8N_2$	120.0688	$C_5H_4N_2O_2$	124.0273
C_8H_{18}	114.1409	C_8H_7N	117.0579	C_8H_8O	120.0575	$C_5H_6N_3O$	124.0511
C_9H_6	114.0470	C_9H_9	117.0705	$C_8H_{10}N$	120.0814	$C_5H_8N_4$	124.0750
115		**118**		C_9H_{12}	120.0939	$C_6H_4O_3$	124.0160
$C_3H_5N_3O_2$	115.0382	$C_2H_4N_3O_3$	118.0253	**121**		$C_6H_6NO_2$	124.0399
$C_3H_7N_4O$	115.0621	$C_2H_6N_4O_2$	118.0491	$C_2H_5N_2O_4$	121.0249	$C_6H_8N_2O$	124.0637
$C_4H_5NO_3$	115.0269	$C_3H_4NO_4$	118.0140	$C_2H_7N_3O_3$	121.0488	$C_6H_{10}N_3$	124.0876
$C_4H_7N_2O_2$	115.0508	$C_3H_6N_2O_3$	118.0379	$C_2H_9N_4O_2$	121.0726	$C_7H_8O_2$	124.0524
$C_4H_9N_3O$	115.0746	$C_3H_8N_3O_2$	118.0617	$C_3H_7NO_4$	121.0375	$C_7H_{10}NO$	124.0763
$C_4H_{11}N_4$	115.0985	$C_3H_{10}N_4O$	118.0856	$C_3H_9N_2O_3$	121.0614	$C_7H_{12}N_2$	124.1001
$C_5H_7O_3$	115.0395	$C_4H_6O_4$	118.0266	$C_3H_{11}N_3O_2$	121.0852	C_8N_2	124.0062
$C_5H_9NO_2$	115.0634	$C_4H_8NO_3$	118.0504	$C_4H_9O_4$	121.0501	$C_8H_{12}O$	124.0888
$C_5H_{11}N_2O$	115.0872	$C_4H_{10}N_2O_2$	118.0743	$C_4H_{11}NO_3$	121.0739	$C_8H_{14}N$	124.1127
$C_5H_{13}N_3$	115.1111	$C_4H_{12}N_3O$	118.0981	$C_5H_5N_4$	121.0515	C_9H_{16}	124.1253
$C_6H_{11}O_2$	115.0759	$C_4H_{14}N_4$	118.1220	$C_6H_5N_2O$	121.0402	**125**	
$C_6H_{13}NO$	115.0998	$C_5H_{10}O_3$	118.0630	$C_6H_7N_3$	121.0641	$C_4H_3N_3O_2$	125.0226
$C_6H_{15}N_2$	115.1236	$C_5H_{12}NO_2$	118.0868	$C_7H_5O_2$	121.0289	$C_4H_5N_4O$	125.0464
$C_7H_{15}O$	115.1123	$C_5H_{14}N_2O$	118.1107	C_7H_7NO	121.0528	$C_5H_5N_2O_2$	125.0351
$C_7H_{17}N$	115.1362	$C_6H_{14}O_2$	118.0994	$C_7H_9N_2$	121.0767	$C_5H_7N_3O$	125.0590
C_9H_7	115.0548	$C_7H_6N_2$	118.0532	C_8H_9O	121.0653	$C_5H_9N_4$	125.0829
116		C_8H_6O	118.0419	$C_8H_{11}N$	121.0892	$C_6H_5O_3$	125.0238
$C_2H_4N_4O_2$	116.0335	C_8H_8N	118.0657	C_9H_{13}	121.1018	$C_6H_7NO_2$	125.0477
$C_3H_4N_2O_3$	116.0222	C_9H_{10}	118.0783	**122**		$C_6H_9N_2O$	125.0715
$C_3H_6N_3O_2$	116.0460	**119**		$C_2H_6N_2O_4$	122.0328	$C_6H_{11}N_3$	125.0954
$C_3H_8N_4O$	116.0699	$C_2H_5N_3O_3$	119.0331	$C_2H_8N_3O_3$	122.0566	$C_7H_9O_2$	125.0603
$C_4H_4O_4$	116.0109	$C_2H_7N_4O_2$	119.0570	$C_2H_{10}N_4O_2$	122.0805	$C_7H_{11}NO$	125.0841
$C_4H_6NO_3$	116.0348	$C_3H_5NO_4$	119.0218	$C_3H_8NO_4$	122.0453	$C_7H_{13}N_2$	125.1080
$C_4H_8N_2O_2$	116.0586	$C_3H_7N_2O_3$	119.0457	$C_3H_{10}N_2O_3$	122.0692	$C_8H_{13}O$	125.0967
$C_4H_{10}N_3O$	116.0825	$C_3H_9N_3O_2$	119.0695	$C_4H_{10}O_4$	122.0579	$C_8H_{15}N$	125.1205
$C_4H_{12}N_4$	116.1063	$C_3H_{11}N_4O$	119.0934	$C_5H_6N_4$	122.0594	C_9H_{17}	125.1331
$C_5H_8O_3$	116.0473	$C_4H_7O_4$	119.0344	$C_6H_4NO_2$	122.0242	**126**	
$C_5H_{10}NO_2$	116.0712	$C_4H_9NO_3$	119.0583	$C_6H_6N_2O$	122.0480	$C_3H_2N_4O_2$	126.0178
$C_5H_{12}N_2O$	116.0950	$C_4H_{11}N_2O_2$	119.0821	$C_6H_8N_3$	122.0719	$C_4H_4N_3O_2$	126.0304
$C_5H_{14}N_3$	116.1189	$C_4H_{13}N_3O$	119.1060	$C_7H_6O_2$	122.0368	$C_4H_6N_4O$	126.0542
$C_6H_{12}O_2$	116.0837	$C_5H_{11}O_3$	119.0708	C_7H_8NO	122.0606	$C_5H_4NO_3$	126.0191
$C_6H_{14}NO$	116.1076	$C_5H_{13}NO_2$	119.0947	$C_7H_{10}N_2$	122.0845	$C_5H_6N_2O_2$	126.0429
$C_6H_{16}N_2$	116.1315	$C_6H_5N_3$	119.0484	$C_8H_{10}O$	122.0732	$C_5H_8N_3O$	126.0668
$C_7H_4N_2$	116.0375	C_7H_5NO	119.0371	$C_8H_{12}N$	122.0970	$C_5H_{10}N_4$	126.0907
$C_7H_{16}O$	116.1202	$C_7H_7N_2$	119.0610	C_9H_{14}	122.1096	$C_6H_6O_3$	126.0317
C_8H_6N	116.0501	C_8H_7O	119.0497	**123**		$C_6H_8NO_2$	126.0555
C_9H_8	116.0626	C_8H_9N	119.0736	$C_2H_7N_2O_4$	123.0406	$C_6H_{10}N_2O$	126.0794
117		C_9H_{11}	119.0861	$C_2H_9N_3O_3$	123.0644	$C_6H_{12}N_3$	126.1032
$C_2H_5N_4O_2$	117.0413	**120**		$C_3H_9NO_4$	123.0532	$C_7H_{10}O_2$	126.0681
$C_3H_3NO_4$	117.0062	$C_2H_6N_3O_3$	120.0410	$C_5H_5N_3O$	123.0433	$C_7H_{12}NO$	126.0919
$C_3H_5N_2O_3$	117.0300	$C_2H_8N_4O_2$	120.0648	$C_5H_7N_4$	123.0672	$C_7H_{14}N_2$	126.1158
$C_3H_7N_3O_2$	117.0539	$C_3H_6NO_4$	120.0297	$C_6H_5NO_2$	123.0320	$C_8H_{14}O$	126.1045
$C_3H_9N_4O$	117.0777	$C_3H_8N_2O_3$	120.0535	$C_6H_7N_2O$	123.0559	$C_8H_{16}N$	126.1284
$C_4H_5O_4$	117.0187	$C_3H_{10}N_3O_2$	120.0774	$C_6H_9N_3$	123.0798	C_9H_{18}	126.1409
$C_4H_7NO_3$	117.0426	$C_3H_{12}N_4O$	120.1012	$C_7H_7O_2$	123.0446	**127**	

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_3H_3N_4O_2$	127.0257	$C_8H_{19}N$	129.1519	$C_4H_{10}N_3O_2$	132.0774	C_8H_8NO	134.0606
$C_4H_5N_3O_2$	127.0382	C_9H_7N	129.0579	$C_4H_{12}N_4O$	132.1012	$C_8H_{10}N_2$	134.0845
$C_4H_7N_4O$	127.0621	$C_{10}H_9$	129.0705	$C_5H_8O_4$	132.0422	$C_9H_{10}O$	134.0732
$C_5H_5NO_3$	127.0269	**130**		$C_5H_{10}NO_3$	132.0661	$C_9H_{12}N$	134.0970
$C_5H_7N_2O_2$	127.0508	$C_3H_4N_3O_3$	130.0253	$C_5H_{12}N_2O_2$	132.0899	$C_{10}H_{14}$	134.1096
$C_5H_9N_3O$	127.0746	$C_3H_6N_4O_2$	130.0491	$C_5H_{14}N_3O$	132.1138	**135**	
$C_5H_{11}N_4$	127.0985	$C_4H_4NO_4$	130.0140	$C_5H_{16}N_4$	132.1377	$C_3H_7N_2O_4$	135.0406
$C_6H_7O_3$	127.0395	$C_4H_6N_2O_3$	130.0379	$C_6H_4N_4$	132.0437	$C_3H_9N_3O_3$	135.0644
$C_6H_9NO_2$	127.0634	$C_4H_8N_3O_2$	130.0617	$C_6H_{12}O_3$	132.0786	$C_3H_{11}N_4O_2$	135.0883
$C_6H_{11}N_2O$	127.0872	$C_4H_{10}N_4O$	130.0856	$C_6H_{14}NO_2$	132.1025	$C_4H_9NO_4$	135.0532
$C_6H_{13}N_3$	127.1111	$C_5H_6O_4$	130.0266	$C_6H_{16}N_2O$	132.1264	$C_4H_{11}N_2O_3$	135.0770
$C_7H_{11}O_2$	127.0759	$C_5H_8NO_3$	130.0504	$C_7H_9N_3$	132.0563	$C_4H_{13}N_3O_2$	135.1009
$C_7H_{13}NO$	127.0998	$C_5H_{10}N_2O_2$	130.0743	$C_7H_{16}O_2$	132.1151	$C_5H_3N_4O$	135.0308
$C_7H_{15}N_2$	127.1236	$C_5H_{12}N_3O$	130.0981	C_8H_6NO	132.0449	$C_5H_{11}O_4$	135.0657
$C_8H_{15}O$	127.1123	$C_5H_{14}N_4$	130.1220	$C_8H_8N_2$	132.0688	$C_5H_{13}NO_3$	135.0896
$C_8H_{17}N$	127.1362	$C_6H_{10}O_3$	130.0630	C_9H_8O	132.0575	$C_6H_5N_3O$	135.0433
C_9H_{19}	127.1488	$C_6H_{12}NO_2$	130.0868	$C_9H_{10}N$	132.0814	$C_6H_7N_4$	135.0672
128		$C_6H_{14}N_2O$	130.1107	$C_{10}H_{12}$	132.0939	$C_7H_5NO_2$	135.0320
$C_3H_4N_4O_2$	128.0335	$C_6H_{16}N_3$	130.1346	**133**		$C_7H_7N_2O$	135.0559
$C_4H_4N_2O_3$	128.0222	$C_7H_4N_3$	130.0406	$C_3H_5N_2O_4$	133.0249	$C_7H_9N_3$	135.0798
$C_4H_6N_3O_2$	128.0460	$C_7H_{14}O_2$	130.0994	$C_3H_7N_3O_3$	133.0488	$C_8H_7O_2$	135.0446
$C_4H_8N_4O$	128.0699	$C_7H_{16}NO$	130.1233	$C_3H_9N_4O_2$	133.0726	C_8H_9NO	135.0684
$C_5H_4O_4$	128.0109	$C_7H_{18}N_2$	130.1471	$C_4H_7NO_4$	133.0375	$C_8H_{11}N_2$	135.0923
$C_5H_6NO_3$	128.0348	$C_8H_6N_2$	130.0532	$C_4H_9N_2O_3$	133.0614	$C_9H_{11}O$	135.0810
$C_5H_8N_2O_2$	128.0586	$C_8H_{18}O$	130.1358	$C_4H_{11}N_3O_2$	133.0852	$C_9H_{13}N$	135.1049
$C_5H_{10}N_3O$	128.0825	C_9H_8N	130.0657	$C_4H_{13}N_4O$	133.1091	$C_{10}H_{15}$	135.1174
$C_5H_{12}N_4$	128.1063	$C_{10}H_{10}$	130.0783	$C_5H_9O_4$	133.0501	**136**	
$C_6H_8O_3$	128.0473	**131**		$C_5H_{11}NO_3$	133.0739	$C_3H_8N_2O_4$	136.0484
$C_6H_{10}NO_2$	128.0712	$C_3H_3N_2O_4$	131.0093	$C_5H_{13}N_2O_2$	133.0978	$C_3H_{10}N_3O_3$	136.0723
$C_6H_{12}N_2O$	128.0950	$C_3H_5N_3O_3$	131.0331	$C_5H_{15}N_3O$	133.1216	$C_3H_{12}N_4O_2$	136.0961
$C_6H_{14}N_3$	128.1189	$C_3H_7N_4O_2$	131.0570	$C_6H_5N_4$	133.0515	$C_4H_{10}NO_4$	136.0610
$C_7H_{12}O_2$	128.0837	$C_4H_5NO_4$	131.0218	$C_6H_{13}O_3$	133.0865	$C_4H_{12}N_2O_3$	136.0848
$C_7H_{14}NO$	128.1076	$C_4H_7N_2O_3$	131.0457	$C_6H_{15}NO_2$	133.1103	$C_5H_2N_3O_2$	136.0147
$C_7H_{16}N_2$	128.1315	$C_4H_9N_3O_2$	131.0695	$C_7H_5N_2O$	133.0402	$C_5H_4N_4O$	136.0386
$C_8H_{16}O$	128.1202	$C_4H_{11}N_4O$	131.0934	$C_7H_7N_3$	133.0641	$C_5H_{12}O_4$	136.0735
$C_8H_{18}N$	128.1440	$C_5H_7O_4$	131.0344	C_8H_7NO	133.0528	$C_6H_4N_2O_2$	136.0273
C_9H_{20}	128.1566	$C_5H_9NO_3$	131.0583	$C_8H_9N_2$	133.0767	$C_6H_6N_3O$	136.0511
$C_{10}H_8$	128.0626	$C_5H_{11}N_2O_2$	131.0821	C_9H_9O	133.0653	$C_6H_8N_4$	136.0750
129		$C_5H_{13}N_3O$	131.1060	$C_9H_{11}N$	133.0892	$C_7H_4O_3$	136.0160
$C_3H_3N_3O_3$	129.0175	$C_5H_{15}N_4$	131.1298	$C_{10}H_{13}$	133.1018	$C_7H_6NO_2$	136.0399
$C_3H_5N_4O_2$	129.0413	$C_6H_{11}O_3$	131.0708	**134**		$C_7H_8N_2O$	136.0637
$C_4H_5N_2O_3$	129.0300	$C_6H_{13}NO_2$	131.0947	$C_3H_6N_2O_4$	134.0328	$C_7H_{10}N_3$	136.0876
$C_4H_7N_3O_2$	129.0539	$C_6H_{15}N_2O$	131.1185	$C_3H_8N_3O_3$	134.0566	$C_8H_8O_2$	136.0524
$C_4H_9N_4O$	129.0777	$C_6H_{17}N_3$	131.1424	$C_3H_{10}N_4O_2$	134.0805	$C_8H_{10}NO$	136.0763
$C_5H_5O_4$	129.0187	$C_7H_5N_3$	131.0484	$C_4H_8NO_4$	134.0453	$C_8H_{12}N_2$	136.1001
$C_5H_7NO_3$	129.0426	$C_7H_{15}O_2$	131.1072	$C_4H_{10}N_2O_3$	134.0692	$C_9H_{12}O$	136.0888
$C_5H_9N_2O_2$	129.0664	$C_7H_{17}NO$	131.1311	$C_4H_{12}N_3O_2$	134.0930	$C_9H_{14}N$	136.1127
$C_5H_{11}N_3O$	129.0903	$C_8H_7N_2$	131.0610	$C_4H_{14}N_4O$	134.1169	$C_{10}H_{16}$	136.1253
$C_5H_{13}N_4$	129.1142	C_9H_7O	131.0497	$C_5H_{10}O_4$	134.0579	**137**	
$C_6H_9O_3$	129.0552	C_9H_9N	131.0736	$C_5H_{12}NO_3$	134.0817	$C_3H_9N_2O_4$	137.0563
$C_6H_{11}NO_2$	129.0790	$C_{10}H_{11}$	131.0861	$C_5H_{14}N_2O_2$	134.1056	$C_3H_{11}N_3O_3$	137.0801
$C_6H_{13}N_2O$	129.1029	**132**		$C_6H_4N_3O$	134.0355	$C_4H_{11}NO_4$	137.0688
$C_6H_{15}N_3$	129.1267	$C_3H_4N_2O_4$	132.0171	$C_6H_6N_4$	134.0594	$C_5H_3N_3O_2$	137.0226
$C_7H_{13}O_2$	129.0916	$C_3H_6N_3O_3$	132.0410	$C_6H_{14}O_3$	134.0943	$C_5H_5N_4O$	137.0464
$C_7H_{15}NO$	129.1154	$C_3H_8N_4O_2$	132.0648	$C_7H_6N_2O$	134.0480	$C_6H_5N_2O_2$	137.0351
$C_7H_{17}N_2$	129.1393	$C_4H_6NO_4$	132.0297	$C_7H_8N_3$	134.0719	$C_6H_7N_3O$	137.0590
$C_8H_{17}O$	129.1280	$C_4H_8N_2O_3$	132.0535	$C_8H_6O_2$	134.0368	$C_6H_9N_4$	137.0829

APPENDIX A (*Continued*)

	FM		FM		FM		FM
$C_7H_5O_3$	137.0238	$C_6H_8N_2O_2$	140.0586	$C_8H_{16}NO$	142.1233	$C_9H_8N_2$	144.0688
$C_7H_7NO_2$	137.0477	$C_6H_{10}N_3O$	140.0825	$C_8H_{18}N_2$	142.1471	$C_9H_{20}O$	144.1515
$C_7H_9N_2O$	137.0715	$C_6H_{12}N_4$	140.1063	$C_9H_6N_2$	142.0532	$C_{10}H_8O$	144.0575
$C_7H_{11}N_3$	137.0954	$C_7H_8O_3$	140.0473	$C_9H_{18}O$	142.1358	$C_{10}H_{10}N$	144.0814
$C_8H_9O_2$	137.0603	$C_7H_{10}NO_2$	140.0712	$C_9H_{20}N$	142.1597	$C_{11}H_{12}$	144.0939
$C_8H_{11}NO$	137.0841	$C_7H_{12}N_2O$	140.0950	$C_{10}H_8N$	142.0657	**145**	
$C_8H_{13}N_2$	137.1080	$C_7H_{14}N_3$	140.1189	$C_{10}H_{22}$	142.1722	$C_4H_5N_2O_4$	145.0249
$C_9H_{13}O$	137.0967	$C_8H_{12}O_2$	140.0837	$C_{11}H_{10}$	142.0783	$C_4H_7N_3O_3$	145.0488
$C_9H_{15}N$	137.1205	$C_8H_{14}NO$	140.1076	**143**		$C_4H_9N_4O_2$	145.0726
$C_{10}H_{17}$	137.1331	$C_8H_{16}N_2$	140.1315	$C_4H_3N_2O_4$	143.0093	$C_5H_7NO_4$	145.0375
138		$C_9H_{16}O$	140.1202	$C_4H_5N_3O_3$	143.0331	$C_5H_9N_2O_3$	145.0614
$C_3H_{10}N_2O_4$	138.0641	$C_9H_{18}N$	140.1440	$C_4H_7N_4O_2$	143.0570	$C_5H_{11}N_3O_2$	145.0852
$C_5H_4N_3O_2$	138.0304	$C_{10}H_6N$	140.0501	$C_5H_5NO_4$	143.0218	$C_5H_{13}N_4O$	145.1091
$C_5H_6N_4O$	138.0542	$C_{10}H_{20}$	140.1566	$C_5H_7N_2O_3$	143.0457	$C_6H_5N_4$	145.0501
$C_6H_4NO_3$	138.0191	$C_{11}H_8$	140.0626	$C_5H_9N_3O_2$	143.0695	$C_6H_{11}NO_3$	145.0739
$C_6H_6N_2O_2$	138.0429	**141**		$C_5H_{11}N_4O$	143.0934	$C_6H_{13}N_2O_2$	145.0978
$C_6H_8N_3O$	138.0668	$C_4H_3N_3O_3$	141.0175	$C_6H_7O_4$	143.0344	$C_6H_{15}N_3O$	145.1216
$C_6H_{10}N_4$	138.0907	$C_4H_5N_4O_2$	141.0413	$C_6H_9NO_3$	143.0583	$C_6H_{17}N_4$	145.1455
$C_7H_6O_3$	138.0317	$C_5H_3NO_4$	141.0062	$C_6H_{11}N_2O_2$	143.0821	$C_7H_5N_4$	145.0515
$C_7H_8NO_2$	138.0555	$C_5H_5N_2O_3$	141.0300	$C_6H_{13}N_3O$	143.1060	$C_7H_{13}O_3$	145.0865
$C_7H_{10}N_2O$	138.0794	$C_5H_7N_3O_2$	141.0539	$C_6H_{15}N_4$	143.1298	$C_7H_{15}NO_2$	145.1103
$C_7H_{12}N_3$	138.1032	$C_5H_9N_4O$	141.0777	$C_7H_{11}O_3$	143.0708	$C_7H_{17}N_2O$	145.1342
$C_8H_{10}O_2$	138.0681	$C_6H_5O_4$	141.0187	$C_7H_{13}NO_2$	143.0947	$C_7H_{19}N_3$	145.1580
$C_8H_{12}NO$	138.0919	$C_6H_7NO_3$	141.0426	$C_7H_{15}N_2O$	143.1185	$C_8H_5N_2O$	145.0402
$C_8H_{14}N_2$	138.1158	$C_6H_9N_2O_2$	141.0664	$C_7H_{17}N_3$	143.1424	$C_8H_7N_3$	145.0641
$C_9H_{14}O$	138.1045	$C_6H_{11}N_3O$	141.0903	$C_8H_{15}O_2$	143.1072	$C_8H_{17}O_2$	145.1229
$C_9H_{16}N$	138.1284	$C_6H_{13}N_4$	141.1142	$C_8H_{17}NO$	143.1311	$C_8H_{19}NO$	145.1467
$C_{10}H_{18}$	138.1409	$C_7H_9O_3$	141.0552	$C_8H_{19}N_2$	143.1549	C_9H_7NO	145.0528
139		$C_7H_{11}NO_2$	141.0790	$C_9H_7N_2$	143.0610	$C_9H_9N_2$	145.0767
$C_4H_3N_4O_2$	139.0257	$C_7H_{13}N_2O$	141.1029	$C_9H_{19}O$	143.1436	$C_{10}H_9O$	145.0653
$C_5H_3N_2O_3$	139.0144	$C_7H_{15}N_3$	141.1267	$C_9H_{21}N$	143.1675	$C_{10}H_{11}N$	145.0892
$C_5H_5N_3O_2$	139.0382	$C_8H_{13}O_2$	141.0916	$C_{10}H_7O$	143.0497	$C_{11}H_{13}$	145.1018
$C_5H_7N_4O$	139.0621	$C_8H_{15}NO$	141.1154	$C_{10}H_9N$	143.0736	**146**	
$C_6H_5NO_3$	139.0269	$C_8H_{17}N_2$	141.1393	$C_{11}H_{11}$	143.0861	$C_4H_6N_2O_4$	146.0328
$C_6H_7N_2O_2$	139.0508	$C_9H_{17}O$	141.1280	**144**		$C_4H_8N_3O_3$	146.0566
$C_6H_9N_3O$	139.0747	$C_9H_{19}N$	141.1519	$C_4H_4N_2O_4$	144.0171	$C_4H_{10}N_4O_2$	146.0805
$C_6H_{11}N_4$	139.0985	$C_{10}H_7N$	141.0579	$C_4H_6N_3O_3$	144.0410	$C_5H_8NO_4$	146.0453
$C_7H_7O_3$	139.0395	$C_{10}H_{21}$	141.1644	$C_4H_8N_4O_2$	144.0648	$C_5H_{10}N_2O_3$	146.0692
$C_7H_9NO_2$	139.0634	$C_{11}H_9$	141.0705	$C_5H_6NO_4$	144.0297	$C_5H_{12}N_3O_2$	146.0930
$C_7H_{11}N_2O$	139.0872	**142**		$C_5H_8N_2O_3$	144.0535	$C_5H_{14}N_4O$	146.1169
$C_7H_{13}N_3$	139.1111	$C_4H_4N_3O_3$	142.0253	$C_5H_{10}N_3O_2$	144.0774	$C_6H_{10}O_4$	146.0579
$C_8H_{11}O_2$	139.0759	$C_4H_6N_4O_2$	142.0491	$C_5H_{12}N_4O$	144.1012	$C_6H_{12}NO_3$	146.0817
$C_8H_{13}NO$	139.0998	$C_5H_4NO_4$	142.0140	$C_6H_8O_4$	144.0422	$C_6H_{14}N_2O_2$	146.1056
$C_8H_{15}N_2$	139.1236	$C_5H_6N_2O_3$	142.0379	$C_6H_{10}NO_3$	144.0661	$C_6H_{16}N_3O$	146.1295
$C_9H_3N_2$	139.0297	$C_5H_8N_3O_2$	142.0617	$C_6H_{12}N_2O_2$	144.0899	$C_7H_6N_4$	146.0594
$C_9H_{15}O$	139.1123	$C_5H_{10}N_4O$	142.0856	$C_6H_{14}N_3O$	144.1138	$C_7H_{14}O_3$	146.0943
$C_9H_{17}N$	139.1362	$C_6H_6O_4$	142.0266	$C_6H_{16}N_4$	144.1377	$C_7H_{16}NO_2$	146.1182
$C_{10}H_{19}$	139.1488	$C_6H_8NO_3$	142.0504	$C_7H_{12}O_3$	144.0786	$C_7H_{18}N_2O$	146.1420
$C_{11}H_7$	139.0548	$C_6H_{10}N_2O_2$	142.0743	$C_7H_{14}NO_2$	144.1025	$C_8H_2O_3$	146.0003
140		$C_6H_{12}N_3O$	142.0981	$C_7H_{16}N_2O$	144.1264	$C_8H_6N_2O$	146.0480
$C_4H_4N_4O_2$	140.0335	$C_6H_{14}N_4$	142.1220	$C_7H_{18}N_3$	144.1502	$C_8H_8N_3$	146.0719
$C_5H_4N_2O_3$	140.0222	$C_7H_{10}O_3$	142.0630	$C_8H_6N_3$	144.0563	$C_8H_{18}O_2$	146.1307
$C_5H_6N_3O_2$	140.0460	$C_7H_{12}NO_2$	142.0868	$C_8H_{16}O_2$	144.1151	$C_9H_6O_2$	146.0368
$C_5H_8N_4O$	140.0699	$C_7H_{14}N_2O$	142.1107	$C_8H_{18}NO$	144.1389	C_9H_8NO	146.0606
$C_6H_4O_4$	140.0109	$C_7H_{16}N_3$	142.1346	$C_8H_{20}N_2$	144.1628	$C_9H_{10}N_2$	146.0845
$C_6H_6NO_3$	140.0348	$C_8H_{14}O_2$	142.0994	C_9H_6NO	144.0449	$C_{10}H_{10}O$	146.0732

