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Mass Spectrometry

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Mass spectrometry has a Janus-like quality in embracing and pursuing both the roles of chemical reactor and analytical instrument. Mass spectrometry in its guise of chemical reactor is probing at ever deeper levels the nature of the chemical reactivity of (radical-)ions. As one of the most sensitive of analytical techniques, mass spectrometry is at the forefront of applied science seeking to rationalize the phenomenological universe at the atomic and molecular level. We have organized the present review according to this duality. Following our initial section discussing techniques, instruments, and computers, we make sharp distinction between the chemistry of organic (radical-)ions and analytical applications in bioorganic chemistry and medicine. The sheer enormity of the number of publications in mass spectrometry, which exceeds 20,000 in the two years 1972 and 1973, demands that we restrict the scope of this review. We choose to

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Robert E. Cox obtained his BSc (Honors Chemistry) at the Queen's University of Belfast in 1966. He then worked for a period with the British Petroleum Co. studying the composition of lipids of microorganisms grown on petroleum fractions. Further academic study and research on the chemistry and geochemistry of acyclic isoprenoid compounds under J. R. Maxwell and G. Eglinton gained for him the degree of PhD from the University of Bristol in 1972. After finishing further research work on the geochemistry of lipids, he joined the staff of the Space Sciences Laboratory, University of California, Berkeley, in 1973. His current interests lie in the application of mass spectrometric techniques to problems in biomedicine.

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cover the chemistry of organic (radical-)ions at the expense of inorganic, organometallic, and surface ion chemistry, since it is the area in which the general principles of gas-phase ion chemistry tend to originate and to develop and in which there has been the largest investment of time, money, and human effort. We choose to cover biochemistry and medicine because of their contemporary importance and because of the stupendous contributions of mass spectrometry to these fields in the past two years. We are also guided in our choice by our own experience and interest. Even though the combined experience of the present three reviewers is wide and diverse, there are still large areas of mass spectrometry in which not one of us has specialist knowledge. We have sought to review in detail the mass spectrometry of natural products, primarily because they illustrate a comprehensive variety of structural types. Compounds tend to be surveyed in biosynthetic rather than chemical categories. We believe our literature search has been close to exhaustive in these areas; however, the number of papers was far too large for all to be usefully included in this review. We have, therefore, emphasized review articles, newer instrumental methods and techniques, fragmentation studies, and extensive reports of mass spectral data. A section is devoted to biomedicine where mass spectrometry is on the verge of extensive clinical application. Mass spectrometry in environmental problems is covered briefly, since a review is in preparation (*1273*). Our literature coverage extends from that previously covered (*267*) (December 1971) up to the most recent issues of journals available at the University of California, Berkeley, as of January 10, 1974. For journals published in the United States or Canada, this generally means coverage up to December 1973. Coverage of European journals is typically up to October or November 1973. We have also included some papers published before December 1971 having special significance to fields of inquiry which were particularly active or important in this two-year period.

The emphasis in our review of gas-phase organic ion chemistry is placed strongly on studies making significant contributions to the understanding of ion chemistry. We cover unimolecular isomerization and decomposition, ion-molecule processes, equilibria and clustering, and techniques of importance. Recent advances in understanding of unimolecular processes have made increasingly clear the necessity of *defining or measuring internal energies and lifetimes of reactant ions*. Gas-phase ion chemistry is now at the stage of measuring the kinetics and energetics for the first few of the myriad of unimolecular processes identified in the past few decades. Stable ion structures are being determined with some degree of certainty and processes are beginning to be discussed in more reliable mechanistic detail. Appearance potential measurements with energy-resolved electron beams, charge exchange tandem mass spectrometry, collision-induced decomposition, crossed beam studies, field ionization kinetics, ion cyclotron resonance, kinetic energy release studies, photoion-photoelectron coincidence studies, and pulsed electron beam trapping studies are methods making important contributions toward understanding unimolecular processes.

It is clear that gas-phase ion chemistry has much to offer in providing answers to problems addressed by traditional physical organic chemistry. Mechanistic analogies between gas- and liquid-phase processes have been studied for some time—*e.g.*, Norrish type II photochemical reaction. Recently, thermodynamic properties determined for gas-phase ionic equilibria have been combined with appropriate solution properties, allowing the latter to be separated into intrinsic and solvation contributions. The results reveal startlingly large solvation contributions. The gas-phase order of amine basicities, for example, follows the inductive effect order revealing that the anomalous order of basicities in solution is due to solvation effects (*43*). The intrinsic order of alcohol acidities has been shown to be the reverse of that measured in solution (*216*); again, solvation is responsible. Gas-phase measurements have shown toluene to be an intrinsically stronger acid than water (*216*). Moreover, solvation itself has been studied directly in the gas-phase (*837, 838*) and thermodynamic properties have been determined for the solvation reactions. We have covered these studies, which often use ion cyclotron resonance or pulsed high pressure mass spectrometers, in some detail.

"Metastable Ions" by Cooks, Beynon, Caprioli, and Lester (*344*) is one of the better books to appear on gas-phase ion chemistry since Field and Franklin (*506*). It contains well-written detailed discussions of theory of

mass spectra, mechanisms, ion structures, energy partitioning, and instrumentation. "Theory of Unimolecular Reactions" by Forst (*519*) is an excellent book giving a detailed description of the theory of mass spectra from the point of view of the chemical kineticist. Unimolecular reactions are also discussed theoretically by Robinson and Holbrook (*1281*). "Biochemical Applications of Mass Spectrometry" edited by Waller (*1563*) remains unparalleled for authority and comprehensive coverage of bioorganic chemistry. McFadden (*1132*) has written an excellent and comprehensive text on gas chromatography–mass spectrometry. Costa and Holmstedt's volume (*350*) on gas chromatography–mass spectrometry in neurobiology is recommended in particular for its authoritative presentation of the mass fragmentography technique. A number of good books have appeared on the theory and interpretation of organic mass spectra, including a second edition of "Interpretation of Mass Spectra" by McLafferty (*1139*), "Introduction to Mass Spectrometry" by Hill (*670*), "Interpretation of Mass Spectra of Organic Compounds" by Hamming and Foster (*628*), "Mass Spectrometry for Organic Chemists" by Johnstone (*797*), and "Principles of Organic Mass Spectrometry" by Williams and Howe (*1594*). Biemann (*154*) has reviewed the elucidation of organic structures by mass spectroscopy. The mass spectra of heterocyclic compounds are comprehensively reviewed in the book by Porter and Baldas (*1203*). An unusually good collection of chapters has been assembled by Maccoll (*1012*) for the volume entitled "Mass Spectrometry" in the MTP International Review Science Series One. Especially recommended are the chapters on Theory of Mass Spectra (Wahrhaftig), Field Ionization (Robertson), Chemical Ionization (Field), Ion Cyclotron Resonance (Drewery, Good, Jennings) and Metastable Ions (Holmes, Benoit). Another volume in the MTP International Review of Science Series Two, again edited by Maccoll (*1013*), should appear in 1974. The volume in the MTP Series One entitled "Chemical Kinetics" edited by Polanyi (*1236*) contains chapters on mass spectrometry, in particular a discussion of unimolecular gas-phase reactions of polyatomic ions by Setser. The comprehensive two-volume set on ion-molecule reactions edited by Franklin (*527*) was described in the 1972 review (*267*). A second volume entitled "Mass Spectrometry" in the Chemical Society's Specialist Periodical Report Series edited by Williams (*1593*) has appeared with chapters by many of the authors contributing to the first volume (*1592*). The overall standard remains high, although there are still chapters which satisfy neither the criteria of authority nor of comprehensiveness in coverage. The mass spectrometry of inorganic and organometallic compounds is comprehensively covered in a book by Litzow and Spalding (*989*) and in the review by Bruce (*253*). Surface ionization is covered by Ionov (*753*). Most recent measurements of atomic masses and fundamental constants are presented by Sanders and Wapstra (*1318*). Spark source mass spectrometry has been reviewed (*251*). The volume edited by Price (*1248*) contains reviews on time-of-flight techniques, in particular on the combination of time-of-flight mass spectrometry and flash photolysis (*987*). The last chapter of this volume seems out of context. Radiofrequency quadrupole mass spectrometry has been reviewed by Lawson and Todd (*945*). Ahearn (*12*) has discussed trace analysis by mass spectrometry. Listing of the literature is provided by the *Mass Spectrometry Bulletin* published monthly from Aldermaston, England (*1035*). The coverage is exhaustive even for Russian and Japanese journals; however, in our experience, the paper titles are useful but the limited keyword listings are of little value. In preparing this review, we used the *Mass Spectrometry Bulletin* only as a listing of titles, for which purpose the Bulletin's coverage is slow when compared to *Current Contents* (*364*). We would suggest that the *Bulletin's* abstracts be made more informative. The most significant papers in mass spectrometry from the point of view of gas-phase ion chemistry tend to appear in *Journal of the American Chemical Society* (*805*), where they number about two per issue (50–60 per volume). Significant papers on physical aspects of gas-phase ion chemistry sometimes appear in *Journal of Chemical Physics* (*806*). Many important papers from the analytical viewpoint appear in *Analytical Chemistry*. Two international journals are devoted entirely to mass spectrometry; these are *International Journal of Mass Spectrometry and Ion Physics* (*751*) and *Organic Mass Spectrometry* (*1188*). A third, *Biomedical Mass Spectrometry* (*158*), will appear in 1974; the necessity and role of this journal is not at all clear. The Mass Spectroscopy Society of Japan publishes a journal entitled *Mass Spectroscopy* in the Japanese language (*1036*).

The major conferences for mass spectrometrists remain the International Conferences now held triennially in Europe and the Annual Conferences on Mass Spectrometry and Allied Topics held in the United States. The 6th International Conference was held in Edinburgh on September 10–14, 1973, and the proceedings will appear as "Advances in Mass Spectrometry, Volume 6," edited by A. R. West (*752*). Hopefully, the volume will be indexed. Proceedings of the American meetings, the 20th of which was held on June 4–10, 1972, in Dallas, Texas, and the 21st on May 20–25, 1973, in San Francisco, Calif., are only produced for delegates and members of the American Society for Mass Spectrometry, and are not presented in the open literature. An important international conference organized by the Mass Spectroscopy Society of Japan was held in Kyoto, Japan, in 1969, and the proceedings were published in 1970 under the title "Recent Developments in Mass Spectroscopy," edited by K. Ogata and T. Hayakawa (*1179*). We hope this meeting is the charter of a new series. An International Symposium on Mass Spectrometry in Biochemistry and Medicine was held in May 1973 in Milan, Italy, and an International Symposium on Gas Chromatography–Mass Spectrometry in May 1972 was held on the Isle of Elba, Italy. There was a session on mass spectrometry at the 9th International Congress of Biochemistry in Stockholm, Sweden, July 1973. National mass spectrometry meetings are held annually in the United Kingdom, West Germany, and Japan. Significant papers on mass spectrometry appeared at the National (*26*) and in many of the divisional meetings of the American Chemical Society and at the Pittsburgh Conference on Analytical Chemistry and Applied Spectroscopy (*1233*). A view of the politics of organizing mass spectrometry conferences has been given by Reed (*1257*).

The advent of several commercially available ion microprobe instruments has begun to heighten interest in the scope of possible applications for the use of ion beams for production of secondary ion ejection, characteristic of the elemental and isotopic composition of three-dimensional surface layers of matter. An excellent discussion of the history and outlook of these techniques has just appeared (*966*). Cameca, Applied Research Laboratory, Hitachi, and AEI have various versions of such instruments on the market which vary from $300 K to less than $100 K, one of which has sophisticated secondary ion mass analysis ion optics of the Mattauch–Herzog geometry (AEI MS-7). For details, the reviews of Honig (*702*), Hurley (*736*) concerning ion production, acceleration, focusing, analysis, beam handling and detection, Liebl (*966*) and Andersen (*29*) should be consulted. The review of Liebl (*966*) mentioned above is an indication of the excellent series which appear monthly in *Analytical Chemistry*. These articles have been collected and augmented for a five-year period by Senzel (*1355*) and are available as a single volume, "Instrumentation in Analytical Chemistry."

An extensive and highly significant field of mass spectrometry involves information which may be obtained through the accurate measurements of the isotopic composition of elements throughout the periodic table. Development of techniques of isotopic mass spectrometry which are aimed at maximization of sensitivity and ultra-high accuracy has been spurred over the past few years as a result of the return of lunar samples by the U.S. Apollo program and the U.S.S.R. Luna 16 and 20 missions. Studies of ages (geochronology), neutron fluences, and elemental analyses benefit enormously from these measurements.

Studies of mass spectrometry of major, minor, and trace element composition, volatile light elements, radiometric age determinations, rare gas chemistry, radionuclides, solar wind and cosmic rays as well as atmosphere and particles and neutron fluences have been reported in the 4th Lunar Science Conference *Proceedings* (3290 pp) (*1249*). References in particular papers therein document the ana-

lytical mass spectrometric techniques employed in the previous nine volumes which report the first three conferences. Particularly impressive reports, made possible through sensitivity improvements directly resulting from the Apollo program, are the special U.S.S.R. Luna 20 issues of *Geochimica et Cosmochimica Acta* (*565*) and *Earth and Planetary Science Letters* (*1007*). A total weight of 623 mg of U.S.S.R. Luna 20 sample was allocated to U.S. investigators to carry out the research presented in 43 papers therein.

Two further exciting reports in cosmochemistry have just appeared which indicate the immense power of isotopic studies in probing the nature of our own solar system and universe. The first was carried out by Clayton, Grossman, and Mayeda (*326*) on the isotopic composition of anhydrous, high-temperature minerals in carbonaceous meteorites measured as CO_2. It was shown that this oxygen was strongly depleted in ^{17}O and ^{18}O compared with all previously studied materials, indicating an admixture with an almost pure ^{16}O component. It is suggested that such a component is indicative of matter of a distinct nucleosynthetic origin, possibly predating our solar system, representing interstellar dust. The second paper, by Gray, Papanastassiou and Wasserburg, (*588*), demonstrates that some inclusions rich in refractory elements in the same meteorite (Pueblito de Allende) contain the lowest and hence most primitive $^{87}Sr/^{86}Sr$ ratio *yet observed*. This observation, possible only because of the remarkable ultra-high precision of this group's computerized mass spectrometry techniques, suggests that these inclusions condensed from the solar nebula earlier than any other material *previously studied*.

TECHNIQUES, INSTRUMENTS, AND COMPUTERS

Innovative Techniques and Instruments. Majer (*1024*) has presented a 32-page review of the basic theory, instrumentation, and application of mass spectrometry with special reference to the development of the equipment and its impact on the scope of application. It is recommended reading.

A new technique for the identification and characterization of neutral fragments formed by electron impact on gaseous molecules has been discussed by Svec and coworkers (*1258, 1504*). A method of multi-channel analysis of ions blown off laser produced plasma is described using a time-of-flight principle (*1190*). Primary processes of photolysis of 1,1′-azopropane have been reported using a high intensity light beam and a collision-free photochemical reactor incorporated into the source of a mass spectrometer (*1623*). A discussion of the validity of plasma chromatographic mass mobility correlations has appeared (*595*). A theoretical study has demonstrated the possibility of a new type of dynamic mass spectrometry for the analysis of macromolecules (*1202*). A method has been proposed which uses deflection plates to act as a mass separator that may be capable of high sensitivity since the repetition frequency is only dependent upon the transit time of the heaviest ion through the deflection plates (*74*). Double beam mass spectrometry has been discussed further, particularly in relation to obtaining accurate mass measurements using ionization techniques where use of an internal standard becomes difficult or impossible or where maximum sample sensitivity in the ion source is required. In the former case, chemical ionization (CI), field ionization (FI), and field desorption (FD) (*52*) present such calibration difficulties using perfluorokerosene.

Mass measurement accuracy using a 21-110B mass spectrometer with a commercial data system AEI DS-30 has been presented (*573*). Unfortunately, these authors have not chosen to enlighten the reader on meaningful assessment of the performance of this mass spectrometer and computer system except by matching the vendor's specifications. This does little to aid a reader's understanding of why the mass measurements obtained show the reported lack of analytical precision. Operational parameters such as sample flow rate, scan rate per decade, dynamic instrument resolution, effective digitization rate, etc., are difficult to ascertain and no mention is made of exactly analogous results obtained using other systems (*264, 271*). Hilmer and Taylor (*671*) have described a high resolution mass spectrometry system with data acquisition on a Raytheon 706 computer and reduction and processing on a Univac 1108. One can obtain a good assessment of the factors involved in limiting the performance from the discussion of the accurate mass data these authors have reported. Methods have been suggested for signal enhancement as applied to high resolution mass spectrometry (*1142, 1197*). Signal averaging at high resolution has been applied to the measurement of ^{15}N in creatinine (*615*). The effect of controlling the temperature of an ion source in a high resolution mass spectrometer is discussed with respect to increasing reproducibility of mass fragmentation patterns for quantitative analysis of petroleum distillates (*252*). Burlingame and coworkers (*266*) have derived a relationship relating the number of ions in a peak to all other operational parameters of a high resolution mass spectrometer system, and have provided experimental data on the effect of resolution and sensitivity on the accuracy of mass and abundance measurement for the MS-902 between resolutions of 2,500 and 30,000. In this paper, preliminary data were also obtained after changing the basic instrument sensitivity by incorporation of the hexapole lens accessory. Taya and Matsuda (*1465, 1466*) have presented the mathematical treatment of third-order transfer matrices for calculation of trajectories considering the fringing fields of an electrostatic hexapole lens, such as referred to above (*266*). The design and performance of the new ultra-high resolution mass spectrometer, the AEI MS-50, has been discussed (*487*). Basic static resolution of 150,000 has been demonstrated. The Daly metastable detector (*372*) is standard equipment as well as four metastable scanning modes, and attention has been paid to the operation of this system on-line to a computer and optimizing sensitivity at high resolution using the hexapole lenses and the Nier–Johnson geometry.

Earlier, the Berkeley group described a unified computer software and hardware approach primarily for the acquisition, manipulation, and display (either on CRT or hard copy) of gas chromatographic–mass spectrometric (GC–MS) data including gas chromatograms (*1402*). This system was called LOGOS. Recently, this group has described LOGOS II (*265, 268, 270*) which is a large scale real-time computer system for multiple instrument mass spectrometry including low and high resolution, GC–low resolution MS, GC–high resolution MS, and low and high resolution spectral file management. A multiplexed 13-bit data rate maximum of 100 KHz is available for real-time mass spectrometry in this system. It also includes a Fourier transform ^{13}C nuclear magnetic resonance (NMR) spectrometer (*1598*). This high-speed real-time system is based on an XDS Sigma-7 computer. A vacuum pyrolysis high sensitivity, high resolution mass spectrometer system has been used for studying the thermal release patterns of volatilizable and/or pyrolyzable gases from mineral separates from lunar fines (*1387, 1615, 1616*) and minerals implanted with ^{13}C, D, and ^{15}N ions of energies (~1 KeV/nucleon) simulating the solar wind. This system is operated on-line to the LOGOS II Sigma-7 computer. Repetitive cyclic scans of high resolution mass spectra (43-sec cycle time) are used to produce exact mass–mass pyrograms from ambient to 1400 °C. Sample flow rates below nanograms/second are sufficient.