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{10}H_{12}N$	146.0970	$C_5H_{15}N_3O_2$	149.1165	$C_9H_{13}NO$	151.0998	$C_6H_{10}N_4O$	154.0856
$C_{11}H_{14}$	146.1096	$C_6H_5N_4O$	149.0464	$C_9H_{15}N_2$	151.1236	$C_7H_6O_4$	154.0266
147		$C_6H_{13}O_4$	149.0814	$C_{10}H_{15}O$	151.1123	$C_7H_8NO_3$	154.0504
$C_4H_7N_2O_4$	147.0406	$C_6H_{15}NO_3$	149.1052	$C_{10}H_{17}N$	151.1362	$C_7H_{10}N_2O_2$	154.0743
$C_4H_9N_3O_3$	147.0644	$C_7H_5N_2O_2$	149.0351	$C_{11}H_{19}$	151.1488	$C_7H_{12}N_3O$	154.0981
$C_4H_{11}N_4O_2$	147.0883	$C_7H_7N_3O$	149.0590	**152**		$C_7H_{14}N_4$	154.1220
$C_5H_9NO_4$	147.0532	$C_7H_9N_4$	149.0829	$C_4H_{12}N_2O_4$	152.0797	$C_8H_{10}O_3$	154.0630
$C_5H_{11}N_2O_3$	147.0770	$C_8H_5O_3$	149.0238	$C_5H_4N_4O_2$	152.0335	$C_8H_{12}NO_2$	154.0868
$C_5H_{13}N_3O_2$	147.1009	$C_8H_7NO_2$	149.0477	$C_6H_4N_2O_3$	152.0222	$C_8H_{14}N_2O$	154.1107
$C_5H_{15}N_4O$	147.1247	$C_8H_9N_2O$	149.0715	$C_6H_6N_3O_2$	152.0460	$C_8H_{16}N_3$	154.1346
$C_6H_{11}O_4$	147.0657	$C_8H_{11}N_3$	149.0954	$C_6H_8N_4O$	152.0699	$C_9H_{14}O_2$	154.0994
$C_6H_{13}NO_3$	147.0896	$C_9H_9O_2$	149.0603	$C_7H_6NO_3$	152.0348	$C_9H_{16}NO$	154.1233
$C_6H_{15}N_2O_2$	147.1134	$C_9H_{11}NO$	149.0841	$C_7H_8N_2O_2$	152.0586	$C_9H_{18}N_2$	154.1471
$C_6H_{17}N_3O$	147.1373	$C_9H_{13}N_2$	149.1080	$C_7H_{10}N_3O$	152.0825	$C_{10}H_{18}O$	154.1358
$C_7H_5N_3O$	147.0433	$C_{10}H_{13}O$	149.0967	$C_7H_{12}N_4$	152.1063	$C_{10}H_{20}N$	154.1597
$C_7H_7N_4$	147.0672	$C_{10}H_{15}N$	149.1205	$C_8H_8O_3$	152.0473	$C_{11}H_8N$	154.0657
$C_7H_{15}O_3$	147.1021	$C_{11}H_{17}$	149.1331	$C_8H_{10}NO_2$	152.0712	$C_{11}H_{22}$	154.1722
$C_7H_{17}NO_2$	147.1260	**150**		$C_8H_{12}N_2O$	152.0950	$C_{12}H_{10}$	154.0783
$C_8H_5NO_2$	147.0320	$C_4H_{10}N_2O_4$	150.0641	$C_8H_{14}N_3$	152.1189	**155**	
$C_8H_7N_2O$	147.0559	$C_4H_{12}N_3O_3$	150.0879	$C_9H_{12}O_2$	152.0837	$C_5H_3N_2O_4$	155.0093
$C_8H_9N_3$	147.0798	$C_4H_{14}N_4O_2$	150.1118	$C_9H_{14}NO$	152.1076	$C_5H_5N_3O_3$	155.0331
$C_9H_7O_2$	147.0446	$C_5H_{12}NO_4$	150.0766	$C_9H_{16}N_2$	152.1315	$C_5H_7N_4O_2$	155.0570
C_9H_9NO	147.0684	$C_5H_{14}N_2O_3$	150.1005	$C_{10}H_{16}O$	152.1202	$C_6H_5NO_4$	155.0218
$C_9H_{11}N_2$	147.0923	$C_6H_4N_3O_2$	150.0304	$C_{10}H_{18}N$	152.1440	$C_6H_7N_2O_3$	155.0457
$C_{10}H_{11}O$	147.0810	$C_6H_6N_4O$	150.0542	$C_{11}H_6N$	152.0501	$C_6H_9N_3O_2$	155.0695
$C_{10}H_{13}N$	147.1049	$C_6H_{14}O_4$	150.0892	$C_{11}H_{20}$	152.1566	$C_6H_{11}N_4O$	155.0934
$C_{11}H_{15}$	147.1174	$C_7H_6N_2O_2$	150.0429	$C_{12}H_8$	152.0626	$C_7H_7O_4$	155.0344
148		$C_7H_8N_3O$	150.0668	**153**		$C_7H_9NO_3$	155.0583
$C_4H_8N_2O_4$	148.0484	$C_7H_{10}N_4$	150.0907	$C_5H_3N_3O_3$	153.0175	$C_7H_{11}N_2O_2$	155.0821
$C_4H_{10}N_3O_3$	148.0723	$C_8H_6O_3$	150.0317	$C_5H_5N_4O_2$	153.0413	$C_7H_{13}N_3O$	155.1060
$C_4H_{12}N_4O_2$	148.0961	$C_8H_8NO_2$	150.0555	$C_6H_5N_2O_3$	153.0300	$C_8H_{11}O_3$	155.0708
$C_5H_{10}NO_4$	148.0610	$C_8H_{10}N_2O$	150.0794	$C_6H_7N_3O_2$	153.0539	$C_8H_{13}NO_2$	155.0947
$C_5H_{12}N_2O_3$	148.0849	$C_8H_{12}N_3$	150.1032	$C_6H_9N_4O$	153.0777	$C_8H_{15}N_2O$	155.1185
$C_5H_{16}N_4O$	148.1325	$C_9H_{10}O_2$	150.0681	$C_7H_5O_4$	153.0187	$C_8H_{17}N_3$	155.1424
$C_6H_4N_4O$	148.0386	$C_9H_{12}NO$	150.0919	$C_7H_7NO_3$	153.0426	$C_9H_{15}O_2$	155.1072
$C_6H_{12}O_4$	148.0735	$C_9H_{14}N_2$	150.1158	$C_7H_9N_2O_2$	153.0664	$C_9H_{17}NO$	155.1311
$C_6H_{14}NO_3$	148.0974	$C_{10}H_{14}O$	150.1045	$C_7H_{11}N_3O$	153.0903	$C_9H_{19}N_2$	155.1549
$C_6H_{16}N_2O_2$	148.1213	$C_{10}H_{16}N$	150.1284	$C_7H_{13}N_4$	153.1142	$C_{10}H_7N_2$	155.0610
$C_7H_6N_3O$	148.0511	$C_{11}H_{18}$	150.1409	$C_8H_9O_3$	153.0552	$C_{10}H_{19}O$	155.1436
$C_7H_8N_4$	148.0750	**151**		$C_8H_{11}NO_2$	153.0790	$C_{10}H_{21}N$	155.1675
$C_7H_{16}O_3$	148.1100	$C_4H_{11}N_2O_4$	151.0719	$C_8H_{13}N_2O$	153.1029	$C_{11}H_7O$	155.0497
$C_8H_6NO_2$	148.0399	$C_4H_{13}N_3O_3$	151.0958	$C_8H_{15}N_3$	153.1267	$C_{11}H_9N$	155.0736
$C_8H_8N_2O$	148.0637	$C_5H_3N_4O_2$	151.0257	$C_9H_{13}O_2$	153.0916	$C_{11}H_{23}$	155.1801
$C_8H_{10}N_3$	148.0876	$C_5H_{13}NO_4$	151.0845	$C_9H_{15}NO$	153.1154	$C_{12}H_{11}$	155.0861
$C_9H_8O_2$	148.0524	$C_6H_3N_2O_3$	151.0144	$C_9H_{17}N_2$	153.1393	**156**	
$C_9H_{10}NO$	148.0763	$C_6H_5N_3O_2$	151.0382	$C_{10}H_{17}O$	153.1280	$C_5H_4N_2O_4$	156.0171
$C_9H_{12}N_2$	148.1001	$C_6H_7N_4O$	151.0621	$C_{10}H_{19}N$	153.1519	$C_5H_6N_3O_3$	156.0410
$C_{10}H_{12}O$	148.0888	$C_7H_5NO_3$	151.0269	$C_{11}H_7N$	153.0579	$C_5H_8N_4O_2$	156.0648
$C_{10}H_{14}N$	148.1127	$C_7H_7N_2O_2$	151.0508	$C_{11}H_{21}$	153.1644	$C_6H_6NO_4$	156.0297
$C_{11}H_{16}$	148.1253	$C_7H_9N_3O$	151.0746	$C_{12}H_9$	153.0705	$C_6H_8N_2O_3$	156.0535
149		$C_7H_{11}N_4$	151.0985	**154**		$C_6H_{10}N_3O_2$	156.0774
$C_4H_9N_2O_4$	149.0563	$C_8H_7O_3$	151.0395	$C_5H_4N_3O_3$	154.0253	$C_6H_{12}N_4O$	156.1012
$C_4H_{11}N_3O_3$	149.0801	$C_8H_9NO_2$	151.0634	$C_5H_6N_4O_2$	154.0491	$C_7H_8O_4$	156.0422
$C_4H_{13}N_4O_2$	149.1040	$C_8H_{11}N_2O$	151.0872	$C_6H_4NO_4$	154.0140	$C_7H_{10}NO_3$	156.0661
$C_5H_{11}NO_4$	149.0688	$C_8H_{13}N_3$	151.1111	$C_6H_6N_2O_3$	154.0379	$C_7H_{12}N_2O_2$	156.0899
$C_5H_{13}N_2O_3$	149.0927	$C_9H_{11}O_2$	151.0759	$C_6H_8N_3O_2$	154.0617	$C_7H_{14}N_3O$	156.1138

APPENDIX A (*Continued*)

	FM		FM		FM		FM
$C_7H_{16}N_4$	156.1377	$C_7H_{14}N_2O_2$	158.1056	$C_7H_{14}NO_3$	160.0974	$C_8H_{10}N_4$	162.0907
$C_8H_{12}O_3$	156.0786	$C_7H_{16}N_3O$	158.1295	$C_7H_{16}N_2O_2$	160.1213	$C_8H_{18}O_3$	162.1256
$C_8H_{14}NO_2$	156.1025	$C_7H_{18}N_4$	158.1533	$C_7H_{18}N_3O$	160.1451	$C_9H_6O_3$	162.0317
$C_8H_{16}N_2O$	156.1264	$C_8H_6N_4$	158.0594	$C_7H_{20}N_4$	160.1690	$C_9H_8NO_2$	162.0555
$C_8H_{18}N_3$	156.1502	$C_8H_{14}O_3$	158.0943	$C_8H_6N_3O$	160.0511	$C_9H_{10}N_2O$	162.0794
$C_9H_6N_3$	156.0563	$C_8H_{16}NO_2$	158.1182	$C_8H_8N_4$	160.0750	$C_9H_{12}N_3$	162.1032
$C_9H_{16}O_2$	156.1151	$C_8H_{18}N_2O$	158.1420	$C_8H_{16}O_3$	160.1100	$C_{10}H_{10}O_2$	162.0681
$C_9H_{18}NO$	156.1389	$C_8H_{20}N_3$	158.1659	$C_8H_{18}NO_2$	160.1338	$C_{10}H_{12}NO$	162.0919
$C_9H_{20}N_2$	156.1628	$C_9H_6N_2O$	158.0480	$C_8H_{20}N_2O$	160.1577	$C_{10}H_{14}N_2$	162.1158
$C_{10}H_6NO$	156.0449	$C_9H_8N_3$	158.0719	$C_9H_6NO_2$	160.0399	$C_{11}H_{14}O$	162.1045
$C_{10}H_8N_2$	156.0688	$C_9H_{18}O_2$	158.1307	$C_9H_8N_2O$	160.0637	$C_{11}H_{16}N$	162.1284
$C_{10}H_{20}O$	156.1515	$C_9H_{20}NO$	158.1546	$C_9H_{10}N_3$	160.0876	$C_{12}H_{18}$	162.1409
$C_{10}H_{22}N$	156.1753	$C_{10}H_6O_2$	158.0368	$C_9H_{20}O_2$	160.1464	**163**	
$C_{11}H_8O$	156.0575	$C_{10}H_8NO$	158.0606	$C_{10}H_8O_2$	160.0524	$C_5H_{11}N_2O_4$	163.0719
$C_{11}H_{10}N$	156.0814	$C_{10}H_{10}N_2$	158.0845	$C_{10}H_{10}NO$	160.0763	$C_5H_{13}N_3O_3$	163.0958
$C_{11}H_{24}$	156.1879	$C_{10}H_{22}O$	158.1672	$C_{10}H_{12}N_2$	160.1001	$C_5H_{15}N_4O_2$	163.1196
$C_{12}H_{12}$	156.0939	$C_{11}H_{10}O$	158.0732	$C_{11}H_{12}O$	160.0888	$C_6H_{13}NO_4$	163.0845
157		$C_{11}H_{12}N$	158.0970	$C_{11}H_{14}N$	160.1127	$C_6H_{15}N_2O_3$	163.1083
$C_5H_5N_2O_4$	157.0249	$C_{12}H_{14}$	158.1096	$C_{12}H_{16}$	160.1253	$C_6H_{17}N_3O_2$	163.1322
$C_5H_7N_3O_3$	157.0488	**159**		**161**		$C_7H_5N_3O_2$	163.0382
$C_5H_9N_4O_2$	157.0726	$C_5H_7N_2O_4$	159.0406	$C_5H_9N_2O_4$	161.0563	$C_7H_7N_4O$	163.0621
$C_6H_7NO_4$	157.0375	$C_5H_9N_3O_3$	159.0644	$C_5H_{11}N_3O_3$	161.0801	$C_7H_{15}O_4$	163.0970
$C_6H_9N_2O_3$	157.0614	$C_5H_{11}N_4O_2$	159.0883	$C_5H_{13}N_4O_2$	161.1040	$C_7H_{17}NO_3$	163.1209
$C_6H_{11}N_3O_2$	157.0852	$C_6H_9NO_4$	159.0532	$C_6H_{11}NO_4$	161.0688	$C_8H_5NO_3$	163.0269
$C_6H_{13}N_4O$	157.1091	$C_6H_{11}N_2O_3$	159.0770	$C_6H_{13}N_2O_3$	161.0927	$C_8H_7N_2O_2$	163.0508
$C_7H_9O_4$	157.0501	$C_6H_{13}N_3O_2$	159.1009	$C_6H_{15}N_3O_2$	161.1165	$C_8H_9N_3O$	163.0746
$C_7H_{11}NO_3$	157.0739	$C_6H_{15}N_4O$	159.1247	$C_6H_{17}N_4O$	161.1404	$C_8H_{11}N_4$	163.0985
$C_7H_{13}N_2O_2$	157.0978	$C_7H_{11}O_4$	159.0657	$C_7H_5N_4O$	161.0464	$C_9H_7O_3$	163.0395
$C_7H_{15}N_3O$	157.1216	$C_7H_{13}NO_3$	159.0896	$C_8H_5N_2O_2$	161.0351	$C_9H_9NO_2$	163.0634
$C_7H_{17}N_4$	157.1455	$C_7H_{15}N_2O_2$	159.1134	$C_8H_7N_3O$	161.0590	$C_9H_{11}N_2O$	163.0872
$C_8H_5N_4$	157.0515	$C_7H_{17}N_3O$	159.1373	$C_8H_9N_4$	161.0829	$C_9H_{13}N_3$	163.1111
$C_8H_{13}O_3$	157.0865	$C_8H_5N_3O$	159.0433	$C_8H_{17}O_3$	161.1178	$C_{10}H_{11}O_2$	163.0759
$C_8H_{15}NO_2$	157.1103	$C_8H_7N_4$	159.0672	$C_8H_{19}NO_2$	161.1416	$C_{10}H_{13}NO$	163.0998
$C_8H_{17}N_2O$	157.1342	$C_8H_{15}O_3$	159.1021	$C_9H_5O_3$	161.0238	$C_{10}H_{15}N_2$	163.1236
$C_8H_{19}N_3$	157.1580	$C_8H_{17}NO_2$	159.1260	$C_9H_7NO_2$	161.0477	$C_{11}H_{15}O$	163.1123
$C_9H_5N_2O$	157.0402	$C_8H_{19}N_2O$	159.1498	$C_9H_9N_2O$	161.0715	$C_{11}H_{17}N$	163.1362
$C_9H_7N_3$	157.0641	$C_8H_{21}N_3$	159.1737	$C_9H_{11}N_3$	161.0954	$C_{12}H_{19}$	163.1488
$C_9H_{17}O_2$	157.1229	$C_9H_5NO_2$	159.0320	$C_{10}H_9O_2$	161.0603	**164**	
$C_9H_{19}NO$	157.1467	$C_9H_7N_2O$	159.0559	$C_{10}H_{11}NO$	161.0841	$C_5H_{12}N_2O_4$	164.0797
$C_9H_{21}N_2$	157.1706	$C_9H_9N_3$	159.0798	$C_{10}H_{13}N_2$	161.1080	$C_5H_{14}N_3O_3$	164.1036
$C_{10}H_7NO$	157.0528	$C_9H_{19}O_2$	159.1385	$C_{11}H_{13}O$	161.0967	$C_5H_{16}N_4O_2$	164.1275
$C_{10}H_9N_2$	157.0767	$C_9H_{21}NO$	159.1624	$C_{11}H_{15}N$	161.1205	$C_6H_4N_4O_2$	164.0335
$C_{10}H_{21}O$	157.1593	$C_{10}H_7O_2$	159.0446	$C_{12}H_{17}$	161.1331	$C_6H_{14}NO_4$	164.0923
$C_{10}H_{23}N$	157.1832	$C_{10}H_9NO$	159.0684	**162**		$C_6H_{16}N_2O_3$	164.1162
$C_{11}H_9O$	157.0653	$C_{10}H_{11}N_2$	159.0923	$C_5H_{10}N_2O_4$	162.0641	$C_7H_6N_3O_2$	164.0460
$C_{11}H_{11}N$	157.0892	$C_{11}H_{11}O$	159.0810	$C_5H_{12}N_3O_3$	162.0879	$C_7H_8N_4O$	164.0699
$C_{12}H_{13}$	157.1018	$C_{11}H_{13}N$	159.1049	$C_5H_{14}N_4O_2$	162.1118	$C_7H_{16}O_4$	164.1049
158		$C_{12}H_{15}$	159.1174	$C_6H_{12}NO_4$	162.0766	$C_8H_6NO_3$	164.0348
$C_5H_6N_2O_4$	158.0328	**160**		$C_6H_{14}N_2O_3$	162.1005	$C_8H_8N_2O_2$	164.0586
$C_5H_8N_3O_3$	158.0566	$C_5H_8N_2O_4$	160.0484	$C_6H_{16}N_3O_2$	162.1244	$C_8H_{10}N_3O$	164.0825
$C_5H_{10}N_4O_2$	158.0805	$C_5H_{10}N_3O_3$	160.0723	$C_6H_{18}N_4O$	162.1482	$C_8H_{12}N_4$	164.1063
$C_6H_8NO_4$	158.0453	$C_5H_{12}N_4O_2$	160.0961	$C_7H_6N_4O$	162.0542	$C_9H_8O_3$	164.0473
$C_6H_{10}N_2O_3$	158.0692	$C_6H_{10}NO_4$	160.0610	$C_7H_{14}O_4$	162.0892	$C_9H_{10}NO_2$	164.0712
$C_6H_{12}N_3O_2$	158.0930	$C_6H_{12}N_2O_3$	160.0848	$C_7H_{16}NO_3$	162.1131	$C_9H_{12}N_2O$	164.0950
$C_6H_{14}N_4O$	158.1169	$C_6H_{14}N_3O_2$	160.1087	$C_7H_{18}N_2O_2$	162.1369	$C_9H_{14}N_3$	164.1189
$C_7H_{10}O_4$	158.0579	$C_6H_{16}N_4O$	160.1325	$C_8H_6N_2O_2$	162.0429	$C_{10}H_{12}O_2$	164.0837
$C_7H_{12}NO_3$	158.0817	$C_7H_{12}O_4$	160.0735	$C_8H_8N_3O$	162.0668	$C_{10}H_{14}NO$	164.1076

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{10}H_{16}N_2$	164.1315	$C_7H_7N_2O_3$	167.0457	$C_8H_{11}NO_3$	169.0739	$C_7H_{13}N_3O_2$	171.1009
$C_{11}H_{16}O$	164.1202	$C_7H_9N_3O_2$	167.0695	$C_8H_{13}N_2O_2$	169.0978	$C_7H_{15}N_4O$	171.1247
$C_{11}H_{18}N$	164.1440	$C_7H_{11}N_4O$	167.0934	$C_8H_{15}N_3O$	169.1216	$C_8H_{11}O_4$	171.0657
$C_{12}H_{20}$	164.1566	$C_8H_7O_4$	167.0344	$C_8H_{17}N_4$	169.1455	$C_8H_{13}NO_3$	171.0896
165		$C_8H_9NO_3$	167.0583	$C_9H_{13}O_3$	169.0865	$C_8H_{15}N_2O_2$	171.1134
$C_5H_{13}N_2O_4$	165.0876	$C_8H_{11}N_2O_2$	167.0821	$C_9H_{15}NO_2$	169.1103	$C_8H_{17}N_3O$	171.1373
$C_5H_{15}N_3O_3$	165.1114	$C_8H_{13}N_3O$	167.1060	$C_9H_{17}N_2O$	169.1342	$C_8H_{19}N_4$	171.1611
$C_6H_5N_4O_2$	165.0413	$C_8H_{15}N_4$	167.1298	$C_9H_{19}N_3$	169.1580	$C_9H_5N_3O$	171.0433
$C_6H_{15}NO_4$	165.1001	$C_9H_{11}O_3$	167.0708	$C_{10}H_7N_3$	169.0641	$C_9H_7N_4$	171.0672
$C_7H_5N_2O_3$	165.0300	$C_9H_{13}NO_2$	167.0947	$C_{10}H_{17}O_2$	169.1229	$C_9H_{15}O_3$	171.1021
$C_7H_7N_3O_2$	165.0539	$C_9H_{15}N_2O$	167.1185	$C_{10}H_{19}NO$	169.1467	$C_9H_{17}NO_2$	171.1260
$C_7H_9N_4O$	165.0777	$C_9H_{17}N_3$	167.1424	$C_{10}H_{21}N_2$	169.1706	$C_9H_{19}N_2O$	171.1498
$C_8H_5O_4$	165.0187	$C_{10}H_{15}O_2$	167.1072	$C_{11}H_7NO$	169.0528	$C_9H_{21}N_3$	171.1737
$C_8H_7NO_3$	165.0426	$C_{10}H_{17}NO$	167.1311	$C_{11}H_9N_2$	169.0767	$C_{10}H_7N_2O$	171.0559
$C_8H_9N_2O_2$	165.0664	$C_{10}H_{19}N_2$	167.1549	$C_{11}H_{21}O$	169.1593	$C_{10}H_9N_3$	171.0798
$C_8H_{11}N_3O$	165.0903	$C_{11}H_7N_2$	167.0610	$C_{11}H_{23}N$	169.1832	$C_{10}H_{19}O_2$	171.1385
$C_8H_{13}N_4$	165.1142	$C_{11}H_{19}O$	167.1436	$C_{12}H_9O$	169.0653	$C_{10}H_{21}NO$	171.1624
$C_9H_9O_3$	165.0552	$C_{11}H_{21}N$	167.1675	$C_{12}H_{11}N$	169.0892	$C_{10}H_{23}N_2$	171.1863
$C_9H_{11}NO_2$	165.0790	$C_{12}H_9N$	167.0736	$C_{12}H_{25}$	169.1957	$C_{11}H_7O_2$	171.0446
$C_9H_{13}N_2O$	165.1029	$C_{12}H_{23}$	167.1801	$C_{13}H_{13}$	169.1018	$C_{11}H_9NO$	171.0684
$C_9H_{15}N_3$	165.1267	$C_{13}H_{11}$	167.0861	**170**		$C_{11}H_{11}N_2$	171.0923
$C_{10}H_{13}O_2$	165.0916	**168**		$C_6H_6N_2O_4$	170.0328	$C_{11}H_{23}O$	171.1750
$C_{10}H_{15}NO$	165.1154	$C_6H_4N_2O_4$	168.0171	$C_6H_8N_3O_3$	170.0566	$C_{11}H_{25}N$	171.1988
$C_{10}H_{17}N_2$	165.1393	$C_6H_6N_3O_3$	168.0410	$C_6H_{10}N_4O_2$	170.0805	$C_{12}H_{11}O$	171.0810
$C_{11}H_{17}O$	165.1280	$C_6H_8N_4O_2$	168.0648	$C_7H_8NO_4$	170.0453	$C_{12}H_{13}N$	171.1049
$C_{11}H_{19}N$	165.1519	$C_7H_6NO_4$	168.0297	$C_7H_{10}N_2O_3$	170.0692	$C_{13}H_{15}$	171.1174
$C_{12}H_7N$	165.0579	$C_7H_8N_2O_3$	168.0535	$C_7H_{12}N_3O_2$	170.0930	**172**	
$C_{12}H_{21}$	165.1644	$C_7H_{10}N_3O_2$	168.0774	$C_7H_{14}N_4O$	170.1169	$C_6H_8N_2O_4$	172.0484
$C_{13}H_9$	165.0705	$C_7H_{12}N_4O$	168.1012	$C_8H_{10}O_4$	170.0579	$C_6H_{10}N_3O_3$	172.0723
166		$C_8H_8O_4$	168.0422	$C_8H_{12}NO_3$	170.0817	$C_6H_{12}N_4O_2$	172.0961
$C_5H_{14}N_2O_4$	166.0954	$C_8H_{10}NO_3$	168.0661	$C_8H_{14}N_2O_2$	170.1056	$C_7H_{10}NO_4$	172.0610
$C_6H_4N_3O_3$	166.0253	$C_8H_{12}N_2O_2$	168.0899	$C_8H_{16}N_3O$	170.1295	$C_7H_{12}H_{12}N_2O_3$	172.0848
$C_6H_6N_4O_2$	166.0491	$C_8H_{14}N_3O$	168.1138	$C_8H_{18}N_4$	170.1533	$C_7H_{14}N_3O_2$	172.1087
$C_7H_6N_2O_3$	166.0379	$C_8H_{16}N_4$	168.1377	$C_9H_6N_4$	170.0594	$C_7H_{16}N_4O$	172.1325
$C_7H_8N_3O_2$	166.0617	$C_9H_{12}O_3$	168.0786	$C_9H_{14}O_3$	170.0943	$C_8H_{12}O_4$	172.0735
$C_7H_{10}N_4O$	166.0856	$C_9H_{14}NO_2$	168.1025	$C_9H_{16}NO_2$	170.1182	$C_8H_{14}NO_3$	172.0974
$C_8H_6O_4$	166.0266	$C_9H_{16}N_2O$	168.1264	$C_9H_{18}N_2O$	170.1420	$C_8H_{16}N_2O_2$	172.1213
$C_8H_8NO_3$	166.0504	$C_9H_{18}N_3$	168.1502	$C_9H_{20}N_3$	170.1659	$C_8H_{18}N_3O$	172.1451
$C_8H_{10}N_2O_2$	166.0743	$C_{10}H_{16}O_2$	168.1151	$C_{10}H_6N_2O$	170.0480	$C_8H_{20}N_4$	172.1690
$C_8H_{12}N_3O$	166.0981	$C_{10}H_{18}NO$	168.1389	$C_{10}H_8N_3$	170.0719	$C_9H_6N_3O$	172.0511
$C_8H_{14}N_4$	166.1220	$C_{10}H_{20}N_2$	168.1628	$C_{10}H_{18}O_2$	170.1307	$C_9H_8N_4$	172.0750
$C_9H_{10}O_3$	166.0630	$C_{11}H_8N_2$	168.0688	$C_{10}H_{20}NO$	170.1546	$C_9H_{16}O_3$	172.1100
$C_9H_{12}NO_2$	166.0868	$C_{11}H_{20}O$	168.1515	$C_{10}H_{22}N_2$	170.1784	$C_9H_{18}NO_2$	172.1338
$C_9H_{14}N_2O$	166.1107	$C_{11}H_{22}N$	168.1753	$C_{11}H_8NO$	170.0606	$C_9H_{20}N_2O$	172.1577
$C_9H_{16}N_3$	166.1346	$C_{12}H_8O$	168.0575	$C_{11}H_{10}N_2$	170.0845	$C_9H_{22}N_3$	172.1815
$C_{10}H_{14}O_2$	166.0994	$C_{12}H_{10}N$	168.0814	$C_{11}H_{22}O$	170.1671	$C_{10}H_6NO_2$	172.0399
$C_{10}H_{16}NO$	166.1233	$C_{12}H_{24}$	168.1879	$C_{11}H_{24}N$	170.1910	$C_{10}H_8N_2O$	172.0637
$C_{10}H_{18}N_2$	166.1471	$C_{13}H_{12}$	168.0939	$C_{12}H_{10}O$	170.0732	$C_{10}H_{10}N_3$	172.0876
$C_{11}H_{18}O$	166.1358	**169**		$C_{12}H_{12}N$	170.0970	$C_{10}H_{20}O_2$	172.1464
$C_{11}H_{20}N$	166.1597	$C_6H_5N_2O_4$	169.0249	$C_{12}H_{26}$	170.2036	$C_{10}H_{22}NO$	172.1702
$C_{12}H_8N$	166.0657	$C_6H_7N_3O_3$	169.0488	$C_{13}H_{14}$	170.1096	$C_{10}H_{24}N_2$	172.1941
$C_{12}H_{22}$	166.1722	$C_6H_9N_4O_2$	169.0726	**171**		$C_{11}H_8O_2$	172.0524
$C_{13}H_{10}$	166.0783	$C_7H_7NO_4$	169.0375	$C_6H_7N_2O_4$	171.0406	$C_{11}H_{10}NO$	172.0763
167		$C_7H_9N_2O_3$	169.0614	$C_6H_9N_3O_3$	171.0644	$C_{11}H_{12}N_2$	172.1001
$C_6H_5N_3O_3$	167.0331	$C_7H_{11}N_3O_2$	169.0852	$C_6H_{11}N_4O_2$	171.0883	$C_{11}H_{24}O$	172.1828
$C_6H_7N_4O_2$	167.0570	$C_7H_{13}N_4O$	169.1091	$C_7H_9NO_4$	171.0532	$C_{12}H_{12}O$	172.0888
$C_7H_5NO_4$	167.0218	$C_8H_9O_4$	169.0501	$C_7H_{11}N_2O_3$	171.0770	$C_{12}H_{14}N$	172.1127

APPENDIX A (*Continued*)

	FM		FM		FM		FM
$C_{13}H_{16}$	172.1253	$C_{11}H_{12}NO$	174.0919	$C_{11}H_{12}O_2$	176.0837	$C_{12}H_{20}N$	178.1597
173		$C_{11}H_{14}N_2$	174.1158	$C_{11}H_{14}NO$	176.1076	$C_{13}H_8N$	178.0657
$C_6H_9N_2O_4$	173.0563	$C_{12}H_{14}O$	174.1045	$C_{11}H_{16}N_2$	176.1315	$C_{13}H_{22}$	178.1722
$C_6H_{11}N_3O_3$	173.0801	$C_{12}H_{16}N$	174.1284	$C_{12}H_{16}O$	176.1202	$C_{14}H_{10}$	178.0783
$C_6H_{13}N_4O_2$	173.1040	$C_{13}H_{18}$	174.1409	$C_{12}H_{18}N$	176.1440	**179**	
$C_7H_{11}NO_4$	173.0688	**175**		$C_{13}H_{20}$	176.1566	$C_6H_{15}N_2O_4$	179.1032
$C_7H_{13}N_2O_3$	173.0927	$C_6H_{11}N_2O_4$	175.0719	**177**		$C_6H_{17}N_3O_3$	179.1271
$C_7H_{15}N_3O_2$	173.1165	$C_6H_{13}N_3O_3$	175.0958	$C_6H_{13}N_2O_4$	177.0876	$C_7H_5N_3O_3$	179.0331
$C_7H_{17}N_4O$	173.1404	$C_6H_{15}N_4O_2$	175.1196	$C_6H_{15}N_3O_3$	177.1114	$C_7H_7N_4O_2$	179.0570
$C_8H_{13}O_4$	173.0814	$C_7H_{13}NO_4$	175.0845	$C_6H_{17}N_4O_2$	177.1353	$C_7H_{17}NO_4$	179.1158
$C_8H_{15}NO_3$	173.1052	$C_7H_{15}N_2O_3$	175.1083	$C_7H_5N_4O_2$	177.0413	$C_8H_5NO_4$	179.0218
$C_8H_{17}N_2O_2$	173.1291	$C_7H_{17}N_3O_2$	175.1322	$C_7H_{15}NO_4$	177.1001	$C_8H_7N_2O_3$	179.0457
$C_8H_{19}N_3O$	173.1529	$C_7H_{19}N_4O$	175.1560	$C_7H_{17}N_2O_3$	177.1240	$C_8H_9N_3O_2$	179.0695
$C_8H_{21}N_4$	173.1768	$C_8H_7N_4O$	175.0621	$C_7H_{19}N_3O_2$	177.1478	$C_8H_{11}N_4O$	179.0934
$C_9H_7N_3O$	173.0590	$C_8H_{15}O_4$	175.0970	$C_8H_5N_2O_3$	177.0300	$C_9H_7O_4$	179.0344
$C_9H_9N_4$	173.0829	$C_8H_{17}NO_3$	175.1209	$C_8H_7N_3O_2$	177.0539	$C_9H_9NO_3$	179.0583
$C_9H_{17}O_3$	173.1178	$C_8H_{19}N_2O_2$	175.1447	$C_8H_9N_4O$	177.0777	$C_9H_{11}N_2O_2$	179.0821
$C_9H_{19}NO_2$	173.1416	$C_8H_{21}N_3O$	175.1686	$C_8H_{17}O_4$	177.1127	$C_9H_{13}N_3O$	179.1060
$C_9H_{21}N_2O$	173.1655	$C_9H_5NO_3$	175.0269	$C_8H_{19}NO_3$	177.1365	$C_9H_{15}N_4$	179.1298
$C_{10}H_5O_3$	173.0238	$C_9H_7N_2O_2$	175.0508	$C_9H_7NO_3$	177.0426	$C_{10}H_{11}O_3$	179.0708
$C_{10}H_7NO_2$	173.0477	$C_9H_9N_3O$	175.0746	$C_9H_9N_2O_2$	177.0664	$C_{10}H_{13}NO_2$	179.0947
$C_{10}H_9N_2O$	173.0715	$C_9H_{11}N_4$	175.0985	$C_9H_{11}N_3O$	177.0903	$C_{10}H_{15}N_2O$	179.1185
$C_{10}H_{11}N_3$	173.0954	$C_9H_{19}O_3$	175.1334	$C_9H_{13}N_4$	177.1142	$C_{10}H_{17}N_3$	179.1424
$C_{10}H_{21}O_2$	173.1542	$C_9H_{21}NO_2$	175.1573	$C_{10}H_9O_3$	177.0552	$C_{11}H_{15}O_2$	179.1072
$C_{10}H_{23}NO$	173.1781	$C_{10}H_7O_3$	175.0395	$C_{10}H_{11}NO_2$	177.0790	$C_{11}H_{17}NO$	179.1311
$C_{11}H_9O_2$	173.0603	$C_{10}H_9NO_2$	175.0634	$C_{10}H_{13}N_2O$	177.1029	$C_{11}H_{19}N_2$	179.1549
$C_{11}H_{11}NO$	173.0841	$C_{10}H_{11}N_2O$	175.0872	$C_{10}H_{15}N_3$	177.1267	$C_{12}H_{19}O$	179.1436
$C_{11}H_{13}N_2$	173.1080	$C_{10}H_{13}N_3$	175.1111	$C_{11}H_{13}O_2$	177.0916	$C_{12}H_{21}N$	179.1675
$C_{12}H_{13}O$	173.0967	$C_{11}H_{11}O_2$	175.0759	$C_{11}H_{15}NO$	177.1154	$C_{13}H_9N$	179.0736
$C_{12}H_{15}N$	173.1205	$C_{11}H_{13}NO$	175.0998	$C_{11}H_{17}N_2$	177.1393	$C_{13}H_{23}$	179.1801
$C_{13}H_{17}$	173.1331	$C_{11}H_{15}N_2$	175.1236	$C_{12}H_{17}O$	177.1280	$C_{14}H_{11}$	179.0861
174		$C_{12}H_{15}O$	175.1123	$C_{12}H_{19}N$	177.1519	**180**	
$C_6H_{10}N_2O_4$	174.0641	$C_{12}H_{17}N$	175.1362	$C_{13}H_{21}$	177.1644	$C_6H_{16}N_2O_4$	180.1111
$C_6H_{12}N_3O_3$	174.0879	$C_{13}H_3O$	175.0184	**178**		$C_7H_6N_3O_3$	180.0410
$C_6H_{14}N_4O_2$	174.1118	$C_{13}H_{19}$	175.1488	$C_6H_{14}N_2O_4$	178.0954	$C_7H_8N_4O_2$	180.0648
$C_7H_{12}NO_4$	174.0766	**176**		$C_6H_{16}N_3O_3$	178.1193	$C_8H_6NO_4$	180.0297
$C_7H_{14}N_2O_3$	174.1005	$C_6H_{12}N_2O_4$	176.0797	$C_6H_{18}N_4O_2$	178.1431	$C_8H_8N_2O_3$	180.0535
$C_7H_{16}N_3O_2$	174.1244	$C_6H_{14}N_3O_3$	176.1036	$C_7H_6N_4O_2$	178.0491	$C_8H_{10}N_3O_2$	180.0774
$C_7H_{18}N_4O$	174.1482	$C_6H_{16}N_4O_2$	176.1275	$C_7H_{16}NO_4$	178.1080	$C_8H_{12}N_4O$	180.1012
$C_7H_{16}N_4O$	174.1244	$C_7H_{14}NO_4$	176.0923	$C_7H_{18}N_2O_3$	178.1318	$C_9H_8O_4$	180.0422
$C_8H_6N_4O$	174.0542	$C_7H_{16}N_2O_3$	176.1162	$C_8H_6N_2O_3$	178.0379	$C_9H_{10}NO_3$	180.0661
$C_8H_{14}O_4$	174.0892	$C_7H_{18}N_3O_2$	176.1400	$C_8H_8N_3O_2$	178.0617	$C_9H_{12}N_2O_2$	180.0899
$C_8H_{16}NO_3$	174.1131	$C_7H_{20}N_4O$	176.1639	$C_8H_{10}N_4O$	178.0856	$C_9H_{14}N_3O$	180.1138
$C_8H_{18}N_2O_2$	174.1369	$C_8H_6N_3O_2$	176.0460	$C_8H_{18}O_4$	178.1205	$C_9H_{16}N_4$	180.1377
$C_8H_{20}N_3O$	174.1608	$C_8H_8N_4O$	176.0699	$C_9H_6O_4$	178.0266	$C_{10}H_{12}O_3$	180.0786
$C_8H_{22}N_4$	174.1846	$C_8H_{16}O_4$	176.1049	$C_9H_8NO_3$	178.0504	$C_{10}H_{14}NO_2$	180.1025
$C_9H_6N_2O_2$	174.0429	$C_8H_{18}NO_3$	176.1287	$C_9H_{10}N_2O_2$	178.0743	$C_{10}H_{16}N_2O$	180.1264
$C_9H_{10}N_4$	174.0907	$C_8H_{20}N_2O_2$	176.1526	$C_9H_{12}N_3O$	178.0981	$C_{10}H_{18}N_3$	180.1502
$C_9H_{18}O_3$	174.1256	$C_9H_6NO_3$	176.0348	$C_9H_{14}N_4$	178.1220	$C_{11}H_{16}O_2$	180.1151
$C_9H_{20}NO_2$	174.1495	$C_9H_8N_2O_2$	176.0586	$C_{10}H_{10}O_3$	178.0630	$C_{11}H_{18}NO$	180.1389
$C_9H_{22}N_2O$	174.1733	$C_9H_{10}N_3O$	176.0825	$C_{10}H_{12}NO_2$	178.0868	$C_{11}H_{20}N_2$	180.1628
$C_{10}H_6O_3$	174.0317	$C_9H_{12}N_4$	176.1063	$C_{10}H_{14}N_2O$	178.1107	$C_{12}H_8N_2$	180.0688
$C_{10}H_8NO_2$	174.0555	$C_9H_{20}O_3$	176.1413	$C_{10}H_{16}N_3$	178.1346	$C_{12}H_{20}O$	180.1515
$C_{10}H_{10}N_2O$	174.0794	$C_{10}H_8O_3$	176.0473	$C_{11}H_{14}O_2$	178.0994	$C_{12}H_{22}N$	180.1753
$C_{10}H_{12}N_3$	174.1032	$C_{10}H_{10}NO_2$	176.0712	$C_{11}H_{16}NO$	178.1233	$C_{13}H_8O$	180.0575
$C_{10}H_{22}O_2$	174.1620	$C_{10}H_{12}N_2O$	176.0950	$C_{11}H_{18}N_2$	178.1471	$C_{13}H_{10}N$	180.0814
$C_{11}H_{10}O_2$	174.0681	$C_{10}H_{14}N_3$	176.1189	$C_{12}H_{18}O$	178.1358	$C_{13}H_{24}$	180.1879

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{14}H_{12}$	180.0939	$C_{13}H_{12}N$	182.0970	$C_{11}H_{22}NO$	184.1702	$C_{10}H_8N_3O$	186.0668
181		$C_{13}H_{26}$	182.2036	$C_{11}H_{24}N_2$	184.1941	$C_{10}H_{10}N_4$	186.0907
$C_7H_5N_2O_4$	181.0249	$C_{14}H_{14}$	182.1096	$C_{12}H_8O_2$	184.0524	$C_{10}H_{18}O_3$	186.1256
$C_7H_7N_3O_3$	181.0488	**183**		$C_{12}H_{10}NO$	184.0763	$C_{10}H_{20}NO_2$	186.1495
$C_7H_9N_4O_2$	181.0726	$C_7H_7N_2O_4$	183.0406	$C_{12}H_{12}N_2$	184.1001	$C_{10}H_{22}N_2O$	186.1733
$C_8H_7NO_4$	181.0375	$C_7H_9N_3O_3$	183.0644	$C_{12}H_{24}O$	184.1828	$C_{10}H_{24}N_3$	186.1972
$C_8H_9N_2O_3$	181.0614	$C_7H_{11}N_4O_2$	183.0883	$C_{12}H_{26}N$	184.2067	$C_{11}H_8NO_2$	186.0555
$C_8H_{11}N_3O_2$	181.0852	$C_8H_9NO_4$	183.0532	$C_{13}H_{12}O$	184.0888	$C_{11}H_{10}N_2O$	186.0794
$C_8H_{13}N_4O$	181.1091	$C_8H_{11}N_2O_3$	183.0770	$C_{13}H_{14}N$	184.1127	$C_{11}H_{12}N_3$	186.1032
$C_9H_9O_4$	181.0501	$C_8H_{13}N_3O_2$	183.1009	$C_{13}H_{28}$	184.2192	$C_{11}H_{22}O_2$	186.1620
$C_9H_{11}NO_3$	181.0739	$C_8H_{15}N_4O$	183.1247	$C_{14}H_{16}$	184.1253	$C_{11}H_{24}NO$	186.1859
$C_9H_{13}N_2O_2$	181.0978	$C_9H_{11}O_4$	183.0657	**185**		$C_{11}H_{26}N_2$	186.2098
$C_9H_{15}N_3O$	181.1216	$C_9H_{13}NO_3$	183.0896	$C_7H_9N_2O_4$	185.0563	$C_{12}H_{10}O_2$	186.0681
$C_9H_{17}N_4$	181.1455	$C_9H_{15}N_2O_2$	183.1134	$C_7H_{11}N_3O_3$	185.0801	$C_{12}H_{12}NO$	186.0919
$C_{10}H_{13}O_3$	181.0865	$C_9H_{17}N_3O$	183.1373	$C_7H_{13}N_4O_2$	185.1040	$C_{12}H_{14}N_2$	186.1158
$C_{10}H_{15}NO_2$	181.1103	$C_9H_{19}N_4$	183.1611	$C_8H_{11}NO_4$	185.0688	$C_{12}H_{26}O$	186.1985
$C_{10}H_{17}N_2O$	181.1342	$C_{10}H_7N_4$	183.0672	$C_8H_{13}N_2O_3$	185.0927	$C_{13}H_{14}O$	186.1045
$C_{10}H_{19}N_3$	181.1580	$C_{10}H_{15}O_3$	183.1021	$C_8H_{15}N_3O_2$	185.1165	$C_{13}H_{16}N$	186.1284
$C_{11}H_7N_3$	181.0641	$C_{10}H_{17}NO_2$	183.1260	$C_8H_{17}N_4O$	185.1404	$C_{14}H_{18}$	186.1409
$C_{11}H_{17}O_2$	181.1229	$C_{10}H_{19}N_2O$	183.1498	$C_9H_{13}O_4$	185.0814	**187**	
$C_{11}H_{19}NO$	181.1467	$C_{10}H_{21}N_3$	183.1737	$C_9H_{15}NO_3$	185.1052	$C_7H_{11}N_2O_4$	187.0719
$C_{11}H_{21}N_2$	181.1706	$C_{11}H_7N_2O$	183.0559	$C_9H_{17}N_2O_2$	185.1291	$C_7H_{13}N_3O_3$	187.0958
$C_{12}H_7NO$	181.0528	$C_{11}H_9N_3$	183.0798	$C_9H_{19}N_3O$	185.1529	$C_7H_{15}N_4O_2$	187.1196
$C_{12}H_9N_2$	181.0767	$C_{11}H_{19}O_2$	183.1385	$C_9H_{21}N_4$	185.1768	$C_8H_{13}NO_4$	187.0845
$C_{12}H_{21}O$	181.1593	$C_{11}H_{21}NO$	183.1624	$C_{10}H_7N_3O$	185.0590	$C_8H_{15}N_2O_3$	187.1083
$C_{12}H_{23}N$	181.1832	$C_{11}H_{23}N_2$	183.1863	$C_{10}H_9N_4$	185.0829	$C_8H_{17}N_3O_2$	187.1322
$C_{13}H_9O$	181.0653	$C_{12}H_7O_2$	183.0446	$C_{10}H_{17}O_3$	185.1178	$C_8H_{19}N_4O$	187.1560
$C_{13}H_{11}N$	181.0892	$C_{12}H_9NO$	183.0684	$C_{10}H_{19}NO_2$	185.1416	$C_9H_7N_4O$	187.0621
$C_{13}H_{25}$	181.1957	$C_{12}H_{11}N_2$	183.0923	$C_{10}H_{21}N_2O$	185.1655	$C_9H_{15}O_4$	187.0970
$C_{14}H_{13}$	181.1018	$C_{12}H_{23}O$	183.1750	$C_{10}H_{23}N_3$	185.1894	$C_9H_{17}NO_3$	187.1209
182		$C_{12}H_{25}N$	183.1988	$C_{11}H_9N_2O$	185.0715	$C_9H_{19}N_2O_2$	187.1447
$C_7H_6N_2O_4$	182.0328	$C_{13}H_{11}O$	183.0810	$C_{11}H_{11}N_3$	185.0954	$C_9H_{21}N_3O$	187.1686
$C_7H_8N_3O_3$	182.0566	$C_{13}H_{13}N$	183.1049	$C_{11}H_{21}O_2$	185.1542	$C_9H_{23}N_4$	187.1925
$C_7H_{10}N_4O_2$	182.0805	$C_{13}H_{27}$	183.2114	$C_{11}H_{23}NO$	185.1781	$C_{10}H_7N_2O_2$	187.0508
$C_8H_8NO_4$	182.0453	$C_{14}H_{15}$	183.1174	$C_{11}H_{25}N_2$	185.2019	$C_{10}H_9N_3O$	187.0746
$C_8H_{10}N_2O_3$	182.0692	**184**		$C_{12}H_9O_2$	185.0603	$C_{10}H_{11}N_4$	187.0985
$C_8H_{12}N_3O_2$	182.0930	$C_7H_8N_2O_4$	184.0484	$C_{12}H_{11}NO$	185.0841	$C_{10}H_{19}O_3$	187.1334
$C_8H_{14}N_4O$	182.1169	$C_7H_{10}N_3O_3$	184.0723	$C_{12}H_{13}N_2$	185.1080	$C_{10}H_{21}NO_2$	187.1573
$C_9H_{10}O_4$	182.0579	$C_7H_{12}N_4O_2$	184.0961	$C_{12}H_{25}O$	185.1906	$C_{10}H_{23}N_2O$	187.1811
$C_9H_{12}NO_3$	182.0817	$C_8H_{10}NO_4$	184.0610	$C_{12}H_{27}N$	185.2145	$C_{10}H_{25}N_3$	187.2050
$C_9H_{14}N_2O_2$	182.1056	$C_8H_{12}N_2O_3$	184.0848	$C_{13}H_{13}O$	185.0967	$C_{11}H_7O_3$	187.0395
$C_9H_{16}N_3O$	182.1295	$C_8H_{14}N_3O_2$	184.1087	$C_{13}H_{15}N$	185.1205	$C_{11}H_9NO_2$	187.0634
$C_9H_{18}N_4$	182.1533	$C_8H_{16}N_4O$	184.1325	$C_{14}H_{17}$	185.1331	$C_{11}H_{11}N_2O$	187.0872
$C_{10}H_6N_4$	182.0594	$C_9H_{12}O_4$	184.0735	**186**		$C_{11}H_{13}N_3$	187.1111
$C_{10}H_{14}O_3$	182.0943	$C_9H_{14}NO_3$	184.0974	$C_7H_{10}N_2O_4$	186.0641	$C_{11}H_{23}O_2$	187.1699
$C_{10}H_{16}NO_2$	182.1182	$C_9H_{16}N_2O_2$	184.1213	$C_7H_{12}N_3O_3$	186.0879	$C_{11}H_{25}NO$	187.1937
$C_{10}H_{18}N_2O$	182.1420	$C_9H_{18}N_3O$	184.1451	$C_7H_{14}N_4O_2$	186.1118	$C_{12}H_{11}O_2$	187.0759
$C_{10}H_{20}N_3$	182.1659	$C_9H_{20}N_4$	184.1690	$C_8H_{12}NO_4$	186.0766	$C_{12}H_{13}NO$	187.0998
$C_{11}H_8N_3$	182.0719	$C_{10}H_6N_3O$	184.0511	$C_8H_{14}N_2O_3$	186.1005	$C_{12}H_{15}N_2$	187.1236
$C_{11}H_{18}O_2$	182.1307	$C_{10}H_8N_4$	184.0750	$C_8H_{16}N_3O_2$	186.1244	$C_{13}H_{15}O$	187.1123
$C_{11}H_{20}NO$	182.1546	$C_{10}H_{16}O_3$	184.1100	$C_8H_{18}N_4O$	186.1482	$C_{13}H_{17}N$	187.1362
$C_{11}H_{22}N_2$	182.1784	$C_{10}H_{18}NO_2$	184.1338	$C_9H_6N_4O$	186.0542	$C_{14}H_{19}$	187.1488
$C_{12}H_8NO$	182.0606	$C_{10}H_{20}N_2O$	184.1577	$C_9H_{14}O_4$	186.0892	**188**	
$C_{12}H_{10}N_2$	182.0845	$C_{10}H_{22}N_3$	184.1815	$C_9H_{16}NO_3$	186.1131	$C_7H_{12}N_2O_4$	188.0797
$C_{12}H_{22}O$	182.1671	$C_{11}H_8N_2O$	184.0637	$C_9H_{18}N_2O_2$	186.1369	$C_7H_{14}N_3O_3$	188.1036
$C_{12}H_{24}N$	182.1910	$C_{11}H_{10}N_3$	184.0876	$C_9H_{20}N_3O$	186.1608	$C_7H_{16}N_4O_2$	188.1275
$C_{13}H_{10}O$	182.0732	$C_{11}H_{20}O_2$	184.1464	$C_{10}H_6N_2O_2$	186.0429	$C_8H_{14}NO_4$	188.0923