High resolution mass spectrometric analysis of solar wind and meteoritic rare gases, carbon compounds, and carbides released by etching of lunar fines with deuterium fluoride has been carried out (*1614*). A debatable paper on photographic *vs.* electrical recording of gas chromatographic effluents at high resolution has appeared (*614*). Another system for automated evaluation of photographically recorded mass spectra has been presented, demonstrating an accuracy of 5–30 millimass units depending upon the mass (*540*). Background in this area of mass spectrometry folklore can be obtained from Desiderio's chapter (*422*). Information on the response of ion sensitive emulsions to light ions, such as hydrogen, helium, and neon has been discussed (*1351*). A trochoidal electron monochromator to improve electron energy resolution has been described (*1075*).

A gas/liquid equilibrium sampling system has been described. It is capable of handling samples consisting of methane up to C_5 hydrocarbons (*1025*). A remotely oper-

ated high temperature vent valve has been described which is able to quickly vent gas chromatographic effluent in certain GC applications (*1073*). A simple device for analog recording of the abundance of selected ions from a combined GC–MS has been described using prostaglandins $PGF_{2\alpha}$ and $PGF_{1\alpha}$ as examples (*840*). Combined dual flame ionization and total ion current detectors on an AEI MS-12 have been discussed with a view toward improving the molecular separator performance (*256*). A time-of-flight mass spectrometer coupled with a 110 liter/sec ion pump has been described for GC–MS applications using a palladium silver alloy separator (*1408*). Digitally-controlled computer-compatible quadrupole (*469*) and magnetic (*613*) instruments have been described.

Detector Developments. Daly *et al.* (*372*) have described an improved version of their ion detector [used on the new AEI MS-50 (*487*)] which has special advantages for the study of metastable ions. The authors claim it produces better peak shapes than an electron multiplier and has been used with an MS-902 on which 1500 samples have been run with no measurable changes in detector characteristics. Further work on the discrimination in electron multipliers for atomic ions by Pottie *et al.* (*1244*) has extended their earlier work (*934*), as well as the recent review by La Lau (*926*). Relative multiplier yields for 62 atoms have been determined.

Spiral electron multipliers (*1243*) and continuous channel electron multipliers (*1047*) have been discussed in detection of positive ions and organic mass spectrometry, respectively. The latter may have advantages for operation with ion counting techniques. A reduction of secondary ion fogging on photographic plates using mass spectrography has been developed for use in semi-conductor analysis (*327*). Some technical details of fitting the heated cover plate to the ion source in a CEC 21-110B mass spectrometer for operation in the chemical ionization mode have been reported (*1177*). A Varian CH-7 mass spectrometer has been adapted for carbon isotope ratios using an ion counting technique (*1328*). Ion counting with peak switching techniques has been discussed (*807*). A pulsed counting method for trace analysis with more than 100 hours counting time made it possible to measure ion current below 10^{-20} A (*1086*). A somewhat futuristic "electronic photoplate" (*1138*) called an electro-optical multichannel ion detector has been described (*177*). Ingle and Crouch (*744, 745*) have discussed linearity and signal-to-noise ratio in photon counting systems in some detail. This may have a bearing on the limiting operation of the Daly detector (*372*). Computer detection of mass spectral peaks by real-time cross correlation has been described (*106*). Resolution enhancement by iterative and Fourier techniques has been presented (*1639*).

A retarding potential difference (RPD) with digital scanning and phase sensitive detection has been presented (*485*). A deconvolution method for identifying peaks in digitized spectra (*243*) and an iterative curve fitting method for chromatographic peaks (*307*) have been described. Work continues in use of on-line computers and electrical detection in connection with spark-source mass spectrometry (*338, 1097, 1098*). Dual electrode mounts and automatic gap control devices have been described (*1019, 1020*).

Precise Isotope Ratio Measurements. A simultaneous capacitive integrative system of two ion beams has been developed, automated, and applied to measure $^{16}O/^{18}O$ with a precision of 10–20 ppm (*766*). A similar system (*101*) has been described for analysis of carbon dioxide. An elaborate treatment of measuring procedures and corrections for high precision mass spectrometric analysis of isotopic abundance ratios of carbon, oxygen, and nitrogen has been reported (*1092*). Modifications of Du Pont 21-491 (*348*) and AEI MS 902 double focusing mass spectrometers for isotope ratio measurements have been reported (*530, 1196*). Two FORTRAN programs for computation of isotope peak intensities in low and high resolution mass spectra have been presented (*1532*). A mathematical model has been presented for calculation of isotope abundance ratio of an isotope cluster and shows how isotope abundance ratios of a label are determined (*719*). An additional formulation has been given by Buddenbaum and Daves (*258*). Another computer program written for the Univac 1108 in NU-ALGOL and FORTRAN 5 for the calculation of isotopic species has been described (*192*). The program output consists of a list of ionic masses and a graphical presentation of the spectrum. An example calculated is octachloro-3-methylene-cyclopentene. The program may be obtained from the authors. Genty has developed a statistical theory for application to the analysis of a mixture of isotopic compounds of the same species, and it is applied to a mixture of hydrogenated, deuterated, and tritiated propanes (*564*). $^{14}N/^{15}N$ determination using nitrogen gas from inorganic and organic samples has been reported (*502*). It should be mentioned that hydrogen, carbon, nitrogen, oxygen, sulfur, and silicon, as well as a multitude of other elements and their isotopic composition, have been studied precisely in returned lunar samples. References to these high-sensitivity procedures and determinations may be found in Volume II of the Proceedings of the Fourth Lunar Science Conference, *Geochim. Cosmochim. Acta* (*1249*). A novel technique for the determination of ^{15}N content of ammonia by chemical ionization mass spectrometry has been published by Field and coworkers (*1011*) which has the advantage of eliminating interference by water in the sample.

Chromatographic–Mass Spectrometric Techniques. Gas chromatography–mass spectrometry has been recently and very thoroughly reviewed by McFadden (*1132*). This book considers in some detail each component of a GC–MS system, their relationship to one another, computer techniques, and gives examples of applications in different fields. General reviews of GC–MS written by Junk (*808*) and Ryhage (*1305*) have also appeared. Available information on interfacial systems is summarized (*1385*). Mass fragmentography (single or multiple ion detection) carried out with GC–MS combinations has attracted widespread interest in the last few years. It has very rapidly become an established method for the detection and quantitation at the subnanogram level, of components present in complex mixtures. The method usually requires selection of an appropriate derivative of a component which has at least one ion of high abundance at a reasonably high m/e value which is, hopefully, unique to that compound. This requires, of course, that the spectrum of the compound in question be known in advance. The technique seems ideally suited for use in combination with CI since a large fraction of the total ion current can be carried by the pseudomolecular ion. The reader is referred to the following publications for more detailed information on the technique: applications in neurobiology (*350*), pharmacology (*785*), and general (*579*). Stable isotope-labeled compounds are frequently used as internal standards and carriers (to minimize adsorptive losses) in GC–MS fragmentographic assays. Murphy (*1117*) has briefly but clearly discussed the precision of assays when use is made of this device.

In metabolic studies, administration of mixed isotope-labeled precursors in appropriate amounts will lead to metabolites, the spectra of which show readily detectable isotope clusters. Use of this technique with GC–MS detection has been described (*214, 872*). The use of gas chromatography when coupled to a CI source with methane as both carrier gas and reactant gas has been described (*48*). A further development has been made which looks especially promising (*174*). Blum and Richter use excess methane reactant gas admixed with low flows of helium (through capillary columns) at the column effluent to record CI spectra. Methane flow may be readily stopped to record EI spectra. A mass spectrometer with an external ionization source (using ^{63}Ni) at atmospheric pressure is described (*705*) and some applications are recorded (*705, 706*). This instrument shows promise for GC and liquid chromatography coupling.

Various groups have explored ways of improving existing GC or GC–MS systems. Devices for solid sample injection are described (*481, 1517*). Capillary columns have been used with a packed pre-column and gas-phase splitter (all-glass) (*567*) or without a splitter (*1413*). Glass capillary columns are now widely used in biochemical research (*1174*) but difficulties are still encountered in coating them. Two similar coating procedures described by German and Horning (*568*) and Blumer (*176*) hold promise for reproducible production of stable films. A hydro-

phobic finely divided silica is deposited with the phase. With the availability of poly-*m*-carborane siloxane polymers (Dexsils) having low bleed levels at temperatures in excess of 300 °C (*1173, 1237*), analyses of compounds equivalent in volatility to n-C_{60} alkane should become easier. The new polar silicone phase, SILAR-5CP (*558*), is stable to at least 250 °C and may find increasing applications in GC–MS. Grayson *et al.* (*591, 592*) have described the lower elution temperatures possible when flow programming is used in GC–MS analyses instead of temperature programming. The technique requires some separator modifications to cope with flow rate changes.

Use of a high speed differentially pumped mass spectrometer has allowed direct coupling of capillary columns (flow up to *ca.* 7 ml/min) (*658*). An arrangement using PTFE shrinkable tubing permits direct coupling of low flow capillaries (<1 ml/min) to a conventional differentially pumped spectrometer, without air leakage (*598*). Glass capillaries have been interfaced through a two-stage jet separator, make-up gas being added to maintain separator efficiency (*1042*). Newer types of separators have been further explored. These include an effusion type with porous silver membranes (*590*) and an electrochemical cell employing palladium alloy diffusion electrodes for use with hydrogen carrier gas (*396*). An adjustable one-stage jet "separator" for use with capillary columns has been evaluated with unusual thoroughness but is stated to give no enrichment (*361*).

Liquid chromatography (LC) has been extensively developed in the last few years, and for the analysis of compounds that cannot be subjected to GC, even by derivatization, a combination of LC and MS techniques may prove a powerful tool. Some preliminary approaches to the problem of interfacing the instruments have been reported (*76, 705, 1005, 1458*). FD methods have been applied to analyze effluents from a liquid chromatograph but this requires manual concentration of the effluent and placement on the emitter (*1339*).

GC analysis of diastereoisomeric derivatives is increasingly used for separation and identification of enantiomers. New derivatization reagents suitable for biological amines and alcohols are described (*233*).

Computer Techniques—Gas Chromatography and Mass Spectrometry. Previous developments in computerization of combination GC–MS techniques have, from the point of view of the ease of the user, fallen into two categories: those where mass spectral scans were only initiated based upon the emergence of a particular gas chromatographic peak and those where mass spectra were continuously scanned at a cycle time small compared to the gas chromatographic peak width. Some of these systems operated on truncated exact masses in real-time, including display of normalized mass spectra during chromatographic runs, others had varying capability limited by either hardware or software by comparison. At the end of each chromatographic run, background peaks could be deleted, total ion current chromatograms displayed and plotted, as well as mass chromatograms of any diagnostic mass peak of interest. This level of capability has permitted computer exploitation of the complete mass spectral data on gas chromatographic effluents and it has become quickly realized that other parameters in total systems (GC–MS–computer) are limiting factors for certain types of applications.

While much has been published on the computer acquisition, processing, and presentation of mass spectral data, only recently have papers started to appear on the application to gas chromatography itself. Three papers are included which discussed computers of widely different types and capabilities. Levine *et al.* (*959*) have described a gas chromatographic mini-computer system using the PDP-8, 4-K core, 12-bit memory, costing about $3000 for the quantification of metabolic profiles in urinary acids and bile salts present in biological fluids. Landowne *et al.* (*931*) have described an XDS Sigma-2 with 36-K core and 3-megabyte disk which is capable of handling 16 instruments; its advantage is its versatility in handling all common problems in gas chromatographic data reduction without requiring selection of special routines for different situations. Schomburg and Ziegler (*1330*) have discussed gas chromatographic application of the Mülheim PDP-10. An additional paper by Henneberg, Casler, and Ziegler (*662*) discusses a computer algorithm for real-time selection of important mass spectra during an on-line GC–MS analysis.

Several papers have been concerned with computer-controlled multiple ion detection with both magnetic and quadrupole mass spectrometers. Some considerations have been given to a comparison of selected ion monitoring and repetitive scanning during GC–MS. It should be mentioned parenthetically that the basic and operational sensitivity of mass spectrometers differ even under allegedly equivalent conditions by at least 3 orders of magnitude. It is certainly the case that where careful and continuous attention is being paid to maximization of sensitivity (measured every morning for example) of an inherently high sensitivity instrument, the analysis which might require specific ion monitoring, *cf.* fragmentographic techniques, in a less sensitive instrument could be carried out by *mass chromatography* even under conditions of high resolution (up to 10,000). This particular fact of life contributes to the folklore of the alleged advantages and disadvantages of differing instruments and techniques, especially when so many of the fragmentographic techniques will ultimately find a role in the hands of researchers and analysts of minimum familiarity with the capabilities and operational maintenance of mass spectrometers. Examples of specific systems include Holland *et al.* (*687*) using *O*-acetyl derivatives of methylglycosides and methyl esters of prostaglandins PGF_2, on an LKB 9000 with a PDP-81; Watson *et al.* (*1218, 1577*) using prostaglandins PGE_2 and $PGF_{2\alpha}$ on LKB 9000 with a PDP-12A; Holmes *et al.* (*699*) using either a PDP-81 or PDP-12 with an LKB 9000 emphasizing analyses in picograms using isotope tracers and *myo*-inositol [trimethylsilyl (TMS)], alanine, and glucose as test compounds; Klein *et al.* (*864*) using a Perkin-Elmer model 270 with a 400 multichannel analyzer, analyzing chenodeoxycholic acid; Elkin *et al.* (*474*) using an LKB 9000 with PDP-12 analyzing tetrachloropyrocatechol, pentachlorophenol, and tetrahydroquinone; Baczynskyj *et al.* (*71*) using an LKB 9000–IBM 1800 and prostaglandin PGE_2 and PGF_2 and 7β,17β-dimethyltestosterone. Comparison of selective ion monitoring and repetitive scanning using an LKB 9000 (*1306*) and using cholestane as a test compound was reported (*1065*). Jenden and Silverman (*787*) reported an analog data processor for multiple specific ion detection using a quadrupole. An interactive display-oriented data system for a quadrupole operated as a GC–MS has been discussed (*368*). Caprioli and Murphy (*511*) have discussed fragmentographic techniques in their determination of abundance of stable isotopes using the quadrupole. Klein *et al.* (*863*) have discussed instrument design, considerations, and clinical applications of stable isotope analyses on chenodeoxycholic acid. For further papers, see the sections on analytical applications.

Computer Techniques in the Handling and Interpretation of Mass Spectra. By far the best review of computerized data acquisition and handling is given by Ward (*1569*). However, in certain instances, the emphasis seems to be misplaced or the statements are lacking authenticity, such as the implication on page 267 that the fundamental techniques and software required for low resolution data acquisition are fundamentally different from those for high resolution. His choice of discussions of practical and theoretical considerations regarding the sources of error in high resolution mass spectrometers, using publications by authors who do not have a track record in solving these difficulties, is sometimes misleading. But, his points regarding the advantages of coding in high level languages such as FORTRAN on 16-bit and longer word computers, and those emphasizing trends toward complete data acquisition, processing, and computer-aided interpretation systems and unified approaches to low and high resolution system software are well taken. However, re page 275, it certainly is easier to obtain accurate mass measurements on small quantities of material by correct use of a data system than by any other known technique. He correctly points out on page 279 a practical problem in ion-source saturation suppression of perfluorokerosene reference compound peaks (see discussion of double beam instrument above).

Some aspects recently developed are of significant prac-

tical advantage in the daily practice of mass spectrometry. These include the work by Heller and coworkers (*653–655*) on an interactive conversational mass spectra search system accessible over telephone lines. The file may be searched in a number of ways including by peaks and intensities, molecular weight, or molecular formula. In addition the complete mass spectrum of any compound on file can be printed out. The system is now available commercially under General Electric's Mark III computer service by the designation Mass Spectral Search System (MSSS) (*563*). In a similar vein, the molecular weight index of the Merck index is now available (*1442*). Lederberg has described a generalized compilation of tables of accurate masses for the rapid calculation of molecular formulas (*947*). He has recently written a generalized treatment of all elemental compositional accurate mass doublets (948). Work continues on the computation of the molecular weight when the molecular ion is not present in the mass spectrum (*778*). Of enormous immediate benefit in the practice of mass spectrometry is the compilation and retrieval of computer files of mass spectra and their maintenance. Many laboratories are seriously concerned and contribute to these file management and retrieval systems. The API project 44 and TRC DATA project catalogs of petroleum-related spectra have been discussed (*1647*). Classification of mass spectral data files has been described for the Aldermaston collection (*1352*). Criteria for the identification of low resolution mass spectra by retrieval from a file continue to be discussed (*105, 328, 494, 922, 1133*). Grotch has continued work on computer identification of mass spectra using highly compressed spectral codes (*605, 606*). Other diagnostic functions and binary encoding have been described (*1057, 1145, 1278, 1279*). A compiler level search algorithm for spectra of mixtures has been reported (*756*). A method has been proposed for identification of GC–MS components using the most intense peaks in the mass spectra (*1459*).

The philosophy and merits of off-line computing in mass spectrometry are discussed with respect to providing efficient service (*796, 953*). Computer programs for presentation of mass spectra on a Cal-Comp 565 plotter are available on request (*1461*).

A considerable amount of interesting work on the statistical clustering approach continues in computer-aided analysis of mass spectra. Isenhour and Justice reviewed this approach recently (*757*). A series of papers has also been published (*111, 112, 495, 528, 809, 901, 1293, 1508*). Computer-aided analysis of organic mass spectra with respect to low resolution GC–MS (*1531*) and the Mülheim PDP-10 system has been described in some detail (*663*). Smith (*1397*) has described a compound classifier based on computer analysis of low resolution mass spectra. In this technique, use is made of ion series spectra derived from sets of authentic mass spectra. Particular applications to geochemical and environmental studies have been emphasized. The applications of artificial intelligence in connection with mass spectrometry continue. One paper points out the possibility that there may be a relationship between the mass spectrum and pharmacological activity of a compound (*1485*). Heuristic programming (*895*) for the generation of primary ions with charge localization has been described (*391*). The primitive operation of this program currently includes: ionization with charge localization; bond homolysis β to a radical site; bond formation between two adjacent radical sites; transfer of a hydrogen atom to a radical site *via* cyclic transition states of various sizes. 5-Diethylaminopentan-2-one was used as a test case. Lederberg, Feigenbaum, Djerassi, and coworkers have made progress in the application of artificial intelligence for chemical inference in the area of mass spectrometry with papers 9–13 in their series (*288, 1033, 1034, 1398, 1400*). Ward (*1569*), and references therein, contains a review of the earlier papers in this series. Work is continuing on the analysis of mixtures of estrogenic steroids (*1398*). Estrogenic steroids are used in the test of a new program called INTSUM (*1400*) which interprets, in terms of all possible fragmentation breaks, the high resolution mass spectral data collected on known compounds and is able to use these rules thus derived to make interpretive suggestions regarding new members of this structural class. The most impressive and far reaching aspect

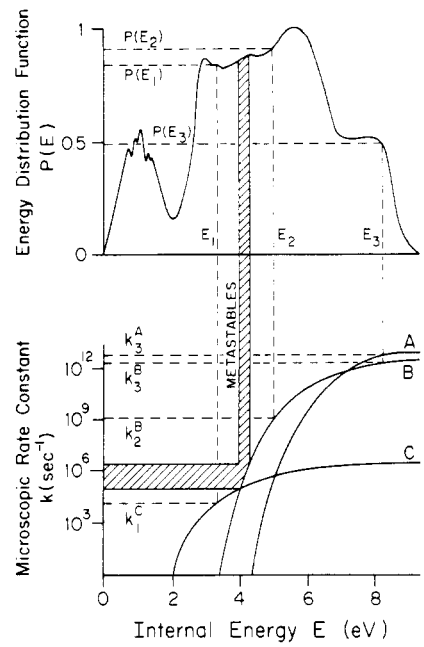

Figure 1. Relationships between internal energy distribution function $P(E)$ for molecular ion and rate curves of microscopic rate constant k against internal energy E. All curves are hypothetical. The shaded bands denote the ranges of internal energies E and microscopic rate constant k associated with metastables. The energies E_1, E_2, and E_3 are arbitrary and have no significance other than to demonstrate how differing internal energies E can induce different reactions

of their effort in this period is the formulation of mathematical and computer tools for the exhaustive generation of cyclic structures and for use in solution of the problem of labeling objects having symmetry (*1033, 1034*). This cyclic structure generator employs "prospective pruning" to avoid duplicate and other undesirable structures. A first attempt has appeared in the application of these techniques in an area other than mass spectrometry and proton nuclear magnetic resonance, namely ^{13}C NMR of tertiary amines (*288*). A non-heuristic application of the original dendritic algorithm to computer determination of structures of branched alkanes from ^{13}C NMR data is described by Burlingame and coworkers (*269*).