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_8H_{16}N_2O_3$	188.1162	**190**		$C_{14}H_9N$	191.0736	$C_{13}H_{21}O$	193.1593
$C_8H_{18}N_3O_2$	188.1400	$C_7H_{14}N_2O_4$	190.0954	$C_{14}H_{23}N$	191.1801	$C_{13}H_{23}N$	193.1832
$C_8H_{20}N_4O$	188.1639	$C_7H_{16}N_3O_3$	190.1193	$C_{15}H_{11}$	191.0861	$C_{14}H_9O$	193.0653
$C_9H_6N_3O_2$	188.0460	$C_7H_{18}N_4O_2$	190.1431	**192**		$C_{14}H_{11}N$	193.0892
$C_9H_8N_4O$	188.0699	$C_8H_6N_4O_2$	190.0491	$C_7H_{16}N_2O_4$	192.1111	$C_{14}H_{25}$	193.1957
$C_9H_{16}O_4$	188.1049	$C_8H_{16}NO_4$	190.1080	$C_7H_{18}N_3O_3$	192.1349	$C_{15}H_{13}$	193.1018
$C_9H_{18}NO_3$	188.1287	$C_8H_{18}N_2O_3$	190.1318	$C_7H_{20}N_4O_2$	192.1588	**194**	
$C_9H_{20}N_2O_2$	188.1526	$C_8H_{20}N_3O_2$	190.1557	$C_8H_6N_3O_3$	192.0410	$C_7H_{18}N_2O_4$	194.1267
$C_9H_{22}N_3O$	188.1764	$C_8H_{22}N_4O$	190.1795	$C_8H_8N_4O_2$	192.0648	$C_8H_6N_2O_4$	194.0328
$C_9H_{24}N_4$	188.2003	$C_9H_8N_3O_2$	190.0617	$C_8H_{18}NO_4$	192.1236	$C_8H_8N_3O_3$	194.0566
$C_{10}H_8N_2O_2$	188.0586	$C_9H_{10}N_4O$	190.0856	$C_8H_{20}N_2O_3$	192.1475	$C_8H_{10}N_4O_2$	194.0805
$C_{10}H_{10}N_3O$	188.0825	$C_9H_{18}O_4$	190.1205	$C_9H_6NO_4$	192.0297	$C_9H_8NO_4$	194.0453
$C_{10}H_{12}N_4$	188.1063	$C_9H_{20}NO_3$	190.1444	$C_9H_8N_2O_3$	192.0535	$C_9H_{10}N_2O_3$	194.0692
$C_{10}H_{20}O_3$	188.1413	$C_9H_{22}N_2O_2$	190.1682	$C_9H_{10}N_3O_2$	192.0774	$C_9H_{12}N_3O_2$	194.0930
$C_{10}H_{22}NO_2$	188.1651	$C_{10}H_8NO_3$	190.0504	$C_9H_{12}N_4O$	192.1012	$C_9H_{14}N_4O$	194.1169
$C_{10}H_{24}N_2O$	188.1890	$C_{10}H_{10}N_2O_2$	190.0743	$C_9H_{20}O_4$	192.1362	$C_{10}H_{10}O_4$	194.0579
$C_{11}H_8O_3$	188.0473	$C_{10}H_{12}N_3O$	190.0981	$C_{10}H_8O_4$	192.0422	$C_{10}H_{12}NO_3$	194.0817
$C_{11}H_{10}NO_2$	188.0712	$C_{10}H_{14}N_4$	190.1220	$C_{10}H_{10}NO_3$	192.0661	$C_{10}H_{14}N_2O_2$	194.1056
$C_{11}H_{12}N_2O$	188.0950	$C_{10}H_{22}O_3$	190.1569	$C_{10}H_{12}N_2O_2$	192.0899	$C_{10}H_{16}N_3O$	194.1295
$C_{11}H_{14}N_3$	188.1189	$C_{11}H_{10}O_3$	190.0630	$C_{10}H_{14}N_3O$	192.1138	$C_{10}H_{18}N_4$	194.1533
$C_{11}H_{24}O_2$	188.1777	$C_{11}H_{12}NO_2$	190.0868	$C_{10}H_{16}N_4$	192.1377	$C_{11}H_{14}O_3$	194.0943
$C_{12}H_{12}O_2$	188.0837	$C_{11}H_{14}N_2O$	190.1107	$C_{11}H_{12}O_3$	192.0786	$C_{11}H_{16}NO_2$	194.1182
$C_{12}H_{14}NO$	188.1076	$C_{11}H_{16}N_3$	190.1346	$C_{11}H_{14}NO_2$	192.1025	$C_{11}H_{18}N_2O$	194.1420
$C_{12}H_{16}N_2$	188.1315	$C_{12}H_{14}O_2$	190.0994	$C_{11}H_{16}N_2O$	192.1264	$C_{11}H_{20}N_3$	194.1659
$C_{13}H_{16}O$	188.1202	$C_{12}H_{16}NO$	190.1233	$C_{11}H_{18}N_3$	192.1502	$C_{12}H_8N_3$	194.0719
$C_{13}H_{18}N$	188.1440	$C_{12}H_{18}N_2$	190.1471	$C_{12}H_{16}O_2$	192.1151	$C_{12}H_{18}O_2$	194.1307
$C_{14}H_{20}$	188.1566	$C_{13}H_{18}O$	190.1358	$C_{12}H_{18}NO$	192.1389	$C_{12}H_{20}NO$	194.1546
189		$C_{13}H_{20}N$	190.1597	$C_{12}H_{20}N_2$	192.1628	$C_{12}H_{22}N_2$	194.1784
$C_7H_{13}N_2O_4$	189.0876	$C_{14}H_{22}$	190.1722	$C_{13}H_8N_2$	192.0688	$C_{13}H_8NO$	194.0606
$C_7H_{15}N_3O_3$	189.1114	$C_{15}H_{10}$	190.0783	$C_{13}H_{20}O$	192.1515	$C_{13}H_{10}N_2$	194.0845
$C_7H_{17}N_4O_2$	189.1353	**191**		$C_{13}H_{22}N$	192.1753	$C_{13}H_{22}O$	194.1671
$C_8H_{15}NO_4$	189.1001	$C_7H_{15}N_2O_4$	191.1032	$C_{14}H_{10}N$	192.0814	$C_{13}H_{24}N$	194.1910
$C_8H_{17}N_2O_3$	189.1240	$C_7H_{17}N_3O_3$	191.1271	$C_{14}H_{24}$	192.1879	$C_{14}H_{10}O$	194.0732
$C_8H_{19}N_3O_2$	189.1478	$C_7H_{19}N_4O_2$	191.1509	$C_{15}H_{12}$	192.0939	$C_{14}H_{12}N$	194.0970
$C_8H_{21}N_4O$	189.1717	$C_8H_7N_4O_2$	191.0570	**193**		$C_{14}H_{26}$	194.2036
$C_9H_7N_3O_2$	189.0539	$C_8H_{17}NO_4$	191.1158	$C_7H_{17}N_2O_4$	193.1189	$C_{15}H_{14}$	194.1096
$C_9H_9N_4O$	189.0777	$C_8H_{19}N_2O_3$	191.1396	$C_7H_{19}N_3O_3$	193.1427	**195**	
$C_9H_{17}O_4$	189.1127	$C_8H_{21}N_3O_2$	191.1635	$C_8H_7N_3O_3$	193.0488	$C_8H_7N_2O_4$	195.0406
$C_9H_{19}NO_3$	189.1365	$C_9H_7N_2O_3$	191.0457	$C_8H_9N_4O_2$	193.0726	$C_8H_9N_3O_3$	195.0644
$C_9H_{21}N_2O_2$	189.1604	$C_9H_9N_3O_2$	191.0695	$C_8H_{19}NO_4$	193.1315	$C_8H_{11}N_4O_2$	195.0883
$C_9H_{23}N_3O$	189.1842	$C_9H_{11}N_4O$	191.0934	$C_9H_7NO_4$	193.0375	$C_9H_9NO_4$	195.0532
$C_{10}H_7NO_3$	189.0426	$C_9H_{19}O_4$	191.1284	$C_9H_9N_2O_3$	193.0614	$C_9H_{11}N_2O_3$	195.0770
$C_{10}H_9N_2O_2$	189.0664	$C_9H_{21}NO_3$	191.1522	$C_9H_{11}N_3O_2$	193.0852	$C_9H_{13}N_3O_2$	195.1009
$C_{10}H_{11}N_3O$	189.0903	$C_{10}H_7O_4$	191.0344	$C_9H_{13}N_4O$	193.1091	$C_9H_{15}N_4O$	195.1247
$C_{10}H_{13}N_4$	189.1142	$C_{10}H_9NO_3$	191.0583	$C_{10}H_9O_4$	193.0501	$C_{10}H_{11}O_4$	195.0657
$C_{10}H_{21}O_3$	189.1491	$C_{10}H_{11}N_2O_2$	191.0821	$C_{10}H_{11}NO_3$	193.0739	$C_{10}H_{13}NO_3$	195.0896
$C_{10}H_{23}NO_2$	189.1730	$C_{10}H_{13}N_3O$	191.1060	$C_{10}H_{13}N_2O_2$	193.0978	$C_{10}H_{15}N_2O_2$	195.1134
$C_{11}H_9O_3$	189.0552	$C_{10}H_{15}N_4$	191.1298	$C_{10}H_{15}N_3O$	193.1216	$C_{10}H_{17}N_3O$	195.1373
$C_{11}H_{11}NO_2$	189.0790	$C_{11}H_{11}O_3$	191.0708	$C_{10}H_{17}N_4$	193.1455	$C_{10}H_{19}N_4$	195.1611
$C_{11}H_{13}N_2O$	189.1029	$C_{11}H_{13}NO_2$	191.0947	$C_{11}H_{13}O_3$	193.0865	$C_{11}H_7N_4$	195.0672
$C_{11}H_{15}N_3$	189.1267	$C_{11}H_{15}N_2O$	191.1185	$C_{11}H_{15}NO_2$	193.1103	$C_{11}H_{15}O_3$	195.1021
$C_{12}H_{13}O_2$	189.0916	$C_{11}H_{17}N_3$	191.1424	$C_{11}H_{17}N_2O$	193.1342	$C_{11}H_{17}NO_2$	195.1260
$C_{12}H_{15}NO$	189.1154	$C_{12}H_{15}O_2$	191.1072	$C_{11}H_{19}N_3$	193.1580	$C_{11}H_{19}N_2O$	195.1498
$C_{12}H_{17}N_2$	189.1393	$C_{12}H_{17}NO$	191.1311	$C_{12}H_{17}O_2$	193.1229	$C_{11}H_{21}N_3$	195.1737
$C_{13}H_{17}O$	189.1280	$C_{12}H_{19}N_2$	191.1549	$C_{12}H_{19}NO$	193.1467	$C_{12}H_7N_2O$	195.0559
$C_{13}H_{19}N$	189.1519	$C_{13}H_{19}O$	191.1436	$C_{12}H_{21}N_2$	193.1706	$C_{12}H_9N_3$	195.0798
$C_{14}H_{21}$	189.1644	$C_{13}H_{21}N$	191.1675	$C_{13}H_9N_2$	193.0767	$C_{12}H_{19}O_2$	195.1385

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{12}H_{21}NO$	195.1624	$C_{11}H_{17}O_3$	197.1178	$C_9H_{15}N_2O_3$	199.1083	$C_{12}H_{28}N_2$	200.2254
$C_{12}H_{23}N_2$	195.1863	$C_{11}H_{19}NO_2$	197.1416	$C_9H_{17}N_3O_2$	199.1322	$C_{13}H_{12}O_2$	200.0837
$C_{13}H_9NO$	195.0684	$C_{11}H_{21}N_2O$	197.1655	$C_9H_{19}N_4O$	199.1560	$C_{13}H_{14}NO$	200.1076
$C_{13}H_{11}N_2$	195.0923	$C_{11}H_{23}N_3$	197.1894	$C_{10}H_7N_4O$	199.0621	$C_{13}H_{16}N_2$	200.1315
$C_{13}H_{23}O$	195.1750	$C_{12}H_9N_2O$	197.0715	$C_{10}H_{15}O_4$	199.0970	$C_{13}H_{28}O$	200.2141
$C_{13}H_{25}N$	195.1988	$C_{12}H_{11}N_3$	197.0954	$C_{10}H_{17}NO_3$	199.1209	$C_{14}H_{16}O$	200.1202
$C_{14}H_{11}O$	195.0810	$C_{12}H_{21}O_2$	197.1542	$C_{10}H_{19}N_2O_2$	199.1447	$C_{14}H_{18}N$	200.1440
$C_{14}H_{13}N$	195.1049	$C_{12}H_{23}NO$	197.1781	$C_{10}H_{21}N_3O$	199.1686	$C_{15}H_{20}$	200.1566
$C_{14}H_{27}$	195.2114	$C_{12}H_{25}N_2$	197.2019	$C_{10}H_{23}N_4$	199.1925	**201**	
$C_{15}H_{15}$	195.1174	$C_{13}H_9O_2$	197.0603	$C_{11}H_7N_2O_2$	199.0508	$C_8H_{13}N_2O_4$	201.0876
196		$C_{13}H_{11}NO$	197.0841	$C_{11}H_9N_3O$	199.0746	$C_8H_{15}N_3O_3$	201.1114
$C_8H_8N_2O_4$	196.0484	$C_{13}H_{13}N_2$	197.1080	$C_{11}H_{11}N_4$	199.0985	$C_8H_{17}N_4O_2$	201.1353
$C_8H_{10}N_3O_3$	196.0723	$C_{13}H_{25}O$	197.1906	$C_{11}H_{19}O_3$	199.1334	$C_9H_{15}NO_4$	201.1001
$C_8H_{12}N_4O_2$	196.0961	$C_{13}H_{27}N$	197.2145	$C_{11}H_{21}NO_2$	199.1573	$C_9H_{17}N_2O_3$	201.1240
$C_9H_{10}NO_4$	196.0610	$C_{14}H_{13}O$	197.0967	$C_{11}H_{23}N_2O$	199.1811	$C_9H_{19}N_3O_2$	201.1478
$C_9H_{12}N_2O_3$	196.0848	$C_{14}H_{15}N$	197.1205	$C_{11}H_{25}N_3$	199.2050	$C_9H_{21}N_4O$	201.1717
$C_9H_{14}N_3O_2$	196.1087	$C_{14}H_{29}$	197.2270	$C_{12}H_9NO_2$	199.0634	$C_{10}H_7N_3O_2$	201.0539
$C_9H_{16}N_4O$	196.1325	$C_{15}H_{17}$	197.1331	$C_{12}H_{11}N_2O$	199.0872	$C_{10}H_9N_4O$	201.0777
$C_{10}H_{12}O_4$	196.0735	**198**		$C_{12}H_{13}N_3$	199.1111	$C_{10}H_{17}O_4$	201.1127
$C_{10}H_{14}NO_3$	196.0974	$C_8H_{10}N_2O_4$	198.0641	$C_{12}H_{23}O_2$	199.1699	$C_{10}H_{19}NO_3$	201.1365
$C_{10}H_{16}N_2O_2$	196.1213	$C_8H_{12}N_3O_3$	198.0879	$C_{12}H_{25}NO$	199.1937	$C_{10}H_{21}N_2O_2$	201.1604
$C_{10}H_{18}N_3O$	196.1451	$C_8H_{14}N_4O_2$	198.1118	$C_{12}H_{27}N_2$	199.2176	$C_{10}H_{23}N_3O$	201.1842
$C_{10}H_{20}N_4$	196.1690	$C_9H_{12}NO_4$	198.0766	$C_{13}H_{11}O_2$	199.0759	$C_{10}H_{25}N_4$	201.2081
$C_{11}H_8N_4$	196.0750	$C_9H_{14}N_2O_3$	198.1005	$C_{13}H_{13}NO$	199.0998	$C_{11}H_7NO_3$	201.0426
$C_{11}H_{16}O_3$	196.1100	$C_9H_{16}N_3O_2$	198.1244	$C_{13}H_{15}N_2$	199.1236	$C_{11}H_9N_2O_2$	201.0664
$C_{11}H_{18}NO_2$	196.1338	$C_9H_{18}N_4O$	198.1482	$C_{13}H_{27}O$	199.2063	$C_{11}H_{11}N_3O$	201.0903
$C_{11}H_{20}N_2O$	196.1577	$C_{10}H_{14}O_4$	198.0892	$C_{13}H_{29}N$	199.2301	$C_{11}H_{13}N_4$	201.1142
$C_{11}H_{22}N_3$	196.1815	$C_{10}H_{16}NO_3$	198.1131	$C_{14}H_{15}O$	199.1123	$C_{11}H_{21}O_3$	201.1491
$C_{12}H_8N_2O$	196.0637	$C_{10}H_{18}N_2O_2$	198.1369	$C_{14}H_{17}N$	199.1362	$C_{11}H_{23}NO_2$	201.1730
$C_{12}H_{10}N_3$	196.0876	$C_{10}H_{20}N_3O$	198.1608	$C_{15}H_{19}$	199.1488	$C_{11}H_{25}N_2O$	201.1968
$C_{12}H_{20}O_2$	196.1464	$C_{10}H_{22}N_4$	198.1846	**200**		$C_{11}H_{27}N_3$	201.2207
$C_{12}H_{22}NO$	196.1702	$C_{11}H_8N_3O$	198.0668	$C_8H_{12}N_2O_4$	200.0797	$C_{12}H_9O_3$	201.0552
$C_{12}H_{24}N_2$	196.1941	$C_{11}H_{10}N_4$	198.0907	$C_8H_{14}N_3O_3$	200.1036	$C_{12}H_{11}NO_2$	201.0790
$C_{13}H_8O_2$	196.0524	$C_{11}H_{18}O_3$	198.1256	$C_8H_{16}N_4O_2$	200.1275	$C_{12}H_{13}N_2O$	201.1029
$C_{13}H_{10}NO$	196.0763	$C_{11}H_{20}NO_2$	198.1495	$C_9H_{14}NO_4$	200.0923	$C_{12}H_{15}N_3$	201.1267
$C_{13}H_{12}N_2$	196.1001	$C_{11}H_{22}N_2O$	198.1733	$C_9H_{16}N_2O_3$	200.1162	$C_{12}H_{25}O_2$	201.1855
$C_{13}H_{24}O$	196.1828	$C_{11}H_{24}N_3$	198.1972	$C_9H_{18}N_3O_2$	200.1400	$C_{12}H_{27}NO$	201.2094
$C_{13}H_{26}N$	196.2067	$C_{12}H_8NO_2$	198.0555	$C_9H_{20}N_4O$	200.1639	$C_{13}H_{13}O_2$	201.0916
$C_{14}H_{12}O$	196.0888	$C_{12}H_{10}N_2O$	198.0794	$C_{10}H_8N_4O$	200.0699	$C_{13}H_{15}NO$	201.1154
$C_{14}H_{14}N$	196.1127	$C_{12}H_{12}N_3$	198.1032	$C_{10}H_{16}O_4$	200.1049	$C_{13}H_{17}N_2$	201.1393
$C_{14}H_{28}$	196.2192	$C_{12}H_{22}O_2$	198.1620	$C_{10}H_{18}NO_3$	200.1287	$C_{14}H_{17}O$	201.1280
$C_{15}H_{16}$	196.1253	$C_{12}H_{24}NO$	198.1859	$C_{10}H_{20}N_2O_2$	200.1526	$C_{14}H_{19}N$	201.1519
197		$C_{12}H_{26}N_2$	198.2098	$C_{10}H_{22}N_3O$	200.1764	$C_{15}H_{21}$	201.1644
$C_8H_9N_2O_4$	197.0563	$C_{13}H_{10}O_2$	198.0681	$C_{10}H_{24}N_4$	200.2003	**202**	
$C_8H_{11}N_3O_3$	197.0801	$C_{13}H_{12}NO$	198.0919	$C_{11}H_8N_2O_2$	200.0586	$C_8H_{14}N_2O_4$	202.0954
$C_8H_{13}N_4O_2$	197.1040	$C_{13}H_{14}N_2$	198.1158	$C_{11}H_{10}N_3O$	200.0825	$C_8H_{16}N_3O_3$	202.1193
$C_9H_{11}NO_4$	197.0688	$C_{13}H_{26}O$	198.1985	$C_{11}H_{12}N_4$	200.1063	$C_8H_{18}N_4O_2$	202.1431
$C_9H_{13}N_2O_3$	197.0927	$C_{13}H_{28}N$	198.2223	$C_{11}H_{20}O_3$	200.1413	$C_9H_6N_4O_2$	202.0491
$C_9H_{15}N_3O_2$	197.1165	$C_{14}H_{14}O$	198.1045	$C_{11}H_{22}NO_2$	200.1651	$C_9H_{16}NO_4$	202.1080
$C_9H_{17}N_4O$	197.1404	$C_{14}H_{16}N$	198.1284	$C_{11}H_{24}N_2O$	200.1890	$C_9H_{18}N_2O_3$	202.1318
$C_{10}H_{13}O_4$	197.0814	$C_{14}H_{30}$	198.2349	$C_{11}N_{26}N_3$	200.2129	$C_9H_{20}N_3O_2$	202.1557
$C_{10}H_{15}NO_3$	197.1052	$C_{15}H_{18}$	198.1409	$C_{12}H_8O_3$	200.0473	$C_9H_{22}N_4O$	202.1795
$C_{10}H_{17}N_2O_2$	197.1291	**199**		$C_{12}H_{10}NO_2$	200.0712	$C_{10}H_8N_3O_2$	202.0617
$C_{10}H_{19}N_3O$	197.1529	$C_8H_{11}N_2O_4$	199.0719	$C_{12}H_{12}N_2O$	200.0950	$C_{10}H_{10}N_4O$	202.0856
$C_{10}H_{21}N_4$	197.1768	$C_8H_{13}N_3O_3$	199.0958	$C_{12}H_{14}N_3$	200.1189	$C_{10}H_{18}O_4$	202.1205
$C_{11}H_7N_3O$	197.0590	$C_8H_{15}N_4O_2$	199.1196	$C_{12}H_{24}O_2$	200.1777	$C_{10}H_{20}NO_3$	202.1444
$C_{11}H_9N_4$	197.0829	$C_9H_{13}NO_4$	199.0845	$C_{12}H_{26}NO$	200.2015	$C_{10}H_{22}N_2O_2$	202.1682