ION CHEMISTRY: UNIMOLECULAR PROCESSES

We restrict our review to the gas-phase chemistry of polyatomic ions; in general we do not cover studies of diatomic or triatomic molecules.

Unimolecular rearrangement and fragmentation reactions are the essential and fundamental foundation of molecular mass spectrometry. It is the charged products of such ionization-induced processes which appear in the mass spectrum.

Theory. The quasi-equilibrium theory (QET) remains the accepted theory for treatment of unimolecular gas-phase reactions of polyatomic ions (*1292, 1557*). Gas-phase ionization imparts internal excitation energy E to the resulting molecular ion. The QET assumes that ionization is rapid compared to subsequent chemical reaction. It is further assumed that, prior to chemical reaction, excited electronic states of the ion cascade to the ground state by radiationless transitions and that the internal energy E is randomized over all internal vibrations and rotations. In which case internal energy E can be described by a distribution function $P(E)$ as in Figure 1. A distribution function approximating to the hypothetical function in Figure 1 might be appropriate for certain molecular ions formed by 70-eV electron impact (EI) or 21.2-eV photon impact (PI). The internal excitation energy E typically leads to a variety of competing unimolecular chemical reactions, the products of which can themselves react further. Each of

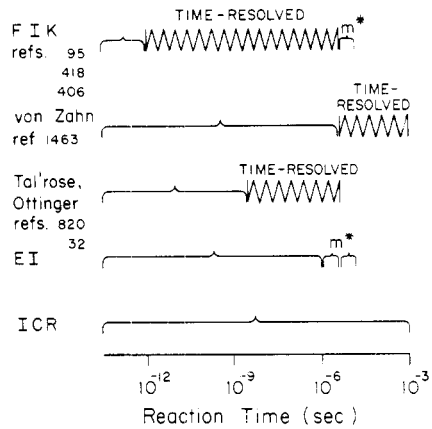

Figure 2. Unimolecular reaction times (ion lifetimes) accessible to various mass spectrometric techniques. Bracketed times indicate that the technique gives an integrated view of all reaction occurring in that time frame

these reactions can be described by a curve of microscopic rate constant k *vs.* internal energy E. In Figure 1, we show such curves for three competing reactions A, B, and C of the hypothetical molecular ion. The distribution of internal energies $P(E)$ gives rise to a distribution of rate constants and of reaction times. Reaction times vary from a minimum generally considered to be in the region of 10^{-13} or 10^{-14} sec (*i.e.*, comparable to molecular vibrations) to presumably infinity. Figure 2 shows the ranges of reaction times accessible to different mass spectrometric techniques. Distinction is made between resolved and integrated views of events. By "resolved," it is meant that reaction can be studied as a function of time; information takes the form of a curve of number of product ions *vs.* time. By "integrated," it is meant that the only information is the *number* of product ions formed (within some long time interval). The distinction is actually quantitative rather than qualitative. For the purposes of studying ion chemistry, a resolved view is desirable. Competition among reactions depends on internal energy. To demonstrate this point, we arbitrarily select three values of the internal energy, E_1, E_2, and E_3 (Figure 1). Molecular ions with internal E_1 can undergo only reaction C at a rate describable by the rate constant k_1^C of value approximately 10^4 sec^{-1} and giving rise to reaction times of 10^{-4} sec. Such reaction times are accessible by ICR or by a specialized technique with long drift tubes such as set up by von Zahn and colleagues (*1462, 1463, 1544*) (see Figure 2). Molecular ions with internal energy E_2 undergo reaction B with a rate constant k_2^B of about 10^9 sec^{-1}. Such a reaction is accessible with most techniques but only field ionization kinetics provides a resolved view (Figure 2). The energy E_2 is sufficient to induce either reaction A or C as well as reaction B, but these reactions are not seen as they are too slow at this energy to compete with reaction B (*i.e.*, $k_2^B \gg k_2^A$ or k_2^C). Those reactions referred to as metastables m^* are reactions with rate constants of 10^5–10^6 sec^{-1} (see Figure 1). In the hypothetical model, both reaction B and C would appear as metastables. At internal energy E_3, both reactions A and B occur although the former predominates (since $k_3^A > k_3^B$). Reaction at E_3 occurs in times of the order of 10^{-13} sec. Assuming no further reaction, the 70-eV electron impact (EI) mass spectrum would contain the products of two of the three reactions (A and B). The intensities would represent the total number of product ions formed within some period of the order of microseconds following ionization. The reaction C would be too slow to make a contribution to the mass spectrum, but would be detected as a metastable transition (along with B).

The QET is a modified form of absolute reaction rate theory and employs the concept of activated complex or transition state. The rate constant k at some internal energy E is obtained from the ratio of the number of energy states of the activated complex with energy $\leq E - E_0$ (E_0 is the activation energy of the reaction) to the number of energy states of the reactant ion at energy E (*1557*), and thus QET is a statistical theory. Available methods for estimating numbers or densities of energy states have been discussed by Forst and Prâšil (*520, 521*). Recently Klots (*866, 867, 869*) and Knewstubb (*874, 876, 877*) have separately pointed out advantages to be gained by invoking the principle of microscopic reversibility and treating ion fragmentation as an ion-neutral collision. The resulting reformulations of the QET emphasize that ion decomposition can give rise to rotations of the separating fragments (*874, 876*) which should tend to enhance fragmentation rates. The reformulations (*877*) establish the necessity of separating free energy of activation into entropy and enthalpy terms (*cf. 406*) and suggest a role for quantum-mechanical tunneling (*866*). Bunker (*261*) has shown how rotational energy of reactants makes important contributions to the internal energy of the activated complex.

While the QET is the most, if not the only, useful theory of mass spectra, it is becoming increasingly clear that the basic tenets as to the rapid energy randomization and rapid decay of excited electronic states are not universally valid. Results from crossed-beam experiments indicate that energy is not randomized prior to loss of $CH_3\cdot$ from the collision-complex $C_4H_8\cdot^+$ (*949*). Excited electronic states of $CO\cdot^+$ (*420*), $H_2O\cdot^+$ (*983*), and $C_2H_2\cdot^+$ (*1449*) formed by EI have lifetimes approaching microseconds or longer. Kinetic measurements on benzene (*32*) in the nanosecond time-frame suggest that $C_4H_4^+$ and $C_3H_3^+$ are formed from an excited electronic state, whereas $C_6H_5^+$ and $C_6H_4^+$ are formed from the ground state. Interpretation of photoionization measurements on benzene (*1291*) supports this view. Results from a longitudinal tandem mass spectrometer indicate that hexan-2-one has an excited electronic state with a lifetime of microseconds (*976*). Emission studies (*544*) reveal that neutral fragments from the decomposition of methylamine ions are formed in excited electronic states. Isolated excited electronic states have been invoked to explain results of charge exchange measurements on *N*-phenylbenzamide (*1509*) and of appearance potential measurements on C_6H_5COX (*123*). Photoelectron/photoion coincidence measurements suggest that isolated excited electronic states are involved in the decomposition of $C_2F_6\cdot^+$ (*1384*).

Quantum-mechanical theories (*23, 24, 1072*) of unimolecular decomposition have been proposed as alternatives to the classical statistical theories. The relationship between a quantum-mechanical approach and the statistical theories has been discussed by Knewstubb (*875*). A stochastic theory of vibrational dissociation has been described (*561*).

Quantum-mechanical calculations of molecular orbital energies of reactant ions, of possible intermediates in decomposition, or even of possible activated complexes have been made with a view either to exploring the extent of the correlation between calculated bond charge densities and fragmentation patterns (*990, 1316, 1319, 1451*) or to elucidating particular features of a fragmentation mechanism (*742, 1204, 1205, 1512*). The molecular orbital approach demands the most accurate methods of calculation and a sensible choice of molecule. It is of questionable value to apply a method as approximate as the extended Hückel to a molecule as complex as estrone (*990*). Attempts to correlate bond dissociation energies derived from appearance potentials with fragmentation patterns have met with only limited success (*467, 468, 1345*). Calculations using the simpler formulations of QET have been useful in rationalizing the fragmentation of certain molecules (*113, 115, 274, 582, 741, 1215, 1320*).

Charge Exchange. Ionization by charge exchange has the unique advantage that known *discrete* amounts of internal energy are imparted to the molecular ion. Theory and mechanism of charge exchange have been discussed (*198, 1026*). By using tandem mass spectrometers, accurate breakdown curves of fragment ion intensities as a function of internal energy can be drawn up (*984*). Nagatani *et al.* (*1150, 1151*) in Japan have reported breakdown curves measured with a tandem mass spectrometer of perpendicular type using *high* kinetic energy bombarding ions. A means of modifying a single-stage mass spectrometer so as to be able to make charge exchange measurements has been described (*1290*). Lindholm (*984*) has

pointed out that, for certain special classes of molecule, appearance potentials of fragments derived from charge exchange breakdown curves tend to occur at energies at which there is a band in the photoelectron spectrum of the molecule concerned. These coincidences exist for certain of the smallest polyatomics (*984*) (*viz.*, NH_3, C_2H_4, C_2H_6, CH_3OH) and for certain monocyclic aromatics [*viz.* benzene (*803*), pyridine (*804*), thiophene (*403*), furan (*402*), pyrrole (*404*), cyclopentadiene (*405*), pyrimidine (*50*), pyridiazine (*51*), pyrazine (*533*), *s*-triazine (*532*), *s*-tetrazine (*534*)]. These experimental coincidences are interpreted (*984*) by correlating ionization of a particular molecular orbital with particular fragmentation reactions on the basis that the bonds suffering the greatest reduction in electron density on vertical ionization will be the ones that subsequently rupture. This implies that energy is not randomized prior to fragmentation and that fragmentation occurs from excited electronic states of the ions. Such conclusions directly contradict the QET approach. These experimental results from charge exchange mass spectrometry and their interpretation which hold such fundamental implication have received little attention, other than from Wahrhaftig (*1557*) who points out that correlations between electron densitites of ionized molecular orbitals and fragmentation do in general not exist.

Appearance Potentials. Electron impact (EI) measurements of appearance potentials can now be made with considerable precision and should lead to accurate heats of formation of ions and radicals becoming available. Photoionization (PI) measurements are reviewed separately in a later section. Lossing (*998*) reports appearance potentials measured with energy-selected monoenergetic electron beams (energy half-widths of better than one-tenth of an eV). One example of their use has been to establish the existence of the cyclopropenyl ion $C_3H_3^+$ with a heat of formation of 256 ± 2 kcal/mole; $C_3H_3^-$ is theoretically the smallest possible aromatic system ($4n + 2$, $n = 0$). Monoenergetic electron beams undoubtedly provide the most precise measurements of appearance potentials (*1452*); however, use of mathematical procedures can refine measurements made without energy analysis of the electron beam. Johnstone and colleagues (*798, 799*) refine their measurements by a computer method referred to as ionization efficiency/energy distribution difference (IE/EDD), which they claim gives values for appearance potentials with an accuracy comparable to that of PI. Using this method, no difference (<0.2 eV) was detected between appearance potentials of certain fragment ions formed in the source and the appearance potentials of fragment ions of those same masses formed in the metastable region (*125*, see also *1176*). If these results are genuine, they indicate that kinetic shifts cannot be easily estimated from measurements of appearance potentials of metastables. The results support the view that kinetic shifts are likely to be no greater than the usual experimental error in measuring appearance potentials or the average thermal internal energy (*640*). A method for determining kinetic shifts directly (*975*), by trapping reactants in the space charge of an electron beam for up to milliseconds and measuring appearance potentials as a function of residence time, promises to throw considerable light on the question of the magnitude of kinetic shifts. It has been suggested that kinetic shifts can be estimated by measuring appearance potentials of fragment ions formed after milliseconds by ion cyclotron resonance (ICR) techniques; however, the reported results do not establish ICR as an accurate method for appearance potential measurements (*600*). Morrison *et al.* (*1100–1102*) use time-averaging and deconvolution to obtain accurate ionization efficiency curves; results are interpreted with the aid of photoelectron spectra. Flesch and Svec have reported a method for the rapid measurement of appearance potentials (*513*) and have pointed out the advantages to deconvoluting ionization efficiency curves (*514*). Finney and Harrison (*510*) report a third-derivative method for determining appearance potentials which they suggest is superior to the second-differential technique (*1099*). Pihlaja, Jalonen and colleagues (*773–776, 1208*) and Loudon and colleagues (*287*) have been concerned with using appearance potential measurements for determinations of ion structure (*774*). Interest in substituent effects (*127, 380, 472, 772, 1231*) has declined sharply in recent years, although good discussions by Benoit (*120–123*) of Hammett correlations in general and with appearance potentials in particular have appeared.

Kinetic Energy Release during Fragmentation. Prolific publication during the past two years by Beynon, Cooks, and colleagues (*340*) and to a lesser extent by Franklin and colleagues (*1354*) has reemphasized the fundamental importance (*867, 868*) of kinetic energy release during ionic fragmentation. The energy release arises from the excess energy above the activation energy (*i.e.*, the internal energy of the activated complex) and from the reverse activation energy (*801*). Using either a time-of-flight method (*631, 632*) or the deflection method (*526, 1354*) of Taubert (*1464*), Franklin and colleagues measure translational energy distributions for the fragment ions from specific dissociation reactions induced by EI. The mean translational energy $\bar{\epsilon}_t$ is calculated from the area beneath the distribution curve (*526, 1354, 1581*) and related to the total excess energy E^* (*i.e.*, internal energy of the activated complex) by the formula (*631*) $\bar{\epsilon}_t = E^*/\alpha N$. N is the number of internal degrees of freedom and α is an empirical constant. The formula has been critically discussed by Klots (*867, 868*). Implicit in the use of the formula is the *assumption that the reverse activation energy is negligible.* This assumption is justified on the grounds that the reactions studied are simple bond cleavages and that, since they occur in the ionization chamber, the reactions must be rapid ($<10^{-6}$ sec) and involve reactant ions of high internal energies. Measured energy releases are typically in the region of a few kcal/mole and the estimated values of excess energies tend to be in the region of 20–50 kcal/mole. The excess energies can be used to correct appearance potential measurements so as to obtain accurate values for heats of formation of ions and radicals (*631, 632, 1354*). The calculated values for heats of formation generally agree well with previous determinations. Franklin and colleagues (*635, 636, 1566*) have also measured kinetic energy release associated with dissociative resonance capture processes. Since the excess energy is known and can be varied, reliable conclusions can be drawn concerning energy partitioning among translational, vibrational, and electronic excitation modes.

Beynon, Cooks, and colleagues estimate energy releases (*80, 152*) associated with specific decomposition processes from the *metastable* peak widths as measured by the Barber–Elliott defocusing technique (*79, 788*). Results are frequently interpreted by assuming that *energy release arises solely from the reverse activation energy* and that the contribution from excess energy is negligible (*800–802*). The assumption is justified on the basis that metastables are reactions of ions of low internal energy. A second point is that the reactions chosen for study tend to be rearrangements (as opposed to direct bond cleavages), which in general are more likely to be associated with significant reverse activation energies. The starting point to the interpretation is diametrically opposed to that assumed by Franklin and colleagues. The energy released during metastable fragmentation can be as high as several hundred kcal/mole as in the *collision-induced* dissociation of H_2^+ (*150, 341*) or as low as a few thousandths of a kcal/mole as with the loss of HCN from the *sym*-triazine molecular ion (*142*). A few kcal/mole is a typical value. Beynon, Cooks, and coworkers (*854*) have recently reported measurements of kinetic energy release as a function of time over the range 4 μsec to 15 μsec; results for the loss of HCN from ionized C_6H_5CN indicate a variation in energy release of 5 meV which is much less than indicated by measurements (*32*) on the kinetics of this reaction. The major significance to date of energy release by metastable fragmentation has been as a mechanistic probe (*140, 340, 800*). Differing energy releases establish the existence of two distinct reaction channels effecting loss of HCHO from anisoles (*340*) and of two distinct reaction channels effecting loss of NO from aromatic nitro compounds (*139*). Differing energy releases establish that there are two ion structures of formula $C_7H_7^+$ formed from ionized toluene, cycloheptatriene, and *tert*-butylbenzene and reacting to lose H· and C_2H_2 in the metastable region (*343*). Holmes (*691*) distinguishes isomeric $H_2CO_2^{\cdot+}$ ions in the mass spectra of ox-

alic and formic acids and isomeric $H_4C_2O_2^{\cdot+}$ ions in the mass spectra of malonic and acetic acids on the basis of metastable peak shapes. Deuterium isotope effects upon energy release for simple bond cleavages to lose H· (D·) are small as theory predicts (*134, 135*). Significant isotope effects upon energy release have been observed for certain reactions effecting loss of H· (D·); these reactions probably involve rearrangement (*134*). The large kinetic energy releases observed for the dissociation of doubly-charged ions into two singly-charged fragments provide a means of calculating effective charge separations for the doubly-charged species by assuming all the energy release to originate from coulombic repulsion (*53, 56, 143*). The magnitude of the charge separation can sometimes elucidate the structure of the ion. Ionization potentials for the formation of doubly-charged ions ($m \rightarrow m^{2+} + 2e$) can be estimated from the difference in kinetic energy between the m^+ and m^{2+} ions involved in the reaction $m^- + N \rightarrow m^{2+} + N + e$ (*339*). The energy releases for metastable decompositions of $C_6H_6^+$ ions from benzene are similar in magnitude to energy releases for decomposition of $C_6H_6^+$ ions formed by charge exchange from doubly-charged $C_6H_6^{2+}$ (*843*). It has been argued (*843*) that both types of $C_6H_6^+$ therefore have the same structure. $C_6H_6^{2+}$ is probably acyclic (*151*) so $C_6H_6^+$ formed from $C_6H_6^{2+}$ by charge exchange is most probably also acyclic. In which case $C_6H_6^+$ formed by ionization of benzene and decomposing in the metastable region is acyclic.