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{10}H_{24}N_3O$	202.1921	$C_8H_{20}N_4O_2$	204.1588	$C_{13}H_{21}N_2$	205.1706	$C_{11}H_{19}N_4$	207.1611
$C_{10}H_{26}N_4$	202.2160	$C_9H_6N_3O_3$	204.0410	$C_{14}H_9N_2$	205.0767	$C_{12}H_{15}O_3$	207.1021
$C_{11}H_8NO_3$	202.0504	$C_9H_8N_4O_2$	204.0648	$C_{14}H_{21}O$	205.1593	$C_{12}H_{17}NO_2$	207.1260
$C_{11}H_{10}N_2O_2$	202.0743	$C_9H_{18}NO_4$	204.1236	$C_{14}H_{23}N$	205.1832	$C_{12}H_{19}N_2O$	207.1498
$C_{11}H_{12}N_3O$	202.0981	$C_9H_{20}N_2O_3$	204.1475	$C_{15}H_9O$	205.0653	$C_{12}H_{21}N_3$	207.1737
$C_{11}H_{14}N_4$	202.1220	$C_9H_{22}N_3O_2$	204.1713	$C_{15}H_{11}N$	205.0892	$C_{13}H_9N_3$	207.0798
$C_{11}H_{22}O_3$	202.1569	$C_9H_{24}N_4O$	204.1952	$C_{15}H_{25}$	205.1957	$C_{13}H_{19}O_2$	207.1385
$C_{11}H_{24}NO_2$	202.1808	$C_{10}H_8N_2O_3$	204.0535	$C_{16}H_{13}$	205.1018	$C_{13}H_{21}NO$	207.1624
$C_{11}H_{26}N_2O$	202.2046	$C_{10}H_{10}N_3O_2$	204.0774	**206**		$C_{13}H_{23}N_2$	207.1863
$C_{12}H_{10}O_3$	202.0630	$C_{10}H_{12}N_4O$	204.1012	$C_8H_{18}N_2O_4$	206.1267	$C_{14}H_9NO$	207.0684
$C_{12}H_{12}NO_2$	202.0868	$C_{10}H_{20}O_4$	204.1362	$C_8H_{20}N_3O_3$	206.1506	$C_{14}H_{11}N_2$	207.0923
$C_{12}H_{14}N_2O$	202.1107	$C_{10}H_{22}NO_3$	204.1600	$C_8H_{22}N_4O_2$	206.1744	$C_{14}H_{23}O$	207.1750
$C_{12}H_{16}N_3$	202.1346	$C_{10}H_{24}N_2O_2$	204.1839	$C_9H_6N_2O_4$	206.0328	$C_{14}H_{25}N$	207.1988
$C_{12}H_{26}O_2$	202.1934	$C_{11}H_8O_4$	204.0422	$C_9H_8N_3O_3$	206.0566	$C_{15}H_{11}O$	207.0810
$C_{13}H_{14}O_2$	202.0994	$C_{11}H_{10}NO_3$	204.0661	$C_9H_{10}N_4O_2$	206.0805	$C_{15}H_{13}N$	207.1049
$C_{13}H_{16}NO$	202.1233	$C_{11}H_{12}N_2O_2$	204.0899	$C_9H_{20}NO_4$	206.1393	$C_{15}H_{27}$	207.2114
$C_{13}H_{18}N_2$	202.1471	$C_{11}H_{14}N_3O$	204.1138	$C_9H_{22}N_2O_3$	206.1631	$C_{16}H_{15}$	207.1174
$C_{14}H_{18}O$	202.1358	$C_{11}H_{16}N_4$	204.1377	$C_{10}H_8NO_4$	206.0453	**208**	
$C_{14}H_{20}N$	202.1597	$C_{11}H_{24}O_3$	204.1726	$C_{10}H_{10}N_2O_3$	206.0692	$C_8H_{20}N_2O_4$	208.1424
$C_{15}H_{22}$	202.1722	$C_{12}H_{12}O_3$	204.0786	$C_{10}H_{12}N_3O_2$	206.0930	$C_9H_8N_2O_4$	208.0484
203		$C_{12}H_{14}NO_2$	204.1025	$C_{10}H_{14}N_4O$	206.1169	$C_9H_{10}N_3O_3$	208.0723
$C_8H_{15}N_2O_4$	203.1032	$C_{12}H_{16}N_2O$	204.1264	$C_{10}H_{22}O_4$	206.1518	$C_9H_{12}N_4O_2$	208.0961
$C_8H_{17}N_3O_3$	203.1271	$C_{12}H_{18}N_3$	204.1502	$C_{11}H_{10}O_4$	206.0579	$C_{10}H_{10}NO_4$	208.0610
$C_8H_{19}N_4O_2$	203.1509	$C_{13}H_{16}O_2$	204.1151	$C_{11}H_{12}NO_3$	206.0817	$C_{10}H_{12}N_2O_3$	208.0848
$C_9H_7N_4O_2$	203.0570	$C_{13}H_{18}NO$	204.1389	$C_{11}H_{14}N_2O_2$	206.1056	$C_{10}H_{14}N_3O_2$	208.1087
$C_9H_{17}NO_4$	203.1158	$C_{13}H_{20}N_2$	204.1628	$C_{11}H_{16}N_3O$	206.1295	$C_{10}H_{16}N_4O$	208.1325
$C_9H_{19}N_2O_3$	203.1396	$C_{14}H_{20}O$	204.1515	$C_{11}H_{18}N_4$	206.1533	$C_{11}H_{12}O_4$	208.0735
$C_9H_{21}N_3O_2$	203.1635	$C_{14}H_{22}N$	204.1753	$C_{12}H_{14}O_3$	206.0943	$C_{11}H_{14}NO_3$	208.0974
$C_9H_{23}N_4O$	203.1873	$C_{15}H_{10}N$	204.0814	$C_{12}H_{16}NO_2$	206.1182	$C_{11}H_{16}N_2O_2$	208.1213
$C_{10}H_7N_2O_3$	203.0457	$C_{15}H_{24}$	204.1879	$C_{12}H_{18}N_2O$	206.1420	$C_{11}H_{18}N_3O$	208.1451
$C_{10}H_9N_3O_2$	203.0695	$C_{16}H_{12}$	204.0939	$C_{12}H_{20}N_3$	206.1659	$C_{11}H_{20}N_4$	208.1690
$C_{10}H_{11}N_4O$	203.0934	**205**		$C_{13}H_8N_3$	206.0719	$C_{12}H_8N_4$	208.0750
$C_{10}H_{19}O_4$	203.1284	$C_8H_{17}N_2O_4$	205.1189	$C_{13}H_{18}O_2$	206.1307	$C_{12}H_{16}O_3$	208.1100
$C_{10}H_{21}NO_3$	203.1522	$C_8H_{19}N_3O_3$	205.1427	$C_{13}H_{20}NO$	206.1546	$C_{12}H_{18}NO_2$	208.1338
$C_{10}H_{23}N_2O_2$	203.1761	$C_8H_{21}N_4O_2$	205.1666	$C_{13}H_{22}N_2$	206.1784	$C_{12}H_{20}N_2O$	208.1577
$C_{10}H_{25}N_3O$	203.1999	$C_9H_7N_3O_3$	205.0488	$C_{14}H_{10}N_2$	206.0845	$C_{12}H_{22}N_3$	208.1815
$C_{11}H_7O_4$	203.0344	$C_9H_9N_4O_2$	205.0726	$C_{14}H_{22}O$	206.1671	$C_{13}H_8N_2O$	208.0637
$C_{11}H_9NO_3$	203.0583	$C_9H_{19}NO_4$	205.1315	$C_{14}H_{24}N$	206.1910	$C_{13}H_{10}N_3$	208.0876
$C_{11}H_{11}N_2O_2$	203.0821	$C_9H_{21}N_2O_3$	205.1553	$C_{15}H_{10}O$	206.0732	$C_{13}H_{20}O_2$	208.1464
$C_{11}H_{13}N_3O$	203.1060	$C_9H_{23}N_3O_2$	205.1791	$C_{15}H_{12}N$	206.0970	$C_{13}H_{22}NO$	208.1702
$C_{11}H_{15}N_4$	203.1298	$C_{10}H_7NO_4$	205.0375	$C_{15}H_{26}$	206.2036	$C_{13}H_{24}N_2$	208.1941
$C_{11}H_{23}O_3$	203.1648	$C_{10}H_9N_2O_3$	205.0614	$C_{16}H_{14}$	206.1096	$C_{14}H_{10}NO$	208.0763
$C_{11}H_{25}NO_2$	203.1886	$C_{10}H_{11}N_3O_2$	205.0852	**207**		$C_{14}H_{12}N_2$	208.1001
$C_{12}H_{11}O_3$	203.0708	$C_{10}H_{13}N_4O$	205.1091	$C_8H_{19}N_2O_4$	207.1345	$C_{14}H_{24}O$	208.1828
$C_{12}H_{13}NO_2$	203.0947	$C_{10}H_{21}O_4$	205.1440	$C_8H_{21}N_3O_3$	207.1584	$C_{14}H_{26}N$	208.2067
$C_{12}H_{15}N_2O$	203.1185	$C_{10}H_{23}NO_3$	205.1679	$C_9H_7N_2O_4$	207.0406	$C_{15}H_{12}O$	208.0888
$C_{12}H_{17}N_3$	203.1424	$C_{11}H_9O_4$	205.0501	$C_9H_9N_3O_3$	207.0644	$C_{15}H_{14}N$	208.1127
$C_{13}H_{15}O_2$	203.1072	$C_{11}H_{11}NO_3$	205.0739	$C_9H_{11}N_4O_2$	207.0883	$C_{15}H_{28}$	208.2192
$C_{13}H_{17}NO$	203.1311	$C_{11}H_{13}N_2O_2$	205.0978	$C_9H_{21}NO_4$	207.1471	$C_{16}H_{16}$	208.1253
$C_{13}H_{19}N_2$	203.1549	$C_{11}H_{15}N_3O$	205.1216	$C_{10}H_9NO_4$	207.0532	**209**	
$C_{14}H_{19}O$	203.1436	$C_{11}H_{17}N_4$	205.1455	$C_{10}H_{11}N_2O_3$	207.0770	$C_9H_9N_2O_4$	209.0563
$C_{14}H_{21}N$	203.1675	$C_{12}H_{13}O_3$	205.0865	$C_{10}H_{13}N_3O_2$	207.1009	$C_9H_{11}N_3O_3$	209.0801
$C_{15}H_9N$	203.0736	$C_{12}H_{15}N$	205.1103	$C_{10}H_{15}N_4O$	207.1247	$C_9H_{13}N_4O_2$	209.1040
$C_{15}H_{23}$	203.1801	$C_{12}H_{17}N_2O$	205.1342	$C_{11}H_{11}O_4$	207.0657	$C_{10}H_{11}NO_4$	209.0688
204		$C_{12}H_{19}N_3$	205.1580	$C_{11}H_{13}NO_3$	207.0896	$C_{10}H_{13}N_2O_3$	209.0927
$C_8H_{16}N_2O_4$	204.1111	$C_{13}H_{17}O_2$	205.1229	$C_{11}H_{15}N_2O_2$	207.1134	$C_{10}H_{15}N_3O_2$	209.1165
$C_8H_{18}N_3O_3$	204.1349	$C_{13}H_{19}NO$	205.1467	$C_{11}H_{17}N_3O$	207.1373	$C_{10}H_{17}N_4O$	209.1404

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{11}H_{13}O_4$	209.0814	$C_{16}H_{18}$	210.1409	$C_{13}H_8O_3$	212.0473	$C_{10}H_{18}N_2O_3$	214.1318
$C_{11}H_{15}NO_3$	209.1052	**211**		$C_{13}H_{10}NO_2$	212.0712	$C_{10}H_{20}N_3O_2$	214.1557
$C_{11}H_{17}N_2O_2$	209.1291	$C_9H_{11}N_2O_4$	211.0719	$C_{13}H_{12}N_2O$	212.0950	$C_{10}H_{22}N_4O$	214.1795
$C_{11}H_{19}N_3O$	209.1529	$C_9H_{13}N_3O_3$	211.0958	$C_{13}H_{14}N_3$	212.1189	$C_{11}H_8N_3O_2$	214.0617
$C_{11}H_{21}N_4$	209.1768	$C_9H_{15}N_4O_2$	211.1196	$C_{13}H_{24}O_2$	212.1777	$C_{11}H_{10}N_4O$	214.0856
$C_{12}H_9N_4$	209.0829	$C_{10}H_{13}NO_4$	211.0845	$C_{13}H_{26}NO$	212.2015	$C_{11}H_{18}O_4$	214.1205
$C_{12}H_{17}O_3$	209.1178	$C_{10}H_{15}N_2O_3$	211.1083	$C_{13}H_{28}N_2$	212.2254	$C_{11}H_{20}NO_3$	214.1444
$C_{12}H_{19}NO_2$	209.1416	$C_{10}H_{17}N_3O_2$	211.1322	$C_{14}H_{12}O_2$	212.0837	$C_{11}H_{22}N_2O_2$	214.1682
$C_{12}H_{21}N_2O$	209.1655	$C_{10}H_{19}N_4O$	211.1560	$C_{14}H_{14}NO$	212.1076	$C_{11}H_{24}N_3O$	214.1921
$C_{12}H_{23}N_3$	209.1894	$C_{11}H_7N_4O$	211.0621	$C_{14}H_{16}N_2$	212.1315	$C_{11}H_{26}N_4$	214.2160
$C_{13}H_9N_2O$	209.0715	$C_{11}H_{15}O_4$	211.0970	$C_{14}H_{28}O$	212.2141	$C_{12}H_8NO_3$	214.0504
$C_{13}H_{11}N_3$	209.0954	$C_{11}H_{17}NO_3$	211.1209	$C_{14}H_{30}N$	212.2380	$C_{12}H_{10}N_2O_2$	214.0743
$C_{13}H_{21}O_2$	209.1542	$C_{11}H_{19}N_2O_2$	211.1447	$C_{15}H_{16}O$	212.1202	$C_{12}H_{12}N_3O$	214.0981
$C_{13}H_{23}NO$	209.1781	$C_{11}H_{21}N_3O$	211.1686	$C_{15}H_{18}N$	212.1440	$C_{12}H_{14}N_4$	214.1220
$C_{13}H_{25}N_2$	209.2019	$C_{11}H_{23}N_4$	211.1925	$C_{15}H_{32}$	212.2505	$C_{12}H_{22}O_3$	214.1569
$C_{14}H_9O_2$	209.0603	$C_{12}H_9N_3O$	211.0746	$C_{16}H_{20}$	212.1566	$C_{12}H_{24}NO_2$	214.1808
$C_{14}H_{11}NO$	209.0841	$C_{12}H_{11}N_4$	211.0985	**213**		$C_{12}H_{26}N_2O$	214.2046
$C_{14}H_{13}N_2$	209.1080	$C_{12}H_{19}O_3$	211.1334	$C_9H_{13}N_2O_4$	213.0876	$C_{12}H_{28}N_3$	214.2285
$C_{14}H_{25}O$	209.1906	$C_{12}H_{21}NO_2$	211.1573	$C_9H_{15}N_3O_3$	213.1114	$C_{13}H_{10}O_3$	214.0630
$C_{14}H_{27}N$	209.2145	$C_{12}H_{23}N_2O$	211.1811	$C_9H_{17}N_4O_2$	213.1353	$C_{13}H_{12}NO_2$	214.0869
$C_{15}H_{13}O$	209.0967	$C_{12}H_{25}N_3$	211.2050	$C_{10}H_{15}NO_4$	213.1001	$C_{13}H_{14}N_2O$	214.1107
$C_{15}H_{15}N$	209.1205	$C_{13}H_9NO_2$	211.0634	$C_{10}H_{17}N_2O_3$	213.1240	$C_{13}H_{16}N_3$	214.1346
$C_{15}H_{29}$	209.2270	$C_{13}H_{11}N_2O$	211.0872	$C_{10}H_{19}N_3O_2$	213.1478	$C_{13}H_{26}O_2$	214.1934
$C_{16}H_{17}$	209.1331	$C_{13}H_{13}N_3$	211.1111	$C_{10}H_{21}N_4O$	213.1717	$C_{13}H_{28}NO$	214.2172
210		$C_{13}H_{23}O_2$	211.1699	$C_{11}H_7N_3O_2$	213.0539	$C_{13}H_{30}N_2$	214.2411
$C_9H_{10}N_2O_4$	210.0641	$C_{13}H_{25}NO$	211.1937	$C_{11}H_9N_4O$	213.0777	$C_{14}H_{14}O_2$	214.0994
$C_9H_{12}N_3O_3$	210.0879	$C_{13}H_{27}N_2$	211.2176	$C_{11}H_{17}O_4$	213.1127	$C_{14}H_{16}NO$	214.1233
$C_9H_{14}N_4O_2$	210.1118	$C_{14}H_{11}O_2$	211.0759	$C_{11}H_{19}NO_3$	213.1365	$C_{14}H_{18}N_2$	214.1471
$C_{10}H_{12}NO_4$	210.0766	$C_{14}H_{13}NO$	211.0998	$C_{11}H_{21}N_2O_2$	213.1604	$C_{15}H_{18}O$	214.1358
$C_{10}H_{14}N_2O_3$	210.1005	$C_{14}H_{15}N_2$	211.1236	$C_{11}H_{23}N_3O$	213.1842	$C_{15}H_{20}N$	214.1597
$C_{10}H_{16}N_3O_2$	210.1244	$C_{14}H_{27}O$	211.2063	$C_{11}H_{25}N_4$	213.2081	$C_{16}H_{22}$	214.1722
$C_{10}H_{18}N_4O$	210.1482	$C_{14}H_{29}N$	211.2301	$C_{12}H_9N_2O_2$	213.0664	**215**	
$C_{11}H_{14}O_4$	210.0892	$C_{15}H_{15}O$	211.1123	$C_{12}H_{11}N_3O$	213.0903	$C_9H_{15}N_2O_4$	215.1032
$C_{11}H_{16}NO_3$	210.1131	$C_{15}H_{17}N$	211.1362	$C_{12}H_{13}N_4$	213.1142	$C_9H_{17}N_3O_3$	215.1271
$C_{11}H_{18}N_2O_2$	210.1369	$C_{15}H_{31}$	211.2427	$C_{12}H_{21}O_3$	213.1491	$C_9H_{19}N_4O_2$	215.1509
$C_{11}H_{20}N_3O$	210.1608	$C_{16}H_{19}$	211.1488	$C_{12}H_{23}NO_2$	213.1730	$C_{10}H_7N_4O_2$	215.0570
$C_{11}H_{22}N_4$	210.1846	**212**		$C_{12}H_{25}N_2O$	213.1968	$C_{10}H_{17}NO_4$	215.1158
$C_{12}H_8N_3O$	210.0668	$C_9H_{12}N_2O_4$	212.0797	$C_{12}H_{27}N_3$	213.2207	$C_{10}H_{19}N_2O_3$	215.1396
$C_{12}H_{10}N_4$	210.0907	$C_9H_{14}N_3O_3$	212.1036	$C_{13}H_9O_3$	213.0552	$C_{10}H_{21}N_3O_2$	215.1635
$C_{12}H_{18}O_3$	210.1256	$C_9H_{16}N_4O_2$	212.1275	$C_{13}H_{11}NO_2$	213.0790	$C_{10}H_{23}N_4O$	215.1873
$C_{12}H_{20}NO_2$	210.1495	$C_{10}H_{14}NO_4$	212.0923	$C_{13}H_{13}N_2O$	213.1029	$C_{11}H_7N_2O_3$	215.0457
$C_{12}H_{22}N_2O$	210.1733	$C_{10}H_{16}N_2O_3$	212.1162	$C_{13}H_{15}N_3$	213.1267	$C_{11}H_9N_3O_2$	215.0695
$C_{12}H_{24}N_3$	210.1972	$C_{10}H_{18}N_3O_2$	212.1400	$C_{13}H_{25}O_2$	213.1855	$C_{11}H_{11}N_4O$	215.0934
$C_{13}H_8NO_2$	210.0555	$C_{10}H_{20}N_4O$	212.1639	$C_{13}H_{27}NO$	213.2094	$C_{11}H_{19}O_4$	215.1284
$C_{13}H_{10}N_2O$	210.0794	$C_{11}H_8N_4O$	212.0699	$C_{13}H_{29}N_2$	213.2332	$C_{11}H_{21}NO_3$	215.1522
$C_{13}H_{12}N_3$	210.1032	$C_{11}H_{16}O_4$	212.1049	$C_{14}H_{13}O_2$	213.0916	$C_{11}H_{23}N_2O_2$	215.1761
$C_{13}H_{22}O_2$	210.1620	$C_{11}H_{18}NO_3$	212.1287	$C_{14}H_{15}NO$	213.1154	$C_{11}H_{25}N_3O$	215.1999
$C_{13}H_{24}NO$	210.1859	$C_{11}H_{20}N_2O_2$	212.1526	$C_{14}H_{17}N_2$	213.1393	$C_{11}H_{27}N_4$	215.2238
$C_{13}H_{26}N_2$	210.2098	$C_{11}H_{22}N_3O$	212.1764	$C_{14}H_{29}O$	213.2219	$C_{12}H_9NO_3$	215.0583
$C_{14}H_{10}O_2$	210.0681	$C_{11}H_{24}N_4$	212.2003	$C_{15}H_{17}O$	213.1280	$C_{12}H_{11}N_2O_2$	215.0821
$C_{14}H_{12}NO$	210.0919	$C_{12}H_8N_2O_2$	212.0586	$C_{15}H_{19}N$	213.1519	$C_{12}H_{13}N_3O$	215.1060
$C_{14}H_{14}N_2$	210.1158	$C_{12}H_{10}N_3O$	212.0825	$C_{16}H_{21}$	213.1644	$C_{12}H_{15}N_4$	215.1298
$C_{14}H_{26}O$	210.1985	$C_{12}H_{12}N_4$	212.1063	**214**		$C_{12}H_{23}O_3$	215.1648
$C_{14}H_{28}N$	210.2223	$C_{12}H_{20}O_3$	212.1413	$C_9H_{14}N_2O_4$	214.0954	$C_{12}H_{25}NO_2$	215.1886
$C_{15}H_{14}O$	210.1045	$C_{12}H_{22}NO_2$	212.1651	$C_9H_{16}N_3O_3$	214.1193	$C_{12}H_{27}N_2O$	215.2125
$C_{15}H_{16}N$	210.1284	$C_{12}H_{24}N_2O$	212.1890	$C_9H_{18}N_4O_2$	214.1431	$C_{12}H_{29}N_3$	215.2363
$C_{15}H_{30}$	210.2349	$C_{12}H_{26}N_3$	212.2129	$C_{10}H_{16}NO_4$	214.1080	$C_{13}H_{11}O_3$	215.0708

APPENDIX A (*Continued*)