Chemical Kinetics. In opening the international conference in London, 1958, Sir Cyril Hinshelwood commented of mass spectrometry "the behavior of molecules in this fragmentation is a new and self-contained chapter of chemical kinetics" (*672*). It is regrettable that some fifteen years later, genuine kinetic data, that is to say rates of reaction as a function of time, are available for so few of the legion of known unimolecular decomposition processes of polyatomic ions; the need for kinetic data is perhaps reflected by the intensity of discussion (*344, 867, 1557*) stimulated by a single paper (*32*) presenting data as to rates of decomposition in the nanosecond time-frame (10^{-9} to 10^{-6} sec). The field ionization kinetics technique is unique in allowing lifetimes of reactant ions to be measured over six orders of magnitude of time from microseconds to picoseconds (*92, 418*) and is discussed separately below. Lifetime measurements at times approaching nanoseconds following electron impact (EI) have been reported by Karachevtsev and Tal'rose (*820, 821*). Ottinger and colleagues (*667, 668, 1191, 1194*) have measured decomposition rates in the nanosecond time-frame for benzonitrile, butane, and heptane ions formed by EI. Recently Andlauer and Ottinger (*31, 32*) have extended their experimental technique so as to measure decomposition rates of benzonitrile, benzene, and thiophene ions formed by charge exchange. The internal energies of the reactants are known and are approximately monoenergetic. The results prove that the reactions $C_6H_6^+ \rightarrow C_6H_5^+ + H$ and $C_6H_6^+ \rightarrow C_4H_4^+ + C_2H_2$ are *not* in competition with each other. A review of ions of short lifetimes is to be published (*401*). Using drift tubes of variable length, von Zahn and Tatarczyk (*1462, 1463, 1544*) have measured the time dependence of decomposition processes of ions formed by EI of alkanes at times between 5 and 500 μsec. The results agree satisfactorily with predictions of QET. The dependences on time for a number of decompositions at times of the order of microseconds (*i.e.*, over just one order of magnitude of time) have been measured using time-of-flight instruments (*1303*). The various kinetic measurements irrefutably establish that many reactive polyatomic ions typically have distributions of lifetimes extending from 10^{-12} sec (and probably shorter) to 10^{-3} sec (and probably longer) and that ionic decompositions are chemical processes describable by statistical (or other) rate theories such as QET.

Field Ionization Kinetics. The field ionization kinetics technique (*92*) provides the necessary information to qualitatively identify the nature of rearrangement and fragmentation reactions in the *picosecond* time-frame (10^{-12} to 10^{-9} sec) and in addition allows the course of each reaction to be followed down to times of the order of microseconds (*406, 407*). Field ionization kinetics affords a time-*resolved* view of the suite of competitive processes induced by ionization (*411*). Rates of reaction and phenomenological rate constants are accessible at times as short as picoseconds and at longer times up to microseconds (*95, 418*). In the past two years, detailed descriptions of methods of calculating lifetimes have appeared (*491, 1227, 1538*). The lifetimes calculated by the method of Viney (*1538*) would appear to be in error by an order of magnitude. The technique is also applicable to dissociations of doubly-charged ions (*99*). Beckey and colleagues (*95, 960–962, 1469*) have shown that the field ionization kinetics data on ionic decompositions (at times from *ca.* 10^{-12} to 10^{-6} sec) do support QET. The rates of ionic decompositions induced by FI are significantly increased by raising the source temperature (*961*) suggesting that some control on the internal energy of reactant ions may be possible in this way.

To successfully apply the field ionization kinetics to problems in ion chemistry demands the use of a double focusing mass spectrometer, so that energy analysis and mass analysis of fragment ions are performed in separate stages (*407, 491*). Measurements should preferably be made by scanning the accelerating voltage rather than the electric sector analyzer voltage (*417, 491*). Using a double-focusing mass spectrometer, Derrick *et al.* (*407, 411*) have been able to throw some light on the nature of processes responsible for the phenomenon of H/D randomization. Isomerization *via* 1,3-allylic hydrogen shifts plays an important role in H/D randomization within alkene ions [*viz.* 2-methylpropene (*410, 412*), 1-butene (*411*), cyclohexene (*408*)]. H/D randomization in ketone ions is arrived at *via* a sequence of rapid hydrogen shifts to and from the carbonyl group and within the hydrocarbon chain (*416*). Derrick and Burlingame (*406*) have emphasized the extent to which the outcome of the competition among various reactions of a molecular ion is dependent upon reaction time and have discussed the factors responsible. There is evidence (*409*) that, in general, five-membered cyclic transition states may tend to be "looser" (*i.e.*, less negative activation entropy) than six-membered. Kinetics of γ-hydrogen rearrangements in hexanal suggest that γ-hydrogen transfer and β-cleavage may be concerted in the process retaining the charge on the oxygen moiety (*415*). Wood *et al.* have demonstrated the usefulness of the concept of charge localization for rationalizing McLafferty rearrangements of acetate esters (*1612*). The field ionization kinetics technique reveals an apparent inverse kinetic isotope effect on fragmentation of 2-methylpropane ions (*414*).

Mechanistic Interpretation of Electron Impact (EI) Mass Spectra. From the viewpoint of mechanistic ion chemistry, the information contained in the 70-eV EI mass spectrum of an unlabeled molecule is setting up questions rather than providing answers. To even approach a position where mechanisms can be postulated necessitates extensive labeling with stable isotopes (D, ^{13}C, ^{18}O, ^{15}N) (*692*), accurate mass measurement to determine atomic composition, metastable measurements, and low electron energy (10–12 eV) mass spectra (*207, 440, 460, 462, 624, 697, 698, 845, 937, 1107, 1365, 1492, 1495, 1613*—these few selected papers typify the better studies of EI mass spectra). Moreover, even this abundant information is often insufficient to provide a secure mechanistic solution, and merely reveals that a process is still more complex than might otherwise have been supposed. The complexity encountered is illustrated by the 7-phenylhept-3-en-2-one *O*-methyloxime ion, in which a sequence of four hydrogen shifts occurs from the oxime to the phenyl moiety so that the neutral naphthalene can be eliminated (*970*). Triple hydrogen rearrangements occur in allyl vinyl ether and thioether ions prior to fragmentation (*834*). Product stability is a major factor directing these, and many other, rearrangements which lead to fragmentation. Further examples of the importance of product stability have been reported in steroid mass spectrometry (*1240*). The important role of functional groups in rearrangement and fragmentation is exemplified by a study of phenyl substituted α,β-unsaturated ketones (*969*). The recently delineated (*1061*) fragmentation pattern of 1,3,5-trinitrobenzene further exemplifies the complexity of EI mass spectra; the highly dendritic form of the pattern is remarkable, bearing in mind the comparative simplicity

of the molecule. An underlying complication in many mass spectra is partial or complete isotopic randomization (*vide infra*) which seems to result from isomerization processes competing with fragmentation.

The first step toward establishing secure mechanisms is the determination of the structure of reactants and products. Many radical-cations (*904*) formed by ionization isomerize prior to fragmentation, for example α,β and β,γ unsaturated esters (*943*) or unsaturated ketones (*429*), so that the structure of the primary reactants need not be obvious. The question of whether or not cyclopropanes undergo ring-opening following ionization illustrates some general points concerning ion structures. The mass spectra of a number of simple isomeric cyclopropanes are identical (*315, 428*). $C_3H_6\cdot^+$ species generated from a number of propenes and cyclopropane appear to have the same propene-type structure when they decompose as metastables. Ion cyclotron resonance studies suggest that cyclopropane retains a cyclic structure following EI (*604*) and that this is the most stable structure of formula $C_3H_6\cdot^+$ (*599*). Heats of formation calculated from equilibrium measurements in a high-pressure ion source support a cyclic structure (*317*). The apparent contradictions among the various measurements seem, however, to have been resolved by evidence from photoionization studies indicating that ring-opening is energy dependent (*1377*). The ring opens at higher energies and presumably prior to unimolecular decomposition reactions, but remains intact at lower energies (*965, 1377*). Another much discussed issue is whether keto or enol is the preferred ion structure (*461*). Deuterium labeling establishes that the $C_6H_5C(OH)CH_2\cdot^+$ ions formed by McLafferty rearrangement in the ketones and *reacting to lose methyl* have the enolic structure (*146, 1489*). Similarly ICR establishes that the $C_6H_6O\cdot^+$ species from both phenetole (*166*) and phenylacetate (*1491*) have the same phenolic structure. Thioamides (*938*) and hydroxycoumarin (*1153*) undergo enethiolization and enolization, respectively, prior to fragmentation. However, ICR establishes that the enolic ion formed by the McLafferty rearrangement in 2-propylcyclopentanone reketonizes to a cyclopentanone-type structure in times of the order of milliseconds (*612*). Thus, there is the possibility that the keto/enol relationship is energy-dependent with perhaps the enol being the high-energy reactive structure and the keto the low-energy stable structure. The structures of $C_7H_7^+$ and $C_7H_8^+$ are very far from being settled (*255, 331, 679, 740, 896, 1349*). All the carbons in $C_7H_7^+$ from cycloheptatriene are equivalent prior to fragmentation (*382*) indicating a tropylium structure. Those ions from *p*-chloroethylbenzene undergoing loss of methyl in the metastable region have rearranged to a tropylium structure (*718*). Recently, however, convincing evidence based on kinetic energy release has appeared to the effect that there are two distinct $C_7H_7^+$ species reacting to lose C_2H_2 in the metastable region (*343*). Moreover, the benzylphenylacetate ion fragments to form two distinct $C_7H_7^+$ species (*681*). Collision-induced metastable measurement (*1604*) establishes that both benzyl $C_6H_5CH_2^+$ and tolyl $C_6H_4CH_3^+$ species have lifetimes of at least 10^{-5} sec. Benzyl ions have been detected in radiolysis experiments (*1620*). $C_7H_8\cdot^+$ species from toluene, cycloheptatriene, and *n*-butylbenzene reacting to lose H in the metastable region have a common structure (*343*). Those $C_7H_8\cdot^+$ species, formed from various precursors by γ-hydrogen rearrangement, which undergo metastable decomposition have a common structure (*963*). All carbons in $C_7H_8\cdot^+$ from toluene become equivalent prior to photodissociation (*448*). On the other hand, ICR results indicate that stable $C_7H_8^+$ ions from toluene, cyclophetatriene, and norbornadiene do not interconvert to an extent more than 10% (*450*) and that stable $C_7H_8^+$ ions from toluene retain their structure ($C_6H_5CH_3\cdot^+$) (*680*). A benztropylium ion has been reported (*1346-1348*). If there is one general point to be drawn from the recent studies of ion structure, it is that ion structure depends very much on internal energy content and the structure of a reactive ion may not be the most stable structure of that formula.

Isotopic randomization is a special instance of isomerization prior to decomposition (*413, 694*). It is especially prevalent prior to metastable decomposition (*790*) and curtails the usefulness of isotopic labeling in metastable studies (*1401*). New instances of isotopic randomization continue to be widely reported (*204, 206, 208, 646, 1416*), particularly with aromatic molecules (*114, 202, 383, 660, 859, 1265, 1309, 1558*). There is complete randomization of both carbons and hydrogens within $C_6H_6\cdot^+$ from benzene (*145*) and within $C_5H_5N^+$ from pyridine (*430*) prior to metastable decomposition. The processes responsible for isotopic randomization are, however, little known or understood, although in aliphatic alkenes and ketones, hydrogen shifts leading to H/D randomization have recently been identified using the field ionization kinetics technique (*406*). H/D randomization in the ethyl carbonium ion (*64*) is due to 1,2-hydrogen shifts with an activation energy of 2 kcal/mole and a frequency factor of 10^{13} sec^{-1} (*1545*). 1,2-Shifts presumably effect H/D randomization in the collision complexes $C_2(H,D)_7$ (*731, 1579*).

Identification and description of cyclic transition states is a major concern in mechanistic mass spectrometry. A review of intramolecular hydrogen transfer reactions in aliphatic hydrocarbons and aromatic compounds has recently appeared (*273*). By far the most common size for cyclic transition states is the six-membered, although five- and seven-membered are also common (*427, 690, 713, 1631*). Numerous four-membered cyclic transition states have been identified (*408, 1124, 1494, 1513*); the suggestion (*196*) that four-membered cyclic transition states are rare seems to be incorrect. A few three-membered cyclic transition states have been reported (*812, 1186*). Cyclic transition states with between eight and fifteen members have been reported (*427, 1268*). The prevalence of six-membered cyclic transition states must reflect the fact that for a ring composed mainly of carbon, six is the energetically preferred size. On the basis of entropy, however, five is preferred over six (*409*), and four is preferred over five (*1124*). Macromolecules react *via* a macrocyclic transition state (*1588*) described as transhelixes (*1307*) or coils (*1059*). Molecular coiling can be viewed as an attempt by a molecule to solvate itself (*1060*). The formation of cyclic ions involves cyclic transition states but, in these cases, attention tends to focus on the cyclic products (*972*). So-called intramolecular dimers (*1103*), such as for example are formed by interaction of the α-naphthyl end groups in (α-naphthyl)-$(CH_2)_n$-(α-naphthyl) ions (n = 3 to 16) (*283*) are an example of macrocyclic ions. Other intramolecular interactions are documented under such titles as neighboring group participation (*1331*), anchimeric assistance (*1214, 1495*), ortho effect (*40, 1493*), and peri effect (*304*). Ring expansion or contraction has a certain fascination. Six-membered cyclic ions expanding to seven-membered have been reported (*718*) and five-membered to six (*1530, 1558*). Conversely, seven-membered cyclic ions contracting to six-membered have been reported (*1270, 1535*) and six-membered to five (*408, 1269*).

We select for special mention two mechanistic problems. Mandelbaum and colleagues (*830*) postulate a concerted mechanism for the retro Diels-Alder reaction of cyclic alkene ions, on the basis that certain cis diketone systems react while their trans isomers do not. Field ionization kinetics results with cyclohexene indicate a concerted mechanism in the picosecond time frame (10^{-12}-10^{-9} sec) and possibly at longer times as well (*408*). Hammerum and Djerassi (*625*) have found, however, that the retro Diels-Alder reaction in simple bicyclic Δ^2 olefins is not influenced by the stereochemistry at the central bond, and interpret this as an argument for a stepwise mechanism. The nature of the retro Diels-Alder reaction (*957*) may depend upon the time-frame considered and, hence, upon the internal energy of the reactant. The loss of water from alcohols, in particular cyclic alcohols, poses severe mechanistic problems which have received considerable attention in the past two years (*15, 279, 305, 334, 608, 696*). The loss of water from straight-chain aliphatic alcohols is *not* a specific 1,4 elimination (*409*) as was previously supposed. Loss of water from cyclohexanol appears to involve a combination of specific and random eliminations (*695*). It has been suggested (*434*) that borneol, isoborneol, and possibly other alcohols as well do *not* lose water, but lose ·OH and H· in a stepwise manner. This novel suggestion has been rejected by certain other workers (*1275*). The suggestion might, however, be the key to

explaining a number of previously inexplicable results concerning loss of 18 mass units from cyclic alcohols.

We have sought to emphasize the advantages and to demonstrate the prevalence of sophisticated double focusing instrumentation with metastable measurement capabilities and of organic syntheses of isotopically labeled compounds. The advantages of high resolution are demonstrated by the incorrect interpretation of loss of 122 mass units from *N,N'*-dibenzoyl-phenylhydrazine as concerted loss of benzamide and a hydrogen atom (*1241*); high resolution measurements establish that the 122 mass units correspond to the elements of benzoic acid (*126*). Many good fundamental studies are of course carried out with much less sophisticated instrumentation (*316, 349, 996, 1369, 1370, 1533*), particularly we note in the Soviet Union. Komarov *et al.* have made a careful study of the effect of temperature on isotope effects in methanes, ethanes, and propanes (*889, 890*) and on the mass spectra of isomeric hydrocarbons (*891*). Chizhov *et al.* (*312*) have quantitatively investigated the transmission effects, across an epoxy ring, of substituent influences on fragmentation. Isaev *et al.* (*755*) have investigated the decomposition of phenol-1-^{13}C under EI. Branton *et al.* (*213*) have reported a careful study of cyclobutanone. Tajima and Tsuchiya (*1453*) have established that $C_5H_5^+$ ions from a number of precursors are typically acyclic. This same group has studied the temperature dependence of decomposition reactions of $C_6H_{12}\cdot^+$ formed directly from 1-hexene and from hexanol by loss of water (*715*).

There have been numerous reports (*20, 345, 353, 507, 627, 1169*) of novel analogies between unimolecular gas-phase ionic reactions and reactions of neutrals induced by photolysis or pyrolysis both in the gas- and liquid-phase. *N*-Benzoyldiarylamine ions undergo a reaction directly analogous to a reverse Chapman rearrangment (*574*). Relationships between stereochemistry of the neutral molecule and the fragmentation of the molecular ion have been extensively explored during the past two years (*15, 279, 305, 334, 377, 390, 608, 936, 1215, 1617*). Unequivocal stereochemical assignments can be made by mass spectrometry using appropriately deuterium labeled compounds (*594, 1016*).

We have omitted an enormous number of papers presenting EI mass spectra and some mechanistic discussion. For many of these papers, the novel feature is that the mass spectra have not previously been reported, and often mechanistic discussion is ill-founded. The novel mass spectra extend and consolidate the analytical capabilities of mass spectrometry. Aldehydes containing cyclopropane rings (*1251*), isonicotinic acid (*1163*), acetals of phenylacetaldehydes (*375*), benzoyloxycyclopentenes (*1390*), trans-cyclopentene-3,5-diol (*1389*), dihydrofurans (*8*), chlorinated toluenes (*908*), nonenes (*1254*), substituted alkynes (*65*), 1,2,3,4,5-pentaphenylpentane-1,5-dione (*201*), *p*-acetophenone ketals (*379*), cyclic fluorethers (*351*), diketopiperazines (*777*), diaminopropane derivatives (*956*), open chain and aromatic $C_9H_{12}O$ alcohols (*897*), methyl 12-dimethylsilyloxyoctadecanoate (*724*), nicotine (*973*), 7-azabicyclo[2.2.1]heptanes (*378*), and benzodioxasilol (*971*) are a few of the more interesting mass spectra to be published in the past two years. Mass spectra of numerous nitrogen heterocyclics have also been reported and discussed in some detail (*63, 164, 165, 276, 352, 860, 1027*).

Metastables. Metastables are fragmentation reactions occurring within a narrow time-window at some time of the order of microseconds following ionization (*693, 790*). A number of novel procedures for the observation of metastables have been described. That known either as DADI (*1043*) or as MIKES (*148*) permits the singling-out and observation of a whole generation of metastable daughter ions characterized by descent from one common precursor (*1267*). DADI or MIKES demands that the magnetic sector precede the electric sector, so that their positions are reversed from the normal configuration (*149, 1551*). The equivalent of DADI or MIKE spectra can be measured on a GEC-AEI MS-30 of normal configuration by scanning the beam deflector plates between the magnet and collector (*1076, 1077*). The authors (*1076, 1077*) whimsically, or perhaps as a facetious comment on excessive use of acronyms, suggest the acronym MAMIES for their technique. It has been pointed out (*75*) that metastable abundances measured by the Major defocusing technique (*1143*) are dependent upon β-slit width.

The emphasis of metastable studies in the period reviewed has been on determination of the structures of ions decomposing in the metastable time-window. Very often an ionized molecule which has delayed for microseconds before decomposing has isomerized in the meantime so that its structure no longer resembles that of the neutral molecule (*1124*). Structures of ions which are themselves the products of fragmentation reactions are still less obvious (*1514*). A general point emerging from ion structure studies is that the structure of an ion decomposing in the metastable time-frame need not be the thermodynamically most stable structure of that ion. Moreover, species decomposing in the metastable region may differ in structure from species of the same formula decomposing at shorter times. The criterion widely employed in metastable ion structure determinations is that of competing metastable transitions (*1360*). If ions of the same elemental composition, but derived from different precursors, undergo the same metastable transitions with the same abundance ratios, they are considered to have a common structure which sometimes can be identified on the basis of this knowledge alone (*370, 791*). The flaw in the method is that ions with the same structure but differing internal energies can give significantly different metastable ratios (*602, 1140, 1497, 1632*). On the basis of the criterion of competing metastable transitions, Williams and colleagues have interpreted metastable abundances measured by the Barber-Elliott defocusing technique (*79*) to explore the extent to which ions of formulas $C_7H_{11}^+$, $C_7H_{10}^+$, $C_8H_{13}^+$, $C_8H_{12}^+$, $C_8H_{10}O^+$, $C_8H_{12}O^+$ (*371*), $C_4H_9O^+$ (*1046*), and $C_9H_{11}^+$ (*1514*) from various precursors isomerize to common structures prior to decomposition in the metastable time-window. A considerably more reliable method for identifying common ion structures is consideration of metastable peak shapes which reflect the kinetic energy released during fragmentation (as already discussed). Kinetic energy release in metastable fragmentations is not strongly dependent upon the internal energy of the reactant ion (*800*). Peak shapes afford a way of distinguishing concerted metastable decomposition (one-step $m_1^+ \rightarrow m_2^+ + N$) from decomposition in two steps ($m_1^+ \rightarrow m_3^+ + N'$ and $m_3^+ \rightarrow m_2^+ + N''$, $N' + N'' \equiv N$), both of which occur within the field-free region (*633*). The mere observation of a metastable transition does *not* establish that the process occurs in a single step (*303, 1401*). Contrary to what has been suggested (*73*), the metastable loss of 28 mass units from an ion derived from carbamazepine 10,11-epoxide is not proof for loss of the $H_2CN\cdot$ radical.

The often large isotope effects exhibited by metastable decompositions can provide insight into the nature of processes occurring in this time-window (*134, 135, 1414*). Deuterium isotope effects on the competing metastables of the $(M -$ ketene$)^+$ ion from acetanilide establish the aniline rather than the cyclohexadieneine as the most probable structure for this ion (*1513*). Metastable abundance ratios support this conclusion (*626*). The $(M -$ ketene$)^+$ ion decomposing at shorter times ($<10^{-6}$ sec) also has the aniline structure (*1494*). Isotope effects indicate that ionized *p*-chloro- and *p*-bromoethylbenzene undergo carbon skeletal rearrangement to tropylium structures prior to loss of Cl· or Br· in the metastable time-window (*718*). There is a strong secondary deuterium isotope effect on the metastable loss of methyl from ionized *tert*-butylbenzene (*1164*); results from ^{13}C-labeling indicate that the $(M - CH_3)^+$ ion formed does not have the phenylated cyclopropane structure discussed by Rylander and Meyerson (*1308*).

Collision-Induced Decomposition. Collision-induced decompositions could become an important method of characterizing ion structure since they afford a convenient means of studying ions which are stable to unimolecular decomposition (*789*). Unimolecular ionic fragmentation is induced by collision with inert neutrals. Collision processes of this type have been extensively studied (*306, 550, 997*) since being postulated many years ago to account for Aston bands (*58*). By introducing a suitable collision gas into the field-free region of a commercial mass spectrometer, the products of the collision-induced decomposition

can be detected as metastables (*141, 789, 1131*). The same metastables at the same abundances indicate a common structure for ions derived from different precursors. The argument is sounder than with competing metastable transitions since decomposition is much less dependent on the internal energy of the reactant ions prior to collision (*1140*). A further advantage of collision-induced decomposition is that the number of decomposition channels is much enhanced, compared to competing metastable transitions, thereby providing more information for structure determination (*1140*). McLafferty and colleagues study collision-induced decomposition with a commercial mass spectrometer of reversed configuration in which the magnet precedes the electric sector (*1551*). The magnetic analyzer is used to select ions of a particular mass which undergo collision with an inert gas in the field-free region between magnet and electric sector. The products of the collision-induced decomposition are kinetic energy analyzed with the electric sector (*cf.* ion kinetic energy spectroscopy). The structures of formulas $C_7H_7^+$ (*1604*), $C_7H_8^{\cdot+}$ (*963, 1141*), $C_2H_5O^+$, $C_3H_6O^{\cdot+}$, $C_7H_8^+$, and $C_{13}H_9^+$ (*1141*), and $C_3H_7O^+$ (*1144*) have been investigated in this way. The acronym CA for "collisional activation" spectra for referring to collision-induced metastables seems unnecessary.

Ion Kinetic Energy Spectroscopy. The major modification to a commercial mass spectrometer necessary for ion kinetic energy spectroscopy (IKE) is installation of an electron multiplier between the electric sector and the magnet (*138, 144*). An IKE spectrum displaying the ionic products of all reactions occurring in the first field-free region is measured with this detector by sweeping the electric sector voltage. The technique was devised by Beynon and colleagues (*138*). IKE spectra are claimed to be detailed "fingerprints" of organic compounds (*143, 147, 1310-1313*). The worth of IKE spectra has, however, been questioned. It has been suggested that their diagnostic use in structure elucidation is strictly limited (*1594*) and that their use in mechanistic studies is tantamount to the use of competing metastable abundances (*717*). Presumably, however, IKE are superior to competing metastable abundances on the basis of sensitivity, since, in the former, ions do not have to traverse the magnetic sector. An IKE study (*55*) of collision-induced processes of rare-gas ions has provided novel and valuable information as to long-lived states of these ions. IKE spectroscopy is not a reliable technique for estimating kinetic energy releases, since peaks in the spectra generally overlap.

Beynon, Cooks, and colleagues have devised several other novel methods of producing spectra. A collision gas is introduced into the first field-free region of a double focusing mass spectrometer. Setting the electric sector at half its normal voltage reveals a spectrum ("$E/2$ mass spectrum") of doubly-charged ions formed by charge stripping reactions $m^+ + N \rightarrow m^{2+} = N + e^-$ (*342*). Setting the electric sector at the negative of its normal voltage produces a "$-E$ mass spectrum" due to reactions $m^+ + N \rightarrow m^- + N^{2+}$ (*844*). Setting the electric sector at twice its normal voltage produces a "$2E$ (or doubly-charged) mass spectrum" due to reactions $m^{2+} + N \rightarrow m^+ + N^+$ (*53, 54, 57*). The "$2E$ spectrum" provides information as to the chemistry of doubly-charged ions (*53, 54, 57, 175*).

ION CHEMISTRY: BIMOLECULAR AND HIGHER MOLECULARITY REACTIONS

Ion-Molecule Reactions. Studies of ion-molecule reactions up until 1971 are covered by the volumes edited by Franklin (*527*) and the review by Friedman and Reuben (*536*). The flowing afterglow method which we mention only as regards equilibria is reviewed by Ferguson (*497*) in the former. A noticeable feature of the literature on ion-molecule reactions in the past two years has been the large proportion of papers concerning ion cyclotron resonance (ICR) spectroscopy (discussed in a separate section below). Experiments with custom-built crossed beam instruments (*423, 664, 1022, 1536, 1611*) and tandem mass spectrometers (*536, 551, 984, 1403*) delve deepest into the nature of ion-molecule processes, however these studies (*1*) tend to fall into categories of atomic and molecular processes which we do not seek to cover in any detail in the present review. Remarkably few studies of polyatomic molecules using tandem mass spectrometers have come to the reviewers' attention, although tandem mass spectrometry offers advantages over even ICR as regards delineation of reaction channels (*420, 1449*). A tandem mass spectrometer at the Brookhaven National Laboratory has, however, been applied to problems of peptide sequencing (*137*) and hormone structure analysis (*136*). Experiments with a tandem mass spectrometer of perpendicular type are in progress at University of Lund, Sweden (*1448*). Single-source electron impact mass spectrometers designed for use at high pressure continue to find extensive and valuable application to ion-molecule studies, even without pulse techniques. Examples are provided by the studies of pentenes (*903*), ethane (*119*), alkylbenzenes (*870*), simple aromatic molecules (*1540*), aliphatic amines (*758*), vinyl fluoride (*1246*), and methane/carbon dioxide (*833*). The ion-molecule reactions in pentanes have been studied and interpreted to characterize pentyl ion structures (*991*); neopentyl ions rearrange to *tert*-pentyl but *sec*-pentyl do not. High pressure in this context means pressures within the range 0.1 to 5 Torr. Intermolecular hydrogen transfers in diethylmalonate have been studied at low pressures (*1599*); the need for higher pressures is obviated by the large cross sections of the reaction. Pulse techniques extend the usefulness of single-source instruments by affording a means of varying residence times. Pulse techniques are readily incorporated with time-of-flight instruments (*1425, 1633*). Harrison and colleagues (*665*) have extended residence times to milliseconds by trapping ions in the space charge of an electron beam of insufficient energy to cause ionization. The ion trapping technique is inspired by that of Bourne and Danby (*193*), which is itself a modification of the technique known as sequential mass spectrometry (*647*). The ion trapping technique has been applied to an investigation of kinetic energy effects on product yields from ion-molecule reactions (*642*) and to studies of the ion-molecule reactions of methane and ethane (*168*), CH_5^+ and $C_2H_5^+$ with polar compounds (*167*), simple oxygen-containing molecules (*166*), and CO/CH_4 and CO_2/CH_4 mixtures (*641*). An "average dipole orientation" theory for treatment of ion-polar molecule collisions has been proposed and tested on charge transfer from rare gas ions to fluorobenzenes and chloroethylenes (*1436*). The theory successfully describes a number of proton transfer reactions [*viz.*, from H_3^+ and CH_5^+ to halogenated ethylenes (*1433*), from CH_5^+ to alkyl chlorides (*1434*), and from $C_4H_9^+$ to alkylamines (*1435*)], and successfully predicts the dependence of the rates of certain ion-polar reactions as measured by ICR on kinetic energy (*199*). A statistical phase space model has been used in computations of cross-sections for reactions of C^- with N_2 and O_2 (*546*). A semi-classical qualitative model for collision-complexes of O_2^+ with neutrals has been described (*688*).

Equilibria. An exciting area of mass spectrometry in the past two years has been the study of gas-phase ionic equilibria and their significance to solution chemistry. Gas-phase ionic equilibrium constants can be accurately measured and thermodynamic properties ($\Delta G°$, $\Delta H°$, $\Delta S°$) calculated. Combining these thermodynamic properties with the appropriate properties from solution, it becomes possible to make a separation into intrinsic (gas-phase) terms and solvation terms. On the basis of gas-phase equilibrium measurements, Arnett, Taft, and others (*43*) have been able to make a complete thermodynamic analysis of the "anomalous order" of amine basicities in solution (NH_3 < primary = secondary > tertiary). Gas-phase measurements (*218*) have established that toluene is intrinsically a stronger acid than either methanol or water, and that the intrinsic order of acidities for alcohols is the reverse of that observed in solution. Equilibrium measurements pertaining to acidities and basicities and to gas-phase solvation are discussed separately below. Other measurements are discussed in the sections on ion cyclotron resonance (ICR) and chemical ionization (CI). The question of dominating importance in all mass spectrometric measurements of equilibria has been whether thermodynamic equilibrium is actually achieved in ion sources. Undoubtedly, steady state concentrations are achieved, but these concentrations may not be the values

that reflect the equilibrium conditions (*398, 535, 836*). The linear van't Hoff plots, the pressure-independence of equilibrium constants, and the reasonable values of calculated thermodynamic properties, inspire confidence that such measurements are most certainly meaningful.

Gas-Phase Basicities and Acidities. Relative gas-phase basicities are determined by measuring equilibrium constants for reactions of the type $M_1H^+ + M_2 \rightleftharpoons M_1 + M_2H^+$ and from these calculating relative basicities ($\Delta G°$). Estimating or neglecting entropy changes ($\Delta S°$) makes proton affinities ($\Delta H°$–Brønsted base strengths) available (*61*). Further treatment of the data yields hydrogen affinities (*61*). Relative gas-phase basicities can be determined quantitatively using the ICR technique (*61, 197*). Accuracies of ≤0.2 kcal/mole for calculated free energy changes have been claimed (*659*). The measurements are undoubtedly this precise, but the accuracy of the basicities is open to doubt for the reasons discussed above that the steady state concentrations may not reflect thermodynamic equilibria. High pressure mass spectrometers (*317, 992, 1626*) and chemical ionization mass spectrometers (*457*) have also been used and afford the advantage that the temperature dependence of equilibrium constants can be investigated. Measuring equilibrium constants at a series of temperatures allows van't Hoff plots to be drawn up. $\Delta H°$ is then obtained directly, and $\Delta S°$ can also be obtained. If the equilibrium constant can be measured only at a single temperature, it is necessary to assume that $\Delta G° \approx \Delta H°$ (*i.e.*, $\Delta S° \approx 0$) in interpreting results; this assumption is made in ICR studies.

The analysis (*43*) of the "anomalous order" of amine basicities in solution has already been mentioned; the gas-phase (intrinsic) basicities of amines determined by ICR follow the inductive effect order (*43*). Gas-phase basicities of amines have attracted considerable attention (*61, 228, 659*). The proton affinities of diamines estimated by Yamdagni and Kebarle (*1626*) with a pulsed high-pressure mass spectrometer are unexpectedly high, and formation of the protonated diamines is accompanied by a large loss of entropy; both facts suggest a cyclic structure with a proton bridge for the protonated diamines (*1626*). Proton affinities (Brønsted base strengths) have been reported for simple alkanes and alkenes (*317*), simple aromatic hydrocarbons (*318*), a wide variety of oxygenated compounds (*759, 992*), water and hydrogen sulfide (*703*), and nitromethane (*910*). Taft and collaborators (*1450*) have established a linear enthalpy/free energy relationship for a series of substituted pyridines between gas-phase proton affinities and aqueous solution basicities. Bohme and colleagues (*657*) have used the flowing afterglow technique to measure equilibrium constants for the reactions $CO_2H^- + CH_4 \rightleftharpoons CH_5^+ + CO_2$ and $N_2OH^+ + CO \rightleftharpoons COH^+ + N_2O$. With this technique, measurements can be made at a series of *well-defined and accurately measured* temperatures; van't Hoff plots can be drawn up and $\Delta H°$ obtained directly without making the assumptions necessary with ICR measurements at a single temperature, that $\Delta G° \approx \Delta H°$.

Relative gas-phase acidities are derived from equilibrium constants measured for reactions of the type $A_1^- + A_2H \rightleftharpoons A_1H + A_2^-$. Electron affinities, proton affinities, and bond strengths can be calculated from the acidities. Brauman and Blair have reported acidities estimated from ICR measurements for carbon acids (*215*), alcohols (*216, 218*), and amines (*217, 219, 222*). The effect of alkyl substituents on gas-phase acidities (*220*) and the acidities of monosubstituted phenols (*1137*) have been investigated by ICR. Yamdagni and Kebarle (*1627*) have reported acidities for carboxylic acids measured with a pulse high-pressure mass spectrometer; the temperature dependence of equilibrium constants could be measured with this instrument and $\Delta S°$ was shown to be approximately zero. The flowing afterglow technique has been used to investigate acidities of alcohols (*183*) and selected Bronsted acids (*184*). This technique has also been used to measure equilibrium constants for the reaction $NH_2^- + H_2 \rightleftharpoons H^- + NH_3$ at a series of temperatures (*182*).

Gas-Phase Solvation or Clustering. Gas-phase solvation or clustering around both positive and negative ions has been studied extensively by Kebarle and colleagues using high-pressure mass spectrometry (*49, 458, 837, 1213, 1624*). Their technique gives residence times in the ion source of milliseconds which is sufficient to establish equilibria at pressures of the order of Torr. Clusters of up to 8 water molecules around a proton have been observed (*838*). The equilibria measured are of the form $H^+(H_2O)_{n-1} + H_2O + M \rightleftharpoons H^+(H_2O)_n + M$. M is an inert third body. Measurements are made at a series of temperatures and give linear van't Hoff plots from which heats and entropies of solvation are obtained. The solvation of negative halide ions by acetonitrile and by water (*1625*), the solvation of proton by methanol and dimethylether (*597*), and the solvation of the ammonium ion by ammonia and water with emphasis on the stability of mixed clusters $(NH_4)^+(NH_3)_n\ (N_2O)_w$ (*1212*) have been investigated. There is sharp disagreement between results of Kebarle and colleagues (*362, 838*) on the proton hydration and results on the same reversible reactions by Field and colleagues (*103, 116*) using the high pressure chemical ionization mass spectrometer (see following sections). Kebarle and colleagues (*362*) suggest that the ion residence times in the Field experiments are too short to establish equilibrium. The suggestion is rejected by Field (*116, 942*). The solvation of alkoxide ions by alcohols (*169*) and the solvation of halide ions by alkyl halides, nitromethane, methanol, and methyl cyanide (*1274*) have been investigated by ICR. These studies yield the order of solvating ability of various neutral molecules, but do not give thermodynamic functions since measurements are made at a single temperature. Clustering of water and methanol around NO^+ have been studied with a PI high-pressure mass spectrometer using the krypton resonance radiation (10.03 eV) (*186, 1122*).

Ion Cyclotron Resonance (ICR) Spectroscopy. From the viewpoint of ion chemistry, ion cyclotron resonance (ICR) (*88, 385, 1609*) has been one of the most active fields within mass spectrometry during the past two years. The central thrust toward elucidating through gas-phase measurements the intrinsic chemistry of ionic processes in solution has been made in ICR. The contributions of ICR to the study of gas-phase acidities and basicities and of gas-phase solvation have already been described. The scope and variety of problems accessible to modern mass spectrometric techniques has been convincingly demonstrated by recent ICR measurements. One remarkable example is the report (*221*) of homogeneous catalysis of an ion-molecule reaction; methanol catalyzes the abstraction of a proton from toluene by the allyl anion. Gas-phase electrophilic aromatic substitution has been measured and discussed in relation to solution reactions by Dunbar, Olah, and colleagues (*452*). The same group (*453*) has measured gas-phase nitration (NO_2^+) and acetylation (CH_3CO^+) of substituted aromatics. Acetylation shows the expected electrophilic substituent effects; however, nitration displays nucleophilic substituent effects. Gas-phase acylation of acetone has been measured and discussed (*1484*). Gas-phase reactions of the methyldiazonium ion $CH_3N_2^+$ have been measured by ICR (*524*); the importance of these studies lies in the light they may be able to throw on diazonium ions in solution (*524*). The occurrence of intramolecular hydrogen bonding in protonated dimethoxyalkanes [$CH_3O(CH_2)_nOCH_3$, $n \geq 5$] has been established from ICR equilibrium measurements on the dimerization reaction (*1103*). Intramolecular hydrogen bonding in protonated diaminoalkane ions has been evaluated quantitatively from consideration of the enhanced gas-phase basicities resulting from the hydrogen bonding (*60, 62*). The proton affinity determinations discussed in the section on basicities provide estimations of carbonium ion stabilities. Beauchamp and coworkers (*1147*) have suggested that equilibrium measurements on halide transfer reactions can afford more accurate estimations of carbonium ion stabilities than measurements on hydride transfers. Strong correlations between gas-phase bimolecular ion chemistry of alkyl halides and the ion chemistry of these species in highly acidic solutions have been revealed by ICR studies of ion-molecule reactions in alkyl halides (*90*); gas-phase nucleophilic displacement reactions which result in the formation of dialkylhalonium ions have been identified. A study (*454*) of the ethane system using 13-eV bombarding electrons to initiate reaction has been undertaken to explore correlations between gas-

phase ion chemistry and ion chemistry in highly acidic media.