	FM		FM		FM		FM
$C_{13}H_{13}NO_2$	215.0947	$C_{11}H_7NO_4$	217.0375	$C_{14}H_{22}N_2$	218.1784	$C_{11}H_{16}N_4O$	220.1325
$C_{13}H_{15}N_2O$	215.1185	$C_{11}H_9N_2O_3$	217.0614	$C_{15}H_{10}N_2$	218.0845	$C_{12}H_{12}O_4$	220.0735
$C_{13}H_{17}N_3$	215.1424	$C_{11}H_{11}N_3O_2$	217.0852	$C_{15}H_{22}O$	218.1671	$C_{12}H_{14}NO_3$	220.0974
$C_{14}H_{15}O_2$	215.1072	$C_{11}H_{13}N_4O$	217.1091	$C_{15}H_{24}N$	218.1910	$C_{12}H_{16}N_2O_2$	220.1213
$C_{14}H_{17}NO$	215.1311	$C_{11}H_{21}O_4$	217.1440	$C_{16}H_{10}O$	218.0732	$C_{12}H_{18}N_3O$	220.1451
$C_{14}H_{19}N_2$	215.1549	$C_{11}H_{23}NO_3$	217.1679	$C_{16}H_{12}N$	218.0970	$C_{12}H_{20}N_4$	220.1690
$C_{15}H_{19}O$	215.1436	$C_{11}H_{25}N_2O_2$	217.1917	$C_{16}H_{26}$	218.2036	$C_{13}H_8N_4$	220.0750
$C_{15}H_{21}N$	215.1675	$C_{11}H_{27}N_3O$	217.2156	$C_{17}H_{14}$	218.1096	$C_{13}H_{16}O_3$	220.1100
$C_{16}H_{23}$	215.1801	$C_{12}H_9O_4$	217.0501	**219**		$C_{13}H_{18}NO_2$	220.1338
216		$C_{12}H_{11}NO_3$	217.0739	$C_9H_{19}N_2O_4$	219.1345	$C_{13}H_{20}N_2O$	220.1577
$C_9H_{16}N_2O_4$	216.1111	$C_{12}H_{13}N_2O_2$	217.0978	$C_9H_{21}N_3O_3$	219.1584	$C_{13}H_{22}N_3$	220.1815
$C_9H_{18}N_3O_3$	216.1349	$C_{12}H_{15}N_3O$	217.1216	$C_9H_{23}N_4O_2$	219.1822	$C_{14}H_{10}N_3$	220.0876
$C_9H_{20}N_4O_2$	216.1588	$C_{12}H_{17}N_4$	217.1455	$C_{10}H_7N_2O_4$	219.0406	$C_{14}H_{20}O_2$	220.1464
$C_{10}H_8N_4O_2$	216.0648	$C_{12}H_{25}O_3$	217.1804	$C_{10}H_9N_3O_3$	219.0644	$C_{14}H_{22}NO$	220.1702
$C_{10}H_{18}NO_4$	216.1236	$C_{12}H_{27}NO_2$	217.2043	$C_{10}H_{11}N_4O_2$	219.0883	$C_{14}H_{24}N_2$	220.1941
$C_{10}H_{20}N_2O_3$	216.1475	$C_{13}H_{13}O_3$	217.0865	$C_{10}H_{21}NO_4$	219.1471	$C_{15}H_{10}NO$	220.0763
$C_{10}H_{22}N_3O_2$	216.1713	$C_{13}H_{15}NO_2$	217.1103	$C_{10}H_{23}N_2O_3$	219.1710	$C_{15}H_{12}N_2$	220.1001
$C_{10}H_{24}N_4O$	216.1952	$C_{13}H_{17}N_2O$	217.1342	$C_{10}H_{25}N_3O_2$	219.1948	$C_{15}H_{24}O$	220.1828
$C_{11}H_8N_2O_3$	216.0535	$C_{13}H_{19}N_3$	217.1580	$C_{11}H_9NO_4$	219.0532	$C_{15}H_{26}N$	220.2067
$C_{11}H_{10}N_3O_2$	216.0774	$C_{14}H_{17}O_2$	217.1229	$C_{11}H_{11}N_2O_3$	219.0770	$C_{16}H_{12}O$	220.0888
$C_{11}H_{12}N_4O$	216.1012	$C_{14}H_{19}NO$	217.1467	$C_{11}H_{13}N_3O_2$	219.1009	$C_{16}H_{14}N$	220.1127
$C_{11}H_{20}O_4$	216.1362	$C_{14}H_{21}N_2$	217.1706	$C_{11}H_{15}N_4O$	219.1247	$C_{16}H_{28}$	220.2192
$C_{11}H_{22}NO_3$	216.1600	$C_{15}H_9N_2$	217.0767	$C_{11}H_{23}O_4$	219.1597	$C_{17}H_{16}$	220.1253
$C_{11}H_{24}N_2O_2$	216.1839	$C_{15}H_{21}O$	217.1593	$C_{11}H_{25}NO_3$	219.1835	**221**	
$C_{11}H_{26}N_3O$	216.2077	$C_{15}H_{23}N$	217.1832	$C_{12}H_{11}O_4$	219.0657	$C_9H_{21}N_2O_4$	221.1502
$C_{11}H_{28}N_4$	216.2316	$C_{16}H_{11}N$	217.0892	$C_{12}H_{13}NO_3$	219.0896	$C_9H_{23}N_3O_3$	221.1741
$C_{12}H_8O_4$	216.0422	$C_{16}H_{25}$	217.1957	$C_{12}H_{15}N_2O_2$	219.1134	$C_{10}H_9N_2O_4$	221.0563
$C_{12}H_{10}NO_3$	216.0661	$C_{17}H_{13}$	217.1018	$C_{12}H_{17}N_3O$	219.1373	$C_{10}H_{11}N_3O_3$	221.0801
$C_{12}H_{12}N_2O_2$	216.0899	**218**		$C_{12}H_{19}N_4$	219.1611	$C_{10}H_{13}N_4O_2$	221.1040
$C_{12}H_{14}N_3O$	216.1138	$C_9H_{18}N_2O_4$	218.1267	$C_{13}H_{15}O_3$	219.1021	$C_{10}H_{23}NO_4$	221.1628
$C_{12}H_{16}N_4$	216.1377	$C_9H_{20}N_3O_3$	218.1506	$C_{13}H_{17}NO_2$	219.1260	$C_{11}H_{11}NO_4$	221.0688
$C_{12}H_{24}O_3$	216.1726	$C_9H_{22}N_4O_2$	218.1744	$C_{13}H_{19}N_2O$	219.1498	$C_{11}H_{13}N_2O_3$	221.0927
$C_{12}H_{26}NO_2$	216.1965	$C_{10}H_8N_3O_3$	218.0566	$C_{13}H_{21}N_3$	219.1737	$C_{11}H_{15}N_3O_2$	221.1165
$C_{12}H_{28}N_2O$	216.2203	$C_{10}H_{10}N_4O_2$	218.0805	$C_{14}H_9N_3$	219.0798	$C_{11}H_{17}N_4O$	221.1404
$C_{13}H_{12}O_3$	216.0786	$C_{10}H_{20}NO_4$	218.1393	$C_{14}H_{19}O_2$	219.1385	$C_{12}H_{13}O_4$	221.0814
$C_{13}H_{14}NO_2$	216.1025	$C_{10}H_{22}N_2O_3$	218.1631	$C_{14}H_{21}NO$	219.1624	$C_{12}H_{15}NO_3$	221.1052
$C_{13}H_{16}N_2O$	216.1264	$C_{10}H_{24}N_3O_2$	218.1870	$C_{14}H_{23}N_2$	219.1863	$C_{12}H_{17}N_2O_2$	221.1291
$C_{13}H_{18}N_3$	216.1502	$C_{10}H_{26}N_4O$	218.2108	$C_{15}H_9NO$	219.0684	$C_{12}H_{19}N_3O$	221.1529
$C_{13}H_{28}O_2$	216.2090	$C_{11}H_8NO_4$	218.0453	$C_{15}H_{11}N_2$	219.0923	$C_{12}H_{21}N_4$	221.1768
$C_{14}H_{16}O_2$	216.1151	$C_{11}H_{10}N_2O_3$	218.0692	$C_{15}H_{23}O$	219.1750	$C_{13}H_9N_4$	221.0829
$C_{14}H_{18}NO$	216.1389	$C_{11}H_{12}N_3O_2$	218.0930	$C_{15}H_{25}N$	219.1988	$C_{13}H_{17}O_3$	221.1178
$C_{14}H_{20}N_2$	216.1628	$C_{11}H_{14}N_4O$	218.1169	$C_{16}H_{11}O$	219.0810	$C_{13}H_{19}NO_2$	221.1416
$C_{15}H_{20}O$	216.1515	$C_{11}H_{22}O_4$	218.1518	$C_{16}H_{13}N$	219.1049	$C_{13}H_{21}N_2O$	221.1655
$C_{15}H_{22}N$	216.1753	$C_{11}H_{24}NO_3$	218.1757	$C_{16}H_{27}$	219.2114	$C_{13}H_{23}N_3$	221.1894
$C_{16}H_{10}N$	216.0814	$C_{11}H_{26}N_2O_2$	218.1996	$C_{17}H_{15}$	219.1174	$C_{14}H_9N_2O$	221.0715
$C_{16}H_{24}$	216.1879	$C_{12}H_{10}O_4$	218.0579	**220**		$C_{14}H_{11}N_3$	221.0954
$C_{17}H_{12}$	216.0939	$C_{12}H_{12}NO_3$	218.0817	$C_9H_{20}N_2O_4$	220.1424	$C_{14}H_{21}O_2$	221.1542
217		$C_{12}H_{14}N_2O_2$	218.1056	$C_9H_{22}N_3O_3$	220.1662	$C_{14}H_{23}NO$	221.1781
$C_9H_{17}N_2O_4$	217.1189	$C_{12}H_{16}N_3O$	218.1295	$C_9H_{24}N_4O_2$	220.1901	$C_{14}H_{25}N_2$	221.2019
$C_9H_{19}N_3O_3$	217.1427	$C_{12}H_{18}N_4$	218.1533	$C_{10}H_8N_2O_4$	220.0484	$C_{15}H_9O_2$	221.0603
$C_9H_{21}N_4O_2$	217.1666	$C_{12}H_{26}O_3$	218.1883	$C_{10}H_{10}N_3O_3$	220.0723	$C_{15}H_{11}NO$	221.0841
$C_{10}H_7N_3O_3$	217.0488	$C_{13}H_{14}O_3$	218.0943	$C_{10}H_{12}N_4O_2$	220.0961	$C_{15}H_{13}N_2$	221.1080
$C_{10}H_9N_4O_2$	217.0726	$C_{13}H_{16}NO_2$	218.1182	$C_{10}H_{22}NO_4$	220.1549	$C_{15}H_{25}O$	221.1906
$C_{10}H_{19}NO_4$	217.1315	$C_{13}H_{18}N_2O$	218.1420	$C_{10}H_{24}N_2O_3$	220.1788	$C_{15}H_{27}N$	221.2145
$C_{10}H_{21}N_2O_3$	217.1553	$C_{13}H_{20}N_3$	218.1659	$C_{11}H_{10}NO_4$	220.0610	$C_{16}H_{13}O$	221.0967
$C_{10}H_{23}N_3O_2$	217.1791	$C_{14}H_{18}O_2$	218.1307	$C_{11}H_{12}N_2O_3$	220.0848	$C_{16}H_{15}N$	221.1205
$C_{10}H_{25}N_4O$	217.2030	$C_{14}H_{20}NO$	218.1546	$C_{11}H_{14}N_3O_2$	220.1087	$C_{16}H_{29}$	221.2270

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{17}H_{17}$	221.1331	$C_{14}H_9NO_2$	223.0634	$C_{11}H_{21}N_4O$	225.1717	$C_{14}H_{28}NO$	226.2172
222		$C_{14}H_{11}N_2O$	223.0872	$C_{12}H_9N_4O$	225.0777	$C_{14}H_{30}N_2$	226.2411
$C_9H_{22}N_2O_4$	222.1580	$C_{14}H_{13}N_3$	223.1111	$C_{12}H_{17}O_4$	225.1127	$C_{15}H_{14}O_2$	226.0994
$C_{10}H_{10}N_2O_4$	222.0641	$C_{14}H_{23}O_2$	223.1699	$C_{12}H_{19}NO_3$	225.1365	$C_{15}H_{16}NO$	226.1233
$C_{10}H_{12}N_3O_3$	222.0879	$C_{14}H_{25}NO$	223.1937	$C_{12}H_{21}N_2O_2$	225.1604	$C_{15}H_{18}N_2$	226.1471
$C_{10}H_{14}N_4O_2$	222.1118	$C_{14}H_{27}N_2$	223.2176	$C_{12}H_{23}N_3O$	225.1842	$C_{15}H_{30}O$	226.2298
$C_{11}H_{12}NO_4$	222.0766	$C_{15}H_{11}O_2$	223.0759	$C_{12}H_{25}N_4$	225.2081	$C_{15}H_{32}N$	226.2536
$C_{11}H_{14}N_2O_3$	222.1005	$C_{15}H_{13}NO$	223.0998	$C_{13}H_9N_2O_2$	225.0664	$C_{16}H_{18}O$	226.1358
$C_{11}H_{16}N_3O_2$	222.1244	$C_{15}H_{27}O$	223.2063	$C_{13}H_{11}N_3O$	225.0903	$C_{16}H_{20}N$	226.1597
$C_{11}H_{18}N_4O$	222.1482	$C_{15}H_{29}N$	223.2301	$C_{13}H_{13}N_4$	225.1142	$C_{16}H_{34}$	226.2662
$C_{11}N_3O_3$	221.9940	$C_{16}H_{15}O$	223.1123	$C_{13}H_{21}O_3$	225.1491	$C_{17}H_{22}$	226.1722
$C_{12}H_{14}O_4$	222.0892	$C_{16}H_{17}N$	223.1362	$C_{13}H_{23}NO_2$	225.1730	**227**	
$C_{12}H_{16}NO_3$	222.1131	$C_{16}H_{31}$	223.2427	$C_{13}H_{25}N_2O$	225.1968	$C_{10}H_{15}N_2O_4$	227.1032
$C_{12}H_{18}N_2O_2$	222.1369	$C_{17}H_{19}$	223.1488	$C_{13}H_{27}N_3$	225.2207	$C_{10}H_{17}N_3O_3$	227.1271
$C_{12}H_{20}N_3O$	222.1608	**224**		$C_{14}H_9O_3$	225.0552	$C_{10}H_{19}N_4O_2$	227.1509
$C_{12}H_{22}N_4$	222.1846	$C_{10}H_{12}N_2O_4$	224.0797	$C_{14}H_{11}NO_2$	225.0790	$C_{11}H_{17}NO_4$	227.1158
$C_{13}H_8N_3O$	222.0668	$C_{10}H_{14}N_3O_3$	224.1036	$C_{14}H_{13}N_2O$	225.1029	$C_{11}H_{21}N_3O_2$	227.1635
$C_{13}H_{10}N_4$	222.0907	$C_{10}H_{16}N_4O_2$	224.1275	$C_{14}H_{15}N_3$	225.1267	$C_{11}H_{23}N_4O$	227.1873
$C_{13}H_{18}O_3$	222.1256	$C_{11}H_{14}NO_4$	224.0923	$C_{14}H_{25}O_2$	225.1855	$C_{12}H_7N_2O_3$	227.0457
$C_{13}H_{20}NO_2$	222.1495	$C_{11}H_{16}N_2O_3$	224.1162	$C_{14}H_{27}NO$	225.2094	$C_{12}H_9N_3O_2$	227.0695
$C_{13}H_{22}N_2O$	222.1733	$C_{11}H_{18}N_3O_2$	224.1400	$C_{14}H_{29}N_2$	225.2332	$C_{12}H_{11}N_4O$	227.0934
$C_{13}H_{24}N_3$	222.1972	$C_{11}H_{20}N_4O$	224.1639	$C_{15}H_{13}O_2$	225.0916	$C_{12}H_{19}O_4$	227.1284
$C_{14}H_{10}N_2O$	222.0794	$C_{12}H_8N_4O$	224.0699	$C_{15}H_{15}NO$	225.1154	$C_{12}H_{21}NO_3$	227.1522
$C_{14}H_{12}N_3$	222.1032	$C_{12}H_{16}O_4$	224.1049	$C_{15}H_{17}N_2$	225.1393	$C_{12}H_{23}N_2O_2$	227.1761
$C_{14}H_{22}O_2$	222.1620	$C_{12}H_{18}NO_3$	224.1287	$C_{15}H_{29}O$	225.2219	$C_{12}H_{25}N_3O$	227.1999
$C_{14}H_{24}NO$	222.1859	$C_{12}H_{20}N_2O_2$	224.1526	$C_{15}H_{31}N$	225.2458	$C_{12}H_{27}N_4$	227.2238
$C_{14}H_{26}N_2$	222.2098	$C_{12}H_{22}N_3O$	224.1764	$C_{16}H_{17}O$	225.1280	$C_{13}H_9NO_3$	227.0583
$C_{15}H_{10}O_2$	222.0681	$C_{12}H_{24}N_4$	224.2003	$C_{16}H_{19}N$	225.1519	$C_{13}H_{11}N_2O_2$	227.0821
$C_{15}H_{12}NO$	222.0919	$C_{13}H_8N_2O_2$	224.0586	$C_{16}H_{33}$	225.2584	$C_{13}H_{13}N_3O$	227.1060
$C_{15}H_{14}N_2$	222.1158	$C_{13}H_{10}N_3O$	224.0825	$C_{17}H_{21}$	225.1644	$C_{13}H_{15}N_4$	227.1298
$C_{15}H_{26}O$	222.1985	$C_{13}H_{12}N_4$	224.1063	**226**		$C_{13}H_{25}NO_2$	227.1886
$C_{15}H_{28}N$	222.2223	$C_{13}H_{20}O_3$	224.1413	$C_{10}H_{14}N_2O_4$	226.0954	$C_{13}H_{27}N_2O$	227.2125
$C_{16}H_{14}O$	222.1045	$C_{13}H_{22}NO_2$	224.1651	$C_{10}H_{16}N_3O_3$	226.1193	$C_{13}H_{29}N_3$	227.2363
$C_{16}H_{16}N$	222.1284	$C_{13}H_{24}N_2O$	224.1890	$C_{10}H_{18}N_4O_2$	226.1431	$C_{14}H_{11}O_3$	227.0708
$C_{16}H_{30}$	222.2349	$C_{13}H_{26}N_3$	224.2129	$C_{11}H_{16}NO_4$	226.1080	$C_{14}H_{13}NO_2$	227.0947
$C_{16}NO$	221.9980	$C_{14}H_{10}NO_2$	224.0712	$C_{11}H_{18}N_2O_3$	226.1318	$C_{14}H_{15}N_2O$	227.1185
$C_{17}H_{18}$	222.1409	$C_{14}H_{12}N_2O$	224.0950	$C_{11}H_{20}N_3O_2$	226.1557	$C_{14}H_{17}N_3$	227.1424
223		$C_{14}H_{14}N_3$	224.1189	$C_{11}H_{22}N_4O$	226.1795	$C_{14}H_{27}O_2$	227.2012
$C_{10}H_{11}N_2O_4$	223.0719	$C_{14}H_{24}O_2$	224.1777	$C_{12}H_8N_3O_2$	226.0617	$C_{14}H_{29}NO$	227.2250
$C_{10}H_{13}N_3O_3$	223.0958	$C_{14}H_{26}NO$	224.2015	$C_{12}H_{10}N_4O$	226.0856	$C_{15}H_{15}O_2$	227.1072
$C_{10}H_{15}N_4O_2$	223.1196	$C_{14}H_{28}N_2$	224.2254	$C_{12}H_{18}O_4$	226.1205	$C_{15}H_{17}NO$	227.1311
$C_{11}H_{13}NO_4$	223.0845	$C_{15}H_{12}O_2$	224.0837	$C_{12}H_{20}NO_3$	226.1444	$C_{15}H_{19}N_2$	227.1549
$C_{11}H_{15}N_2O_3$	223.1083	$C_{15}H_{14}NO$	224.1076	$C_{12}H_{22}N_2O_2$	226.1682	$C_{15}H_{31}O$	227.2376
$C_{11}H_{17}N_3O_2$	223.1322	$C_{15}H_{16}N_2$	224.1315	$C_{12}H_{24}N_3O$	226.1929	$C_{15}H_{33}N$	227.2615
$C_{11}H_{19}N_4O$	223.1560	$C_{15}H_{28}O$	224.2141	$C_{12}H_{26}N_4$	226.2160	$C_{16}H_{19}O$	227.1436
$C_{12}H_7N_4O$	223.0621	$C_{15}H_{30}N$	224.2380	$C_{13}H_{10}N_2O_2$	226.0743	$C_{16}H_{21}N$	227.1675
$C_{12}H_{15}O_4$	223.0970	$C_{16}H_{16}O$	224.1202	$C_{13}H_{12}N_3O$	226.0981	$C_{17}H_{23}$	227.1801
$C_{12}H_{17}NO_3$	223.1209	$C_{16}H_{18}N$	224.1440	$C_{13}H_{14}N_4$	226.1220	**228**	
$C_{12}H_{19}N_2O_2$	223.1447	$C_{16}H_{32}$	224.2505	$C_{13}H_{22}O_3$	226.1569	$C_{10}H_{16}N_2O_2$	228.1111
$C_{12}H_{21}N_3O$	223.1686	$C_{17}H_{20}$	224.1566	$C_{13}H_{24}NO_2$	226.1808	$C_{10}H_{18}N_3O_3$	228.1349
$C_{12}H_{23}N_4$	223.1925	**225**		$C_{13}H_{26}N_2O$	226.2046	$C_{10}H_{20}N_4O_2$	228.1588
$C_{13}H_9N_3O$	223.0746	$C_{10}H_{13}N_2O_4$	225.0876	$C_{13}H_{28}N_3$	226.2285	$C_{11}H_8N_4O_2$	228.0648
$C_{13}H_{11}N_4$	223.0985	$C_{10}H_{15}N_3O_3$	225.1114	$C_{14}H_{10}O_3$	226.0630	$C_{11}H_{18}NO_4$	228.1236
$C_{13}H_{19}O_3$	223.1334	$C_{10}H_{17}N_4O_2$	225.1353	$C_{14}H_{12}NO_2$	226.0868	$C_{11}H_{20}N_2O_3$	228.1475
$C_{13}H_{21}NO_2$	223.1573	$C_{11}H_{15}NO_4$	225.1001	$C_{14}H_{14}N_2O$	226.1107	$C_{11}H_{22}N_3O_2$	228.1713
$C_{13}H_{23}N_2O$	223.1811	$C_{11}H_{17}N_2O_3$	225.1240	$C_{14}H_{16}N_3$	226.1346	$C_{11}H_{24}N_4O$	228.1952
$C_{13}H_{25}N_3$	223.2050	$C_{11}H_{19}N_3O_2$	225.1478	$C_{14}H_{26}O_2$	226.1934	$C_{12}H_8N_2O_3$	228.0535

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{12}H_{12}N_4O$	228.1012	$C_{14}H_{15}NO_2$	229.1103	$C_{10}H_{23}N_4O_2$	231.1822	$C_{13}H_{20}N_4$	232.1690
$C_{12}H_{20}O_4$	228.1362	$C_{14}H_{17}N_2O$	229.1342	$C_{11}H_7N_2O_4$	231.0406	$C_{13}H_{28}O_3$	232.2039
$C_{12}H_{22}NO_3$	228.1600	$C_{14}H_{19}N_3$	229.1580	$C_{11}H_9N_3O_3$	231.0644	$C_{14}H_{16}O_3$	232.1100
$C_{12}H_{24}N_2O_2$	228.1839	$C_{14}H_{29}O_2$	229.2168	$C_{11}H_{11}N_4O_2$	231.0883	$C_{14}H_{18}NO_2$	232.1338
$C_{12}H_{26}N_3O$	228.2077	$C_{14}H_{31}NO$	229.2407	$C_{11}H_{21}NO_4$	231.1471	$C_{14}H_{20}N_2O$	232.1577
$C_{12}H_{28}N_4$	228.2316	$C_{15}H_{17}O_2$	229.1229	$C_{11}H_{23}N_2O_3$	231.1710	$C_{14}H_{22}N_3$	232.1815
$C_{13}H_8O_4$	228.0422	$C_{15}H_{19}NO$	229.1467	$C_{11}H_{25}N_3O_2$	231.1948	$C_{15}H_{10}N_3$	232.0876
$C_{13}H_{10}NO_3$	228.0661	$C_{15}H_{21}N_2$	229.1706	$C_{11}H_{27}N_4O$	231.2187	$C_{15}H_{20}O_2$	232.1464
$C_{13}H_{12}N_2O_2$	228.0899	$C_{16}H_{21}O$	229.1593	$C_{12}H_9NO_4$	231.0532	$C_{15}H_{22}NO$	232.1702
$C_{13}H_{14}N_3O$	228.1138	$C_{16}H_{23}N$	229.1832	$C_{12}H_{11}N_2O_3$	231.0770	$C_{15}H_{24}N_2$	232.1941
$C_{13}H_{24}O_3$	228.1726	$C_{17}H_9O$	229.0653	$C_{12}H_{13}N_3O_2$	231.1009	$C_{16}H_{10}NO$	232.0768
$C_{13}H_{26}NO_2$	228.1965	$C_{17}H_{11}N$	229.0892	$C_{12}H_{15}N_4O$	231.1247	$C_{16}H_{12}N_2$	232.1001
$C_{13}H_{28}N_2O$	228.2203	$C_{18}H_{13}$	229.1018	$C_{12}H_{23}O_4$	231.1597	$C_{16}H_{24}O$	232.1828
$C_{13}H_{30}N_3$	228.2442	**230**		$C_{12}H_{25}NO_3$	231.1835	$C_{16}H_{26}N$	232.2067
$C_{14}H_{12}O_3$	228.0786	$C_{10}H_{18}N_2O_4$	230.1267	$C_{12}H_{27}N_2O_2$	231.2074	$C_{17}H_{12}O$	232.0888
$C_{14}H_{14}NO_2$	228.1025	$C_{10}H_{20}N_3O_3$	230.1506	$C_{12}H_{29}N_3O$	231.2312	$C_{17}H_{14}N$	232.1127
$C_{14}H_{16}N_2O$	228.1264	$C_{10}H_{22}N_4O_2$	230.1744	$C_{13}H_{11}O_4$	231.0657	$C_{17}H_{28}$	232.2192
$C_{14}H_{18}N_3$	228.1502	$C_{11}H_8N_3O_3$	230.0566	$C_{13}H_{13}NO_3$	231.0896	$C_{18}H_{16}$	232.1253
$C_{14}H_{28}O_2$	228.2090	$C_{11}H_{10}N_4O_2$	230.0805	$C_{13}H_{15}N_2O_2$	231.1134	**233**	
$C_{14}H_{30}NO$	228.2329	$C_{11}H_{20}NO_4$	230.1393	$C_{13}H_{17}N_3O$	231.1373	$C_{10}H_{23}N_3O_3$	233.1741
$C_{14}H_{32}N_2$	228.2567	$C_{11}H_{22}N_2O_3$	230.1631	$C_{13}H_{19}N_4$	231.1611	$C_{10}H_{25}N_4O_2$	233.1979
$C_{15}H_{16}O_2$	228.1151	$C_{11}H_{24}N_3O_2$	230.1870	$C_{14}H_{15}O_3$	231.1021	$C_{11}H_9N_2O_4$	233.0563
$C_{15}H_{18}NO$	228.1389	$C_{11}H_{26}N_4O$	230.2108	$C_{14}H_{17}NO_2$	231.1260	$C_{11}H_{11}N_3O_3$	233.0801
$C_{15}H_{20}N_2$	228.1628	$C_{12}H_8NO_4$	230.0453	$C_{14}H_{19}N_2O$	231.1498	$C_{11}H_{23}NO_4$	233.1628
$C_{15}H_{32}O$	228.2454	$C_{12}H_{10}N_2O_3$	230.0692	$C_{14}H_{21}N_3$	231.1737	$C_{11}H_{25}N_2O_3$	233.1866
$C_{16}H_{20}O$	228.1515	$C_{12}H_{12}N_3O_2$	230.0930	$C_{15}H_9N_3$	231.0798	$C_{11}H_{27}N_3O_2$	233.2105
$C_{16}H_{22}N$	228.1753	$C_{12}H_{14}N_4O$	230.1169	$C_{15}H_{19}O_2$	231.1385	$C_{12}H_{11}NO_4$	233.0688
$C_{17}H_{10}N$	228.0814	$C_{12}H_{22}O_4$	230.1518	$C_{15}H_{21}NO$	231.1624	$C_{12}H_{13}N_2O_3$	233.0927
$C_{17}H_{24}$	228.1879	$C_{12}H_{24}NO_3$	230.1757	$C_{15}H_{23}N_2$	231.1863	$C_{12}H_{15}N_3O_2$	233.1165
$C_{18}H_{12}$	228.0939	$C_{12}H_{26}N_2O_2$	230.1996	$C_{16}H_9NO$	231.0684	$C_{12}H_{17}N_4O$	233.1404
229		$C_{12}H_{28}N_3O$	230.2234	$C_{16}H_{11}N_2$	231.0923	$C_{12}H_{25}O_4$	233.1753
$C_{10}H_{17}N_2O_4$	229.1189	$C_{12}H_{30}N_4$	230.2473	$C_{16}H_{23}O$	231.1750	$C_{12}H_{27}NO_3$	233.1992
$C_{10}H_{19}N_3O_3$	229.1427	$C_{13}H_{10}O_4$	230.0579	$C_{17}H_{11}O$	231.0810	$C_{13}H_{13}O_4$	233.0814
$C_{10}H_{21}N_4O_2$	229.1666	$C_{13}H_{12}NO_3$	230.0817	$C_{17}H_{13}N$	231.1049	$C_{13}H_{15}NO_3$	233.1052
$C_{11}H_7N_3O_3$	229.0488	$C_{13}H_{14}N_2O_2$	230.1056	$C_{17}H_{27}$	231.2114	$C_{13}H_{17}N_2O_2$	233.1291
$C_{11}H_9N_4O_2$	229.0726	$C_{13}H_{16}N_3O$	230.1295	$C_{18}H_{15}$	231.1174	$C_{13}H_{19}N_3O$	233.1529
$C_{11}H_{19}NO_4$	229.1315	$C_{13}H_{18}N_4$	230.1533	**232**		$C_{13}H_{21}N_4$	233.1768
$C_{11}H_{21}N_2O_3$	229.1553	$C_{13}H_{26}O_3$	230.1883	$C_{10}H_{20}N_2O_4$	232.1424	$C_{14}H_9N_4$	233.0829
$C_{11}H_{23}N_3O_2$	229.1791	$C_{13}H_{28}NO_2$	230.2121	$C_{10}H_{22}N_3O_3$	232.1662	$C_{14}H_{17}O_3$	233.1178
$C_{11}H_{25}N_4O$	229.2030	$C_{13}H_{30}N_2O$	230.2360	$C_{10}H_{24}N_4O_2$	232.1901	$C_{14}H_{19}NO_2$	233.1416
$C_{12}H_9N_2O_3$	229.0614	$C_{14}H_{14}O_3$	230.0943	$C_{11}H_8N_2O_4$	232.0484	$C_{14}H_{21}N_2O$	233.1655
$C_{12}H_{11}N_3O_2$	229.0852	$C_{14}H_{16}NO_2$	230.1182	$C_{11}H_{10}N_3O_3$	232.0723	$C_{15}H_9N_2O$	233.0715
$C_{12}H_{13}N_4O$	229.1091	$C_{14}H_{18}N_2O$	230.1420	$C_{11}H_{12}N_4O_2$	232.0961	$C_{15}H_{11}N_3$	233.0954
$C_{12}H_{21}O_4$	229.1440	$C_{14}H_{20}N_3$	230.1659	$C_{11}H_{22}NO_4$	232.1549	$C_{15}H_{21}O_2$	233.1542
$C_{12}H_{23}NO_3$	229.1679	$C_{14}H_{30}O_2$	230.2247	$C_{11}H_{24}N_2O_3$	232.1788	$C_{15}H_{23}NO$	233.1781
$C_{12}H_{25}N_2O_2$	229.1917	$C_{15}H_{18}O_2$	230.1307	$C_{11}H_{26}N_3O_2$	232.2026	$C_{15}H_{25}N_2$	233.2019
$C_{12}H_{27}N_3O$	229.2156	$C_{15}H_{20}NO$	230.1546	$C_{11}H_{28}N_4O$	232.2265	$C_{16}H_9O_2$	233.0603
$C_{12}H_{29}N_4$	229.2394	$C_{15}H_{22}N_2$	230.1784	$C_{12}H_{10}NO_4$	232.0610	$C_{16}H_{11}NO$	233.0841
$C_{13}H_9O_4$	229.0501	$C_{16}H_{10}N_2$	230.0845	$C_{12}H_{12}N_2O_3$	232.0848	$C_{16}H_{13}N_2$	233.1080
$C_{13}H_{11}NO_3$	229.0739	$C_{16}H_{22}O$	230.1671	$C_{12}H_{14}N_3O_2$	232.1087	$C_{16}H_{25}O$	233.1906
$C_{13}H_{13}N_2O_2$	229.0978	$C_{16}H_{24}N$	230.1910	$C_{12}H_{16}N_4O$	232.1325	$C_{16}H_{27}N$	233.2145
$C_{13}H_{15}N_3O$	229.1216	$C_{17}H_{10}O$	230.0732	$C_{12}H_{24}O_4$	232.1675	$C_{17}H_{13}O$	233.0967
$C_{13}H_{17}N_4$	229.1455	$C_{17}H_{12}N$	230.0970	$C_{12}H_{26}NO_3$	232.1914	$C_{17}H_{15}N$	233.1205
$C_{13}H_{25}O_3$	229.1804	$C_{17}H_{26}$	230.2036	$C_{12}H_{28}N_2O_2$	232.2152	$C_{17}H_{29}$	233.2270
$C_{13}H_{27}NO_2$	229.2043	$C_{18}H_{14}$	230.1096	$C_{13}H_{12}O_4$	232.0735	$C_{18}H_{17}$	233.1331
$C_{13}H_{29}N_2O$	229.2281	**231**		$C_{13}H_{14}NO_3$	232.0974	**234**	
$C_{13}H_{31}N_3$	229.2520	$C_{10}H_{19}N_2O_4$	231.1345	$C_{13}H_{16}N_2O_2$	232.1213	$C_{10}H_{22}N_2O_4$	234.1580
$C_{14}H_{13}O_3$	229.0865	$C_{10}H_{21}N_3O_3$	231.1584	$C_{13}H_{18}N_3O$	232.1451	$C_{10}H_{24}N_3O_3$	234.1819