The attractive features of ICR for ion-molecule studies are the long residence times of milliseconds and the double resonance technique for delineating reaction channels. Absolute rate constants can be calculated from power absorptions (*35, 277, 335, 835, 1125, 1127, 1146*). The dependence of reaction rates upon ion kinetic energy can be determined by pulse techniques (*1136*). We would bring attention to the expert comments of Drewery, Goode, and Jennings (*446*) to the effect that theoretical analysis of ICR currently outstrips experimental technique. These authors emphasize the need for caution in interpreting double resonance experiments and point out difficulties so often glossed over by other workers in obtaining either relative or absolute rate constants from ICR measurements. Possible pitfalls in interpreting double resonance results have also been discussed by Beauchamp and coworkers (*529*) and by McAllister (*1127, 1128*). The ion-molecule reactions in β-substituted alcohols (*853*), ammonia (*732, 1030*), 1,1-difluoroethylene (*1186*), various perfluorocarbons (*1437*), 2-butanol (*89*), acetone (*1017*), vinyl chloride and fluoride (*36*), acetaldehyde (*1502*), perdeuteromethane (*548*), and nitrogen (*770*) have been studied by ICR. In unraveling the complexities of ion-molecule reaction sequences in mixtures of compounds, ICR has a decisive advantage over single-source high pressure mass spectrometers. The following binary mixtures have been investigated by ICR: CH_4/H_2O, CH_4/H_2S, and CH_4/NH_3 (*734*); H_2/CO and D_2/CO (*1502*); H_2/D_2 (*329*); H_3^+ and neutrals (*733*); H_2/CO_2 (*1404*); N_2O/H_2 and N_2O/CH_4 (*1127*); CH_4/CD_4 (*731*); H_2/CO_2, H_2/CO, and H_2/N_2 (*1126*); C_2HF_3/C_2H_4 (*37*), and C_2H_4/fluoroethylenes (*500*). The propene/deuteropropene and propene/cyclopropane systems have been the objects of detailed study (*196*); the formation of $C_6H_{12}^+$ and its subsequent unimolecular reactions *via* 1,2- and 1,4-hydrogen shifts are discussed. A phase coherent pulsed ICR method for determining ion-molecule frequencies and their dependence on kinetic energy has been proposed (*967*) on the grounds of being easier and more accurate than more established methods (*87, 730, 1609*). Buttrill (*278*) has investigated temperature-effects on rates of ion-molecule collisions. Equations of motions which account for the periods of seconds an ion resides in a trapped-ion cell (*1135*) have been derived (*1361*). A new detector for use in ICR spectroscopy has been described (*735*).

ICR has been used in ion structure determination (*599, 612, 680, 1166, 1491*). The aim has been to characterize a particular structure by its ion-molecule reactions. In this role, ICR is a companion to such methods as collision-induced metastables, competing metastable abundances, metastable peak shapes, and ion kinetic energy spectroscopy. Like collision-induced metastables, the ICR method can probe the structure of ions stable with respect to unimolecular decomposition. McLafferty and coworkers (*1123*) have studied propyl ion structures and have shown that n-$C_3H_7^+$ ions isomerize to *sec*-$C_3H_7^+$ ions. Tomer and Djerassi (*1490*) have established that $C_2H_4S\cdot^-$ ions formed from pentylthiovinyl ether *via* hydrogen transfer from the 2-position have the thioacetaldehyde structure, whereas the $C_2H_4S\cdot^+$ ions formed *via* transfer from the 3- and 4-positions have the vinylthiol structure. Neutral isomers of formula C_5H_{10} have been distinguished on the basis of their reactions with ionized 1,3-butadiene (ionizing energy 10.9 eV) (*603*). By exploiting the long residence times of ICR, it has been shown that the major reaction of ionized 1,5-hexadiyne is loss of hydrogen in times of the order of milliseconds (*601*).

Dunbar and others (*447–451, 906, 907*) have used ICR to monitor cationic photodissociation processes. Photodissociation has recently been reviewed by Durup (*456*). Ions are produced by low energy electron impact and trapped in the ICR cell for periods of seconds. Irradiation with photons of variable wavelength produced photodissociation spectra of ion current as a function of photon energy. The technique has been used for ion structure determination (*448, 450*).

ION CHEMISTRY: IONIZATION TECHNIQUES

Fourteen methods of molecular ionization have been reviewed by Milne and Lacey (309 references) (*1081*). Comparison of electron ionization (EI), field ionization (FI), field desorption (FD), and chemical ionization (CI) for various types of compounds has been included, as well as a detailed treatment of FI, FD, and CI applications thus far.

Chemical Ionization (CI). The growth rate of chemical ionization (CI) since its conception in 1966 (*1112*) must be unprecedented for an analytical technique. Within the space of seven years, it has passed through six of the seven ages of an analytical method proposed in the recent editorial by Laitinen (*925*). Papers in which the emphasis rests on fragmentation mechanisms following CI (*516, 725, 1062, 1063, 1130*) are nowadays far outnumbered by the legion of papers dealing with analytical applications of CI in biochemistry, biology, and medicine (see later sections). CI mass spectrometry in structural analysis has been reviewed (*515*). There have been relatively few papers reporting advances in the basic instrumentation of CI mass spectrometry (*292, 549, 682, 683, 1430*). Advances have been made as regards novel reagent gases as alternatives to the standard methane or isobutane. Reagent gases without acidic hydrogens effect charge exchange and the amount of fragmentation depends on the recombination energy of the reagent gas ions (*470*). Two component reagent gases have been suggested (*47, 727*). With Ar^+/H_3O^+ (*727*), Ar^+ effects charge change and produces a fragmentation pattern, while H_3O^+ transfers a proton to the sample molecules and identifies the molecular weight. Ammonia (*459*), deuterated water (*726*), nitric oxide (*728*), and tetramethylsilane (*1178*) each possesses some desirable quality when used as a reagent gas. It appears that reagent gases can be chosen to suit the sample, and that the nature of the CI mass spectrum can be varied almost at will to provide different kinds of information by proper variation of the reagent gas. An ICR cell has been used for chemical ionization (*330*); the long residence times mean that lower pressures are required to produce CI conditions.

Field (*503, 504*) has shown how kinetic measurements on unimolecular ionic decompositions can be carried out with the CI mass spectrometer. The measurements yield kinetic data analogous to data from thermal unimolecular gas-phase reactions (*124*), although the true significance of the CI results is not yet wholly clear (*1053*). Interpretation of the measurements rests on the assumption that sufficient collisions occur prior to decomposition to establish a Boltzmann internal energy distribution. Typical calculated residence times are of the order of 10 μsec and source pressures are estimated to be of the order of Torr (*505*). It has, however, been suggested by other workers (*297, 1412*) that these calculated residence times are longer than the true residence times. Given a Boltzmann distribution, rate constants for decomposition can be calculated using conventional rate expressions (*503, 504*). Plotting the calculated rate constants *vs.* temperature gives linear Arrhenius plots, from which activation energies and preexponential factors are obtained. Among the reactions studied are the unimolecular decomposition of protonated tertiary alkyl acetates and other esters to form the alkyl carbonium ions (*940, 941*); calculated activation energies are around 8–9 kcals and preexponential factors are around 10^{10}–10^{-12} sec^{-1}. The calculated rate constants are independent of pressure which is consistent with equilibrium being established in the source (*942*). A number of other systems (*505*) have been investigated including amino acids (*1055*).

CI has also been applied by Field to equilibrium studies (*505*). There is convincing evidence that reversible reactions occur in the CI source (*503*), but it is less certain that the reactions reach equilibrium (*441, 1053*). Linear van't Hoff plots have been obtained for a number of association reactions and from these plots free energies, enthalpies, and entropies have been calculated (*116–118, 503, 504*). A disturbing or intriguing feature of these results, depending on one's point of view, is that the calculated values of $\Delta S°$ for certain of these reactions involving association of two molecules have been found to be positive (*505*). The formation of protonated benzylacetate dimer from protonated benzylacetate and benzylacetate is one such reaction (*503, 504*). The loss of three translational degrees of freedom should give a large negative $\Delta S°$. The CI method has also been applied to reversible reactions of the type (*1409*).

$$t\text{-}C_4H_9^+ + i\text{-}C_5H_{12} \rightleftharpoons t\text{-}C_5H_{11}^+ + i\text{-}C_4H_{10}$$

Negative chemical ionization has been explored by Dougherty *et al.* (*439, 441*). Negative chemical ionization can be viewed as an extension of the technique of adding nonreactive gas to enhance negative ionization cross sections (*442*). It is suggested (*159*) that, for analytical applications, negative chemical ionization complements positive chemical ionization.

Field Ionization (FI). The future of field ionization (FI) as an analytical technique is difficult to forecast. In a recent review (*27*) in *Analytical Chemistry*, it was suggested that FI [as distinct from field desorption (FD), which is discussed separately below] will become a standard technique in many laboratories that previously had never used mass spectrometry and will become as universally employed as gas chromatography. The fundamental problem that FI sensitivities for individual members of multicomponent mixtures are dependent on the nature of the other components has yet, however, to be faced and solved (*92, 400*). Moreover, analytical applications of FI (*554, 1343, 1350, 1422, 1496*) (covered more fully in later sections) in the past two years have not been numerous in comparison to some other techniques, for example CI or even FD. Analytical capabilities of FI continue, however, to be improved by instrumental advances (*94, 1568*) which could result in more extensive analytical application. Effective conditioning or activation of emitters to produce stable and inert protrusions of up to 40 μm in length can be achieved by suitable treatment with benzonitrile at high temperatures (*93, 96, 1333*). The protrusions are conducting and presumably composed of carbon (*1333*), in contrast to protrusions grown at low temperatures which are composed of semiconducting organic polymers (*419*). Yet it is still doubtful whether any conditioning technique is sufficiently reliable for routine application (*81*). A novel multitip FI source (*4, 5, 27, 246*) with about 1000 tips deposited 25 μm apart by evaporation techniques could represent a major advance in source design; the source has been applied to analytical problems in a number of diverse fields (*27, 1350, 1422*). An ingenious electrohydrodynamic source, in which the extremely high field strengths necessary for FI are produced by interaction between liquid metal droplets and an electrostatic field, has been devised; however, its application is probably limited to liquid metals and compounds soluble therein (*332, 333, 488*).

The more physical aspects of FI attract considerable interest. An excellent review has been given by Robertson (*1277*). Field emission and ionization in condensed phases has been reviewed by Gomer (*575*). Müller's group has recently measured with the field ion atom probe (*1108, 1443*) the kinetic energy spectrum of field ions formed at a single atomic site (*1109*). A number of novel theoretical treatments of the FI process have appeared (*38, 295, 780*). Mechanistic discussions of FI mass spectra (as distinct from field ionization kinetics) have appeared (*1074*) including one study using extensive deuterium labeling (*248*). Beckey and Röllgen (*100, 1286, 1287*) have carried out careful studies of the chemical processes occurring at the surface of FI emitters; their novel pulsed desorption technique (*1288*) seems to hold considerable promise for such studies. Dimer formed from two components of a mixture (*e.g.*, aniline–nitrobenzene) have been observed in FI mass spectra (*97*). Hammett correlations in FI mass spectra have been pointed out and discussed (*98, 1228, 1229*).

Field Desorption (FD). Enormous interest is currently focused on the field desorption technique developed in Beckey's laboratories (*93, 1337*). The technique seeks to remove the most fundamental limitation of mass spectrometry by producing mass spectra from thermally unstable *nonvolatile* compounds. The emitter is dipped in a solution of the sample, thereby depositing nanogram quantities of the sample onto the emitter. The emitter is then placed in the mass spectrometer where a spectrum is produced from the absorbed sample by simultaneously applying a very high field and by heating the emitter (*1603*). The key to success with the technique lies in conditioning the emitter so as to enhance its surface area and, hence, the amount of sample it can absorb. Conditioning is discussed under field ionization. The mass spectra produced by field desorption almost invariably display molecular ions and little fragmentation. Although almost all reported studies of field desorption originate from the same laboratory, there seems little doubt that field desorption is a powerful technique for measuring molecular weights. Aside from molecular weight determination, it has not been established that field desorption has any advantages for structure elucidation, although work with macromolecules looks promising. Routine calibration of mass scales for accurate mass measurements could be a problem with single beam instruments (*1044*); the problem might be alleviated with dual-beam instruments such as the GEC-AEI MS-30 (*1591*). The reviewers feel that it remains to be seen whether or not field desorption will be economically viable for routine analysis, if the information provided is limited to molecular weight determination. Field desorption has to date been applied to studies of nucleosides and nucleotides (*1335*), purine bases (*1333*), amino acids (*1602*), peptides (*1601*), pesticides (*1336, 1344*), drug metabolites (*1334*), substituted sultams (*1342*), disodium salts of aldohexose phosphates (*1340*), antibiotics (*1272*), stereoisomeric glycosides (*954*), and quaternary ammonium salts (*226*). A recent innovation has been pyrolysis (*1058*) of samples *in situ* on the emitter. The high field is applied at the same time to give a field desorption spectrum of the pyrolysis products. The pyrolysis method has been applied to bacteria, deoxyribonucleic acid, and even tissue and blood cells (*1338, 1341*).

Negative Ions. A comprehensive review by Dillard (*433*), which has recently appeared, removes much of the burden from the present reviewers. We have been selective in our coverage and, in particular, do not attempt to exhaustively review inorganic negative ions (*571, 1386*). Efforts continue to develop 70-eV EI negative ion mass spectra as a method of analysis and structure elucidation (*205, 761, 849, 1635*). Negative ion mass spectra can be measured on most mass spectrometers by appropriate adjustment to the polarities of certain potentials (*1634*). The intensities in the mass spectra are, however, low. Skeletal rearrangements have been reported in the negative ion mass spectra of ylides (*19, 22*). Todd and colleagues (*21, 1486*) have discussed a qualitative theory devised to rationalize 70-eV EI negative ion mass spectra. Negative molecular ions in these spectra arise from secondary electrons (*1129*). The reviewers note that *identical* descriptions of the 70-eV EI mass spectra of deuterated methanols were submitted and published by the principal author in *two* separate journals (*1480, 1481*). Doubly-charged negative fluorine ions have been observed in the EI mass spectrum of CF_3Cl (*14*). Decomposition reactions of negative ions can be induced by collision with neutrals (*203*).

Ionization efficiency curves measured at low electron energies (0–20 eV) have been reported for negative ions from carbon dioxide (*300*), nidocarboranes (*244*), nitriles (*1505*), cyclic hydrocarbons (*531*), cyclic anhydrides (*347*) and nitromethane (*431*). The results are discussed in terms of the three general mechanisms of negative ion formation—resonance capture, dissociative resonance capture, and ion-pair formation mechanisms. Accurate appearance potentials have been measured by the retarding potential difference method for ions formed from perfluorocyclobutane by dissociative resonance capture (*974*). Thynne and colleagues (*634, 637–639, 1018, 1483*) have resolved structure in ionization efficiency curves by deconvolution procedures. Electron capture processes in BF_3 and BCl_3 have been studied by both electron swarm and pulsed retarding potential difference electron beam techniques (*1426*). Translational energies of ions (*635*) formed by resonance electron-capture processes in CO, CO_2, NO, and SO_2 (*636*) and in CF_4 and SiF_4 (*1566*) have been measured by Franklin and coworkers as a function of excess energy. Time-of-flight mass spectrometers have been widely used to measure autodetachment lifetimes (*347, 431, 531, 848, 1479, 1483*). The effects of temperature on ionization efficiency curves for ions from SF_6 (*977*) and on electron capture by polyatomic molecules at low energies (<0.2 eV) (*1410*) have been investigated. The potentials of tetracyanoethylene (*229*) and tungsten hexafluoride (*1482*) as scavengers have been assessed. The photodetachment of electrons from tetracyanoethylene ions has been re-

ported (*1010*). Some studies of negative ion-molecule reactions have been reported (*432, 1031, 1368*) (other studies were covered in the sections of acidities, solvation, and chemical ionization).

Photoionization (PI). The amount of energy available for photoionization is known precisely. The energy deposition function for the molecular ion is reflected by the photoelectron spectrum; an indication of recent progress in photoelectron spectroscopy is provided by the reports of the Sussex (*493*) and Asilomar (*1372*) meetings. For these reasons, photoionization is suited to detailed studies of atomic and molecular processes such as the studies by Berkowitz, Chupka, and colleagues on NO (*851*), N_2O (*852*), HOF (*128*), and F_2O (*129*). The photoelectron spectrum of a molecule is only a crude approximation to the internal energy distribution function of the molecular ion following EI (*746*); the energy deposition functions for EI and PI have been shown to differ in the cases of toluene (*1415*) and decene (*794*). Meisels *et al.* (*1051, 1052*) have shown, however, that more reasonable approximations to the internal energy distribution function following EI can be obtained from considering photoionization cross-sections together with photoelectron spectra. Photoion/photoelectron coincidence studies which correlate the nature of the fragmentation of the molecular ion with internal energy constitute one of the most promising areas of mass spectrometry (*1384*). Eland and Danby (*374, 473*) have described two types of experiment. In one type, the excitation energies at which a particular ion mass is formed are measured; in the other, the ion masses formed at a particular excitation energy are measured. Brehm *et al.* have discussed coincidence measurements on SO_2 (*224*) and CS_2 (*225*). Stockbauer and Ingram (*1423, 1424*) have reported and discussed coincidence measurements on CD_4, CH_4, C_2D_6, and C_2H_6; the results accord with QET.

Rosenstock *et al.* (*1291*) have considered the significance to QET of PI data on the fragmentation of benzene; they conclude that some decomposition occurs from isolated excited electronic states. PI studies of the fragmentation of benzyl chloride (*16*) and of hetero aromatic alcohols and aromatic amines (*1242*) have been described. A considerable number of fine PI measurements with the National Bureau of Standards high-pressure mass spectrometer on ion-molecule reactions have been reported by Sieck, Ausloos, and colleagues (*1376, 1377, 1381, 1382*). Ion-molecule reactions of acetone (*1374*), isopropanol (*578*), methylcyclopropane and cyclobutane (*965*), 1-butene, 2-butene, and 2-methylpropene (*1375, 1380*), and nitrous oxide (*1378*) have been studied with one objective being to determine the structures of the reactant ions. A comparison has been made of photoionization and Penning ionization of simple hydrocarbons (*1379*). PI studies of ion-molecule reactions have been reported from other laboratories (*758, 903, 1122, 1356*).

ANALYTICAL APPLICATIONS IN BIOMEDICINE

Uses of Stable Isotopes in Biomedical Research. There has been a considerable revival of interest in the use of stable isotopes such as ^{13}C, ^{2}H, ^{15}N, and ^{18}O in the life sciences and medicine. This is largely because of their increased availability in the form of simple organic molecules and because of the development of Fourier transform ^{13}C NMR and mass spectrometric techniques for their detection in tracer experiments. The relative nontoxicity of these isotopes compared to radioactive ones is of great advantage in experiments carried out with human beings. Matwiyoff and Ott (*1041*) have recently reviewed the uses of stable isotopes, notably ^{13}C in these fields, describing large scale production methods, improved analytical instrument techniques, and examples of uses. A short review by Knapp and Gaffney (*871*) discusses the advantages of using stable isotopes over their radioactive counterparts in clinical pharmacology.

Some recent reports give an idea of the relative innocuous nature of stable isotopes. Two weanling mice developed apparently normally on a ^{13}C-labeled diet until their body carbon content increased to *ca.* 60% ^{13}C (*1193*). In another study, dealing with cholesterol metabolism in rats, the animals were fed water containing 10% D_2O for a considerable period with only minimal toxic effects (*1220*). In humans, deuterated amino acids have been administered in studies of metabolic disorders such as phenylketonuria and "sweaty feet syndrome" with mass spectrometric determination of products (*365–367*). Stable isotope-labeling has also been used to study gluconeogenesis and glucose utilization in children (*155*). ^{15}N-lysine has been administered to people suffering from chronic enterocolitis and nitrogen isotopes in excreted products analyzed by MS methods (*107*). Tyrosine metabolism in rat brain in the presence of an ^{18}O atmosphere has been followed using fragmentographic determination of hydroxylated products (*1353*). Rats with a bile fistula have been fed D-labeled ethanol and the incorporation of the label into cholesterol and bile acids followed by mass spectrometry (*359, 360*). A further study has used both ^{13}C- and D-labeled ethanol with ^{13}C NMR examination of products and ^{2}H, ^{1}H decoupling (*1597*). ^{13}C NMR and mass spectrometry may play complementary roles in studies of this type. The former technique still lacks the sensitivity of the latter and is not good for quantitative determination of label incorporation but can accurately determine sites of incorporation for ^{13}C. Mass spectrometry, however, can give accurate quantitation of isotope incorporation on small amounts of material but may be less specific in defining sites of incorporation, especially for deuterium.

Among MS techniques recently proposed for use in this area are ones for analysis of the isotope ratio of expired CO_2 following ^{13}C-labeled compound intake (*1134*) and for GC-MS recognition of metabolites produced from mixed ^{1}H, ^{2}H-labeled compounds (*872*).

For preparation of labeled biological compounds, convenient methods are described in the *Journal of Labelled Compounds* (Presses Académiques Européennes, Brussels, Belgium).

Many other examples of the uses of stable isotopes in fragmentographic quantitation, in elucidating fragmentation mechanisms, and in tracer experiments, may be found in later sections of this review.

Screening of Body Fluids and Tissues for Metabolic and Other Disorders. Inherited disorders of metabolism may often manifest themselves by accumulation of particular metabolites in body tissues or physiological fluids. Existing clinical tests can detect known disorders by identifying individual compounds; enzyme assays, more time consuming, can detect specific defects given some prior knowledge of which metabolic pathway is affected. Pioneering work by the group of Jellum and Eldjarn has however shown the applicability of GC–MS in determining a whole suite of compounds with great specificity in a single analysis of a body fluid. Applied to urine, this procedure can detect many of the existing metabolic errors and has been responsible for uncovering several previously unknown ones. Groups in several countries now use such screening procedures, see *e.g.* (*576, 617, 704, 738, 782, 930, 944, 1090, 1524, 1595, 1608*). The use of computers in the acquisition and analysis of data is particularly valuable in such work (*704, 738, 783*). Analysis by GC–MS of amniotic fluid (*617*) or by pyrolysis GC of fetal cells (*1263*) may be used to detect inherited biochemical abnormalities before birth.

Much work has still to be done to establish the best methods for determination of suites of compounds and to identify normal components of urine. Several groups have used a variety of gas-phase methods to determine α-keto acids, important in some acidemias. These compounds have been recently analyzed as free acids (*577*) and silylated oximes (*930, 1419*). The structures of silylated quinoxalinol derivatives have been further explored (*539*). For other aliphatic and aromatic acids, methyl or trimethylsilyl esters are most commonly used. For GC–MS analysis of amino acids in urine, alternative procedures to those already described (*782*) have been proposed (*170, 1595*). A procedure usable for urinary sugar alcohols is described (*616, 1090*). Urinary anthranilic acid and kynurenine may be estimated by GC methods (*675, 1161*). Variations in the urinary acid profiles of normal young adults on a controlled diet have been studied (*1608*) and the effects of ethanol ingestion noted (*958, 1607*). Levels of glutarate have been estimated by GC–MS (*950*). Branched short

chain diacids (*1225*) and aldonic and deoxyaldonic acids (*944*) are present in urine.

Exploration of metabolic abnormalities in patients with known metabolic disorders continues, covering β-hydroxy-*n*-valeric acid in a patient with propionic and methylmalonic acidemia (*1428*), branched chain and odd carbon number fatty acids in glycerolipids in a case of methylmalonic aciduria (*858*), monounsaturated dicarboxylic acids in a child with metabolic acidosis (*191*), 2-hydroxybutyric acid in patients having lactic acidosis (*1224*), adipic and suberic acids in ketotic patients (*1223*), tiglylglycine in a child with β-methylcrotonylglycinuria (*576*), methylcitrate in patients with propionic acidemia (*33*) and branched chain α-keto acids from patients with maple syrup urine disease (*577*).

These screening procedures may ultimately find use in diagnosis of disease states other than metabolic disorders. Several papers have described abnormal excretion of compounds in certain patients but an understanding of biochemical manifestations of disease is at a very primitive stage. For example, in a GC–MS analysis of urinary volatile metabolites from patients with diabetes mellitus, it has been found that certain compounds including pyrazines and lower alcohols, are consistently elevated (*1645*). Cerebrospinal fluid of other diabetics contains 1,5-anhydroglucitol (*1232*). GC–MS methods for analysis of volatiles of breath and urine have been described by another group (*1039, 1470*) but only analyses of "normals" are reported. Origins of other compounds detected in urine of sick people such as 3-methylxanthine (*1524*) and β-*p*-hydroxyphenylhydracrylic acid (*1553*) remain uncertain. It has been suggested that monitoring of the urinary levels of polyamines such as spermidine, spermine, and putrescine may be useful for the prognosis of cancer and a GC–MS method is proposed for quantitation of these (*397*).

Neurobiology. The sensitivity and specificity of mass spectral methods, notably GC–MS, appears to have great appeal for workers in neurochemistry, interested in the determination of biogenic amines and metabolites at the sub-nanogram level (see *350*). Several recent papers have been devoted to examinations of derivatization methods for amines and to studying their fragmentations. The spectra of underivatized DOPA and analogs (*1516*) and the CI spectra of a variety of biogenic amines (*1080*) are discussed. Recent reports on mass spectral or electron capture assays have described use of a variety of derivatives including perfluoroacyl (*44, 290, 386, 899*), perfluoroaryl (*1088*), acetyl (*354*), isothiocyanates (*1159*), TMS (*1156*) and reaction products with fluorescamine (*1155*). Various derivatives for GC–MS of catecholamines have been explored (*1239*). Fragmentographic assays have been developed for several primary amines (*829*), norepinephrine and dopamine (*899*), four indole alkylamines (*290*), *N,N*-dimethyltryptamine (*1560, 1618*), choline and acetylcholine (*786*), and tetrahydropapaveroline (*25*).

Melatonin has been identified in chicken blood by GC–MS (*1216*) and levels in rat pineal glands measured (*386*). Four indolealkylamines including melatonin, have also been measured in rat pineals (*290*). The action of indoleamine-*N*-methyltransferase has been investigated by MS methods (*1157, 1559*). Concentrations of *N,N*-dimethyltryptamine in "normal" and psychiatric patients have been examined (*1618*). Bufotenin is present in the urine of some patients with schizophrenia or infantile autism (*1156*). Following an earlier report, a search has been made by GC–MS for the presence of *trans*-3-methyl-2-hexenoic acid in the sweat of schizophrenics (*580*). The compound was detected but is also present in "normal" sweat.

Methods described above for urine acid screening detect a variety of aromatic acids, many of which are metabolites of amines. Levels of such compounds in body tissues and fluids have attracted interest in relation to neurochemistry. Fragmentographic assays for 4-hydroxy-3-methoxyphenylacetic acid (*133, 369, 1392, 1393*), indole-3-acetic acid (*132*), 5-hydroxyindole-3-acetic acid (*131*) and 4-hydroxy-3-methoxyphenylglycol (*209*) are reported. Perfluoroacyl derivatives are preferred. Metabolites of DOPA and other amines have been further studied (*1106, 1552, 1573*). A GC–MS method failed to detect benzoyl sarcosine in normal urine (*933*). A study of urinary acids in a patient with periodic catatonia showed interesting fluctuations in the levels of tartrate, malate, *m*-quinol, and 3,4-dihydroxybutyrate (*951*).

Pharmacology. GC-MS methods appear to have become those of choice in detection, measurement, and metabolic studies of drugs. A recent review by Jenden and Cho (*785*) (191 references) covers applications of the technique in pharmacology and toxicology. A shorter review by Prox (*1250*) gives some examples of the uses of mass spectrometry in drug metabolism studies. GC–MS detection and quantitation of addictives and hallucinogens is described (*700*) while fragmentography is briefly described in the review by Watson of newer analytical techniques in pharmacology (*1574*). The utility of GC–MS computer systems is described in papers by Horning *et al.*, (*709*) (for measurement of drugs and their metabolites in body fluids) and by Finkle *et al.* (*509*) (for rapid identification of drugs of abuse). CI methods are also finding applications in drug studies (*709, 1250, 1315*). Fragmentography with the use of a CI source may find increasing applications in the measurement of low concentrations of drugs with the possibility of using the highly specific and abundant quasi-molecular ions (*709, 1580*). A rapid and simple method for the extraction of neutral and basic drugs from plasma is described, which uses isopropanol extraction from diluted plasma saturated with potassium carbonate (*707*). Ting *et al.* (*1485*) have proposed a relation between the fragmentation patterns of drugs and their pharmacological actions.

Fragmentographic methods have been employed to monitor therapeutic levels of drugs in plasma, *e.g.*, imipramine (*537*), carbamazepine (*1199*), and indoramin (*443*). GC with electron capture detection may compete with fragmentography in quantitating drugs (if halogenated derivatives are used) but GC–MS is still useful in confirming the nature of derivatized products (*109, 435*). Examples of studies of the metabolism of clinically used drugs in man and animals by GC–MS methods are as follows: nortriptyline (*872*), propranolol (*1562*), doriden (*1421*), methsuximide (*708, 1111*), dilantin (*298*), cambendazole (*1518*), hydralazine (*1643*), lidocaine (*1431*), methaqualone (*189*), digoxin (*1575*), codeine (*463*), glycerylguaiacolate (*1521*), phentermine (*314*), alclofenac (*1289*), and hexamethylmelamine (*795*).

Toxic metabolites that may be produced by ingestion of propenylbenzene derivatives present in flavors and spices have been examined using GC combined with a CI mass spectrometer (*1192*). Plasticisers such as phthalates are now frequently found in blood. A study has been made of the metabolism of diethylhexylphthalate by rats (*18*). EI spectra of many compounds of this type do not exhibit molecular ions and CI methods are useful in obtaining quasi-molecular ions (*18, 490*). Pyrazoles are potent inhibitors of certain enzymes and it has been shown that these compounds are amenable to GC–MS analysis (*1304*).

For GC–MS of barbiturates, the 1,3-dimethyl derivatives have been most widely employed. For the derivatization of these compounds, trimethylanilinium hydroxide appears to be the reagent of choice (*444, 1395*) [though see (*1476*)]. GC retention times and principal fragment ions for nineteen barbiturates (as 1,3-dimethyl derivatives) are recorded (*1395*). Metabolites of amylobarbitone (*444*) and allobarbital (*1078*) are described and may be quantified by fragmentography. The fragmentations of some *N*-substituted barbitals and their TMS derivatives have been described recently, and it is claimed that the latter derivatives can be used to distinguish isomeric barbiturates (*1576*). The identification of barbiturates in mixtures using a direct probe is described (*1282*). FI spectra of underivatized barbiturates can give some information on the nature of substituents in addition to the molecular weights (*282*).

Street drugs continue to be studied with forensic and metabolic interest. Mass spectral techniques have been used for the identification of heroin in suspected material (*1152*), for the detection of 2,5-dimethoxy-4-methylamphetamine (*538*), amphetamine (*313, 815*), *p*-hydroxyamphetamine (*108*), amphetamines and hallucinogens (*211*), and lysergic acid diethylamide (*1572*). Some of the above articles describe quantitation by mass fragmentography. Perfluoroacyl derivatives appear to be the most popular

for analysis of the amphetamines. GC–MS has also been used to identify metabolic products of methamphetamine (*281*), amphetamine (*91*), and methadone (*83, 1439*). The chemistry of cannabis is being exhaustively explored and reported, ranging from the contents of the plant and extracts thereof (*425, 426, 496, 501, 1510, 1511, 1549, 1550*) to the metabolism of cannabinoids (*275, 1561*). The CI spectra of cannabinoids have been discussed (*1394*).

Glucuronide conjugates are important in the metabolism of drugs of many kinds and several mass spectral techniques may be feasible for their analysis: GC–MS (*156, 566*), direct probe (*1211, 1475, 1477*), and CI (*299*). In these studies, the glucuronic acid moiety has been derivatized in various ways, including methyl esterification-acetylation, methyl esterification-trimethylsilylation and permethylation. Pyrines and xanthines have also been studied by GC–MS (*814, 818, 1091*). These compounds are sometimes used in the doping of racehorses and mass fragmentographic techniques may be used for their estimation. Two new metabolites of caffeine are reported (*1255*).

^{14}C-labeled drugs with high specific activity are occasionally employed and MS may be used to determine their activities (*1520*). The method is illustrated for cambendazole. The stereochemistry of alkyl-substituted 6,7-benzomorphans can be assigned by examination of the mass spectra (*1534*).

Steroids. This section is reserved for studies of sterols and bile acids in mammals using mass spectral methods. More general aspects of the mass spectrometry of steroids are covered in the section on natural products.

A testosterone metabolite, 5α-androstane-3β,17β-diol has been identified in human urine (*130*). Twelve estrogens in urine of pregnancy have been quantitatively determined using mass fragmentography (*11*). Major C_{19} and C_{21} steroids have been determined in urine and feces from two women with intrahepatic cholestasis in late pregnancy, before and after administration of phthalylsulfathiazol (*483*). The metabolism of androstenedione in human fetal liver has been investigated (*988*). Another study on the fetus has examined the biosynthesis of epitestosterone and the metabolism of testosterone (*1234*). Estrogens in human placental tissue at term have been identified and quantitated (*771*) and the metabolism of androstenedione and testosterone in placental preparations examined (*214*). The changing pattern of steroid excretion during infancy has been further explored (*421, 611, 1357*). A 1,3,16-trihydroxypregnan-20-one has been found to be predominant in the urine of a newborn anencephalic infant (*480*), and two pregnanetetrols have been isolated from the urine of a girl having congenital adrenal hyperplasia (*619*). Plasma neutral steroid sulfates and urinary neutral steroid sulfates and glucuronides have also been determined in children with this type of disorder (*1537*). GC–MS techniques have been applied in a study of the metabolism of steroid contraceptives (*1420*).

16α-Hydroxy-2-methoxyestrone has been identified in rat bile using fragmentations of the diacetate derivative (*1571*). GC–MS methods have made possible the identification of monohydroxy bile acids in plasma of pregnant women with intrahepatic cholestasis (*70*), of 3β-hydroxy-5-cholenoic acid in meconium (*69*), and of the latter acid, lithocholic acid and ursodeoxycholic acid in the urine of patients with liver disorders (*68*). MS methods have assisted in studies of D incorporation into bile acids and cholesterol in rats with a bile fistula given D-labeled ethanol (*359, 360*). The metabolism of 5α-cholestane-3β, 26-diol and 5α-cholestane-3β,7α, 26-triol in rats with a bile fistula has also been examined (*1168*). GC–MS of trifluoroacetylated methyl ester derivatives has been used in the identification of lithocholic acid and other bile acids in the serum of healthy persons (*1217*). Human serum contains cholesterol-α-oxide and other minor sterols (*589*). A mass spectral method for identification and quantitation of dietary and fecal neutral sterols has been described (*678*) and applied in a study of the dynamic aspects of cholesterol metabolism in rats using D_2O administration (*1219*). A study of the biosynthesis of lipophile steroid sulfoconjugates from steroid sulfates in guinea pig liver preparations is reported (*919*).

Structural elucidations of various metabolites of vitamin D_3 have used MS methods (*569, 648, 685, 686*).

Prostaglandins. There has been extensive work on the use of GC–MS for identification and quantitation of prostaglandins and their metabolites. Quantitation by the use of deuterated analogs as carriers and internal standards is widely used (*66, 593, 620, 687, 841*). For certain compounds, notably methyl ester-TMS ether derivatives, use of isotopic carriers may not be necessary due to the thermal stability and low polarity of these (*1446, 1447*). ω-Homo or ω-nor analogs of compounds being measured may also be used as internal standards for fragmentographic assays (*1070*). A variety of derivatives for GC—MS of prostaglandins has been used depending on the functional groups present. These derivatives include TMS (*585, 586, 841, 1446, 1447*), acetyl (*593, 687*), butylboronate (*841*), and heptafluorobutyryl (*1068*) for hydroxyl groups, and methoximes for ketone groups (*584, 585, 593, 620*). In the above reports, methyl esters have been most frequently used for derivatization of carboxylic acid groups. Fragmentations of some derivatives of prostaglandins of the A series (*1069*), B series (*1067*), E series (*1066*) and F series (*1064*) have been studied using high resolution and D-labeling.

The metabolism of prostaglandins of the F series in men and women (*584–586, 620*) and that of prostaglandins of the E type in the guinea pig (*621*) has been investigated using MS methods. A study has been made of the biosynthesis of prostaglandin D_1 (*523*); spectra of the compound and of reduced and dehydrated analogs are reported.

Miscellaneous. Muysers and Smidt (*1121*) have reviewed mass spectral methods for the analysis of respired gases with reference to lung physiology. Porphyrins and hemes are important metabolically and methods for their analysis proposed (*1023, 1429*). Reports have also appeared on elucidations of glycosphingolipids (*486, 823, 1373, 1417*), peptide hormones (*227, 262, 263, 986*) and of sugars in urine (*1008, 1009*). A metabolite of biotin is described (*157*). High resolution mass fragmentography using a direct insertion probe has been used to measure concentrations of various purines in tissues in studies related to gout (*1207, 1407*).

ANALYTICAL APPLICATIONS TO NATURAL PRODUCTS

Alkaloids, Porphyrins. GC–MS methods have been used to obtain the spectra of TMS derivatives of some disubstituted pyridines and quinolines (*1519*). Other alkaloids that have been identified using this technique include anagyrine (*839*), analogs of mescaline (*819*), and *Amaryllidaceae* types (*1079*).