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{10}H_{26}N_4O_2$	234.2057	$C_{15}H_{13}N_3$	235.1111	$C_{12}H_{21}N_4O$	237.1717	$C_{15}H_{30}N_2$	238.2411
$C_{11}H_{10}N_2O_4$	234.0641	$C_{15}H_{23}O_2$	235.1699	$C_{13}H_9N_4O$	237.0777	$C_{16}H_{14}O_2$	238.0994
$C_{11}H_{12}N_3O_3$	234.0879	$C_{15}H_{25}NO$	235.1937	$C_{13}H_{17}O_4$	237.1127	$C_{16}H_{16}NO$	238.1233
$C_{11}H_{14}N_4O_2$	234.1118	$C_{15}H_{27}N_2$	235.2176	$C_{13}H_{19}NO_3$	237.1365	$C_{16}H_{18}N_2$	238.1471
$C_{11}H_{24}NO_4$	234.1706	$C_{16}H_{11}O_2$	235.0759	$C_{13}H_{21}N_2O_2$	237.1604	$C_{16}H_{30}O$	238.2298
$C_{11}H_{26}N_2O_3$	234.1945	$C_{16}H_{13}NO$	235.0998	$C_{13}H_{23}N_3O$	237.1842	$C_{16}H_{32}N$	238.2536
$C_{12}H_{12}NO_4$	234.0766	$C_{16}H_{15}N_2$	235.1236	$C_{13}H_{25}N$	237.2081	$C_{17}H_{18}O$	238.1358
$C_{12}H_{14}N_2O_3$	234.1005	$C_{16}H_{27}O$	235.2063	$C_{14}H_9N_2O_2$	237.0664	$C_{17}H_{20}N$	238.1597
$C_{12}H_{16}N_3O_2$	234.1244	$C_{16}H_{29}N$	235.2301	$C_{14}H_{11}N_3O$	237.0903	$C_{17}H_{34}$	238.2662
$C_{12}H_{18}N_4O$	234.1482	$C_{17}H_{15}O$	235.1123	$C_{14}H_{13}N_4$	237.1142	$C_{18}H_{22}$	238.1722
$C_{12}H_{26}O_4$	234.1832	$C_{17}H_{17}N$	235.1362	$C_{14}H_{21}O_3$	237.1491	**239**	
$C_{13}H_{14}O_4$	234.0892	$C_{17}H_{31}$	235.2427	$C_{14}H_{23}NO_2$	237.1730	$C_{11}H_{15}N_2O_4$	239.1032
$C_{13}H_{16}NO_3$	234.1131	$C_{18}H_{19}$	235.1488	$C_{14}H_{25}N_2O$	237.1968	$C_{11}H_{17}N_3O_3$	239.1271
$C_{13}H_{18}N_2O_2$	234.1369	**236**		$C_{14}H_{27}N_3$	237.2207	$C_{11}H_{19}N_4O_2$	239.1509
$C_{13}H_{20}N_3O$	234.1608	$C_{10}H_{24}N_2O_4$	236.1737	$C_{15}H_9O_3$	237.0552	$C_{12}H_{17}NO_4$	239.1158
$C_{13}H_{22}N_4$	234.1846	$C_{11}H_{12}N_2O_4$	236.0797	$C_{15}H_{11}NO_2$	237.0790	$C_{12}H_{19}N_2O_3$	239.1396
$C_{14}H_{10}N_4$	234.0907	$C_{11}H_{14}N_3O_3$	236.1036	$C_{15}H_{13}N_2O$	237.1029	$C_{12}H_{21}N_3O_2$	239.1635
$C_{14}H_{18}O_3$	234.1256	$C_{11}H_{16}N_4O_2$	236.1275	$C_{15}H_{15}N_3$	237.1267	$C_{12}H_{23}N_4O$	239.1873
$C_{14}H_{20}NO_2$	234.1495	$C_{12}H_2N_3O_3$	236.0096	$C_{15}H_{25}O_2$	237.1855	$C_{13}H_9N_3O_2$	239.0695
$C_{14}H_{22}N_2O$	234.1733	$C_{12}H_4N_4O_2$	236.0335	$C_{15}H_{27}NO$	237.2094	$C_{13}H_{11}N_4O$	239.0934
$C_{14}H_{24}N_3$	234.1972	$C_{12}H_{14}NO_4$	236.0923	$C_{15}H_{29}N_2$	237.2332	$C_{13}H_{19}O_4$	239.1284
$C_{15}H_{10}N_2O$	234.0794	$C_{12}H_{16}N_2O_3$	236.1162	$C_{16}H_{13}O_2$	237.0916	$C_{13}H_{21}NO_3$	239.1522
$C_{15}H_{12}N_3$	234.1032	$C_{12}H_{18}N_3O_2$	236.1400	$C_{16}H_{15}NO$	237.1154	$C_{13}H_{23}N_2O_2$	239.1761
$C_{15}H_{22}O_2$	234.1620	$C_{12}H_{20}N_4O$	236.1639	$C_{16}H_{17}N_2$	237.1393	$C_{13}H_{25}N_3O$	239.1999
$C_{15}H_{24}NO$	234.1859	$C_{13}H_8N_4O$	236.0699	$C_{16}H_{29}O$	237.2219	$C_{13}H_{27}N_4$	239.2238
$C_{15}H_{26}N_2$	234.2098	$C_{13}H_{16}O_4$	236.1049	$C_{16}H_{31}N$	237.2458	$C_{14}H_9NO_3$	239.0583
$C_{16}H_{10}O_2$	234.0681	$C_{13}H_{18}NO_3$	236.1287	$C_{17}H_{17}O$	237.1280	$C_{14}H_{11}N_2O_2$	239.0821
$C_{16}H_{12}NO$	234.0919	$C_{13}H_{20}N_2O_2$	236.1526	$C_{17}H_{19}N$	237.1519	$C_{14}H_{13}N_3O$	239.1060
$C_{16}H_{14}N_2$	234.1158	$C_{13}H_{22}N_3O$	236.1764	$C_{17}H_{33}$	237.2584	$C_{14}H_{15}N_4$	239.1298
$C_{16}H_{26}O$	234.1985	$C_{13}H_{24}N_4$	236.2003	$C_{18}H_{21}$	237.1644	$C_{14}H_{23}O_3$	239.1648
$C_{16}H_{28}N$	234.2223	$C_{14}H_{10}N_3O$	236.0825	**238**		$C_{14}H_{25}NO_2$	239.1886
$C_{17}H_{16}N$	234.1284	$C_{14}H_{12}N_4$	236.1063	$C_{11}H_{14}N_2O_4$	238.0954	$C_{14}H_{27}N_2O$	239.2125
$C_{17}H_{30}$	234.2349	$C_{14}H_{20}O_3$	236.1413	$C_{11}H_{16}N_3O_3$	238.1193	$C_{14}H_{29}N_3$	239.2363
$C_{18}H_{18}$	234.1409	$C_{14}H_{22}NO_2$	236.1651	$C_{11}H_{18}N_4O_2$	238.1431	$C_{15}H_{11}O_3$	239.0708
235		$C_{14}H_{24}N_2O$	236.1890	$C_{12}H_{16}NO_4$	238.1080	$C_{15}H_{13}NO_2$	239.0947
$C_{10}H_{23}N_2O_4$	235.1659	$C_{14}H_{26}N_3$	236.2129	$C_{12}H_{18}N_2O_3$	238.1318	$C_{15}H_{15}N_2O$	239.1185
$C_{10}H_{25}N_3O_3$	235.1897	$C_{15}H_{10}NO_2$	236.0712	$C_{12}H_{20}N_3O_2$	238.1557	$C_{15}H_{17}N_3$	239.1424
$C_{11}H_{11}N_2O_4$	235.0719	$C_{15}H_{12}N_2O$	236.0950	$C_{12}H_{22}N_4O$	238.1795	$C_{15}H_{27}O_2$	239.2012
$C_{11}H_{13}N_3O_3$	235.0958	$C_{15}H_{14}N_3$	236.1189	$C_{13}H_8N_3O_2$	238.0617	$C_{15}H_{29}NO$	239.2250
$C_{11}H_{15}N_4O_2$	235.1196	$C_{15}H_{24}O_2$	236.1777	$C_{13}H_{10}N_4O$	238.0856	$C_{15}H_{31}N_2$	239.2489
$C_{11}H_{25}NO_4$	235.1784	$C_{15}H_{26}NO$	236.2015	$C_{13}H_{18}O_4$	238.1205	$C_{16}H_{15}O_2$	239.1072
$C_{12}H_{13}NO_4$	235.0845	$C_{15}H_{28}N_2$	236.2254	$C_{13}H_{20}NO_3$	238.1444	$C_{16}H_{17}NO$	239.1311
$C_{12}H_{15}N_2O_3$	235.1083	$C_{16}H_{12}O_2$	236.0837	$C_{13}H_{22}N_2O_2$	238.1682	$C_{16}H_{19}N_2$	239.1549
$C_{12}H_{17}N_3O_2$	235.1322	$C_{16}H_{14}NO$	236.1076	$C_{13}H_{24}N_3O$	238.1921	$C_{16}H_{31}O$	239.2376
$C_{12}H_{19}N_4O$	235.1560	$C_{16}H_{16}N_2$	236.1315	$C_{13}H_{26}N_4$	238.2160	$C_{16}H_{33}N$	239.2615
$C_{13}H_{15}O_4$	235.0970	$C_{16}H_{28}O$	236.2141	$C_{14}H_{10}N_2O_2$	238.0743	$C_{17}H_{19}O$	239.1436
$C_{13}H_{17}NO_3$	235.1209	$C_{16}H_{30}N$	236.2380	$C_{14}H_{12}N_3O$	238.0981	$C_{17}H_{21}N$	239.1675
$C_{13}H_{19}N_2O_2$	235.1447	$C_{17}H_{16}O$	236.1202	$C_{14}H_{14}N_4$	238.1220	$C_{17}H_{35}$	239.2740
$C_{13}H_{21}N_3O$	235.1686	$C_{17}H_{18}N$	236.1440	$C_{14}H_{22}O_3$	238.1569	$C_{18}H_{23}$	239.1801
$C_{13}H_{23}N_4$	235.1925	$C_{17}H_{32}$	236.2505	$C_{14}H_{24}NO_2$	238.1808	**240**	
$C_{14}H_9N_3O$	235.0746	$C_{18}H_{20}$	236.1566	$C_{14}H_{26}N_2O$	238.2046	$C_{11}H_{16}N_2O_4$	240.1111
$C_{14}H_{11}N_4$	235.0985	**237**		$C_{14}H_{28}N_3$	238.2285	$C_{11}H_{18}N_3O_3$	240.1349
$C_{14}H_{19}O_3$	235.1334	$C_{11}H_{13}N_2O_4$	237.0876	$C_{15}H_{10}O_3$	238.0630	$C_{11}H_{20}N_4O_2$	240.1588
$C_{14}H_{21}NO_2$	235.1573	$C_{11}H_{15}N_3O_3$	237.1114	$C_{15}H_{12}NO_2$	238.0868	$C_{12}H_8N_4O_2$	240.0648
$C_{14}H_{23}N_2O$	235.1811	$C_{11}H_{17}N_4O_2$	237.1353	$C_{15}H_{14}N_2O$	238.1107	$C_{12}H_{18}NO_4$	240.1236
$C_{14}H_{25}N_3$	235.2050	$C_{12}H_{15}NO_4$	237.1001	$C_{15}H_{16}N_3$	238.1346	$C_{12}H_{20}N_2O_3$	240.1475
$C_{15}H_9NO_2$	235.0634	$C_{12}H_{17}N_2O_3$	237.1240	$C_{15}H_{26}O_2$	238.1934	$C_{12}H_{22}N_3O_2$	240.1713
$C_{15}H_{11}N_2O$	235.0872	$C_{12}H_{19}N_3O_2$	237.1478	$C_{15}H_{28}NO$	238.2172	$C_{12}H_{24}N_4O$	240.1952

APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{13}H_8N_2O_3$	240.0535	$C_{15}H_{17}N_2O$	241.1342	$C_{17}H_{24}N$	242.1910	$C_{12}H_{24}N_2O_3$	244.1788
$C_{13}H_{10}N_3O_2$	240.0774	$C_{15}H_{19}N_3$	241.1580	$C_{18}H_{10}O$	242.0732	$C_{12}H_{26}N_3O_2$	244.2026
$C_{13}H_{12}N_4O$	240.1012	$C_{15}H_{29}O_2$	241.2168	$C_{18}H_{12}N$	242.0970	$C_{12}H_{28}N_4O$	244.2265
$C_{13}H_{20}O_4$	240.1362	$C_{15}H_{31}NO$	241.2407	$C_{18}H_{26}$	242.2036	$C_{13}H_{10}NO_4$	244.0610
$C_{13}H_{22}NO_3$	240.1600	$C_{15}H_{33}N_2$	241.2646	$C_{19}H_{14}$	242.1096	$C_{13}H_{12}N_2O_3$	244.0848
$C_{13}H_{24}N_2O_2$	240.1839	$C_{16}H_{17}O_2$	241.1229	**243**		$C_{13}H_{14}N_3O_2$	244.1087
$C_{13}H_{28}N_4$	240.2316	$C_{16}H_{19}NO$	241.1467	$C_{11}H_{19}N_2O_4$	243.1345	$C_{13}H_{16}N_4O$	244.1325
$C_{14}H_8O_4$	240.0422	$C_{16}H_{21}N_2$	241.1706	$C_{11}H_{21}N_3O_3$	243.1584	$C_{13}H_{24}O_4$	244.1675
$C_{14}H_{10}NO_3$	240.0661	$C_{16}H_{33}O$	241.2533	$C_{11}H_{23}N_4O_2$	243.1822	$C_{13}H_{26}NO_3$	244.1914
$C_{14}H_{12}N_2O_2$	240.0899	$C_{16}H_{35}N$	241.2771	$C_{12}H_7N_2O_4$	243.0406	$C_{13}H_{28}N_2O_2$	244.2152
$C_{14}H_{14}N_3O$	240.1138	$C_{17}H_{21}O$	241.1593	$C_{12}H_9N_3O_3$	243.0644	$C_{13}H_{30}N_3O$	244.2391
$C_{14}H_{16}N_4$	240.1377	$C_{17}H_{23}N$	241.1832	$C_{12}H_{11}N_4O_2$	243.0883	$C_{13}H_{32}N_4$	244.2629
$C_{14}H_{24}O_3$	240.1726	$C_{18}H_{25}$	241.1957	$C_{12}H_{21}NO_4$	243.1471	$C_{14}H_{12}O_4$	244.0735
$C_{14}H_{26}NO_2$	240.1965	**242**		$C_{12}H_{23}N_2O_3$	243.1710	$C_{14}H_{14}NO_3$	244.0974
$C_{14}H_{28}N_2O$	240.2203	$C_{11}H_{18}N_2O_4$	242.1267	$C_{12}H_{25}N_3O_2$	243.1948	$C_{14}H_{16}N_2O_2$	244.1213
$C_{14}H_{30}N_3$	240.2442	$C_{11}H_{20}N_3O_3$	242.1506	$C_{12}H_{27}N_4O$	243.2187	$C_{14}H_{18}N_3O$	244.1451
$C_{15}H_{12}O_3$	240.0786	$C_{11}H_{22}N_4O_2$	242.1744	$C_{13}H_9NO_4$	243.0532	$C_{14}H_{20}N_4$	244.1690
$C_{15}H_{14}NO_2$	240.1025	$C_{12}H_8N_3O_3$	242.0566	$C_{13}H_{11}N_2O_3$	243.0770	$C_{14}H_{28}O_3$	244.2039
$C_{15}H_{16}N_2O$	240.1264	$C_{12}H_{10}N_4O_2$	242.0805	$C_{13}H_{13}N_3O_2$	243.1009	$C_{14}H_{30}NO_2$	244.2278
$C_{15}H_{18}N_3$	240.1502	$C_{12}H_{20}NO_4$	242.1393	$C_{13}H_{15}N_4O$	243.1247	$C_{14}H_{32}N_2O$	244.2516
$C_{15}H_{28}O_2$	240.2090	$C_{12}H_{22}N_2O_3$	242.1631	$C_{13}H_{23}O_4$	243.1597	$C_{15}H_{16}O_3$	244.1100
$C_{15}H_{30}NO$	240.2329	$C_{12}H_{24}N_3O_2$	242.1870	$C_{13}H_{25}NO_3$	243.1835	$C_{15}H_{18}NO_2$	244.1338
$C_{15}H_{32}N_2$	240.2567	$C_{12}H_{26}N_4O$	242.2108	$C_{13}H_{27}N_2O_2$	243.2074	$C_{15}H_{20}N_2O$	244.1577
$C_{16}H_{16}O_2$	240.1151	$C_{13}H_8NO_4$	242.0453	$C_{13}H_{29}N_3O$	243.2312	$C_{15}H_{22}N_3$	244.1815
$C_{16}H_{20}N_2$	240.1628	$C_{13}H_{10}N_2O_3$	242.0692	$C_{13}H_{31}N_4$	243.2551	$C_{15}H_{32}O_2$	244.2403
$C_{16}H_{18}NO$	240.1389	$C_{13}H_{12}N_3O_2$	242.0930	$C_{14}H_{11}O_4$	243.0657	$C_{16}H_{10}N_3$	244.0876
$C_{16}H_{32}O$	240.2454	$C_{13}H_{14}N_4O$	242.1169	$C_{14}H_{13}NO_3$	243.0896	$C_{16}H_{20}O_2$	244.1464
$C_{16}H_{34}N$	240.2693	$C_{13}H_{22}O_4$	242.1518	$C_{14}H_{15}N_2O_2$	243.1134	$C_{16}H_{22}NO$	244.1702
$C_{17}H_{20}O$	240.1515	$C_{13}H_{24}NO_3$	242.1757	$C_{14}H_{17}N_3O$	243.1373	$C_{16}H_{24}N_2$	244.1941
$C_{17}H_{22}N$	240.1753	$C_{13}H_{26}N_2O_2$	242.1996	$C_{14}H_{19}N_4$	243.1611	$C_{17}H_{10}NO$	244.0763
$C_{17}H_{36}$	240.2819	$C_{13}H_{28}N_3O$	242.2234	$C_{14}H_{27}O_3$	243.1961	$C_{17}H_{12}N_2$	244.1001
$C_{18}H_{24}$	240.1879	$C_{13}H_{30}N_4$	242.2473	$C_{14}H_{29}NO_2$	243.2199	$C_{17}H_{24}O$	244.1828
241		$C_{14}H_{10}O_4$	242.0579	$C_{14}H_{31}N_2O$	243.2438	$C_{17}H_{26}N$	244.2067
$C_{11}H_{17}N_2O_4$	241.1189	$C_{14}H_{12}NO_3$	242.0817	$C_{14}H_{33}N_3$	243.2677	$C_{18}H_{12}O$	244.0888
$C_{11}H_{19}N_3O_3$	241.1427	$C_{14}H_{14}N_2O_2$	242.1056	$C_{15}H_{15}O_3$	243.1021	$C_{18}H_{14}N$	244.1127
$C_{11}H_{21}N_4O_2$	241.1666	$C_{14}H_{16}N_3O$	242.1295	$C_{15}H_{17}NO_2$	243.1260	$C_{18}H_{28}$	244.2192
$C_{12}H_{19}NO_4$	241.1315	$C_{14}H_{18}N_4$	242.1533	$C_{15}H_{19}N_2O$	243.1498	$C_{19}H_{16}$	244.1253
$C_{12}H_{21}N_2O_3$	241.1553	$C_{14}H_{26}O_3$	242.1883	$C_{15}H_{21}N_3$	243.1737	**245**	
$C_{12}H_{23}N_3O_2$	241.1791	$C_{14}H_{28}NO_2$	242.2121	$C_{15}H_{31}O_2$	243.2325	$C_{11}H_{21}N_2O_4$	245.1502
$C_{12}H_{25}N_4O$	241.2030	$C_{14}H_{30}N_2O$	242.2360	$C_{15}H_{33}NO$	243.2564	$C_{11}H_{23}N_3O_3$	245.1741
$C_{13}H_{11}N_3O_2$	241.0852	$C_{14}H_{32}N_3$	242.2598	$C_{16}H_{19}O_2$	243.1385	$C_{11}H_{25}N_4O_2$	245.1979
$C_{13}H_{13}N_4O$	241.1091	$C_{15}H_{14}O_3$	242.0943	$C_{16}H_{21}NO$	243.1624	$C_{12}H_9N_2O_4$	245.0563
$C_{13}H_{21}O_4$	241.1440	$C_{15}H_{16}NO_2$	242.1182	$C_{16}H_{23}N_2$	243.1863	$C_{12}H_{11}N_3O_3$	245.0801
$C_{13}H_{25}N_2O_2$	241.1679	$C_{15}H_{18}N_2O$	242.1420	$C_{17}H_{23}O$	243.1750	$C_{12}H_{13}N_4O_2$	245.1040
$C_{13}H_{25}N_2O_2$	241.1917	$C_{15}H_{20}N_3$	242.1659	$C_{17}H_{25}N$	243.1988	$C_{12}H_{23}NO_4$	245.1628
$C_{13}H_{27}N_3O$	241.2156	$C_{15}H_{30}O_2$	242.2247	$C_{18}H_{11}O$	243.0810	$C_{12}H_{25}N_2O_3$	245.1866
$C_{13}H_{29}N_4$	241.2394	$C_{15}H_{32}NO$	242.2485	$C_{18}H_{13}N$	243.1049	$C_{12}H_{27}N_3O_2$	245.2105
$C_{14}H_{11}NO_3$	241.0739	$C_{15}H_{34}N_2$	242.2724	$C_{18}H_{27}$	243.2114	$C_{12}H_{29}N_4O$	245.2343
$C_{14}H_{13}N_2O_2$	241.0978	$C_{16}H_{18}O_2$	242.1307	$C_{19}H_{15}$	243.1174	$C_{13}H_{11}NO_4$	245.0688
$C_{14}H_{15}N_3O$	241.1216	$C_{16}H_{20}NO$	242.1546	**244**		$C_{13}H_{13}N_2O_3$	245.0927
$C_{14}H_{17}N_4$	241.1445	$C_{16}H_{22}N_2$	242.1784	$C_{11}H_{20}N_2O_4$	244.1424	$C_{13}H_{15}N_3O_2$	245.1165
$C_{14}H_{25}O_3$	241.1804	$C_{16}H_{34}O$	242.2611	$C_{11}H_{22}N_3O_3$	244.1662	$C_{13}H_{17}N_4O$	245.1404
$C_{14}H_{27}NO_2$	241.2043	$C_{16}H_{18}O_2$	242.1307	$C_{11}H_{24}N_4O_2$	244.1901	$C_{13}H_{25}O_4$	245.1753
$C_{14}H_{29}N_2O$	241.2281	$C_{16}H_{20}NO$	242.1546	$C_{12}H_8N_2O_4$	244.0484	$C_{13}H_{27}NO_3$	245.1992
$C_{14}H_{31}N_3$	241.2520	$C_{16}H_{22}N_2$	242.1784	$C_{12}H_{10}N_3O_3$	244.0723	$C_{13}H_{29}N_2O_2$	245.2230
$C_{15}H_{13}O_3$	241.0865	$C_{16}H_{34}O$	242.2611	$C_{12}H_{12}N_4O_2$	244.0961	$C_{13}H_{31}N_3O$	245.2469
$C_{15}H_{15}NO_2$	241.1103	$C_{17}H_{22}O$	242.1871	$C_{12}H_{22}NO_4$	244.1549	$C_{14}H_{13}O_4$	245.0814

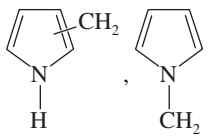
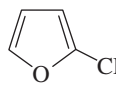
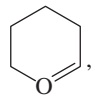
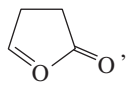
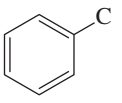
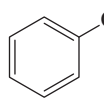
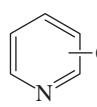
APPENDIX A (*Continued*)

FM		FM		FM		FM	
$C_{14}H_{15}NO_3$	245.1052	$C_{16}H_{26}N_2$	246.2098	$C_{12}H_{14}N_3O_3$	248.1036	$C_{15}H_{25}N_2O$	249.1968
$C_{14}H_{17}N_2O_2$	245.1291	$C_{17}H_{10}O_2$	246.0681	$C_{12}H_{16}N_4O_2$	248.1275	$C_{15}H_{27}N_3$	249.2207
$C_{14}H_{19}N_3O$	245.1529	$C_{17}H_{12}NO$	246.0919	$C_{12}H_{26}NO_4$	248.1863	$C_{16}H_{11}NO_2$	249.0790
$C_{14}H_{21}N_4$	245.1768	$C_{17}H_{14}N_2$	246.1158	$C_{12}H_{28}N_2O_3$	248.2101	$C_{16}H_{13}N_2O$	249.1029
$C_{14}H_{29}O_3$	245.2117	$C_{17}H_{26}O$	246.1985	$C_{13}H_{14}NO_4$	248.0923	$C_{16}H_{15}N_3$	249.1267
$C_{14}H_{31}NO_2$	245.2356	$C_{17}H_{28}N$	246.2223	$C_{13}H_{16}N_2O_3$	248.1162	$C_{16}H_{25}O_2$	249.1855
$C_{15}H_{17}O_3$	245.1178	$C_{18}H_{14}O$	246.1045	$C_{13}H_{18}N_3O_2$	248.1400	$C_{16}H_{27}NO$	249.2094
$C_{15}H_{19}NO_2$	245.1416	$C_{18}H_{16}N$	246.1284	$C_{13}H_{20}N_4O$	248.1639	$C_{16}H_{29}N_2$	249.2332
$C_{15}H_{21}N_2O$	245.1655	$C_{18}H_{30}$	246.2349	$C_{13}H_{28}O_4$	248.1988	$C_{17}H_{13}O_2$	249.0916
$C_{15}H_{23}N_3$	245.1894	$C_{19}H_{18}$	246.1409	$C_{14}H_{16}O_4$	248.1049	$C_{17}H_{15}NO$	249.1154
$C_{16}H_9N_2O$	245.0715	**247**		$C_{14}H_{20}N_2O_2$	248.1526	$C_{17}H_{17}N_2$	249.1393
$C_{16}H_{11}N_3$	245.0954	$C_{11}H_{23}N_2O_4$	247.1659	$C_{14}H_{22}N_3O$	248.1764	$C_{17}H_{29}O$	249.2219
$C_{16}H_{21}O_2$	245.1542	$C_{11}H_{25}N_3O_3$	247.1897	$C_{14}H_{24}N_4$	248.2003	$C_{17}H_{31}N$	249.2458
$C_{16}H_{23}NO$	245.1781	$C_{11}H_{27}N_4O_2$	247.2136	$C_{15}H_{10}N_3O$	248.0825	$C_{18}H_{17}O$	249.1280
$C_{16}H_{25}N_2$	245.2019	$C_{12}H_{11}N_2O_4$	247.0719	$C_{15}H_{12}N_4$	248.1063	$C_{18}H_{19}N$	249.1519
$C_{17}H_{11}NO$	245.0841	$C_{12}H_{13}N_3O_3$	247.0958	$C_{15}H_{20}O_3$	248.1413	$C_{18}H_{33}$	249.2584
$C_{17}H_{13}N_2$	245.1080	$C_{12}H_{15}N_4O_2$	247.1196	$C_{15}H_{22}NO_2$	248.1651	$C_{19}H_{21}$	249.1644
$C_{17}H_{25}O$	245.1906	$C_{12}H_{25}NO_4$	247.1784	$C_{15}H_{24}N_2O$	248.1890	**250**	
$C_{17}H_{27}N$	245.2145	$C_{12}H_{27}N_2O_3$	247.2023	$C_{15}H_{26}N_3$	248.2129	$C_{11}H_{26}N_2O_4$	250.1894
$C_{18}H_{13}O$	245.0967	$C_{12}H_{29}N_3O_2$	247.2261	$C_{16}H_{10}NO_2$	248.0712	$C_{12}H_{14}N_2O_4$	250.0954
$C_{18}H_{15}N$	245.1205	$C_{13}H_{13}NO_4$	247.0845	$C_{16}H_{12}N_2O$	248.0950	$C_{12}H_{16}N_3O_3$	250.1193
$C_{18}H_{29}$	245.2270	$C_{13}H_{15}N_2O_3$	247.1083	$C_{16}H_{14}N_3$	248.1189	$C_{12}H_{18}N_4O_2$	250.1431
$C_{19}H_{17}$	245.1331	$C_{13}H_{17}N_3O_2$	247.1322	$C_{16}H_{24}O_2$	248.1777	$C_{13}H_{16}NO_4$	250.1080
246		$C_{13}H_{19}N_4O$	247.1560	$C_{16}H_{26}NO$	248.2015	$C_{13}H_{18}N_2O_3$	250.1318
$C_{11}H_{22}N_2O_4$	246.1580	$C_{13}H_{27}O_4$	247.1910	$C_{16}H_{28}N_2$	248.2254	$C_{13}H_{20}N_3O_2$	250.1557
$C_{11}H_{24}N_3O_3$	246.1819	$C_{13}H_{29}NO_3$	247.2148	$C_{17}H_{12}O_2$	248.0837	$C_{13}H_{22}N_4O$	250.1795
$C_{11}H_{26}N_4O_2$	246.2057	$C_{14}H_{15}O_4$	247.0970	$C_{17}H_{14}NO$	248.1076	$C_{14}H_{10}N_4O$	250.0856
$C_{12}H_{10}N_2O_4$	246.0641	$C_{14}H_{17}NO_3$	247.1209	$C_{17}H_{16}N_2$	248.1315	$C_{14}H_{20}NO_3$	250.1444
$C_{12}H_{12}N_3O_3$	246.0879	$C_{14}H_{19}N_2O_2$	247.1448	$C_{17}H_{28}O$	248.2141	$C_{14}H_{22}N_2O_2$	250.1682
$C_{12}H_{14}N_4O_2$	246.1118	$C_{14}H_{21}N_3O$	247.1686	$C_{17}H_{30}N$	248.2380	$C_{14}H_{24}N_3O$	250.1921
$C_{12}H_{24}NO_4$	246.1706	$C_{14}H_{23}N_4$	247.1925	$C_{18}H_{16}O$	248.1202	$C_{14}H_{26}N_4$	250.2160
$C_{12}H_{26}N_2O_3$	246.1945	$C_{15}H_9N_3O$	247.0746	$C_{18}H_{18}N$	248.1440	$C_{15}H_{10}N_2O_2$	250.0743
$C_{12}H_{28}N_3O_2$	246.2183	$C_{15}H_{11}N_4$	247.0985	$C_{18}H_{32}$	248.2505	$C_{15}H_{12}N_3O$	250.0981
$C_{12}H_{30}N_4O$	246.2422	$C_{15}H_{19}O_3$	247.1334	$C_{19}H_{20}$	248.1566	$C_{15}H_{14}N_4$	250.1220
$C_{13}H_{12}NO_4$	246.0766	$C_{15}H_{21}NO_2$	247.1573	**249**		$C_{15}H_{22}O_3$	250.1569
$C_{13}H_{14}N_2O_3$	246.1005	$C_{15}H_{23}N_2O$	247.1811	$C_{11}H_{25}N_2O_4$	249.1815	$C_{15}H_{24}NO_2$	250.1808
$C_{13}H_{16}N_3O_2$	246.1244	$C_{15}H_{25}N_3$	247.2050	$C_{11}H_{27}N_3O_3$	249.2054	$C_{15}H_{26}N_2O$	250.2046
$C_{13}H_{18}N_4O$	246.1482	$C_{16}H_{11}N_2O$	247.0872	$C_{12}H_{13}N_2O_4$	249.0876	$C_{15}H_{28}N_3$	250.2285
$C_{13}H_{26}O_4$	246.1832	$C_{16}H_{13}N_3$	247.1111	$C_{12}H_{15}N_3O_3$	249.1114	$C_{16}H_{10}O_3$	250.0630
$C_{13}H_{28}NO_3$	246.2070	$C_{16}H_{23}O_2$	247.1699	$C_{12}H_{17}N_4O_2$	249.1353	$C_{16}H_{12}NO_2$	250.0868
$C_{13}H_{30}N_2O_2$	246.2309	$C_{16}H_{25}NO$	247.1937	$C_{12}H_{27}NO_4$	249.1941	$C_{16}H_{14}N_2O$	250.1107
$C_{14}H_{14}O_4$	246.0892	$C_{16}H_{27}N_2$	247.2176	$C_{13}H_{15}NO_4$	249.1001	$C_{16}H_{16}N_3$	250.1346
$C_{14}H_{16}NO_3$	246.1131	$C_{17}H_{11}O_2$	247.0759	$C_{13}H_{17}N_2O_3$	249.1240	$C_{16}H_{26}O_2$	250.1934
$C_{14}H_{18}N_2O_2$	246.1369	$C_{17}H_{13}NO$	247.0998	$C_{13}H_{19}N_3O_2$	249.1478	$C_{16}H_{28}NO$	250.2172
$C_{14}H_{20}N_3O$	246.1608	$C_{17}H_{15}N_2$	247.1236	$C_{13}H_{21}N_4O$	249.1717	$C_{16}H_{30}N_2$	250.2411
$C_{14}H_{22}N_4$	246.1846	$C_{17}H_{27}O$	247.2063	$C_{14}H_9N_4O$	249.0777	$C_{17}H_{14}O_2$	250.0994
$C_{l4}H_{30}O_3$	246.2196	$C_{17}H_{29}N$	247.2301	$C_{14}H_{17}O_4$	249.1127	$C_{17}H_{16}NO$	250.1233
$C_{15}H_{10}N_4$	246.0907	$C_{18}H_{15}O$	247.1123	$C_{14}H_{19}NO_3$	249.1365	$C_{17}H_{18}N_2$	250.1471
$C_{15}H_{18}O_3$	246.1256	$C_{18}H_{17}N$	247.1362	$C_{14}H_{21}N_2O_2$	249.1604	$C_{17}H_{30}O$	250.2298
$C_{15}H_{20}NO_2$	246.1495	$C_{18}H_{31}$	247.2427	$C_{14}H_{23}N_3O$	249.1842	$C_{17}H_{32}N$	250.2536
$C_{15}H_{22}N_2O$	246.1733	$C_{19}H_{19}$	247.1488	$C_{14}H_{25}N_4$	249.2081	$C_{18}H_{18}O$	250.1358
$C_{15}H_{24}N_3$	246.1972	**248**		$C_{15}H_9N_2O_2$	249.0664	$C_{18}H_{20}N$	250.1597
$C_{16}H_{10}N_2O$	246.0794	$C_{11}H_{24}N_2O_4$	248.1737	$C_{15}H_{11}N_3O$	249.0903	$C_{18}H_{34}$	250.2662
$C_{16}H_{12}N_3$	246.1032	$C_{11}H_{26}N_3O_3$	248.1976	$C_{15}H_{13}N_4$	249.1142	$C_{19}H_{22}$	250.1722
$C_{16}H_{22}O_2$	246.1620	$C_{11}H_{28}N_4O_2$	248.2214	$C_{15}H_{21}O_3$	249.1491		
$C_{16}H_{24}NO$	246.1859	$C_{12}H_{12}N_2O_4$	248.0797	$C_{15}H_{23}NO_2$	249.1730		

APPENDIX B COMMON FRAGMENT IONS

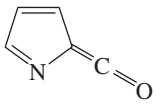
All fragments listed bear +1 charges. To be used in conjunction with Appendix C. Not all members of homologous and isomeric series are given. The list is meant to be suggestive rather than exhaustive. Appendix II of Hamming and Foster (1972), Table A-7 of McLafferty and Turecek's (1993) interpretative book, and the high-resolution ion data of McLafferty and Venkataraghavan (1982) are recommended as supplements.

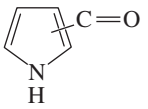
***m/z* Ions**[a]

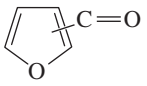
14 CH_2
15 CH_3
16 O
17 OH
18 H_2O, NH_4
19 F, H_3O
26 $C{\equiv}N$, C_2H_2
27 C_2H_3
28 C_2H_4, CO, N_2 (air), $CH{=}NH$
29 C_2H_5, CHO
30 CH_2NH_2, NO
31 CH_2OH, OCH_3
32 O_2 (air)
33 SH, CH_2F
34 H_2S
35 ^{35}Cl[b]
36 $H^{35}Cl$[b]
39 C_3H_3
40 $CH_2C{=}N$, Ar (air)
41 C_3H_5, $CH_2C{=}N$ + H, C_2H_2NH
42 C_3H_6, C_2H_2O
43 C_3H_7, $CH_3C{=}O$, C_2H_5N
44 $CH_2C(=O)H$ + H, CH_3CHNH_2, CO_2 (air), $NH_2C{=}O$, $(CH_3)_2N$
45 $CH_3CH(OH)$, CH_2CH_2OH, CH_2OCH_3, $C(=O)OH$
46 NO_2
47 CH_2SH, CH_3S
48 CH_3S + H
49 $CH_2{}^{35}Cl$[b]
51 CH_2F_2, C_4H_3
53 C_4H_5
54 $CH_2CH_2C{\equiv}N$
55 C_4H_7, $CH_2{=}CHC{=}O$
56 C_4H_8
57 C_4H_9, $C_2H_5C{=}O$
58 $CH_3C(=O)CH_2$ + H, $C_2H_5CHNH_2$, $(CH_3)_2NCH_2$, $C_2H_5NHCH_2$, C_2H_5S
59 $(CH_3)_2COH$, $CH_2OC_2H_5$, CO_2CH_3, $NH_2C(=O)CH_2$ + H, CH_3OCHCH_3, CH_3CHCH_2OH, C_2H_5CHOH
60 CH_2CO_2H + H, CH_2ONO
61 CH_3CO_2 + 2H, CH_2CH_2SH, CH_2SCH_3
65 C_5H_5
66 H_2S_2,  $\equiv C_5H_6$
67 C_5H_7
68 $CH_2CH_2CH_2C{\equiv}N$
69 C_5H_9, CF_3, $CH_3CH{=}CHC{=}O$, $CH_2{=}C(CH_3)C{=}O$
70 C_5H_{10}
71 C_5H_{11}, $C_3H_7C{=}O$
72 $C_2H_5C(=O)CH_2$ + H, $C_3H_7CHNH_2$, $(CH_3)_2N{=}C{=}O$, $C_2H_5NHCHCH_3$ and isomers
73 Homologs of 59, $(CH_3)_3Si$
74 $CH_2CO_2CH_3$ + H
75 $CO_2C_2H_5$ + 2H, $C_2H_5CO_2$ + 2H, $CH_2SC_2H_5$, $(CH_3)_2CSH$, $(CH_3O)_2CH$, $(CH_3)_2SiOH$
76 C_6H_4 (C_6H_4XY)
77 C_6H_5 (C_6H_5X)
78 C_6H_5 + H
79 C_6H_5 + 2H, ^{79}Br[b]
80 CH_3SS + H, $H^{79}Br$[b], 
81  CH_2, C_6H_9
82 $(CH_2)_4C{\equiv}N$, C_6H_{10}, $C^{35}Cl_2$[b]
83 C_6H_{11}, $CH^{35}Cl_2$[b], 
85  ,  , C_6H_{13}, $C_4H_9C{=}O$, $Cl^{35}ClF_2$[b]
86 $C_3H_7C(=O)CH_2$ + H, $C_4H_9CHNH_2$ and isomers
87 $C_3H_7CO_2$, Homologs of 73, $CH_2CH_2CO_2CH_3$
88 $CH_2CO_2C_2H_5$ + H
89 $CO_2C_3H_7$ + 2H, 
90  , CH_3CHONO_2
91 $(C_6H_5)CH_2$, $(C_6H_5)CH$ + H, $(C_6H_5)C$ + 2H, $(CH_2)_4{}^{35}Cl$[b], $(C_6H_5)N$
92  CH_2, $(C_6H_5)CH_2$ + H

APPENDIX B (*Continued*)

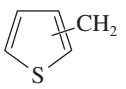
***m/z* Ions**[a]

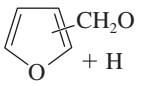
93 $CH_2{}^{79}Br$[b], C_7H_9, $(C_6H_5)O$, 

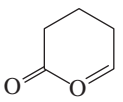
94 $(C_6H_5)O$ + H, 

95 

96 $(CH_2)_5C{\equiv}N$

97 C_7H_{13}, 

98 

99 C_7H_{15}, $C_6H_{11}O$, 

100 $C_4H_9C(=O)CH_2$ + H, $C_5H_{11}CHNH_2$

101 $CO_2C_4H_9$

102 $CH_2CO_2C_2H_7$ + H

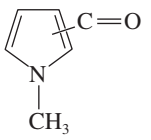
103 $CO_2C_4H_9$ + 2H, $C_5H_{11}S$, $CH(OCH_2CH_3)_2$

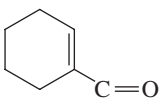
104 $C_2H_5CHONO_2$

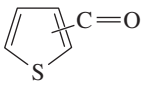
105 $C_6H_5C{=}O$, $C_6H_5CH_2CH_2$, $C_6H_5CHCH_3$

106 $C_6H_5NHCH_2$

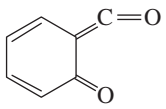
107 $C_6H_5CH_2O$, $HO(C_6H_4)CH_2$, $C_2H_4{}^{79}Br$[b]

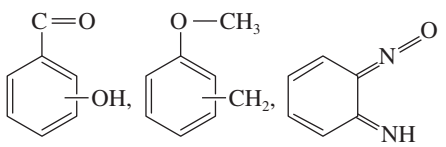
108 $C_6H_5CH_2O$ + H, 

109 

111 

119 CF_3CF_2, $(C_6H_5)C(CH_3)_2$, $CH_3CH(C_6H_4)CH_3$, $CO(C_6H_4)CH_3$

120 

121 C_9H_{13}, 

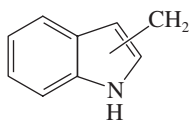
122 $C_6H_5CO_2$ + H

123 $F(C_6H_4)C{=}O$, $C_6H_5CO_2$ + 2H

125 C_6H_5SO

127 I

128 HI

130 

131 C_3F_5, $C_6H_5CH{=}CHC{=}O$

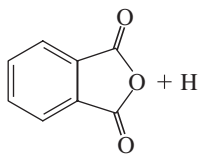
135 $(CH_2)_4{}^{79}Br$[b]

138 $CO_2(C_6H_4)OH$ + H

139 $^{35}Cl(C_6H_4)C{=}O$[b]

141 CH_2I

147 $(CH_3)_2Si{=}O{-}Si(CH_3)_3$

149 

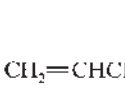
154 $(C_6H_5)_2$

[a] Ions indicated as a fragment + *n*H (*n* + 1,2,3, . . .) are ions that arise via rearrangement involving hydrogen transfer.

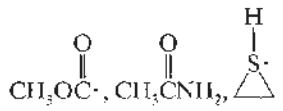
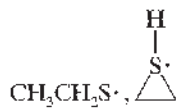
[b] Only the more abundant isotope is indicated.

APPENDIX C COMMON FRAGMENTS LOST

This list is suggestive rather than comprehensive. It should be used in conjunction with Appendix B. Table 5-19 of Hamming and Foster (1972) and Table A-5 of McLafferty and Turecek (1993) are recommended as supplements. All of these fragments are lost as neutral species.

Molecular Ion Minus	Fragment Lost (Inference Structure)
1	H·
2	2H·
15	CH_3·
16	O ($ArNO_2$, amine oxides, sulfoxides); ·NH_2 (carboxamides, sulfonamides)
17	HO·
18	H_2O (alcohols, aldehydes, ketones)
19	F·
20	HF
26	CH≡CH, ·C≡N
27	CH_2=CH·, HC≡N (aromatic nitrites, nitrogen heterocycles)
28	CH_2=CH_2, CO, (quinones) (HCN + H)
29	CH_3CH_2·, (ethyl ketones, $ArCH_2CH_2CH_3$), ·CHO
30	NH_2CH_2·, CH_2O ($ArOCH_3$), NO ($ArNO_2$), C_2H_6
31	·OCH_3(methyl esters), ·CH_2OH, CH_3NH_2
32	CH_3OH, S
33	HS· (thiols), (·CH_3 and H_2O)
34	H_2S (thiols)
35	Cl·
36	HCl, $2H_2O$
37	H_2Cl (or HCl + H)
38	C_3H_2, C_2N, F_2
39	C_3H_3, HC_2N
40	CH_3C≡CH
41	CH_2=$CHCH_2$·
42	CH_2=$CHCH_3$, CH_2=C=O,  CH_2, NCO, $NCNH_2$
43	C_3H_7· (propyl ketones, $ArCH_2$—C_3H_7), CH_3  · (methyl ketones, CH_3  G, where G = various functional groups), CH_2=CH—O·, (CH_3· and CH_2=CH_2), HCNO
44	CH_2=CHOH, CO_2 (esters, anhydrides), N_2O, $CONH_2$, $NHCH_2CH_3$
45	CH_3CHOH, CH_3CH_2O· (ethyl esters), CO_2H, $CH_3CH_2NH_2$
46	(H_2O and CH_2=CH_2), CH_3CH_2OH, ·NO_2 ($ArNO_2$)
47	CH_3S·
48	CH_3SH, SO (sulfoxides), O_3
49	·CH_2Cl
51	·CHF_2
52	C_4H_4, C_2N_2
53	C_4H_5
54	CH_2=CH—CH=CH_2
55	CH_2=$CHCHCH_3$

APPENDIX C (*Continued*)

Molecular Ion Minus	Fragment Lost (Inference Structure)
56	$CH_2{=}CHCH_2CH_3$, $CH_3CH{=}CHCH_3$, 2CO
57	$C_4H_9\cdot$ (butyl ketones), C_2H_5CO (ethyl ketones, EtC=OG, G = various structural units)
58	$\cdot NCS$, (NO + CO), CH_3COCH_3, C_4H_{10}
59	$CH_3OC\cdot$, CH_3CNH_2, 
60	C_3H_7OH, $CH_2{=}C(OH)_2$ (acetate esters)[a]
61	$CH_3CH_2S\cdot$, 
62	(H_2S and $CH_2{=}CH_2$)
63	$\cdot CH_2CH_2Cl$
64	C_5H_4, S_2, SO_2
68	$CH_2{=}C(CH_3){-}CH{=}CH_2$
69	$CF_3\cdot$, $C_5H_9\cdot$
71	$C_5H_{11}\cdot$
73	$CH_3CH_2OC\cdot$
74	C_4H_9OH
75	C_6H_3
76	C_6H_4, CS_2
77	C_6H_5, CS_2H
78	C_6H_6, CS_2H_2, C_5H_4N
79	$Br\cdot$, C_5H_5N
80	HBr
85	$\cdot CClF_2$
100	$CF_2{=}CF_2$
119	$CF_3{-}CF_2\cdot$
122	C_6H_5COOH
127	$I\cdot$
128	HI

[a] McLafferty rearrangement.