The fragmentations of some nicotine *N*-oxides and tetrahydrooxazines have been considered (*1332*). The biosyntheses of pyridine alkaloids in *Tripterygium wilfordii* (*952*) and of nicotine analogs in a *Nicotiana* sp. (*1298*) have been investigated, MS methods being used to identify products. New alkaloids recently elucidated having pyridine or piperidine rings, include 4-desoxyevonine (*259*), pyrindicin from *Streptomyces griseofluvus* (*1187*), a 1-pyrindine from a fungus (*609*), and prosopine and prosopinine (*847*). Sulfur-containing nupharidines have been identified (*927*) and anagyrine in teratogenic lupins (*839*).

Inoue *et al.* (*748*) have studied the fragmentations of nine lysergic acid derivatives using D-labeling. New indole-containing alkaloids include vincadine from an *Amsonia* sp. (*1646*), geissovelline from a *Geissospermum* sp. (*1093*), raucaffrinoline from a *Rauwolfia* sp. (*59*), talpinine and talcarpine from a *Pleiocarpa* sp. (*1154*), and indolepyridine types from a *Nauclea* sp. (*1118*). *N*-Oxides of oxindoles have been identified in an *Uncaria* sp. (*1230*). A structure is proposed for haplophytine, deduced in part from MS data (*1630*).

The mass spectra of some tropane and tropidine derivatives have been discussed (*424*). Novel pyrrolidine ring-containing alkaloids include harringtonine and derivatives from a *Cephalotaxus* sp. (*1245*) and hammarbine and related compounds (*985*). In the latter report, GC–MS of the derived alditol acetate served to identify hammarbine as a β-D-glucopyranoside. Completion of the structure of isoline (*355*) has relied extensively on MS data.

The mass spectra of some quinolizidine alkaloids from a *Lythrum* sp. have been studied in some detail using high resolution and D-labeling methods (*542*). A new ketonic quinoline has been isolated from an *Orixa* sp. (*438*).

An investigation of the M − 92 ion in the spectrum of 8-benzyloxytetrahydroisoquinoline has been made using metastable ion analysis and D-labeling (*303*). New syntheses of some tetrahydroisoquinoline cactus alkaloids are presented with some MS data given (*241*). New alkaloids recently described containing isoquinoline systems include hernandonine (*547*), erythrinine (*762*), and bisbenzylisoquinoline types from a *Pycnarrhena* sp. (*1391*). GC–MS of the TMS derivatives has served to identify two novel amino acid analogs of mescaline (*819*). A new pavinane group alkaloid is described (*346*).

GC–MS methods may be used to identify *Amaryllidaceae* alkaloids (*1079*). High resolution and isotope-labeling studies have been carried out on *Amaryllidaceae* alkaloids of the crinine series (*993, 995*).

Fragmentations of indolinocodeine and derivatives thereof have been explored using high resolution and D-labeling methods (*3*). 16-Hydroxythebaine has been isolated from opium (*230*).

Macrocyclic peptide alkaloids have attracted interest recently, some having antitumor properties. A complete analysis of the high resolution spectrum of a frangulanine-type (discarine A) has been made (*1032*). Mass spectral methods have been extensively used in the elucidation of this type of structure (*161, 1498–1500, 1567*). A glutarimide peptide has been identified as a constituent of a *Croton* sp. (*920*).

Some features of the spectra of lycoctonine alkaloids have been discussed (*1638*). New steroidal alkaloids bearing pyridine rings have been isolated from a *Marsdenia* sp. (*562, 1440*).

The spectra of porphyrins are discussed (*1054*) as are those of the TMS derivatives of some hydroxyporphyrins (*302*). Reductive degradation with hydriodic acid may be used to cleave porphyrins to pyrroles which, suitably derivatized, can be analyzed by GC–MS (*1023, 1429*).

Flavonoids, Coumarins, Phenols. The CI spectra of several flavonoids have been recorded using isobutane, H_2, and D_2 as reagent gases (*325*). The spectra show abundant quasi-molecular ions and metastables and possess certain structurally significant fragment ions. A combination of EI and CI methods has been used by another group (*781*) in characterizing products of oxidation of dihydrogossypetin by a *Pseudomonas* sp. For characterization of flavonoid glycosides, mass spectrometry of permethylated derivatives has found favor (*1325, 1556*). Perdeuteriomethylation followed by complete hydrolysis and GC–MS analysis of the derived partially-methylated alditol acetates (*1327*) can give much information on the sugar content and the interglycosidic linkages. A spectrum of the aglycone moiety (ethylated with diazoethane) gives further information as to the position of the sugars in the original molecule (*1326*). Various hydroxy-flavones have been analyzed by GC–MS (*1171*); fragmentation data are not reported.

The mass spectra of 2′-hydroxychalcones and the corresponding 2-phenylchrom-4-ones are essentially identical and Van de Sande *et al.* (*1522*) conclude that an intramolecular equilibrium exists between a chalcone-type and a flavanone-type molecular ion. The spectra of 4-chromanone derivatives (*909*) and of flavones bearing C-isoprenoid groups (*1253*) are discussed.

The isoflavonoids of a *Dalbergia* sp. (*436*) and methoxylated flavonoids from *Artemisia* spp. (*1283*) have been characterized, the structure of phellodendroside from *Phellodendron japonicum* revised (*596*), and the structures of two biflavonoids described (*7, 979, 1256*) using mass spectral information. Glycosides of polymethoxyflavonols have been found in an *Ipomopsis* sp. (*1405*), chromone glucosides in lichens (*720*), flavone-C-glycosides in a *Linum* sp. (*1554*), and isoflavonoid glycosides in a *Dalbergia* sp. (*10*). The distribution, isolation and structure elucidation of some plant procyanidins is described (*1478*). A new neoflavonoid is present in *Dalbergia stevensonii* (*437*).

The diagnostic utility of the spectra of 7-methoxycoumarins having isoprenoid sidechains at C_6 (*1014*) and those of 3,4-dialkoxyfurocoumarins (*1015*) have been explored. Fragmentations of linear monoxy- and monoacyloxy-dihydrofurocoumarins (*1640*) and of 4-phenylcoumarins (*1120*) are discussed. An extensive mass spectral investigation of the 4-alkyl- and 4-phenylcoumarins of *Mammea americana* has been made (*358*); these compounds can be analyzed by GC–MS without derivatization (*553*). New coumarins include a 4-alkyl-type from a *Calophyllum* sp. (*291*), a coumarin epoxide from a *Thamnosma* sp. (*921*), asperentin from an *Aspergillus* sp. (*607*), and an isocoumarin metabolite of an *Alternaria* sp. (*813*).

The fragmentations of xanthone, monohydroxyxanthone, and monomethoxyxanthone have been examined using isotope labeling and metastable ion analysis (*40*). Lorostemin is a new xanthone from *Lorostemon* spp. (*223*).

Mass spectral data have been extensively used in the elucidation of two new depsidones from a lichen (*357*). The use of the mass spectra in identifying phloroglucinols in plants is discussed (*999*). The fragmentations of catechol esters are described (*1445*). GC–MS studies of other phenolic compounds are reported (*669, 1094, 1247*). The relation of the mass spectral fragmentations to the stereochemical features of secalonic acids (phenolic fungal metabolites) has been explored (*716*). Phenolic metabolites of an *Aspergillus* sp. (*78*) and of a *Scytalidium* sp. (*508*) have been described, also pigments of a *Suillus* fungus (*465*) and of a crinoid (*82*). Tocopherols and tocotrienols may be estimated in vegetable oils by GC–MS analysis of the TMS derivatives (*583*). The spectra of free tocopherols and of their acetates have been reported (*1321*).

Isoprenoids. Complex mixtures of terpenoids in oils may conveniently be characterized by GC–MS methods. Some of the major components (monoterpenes) in spike oil have been identified in this manner (*912*). Fragmentations of natural pyrethrins are described (*1210*).

GC–MS has allowed identification of nine sesquiterpenoid hydrocarbons (all structures previously known) in a liverwort (*1040*). MS methods have also been used in the structural elucidations of new sesquiterpene alcohols including α-copaene-11-ol and 8-acetoxyelemol (*1181*), pygmol from an *Artemisia* sp. (*754*) and a brominated alcohol, oppositol, from a red alga (*618*). Novel sesquiterpenoid lactones isolated include ones having antileukemic properties, liatrin (*916*), eriolangin and eriolanin (*914*). CI with methane reagent gas was used to obtain the molecular weights of the latter compounds. Other new sesquiterpenoid lactones are ones from a *Lactarius* sp. (*1021*) and viscidulins (*1359*). Liedtke and Djerassi (*968*) have studied fragmentations of terpenoid esters of the juvenile hormone type using high resolution and D-labeling methods. Fragmentography using a D-labeled analog as internal standard and carrier, has been employed to measure concentrations of juvenile hormone in *Hyalophora* moths (*153*).

MacMillan *et al.* make extensive use of GC–MS in studies of the plant growth substances, the gibberellins (*86, 194*). A GC–MS method is described for the determination of specific activity of ^{14}C-labeled *ent*-kaurenes and kaurenoic acids (*195*). New metabolites of *Gibberella fujikuroi* include 3β,7β-dihydroxykaurenolide (*84*). GC–MS has been used to follow changes in diterpene composition during growth of an *Isodon* sp. (*541*). Rearranged labdanes of a *Hymenaea* sp. are described (*846*) as are diterpene metabolites of a *Cyathus* sp. (*67*). Spectra of some acetals related to manool display a novel expulsion of CH_3CO_2H or its equivalent (*587*). Fragmentations of eleven analogs of vitamin A are discussed (*1260*). Extensive use of MS methods has been made in the elucidations of the structures of eleven new diterpenes, derivatives of sandaracopimar-15-en-8β-ol, isolated from species of *Garuleum* and *Osteospermum* (*179*). Chlorophyll from the purple photosynthetic bacterium *Rhodospirillum rubrum* is an ester of all-*trans*-geranylgeraniol and not phytol, as is the case with most chlorophylls (*835*). It was found that chlorophyll heated on a direct insertion probe produced ions characteristic of the esterifying alcohol.

New furanoterpenoids isolated include vicinin-3 and vicinin-4 from an *Ircinia* sp. and furospongin-3 and furospongin-4 from *Spongia officinalis* (*323*). The furospongins are sesterterpenoids. Other new C_{25} terpenes are cheilarinosin from *Cheilanthes farinosa* (*765*) and deoxoscalarin (*322*).

MS methods have recently played minor roles in further studies of the biosynthesis of isoprenoids, being used mainly to characterize reaction products. Thus, the specificities of isopentenyl pyrophosphate isomerase from pig liver (*902*) and that of a pig liver preparation converting farnesylpyrophosphate into squalene (*1180*), have been examined. A study of the biosynthesis of fusidic acid in relation to the mechanism of the oxidative cyclization of squalene is reported (*464*). Total syntheses of triterpenoids based on "biogenetic-type" reactions from squalene and farnesol derivatives have been further explored, with MS characterization of products (*1528, 1529*). *Halobacterium cutirubrum* contains di- and tetrahydrosqualenes and the positions of saturation have now been firmly established (*905*). New tetra- and pentacyclic triterpenes isolated include lup-20(29)-ene-3β,11β-diol from a *Dodonaea* sp. (*570*), inotodiol (a corrected structure) (*399*), polypunonic acid (*393*), a dammarane triol (*1149*), alphitexolide from an *Alphitonia* sp. (*210*), daturadiol and daturaolone from a *Datura* sp. (*884*), and maitenin, a quinone, from a *Maytenus* sp. (*392*). α- and β-Amyrin were identified in a blue-green alga by GC–MS methods (*518*). A furanoid undecanortriterpene is described (*296*).

Interesting new C_{35} pentacyclic terpenes have been identified in *Acetobacter xylinum* (*522*). These are hopane derivatives substituted by a 5-carbon chain, bearing four vicinal hydroxyl groups.

Mass spectral data are extensively used in the structural elucidation of carotenoids. A review by Foppen (*517*) includes details of fragmentation of individual compounds, while a more recent review (*964*) discusses briefly the role of mass spectrometry in this field. Factors affecting the intensity ratio of the M − 92 and M − 106 ions in the mass spectra of carotenoids are discussed (*525*). New bacterial carotenoids include C_{50} mono- and diglucosides (*46*) and conjugated carbonyl types (*34*). The structure of aleuriaxanthin is described with discussion of its spectrum (*45*). Carotene epoxides have been identified in tomatoes (*110*). Incorporation of ^{14}C-labeled mevalonate into chlorobactene has been examined with the product and derivatives thereof, characterized by mass spectrometry (*1104*).

MS methods have been used to identify dolichols and ubiquinones isolated from cultures of *Phytophthora cactorum* containing [2-^{14}C]-mevalonate (*1266*). 6-Methoxy-2-nonaprenylphenol has been identified as an intermediate in the biosynthesis of ubiquinone-9 in the rat (*1175*).

Steroids. Brooks and Middleditch (*239*) have recently reviewed the mass spectrometry of steroids quite comprehensively (324 references, including some appearing in 1972). A review by Novotny (in Czech, 245 references) has appeared (*1172*) covering the gas chromatography of steroids with some mention of derivatization techniques and GC–MS methods. CI of TMS ethers of bile acids using nitric oxide with nitrogen, argon or helium as reagent gas, gives much enhanced quasi-molecular ions (*784*); the EI spectra give molecular ions of very low or negligible abundance. CI has also been applied to 17-hydroxysteroids (*1063*) and to steroidal amino alcohols (*994*). In the latter report, specific fragmentations such as loss of water from the quasi-molecular ion, are discussed in terms of conformational equilibria. Applications of computer interpretation to the mass spectra of estrogenic steroids are reported (*1398–1400*). Computer procedures for acquisition and evaluation of GC–MS data on TMS and methoxime-TMS derivatives of steroids have been discussed (*1261, 1262*). The "twin ion" technique for recognition from their mass spectra of metabolites of isotope-labeled compounds is described in a GC–MS study of intermediates in estrogen biosynthesis (*214*). Isotope (^{14}C) dilution is used in a method for determination of aldosterone in plasma by GC–MS (*1383*). Twelve estrogens in urine of pregnancy may be quantitated by mass fragmentography (*11*). Procedures for isolation and identification by GC–MS of urinary estrogens are described (*1455*).

Various types of derivatives suitable for analysis of corticosteroids have been described. Recent papers survey cyclic boronates (*240*) and methoxime–TMS types (*1471, 1473*) while one (*72*) compares methoxime–TMS, cyclic boronates, dimethylsiliconides, and oxetanones. Methoxime–TMS derivatives of the 17α,21-diol-20-one side chain appear to be preferred but it has been suggested that the di-TMS ether–enol-TMS ether may be an alternative (*293, 294*). The method used to prepare these does not silylate hindered hydroxyl groups while 3-keto groups do not quantitatively form enol-TMS derivatives. Hydroxyl groups in steroids may also be converted to chloromethyldimethylsilyl ethers (*238, 301*). These have longer GC retention times compared to TMS derivatives, may be useful in distinguishing certain stereoisomeric pairs, and chlorine-containing fragment ions in the spectra are easily recognized from the isotope patterns. Dimethylsilyl ethers of hydroxysteroids are reported (*722*), and it has been shown that the dimethylphosphinic ester of estrone has good GC properties (*1541*). Heptafluorobutyryl esters have also been described (*387, 388*). Retention data and fragmentations for various 24-ethylidene sterols and of their acetate and TMS ether derivatives are reported (*237*); the stereochemistry at C_{28} may be deduced from the spectra of the acetates. A further compilation of data (for TMS ethers of sixteen sterols, six cholestanediols, six cholestenediols, and one cholestanetriol) is given (*236*). The fragmentations of a wide range of Δ^5-3β-hydroxy C_{19} steroids as TMS ethers have been explored using high resolution and isotope-labeling data (*235*). The origins of specific ions in the spectra of TMS derivatives have been investigated, also using stable isotope labeling (*234, 1546–1548*). The fragmentations of alkyl ethers of some 3-hydroxy-steroids (*1160*) and of steroidal 3,5- and 4,5-diols and of their acetates and ketols (*1619*) are discussed. A method for determination of vitamins D in a mixture utilizes the fragmentations of the tetracyanoethylene adducts (*1507*).

The specificity of fragmentations of the steroid skeleton in relation to structural features such as double bond position, stereochemistry of ring junctions and substituents, etc. has been described in several papers (*479, 623, 862, 1028, 1056, 1240, 1295, 1323, 1364, 1487*). Specific D-labeling is extremely valuable and has been repeatedly used in studies of this type.

Novel steroids isolated include many from marine sources. The unusual $\Delta^{9(11)}$ double bond is represented in 5α-pregn-9(11)-ene-3β,6α-diol-20-one (*1366, 1371*) and in three compounds containing the rare 23-oxo group, 5α-cholesta-9(11),20(22)-diene-3β,6α-diol-23-one (*1366*), 5α-cholesta-9(11),24-diene-3β,6α-diol-23-one and 5α-cholest-9(11)-ene-3β,6α-diol-23-one (*1406*). These compounds were all isolated from starfish toxins. Other new marine sterols described are 24-*nor*-7,22-diene and 24-*nor*-5,22-diene types (*482, 880*). Goad *et al.* (*572, 1396*) have described the sterol composition of several kinds of marine life using GC–MS. Sponges have been the source of sterols having a novel pattern of side chain alkylation (*394*); these compounds are 26-methyl homologs of 24-methyl and 24-methylene cholesterol.

GC–MS has been used in investigations of the sterol composition of *Scenedesmus obliquus* grown in H_2O and D_2O (*104*) and of lichens (*1610*). A novel C_{28} triene, ergosta-5,8,22-trien-3β-ol has been isolated from the lichen *Xanthoria parietina* (*955*). Novel cyclopropyl sterols include 14α-methyl-9β,19-cyclo-5α-ergost-24(28)-en-3β-ol from *Musa sapientum* (*873*) and 4α,14α-dimethyl-24-ethyl-9:19-cyclocholest-25-en-3β-ol from *Trichosantes palmata* (*883*). 4α-Methyl sterols have been identified in the pitcher plant by GC-MS (*1565*) and the technique has also been applied to studies of the sterol composition of 19 vegetable oils (*763*) and of the slash pine (*939*). Several of the above studies have employed GC–MS of the free sterols.

MS methods have assisted in the identification of the 2-cinnamate esters of β-ecdysone, polypodine B, ponasterone C, and dacrysterone in the bark of *Dacrydium intermedium* (*1299, 1300*) and of phytoecdysones and iridoids from a *Vitex* sp. (*1271*). Ikekawa *et al.* (*743*) have given extensive data on the spectra of TMS ethers of phytoecdysones and use the heptafluorobutyryl derivatives for quantitation by electron capture GC. Zooecdysones may be quantitatively determined by fragmentography of the TMS derivatives (*1087*); the method was applied to silkworm pupae.

Sterol glucosides in plants may be converted to the per-TMS derivatives and subjected to GC–MS (*923*). These derivatives have somewhat long retention times and lack

molecular ions. It is stated by Knights (*878*) that the pertrifluoroacetylated compounds have better GC and MS properties (including more abundant molecular ions). The spectra of TMS derivatives of some cardiac aglycones and monoglycosides are discussed (*492*) as are the fragmentations of bufadienolides (toad poisons) (*249, 250*). Both EI and FI methods have found application in the study of cardenolides and their glycosides (*247*). Fragmentations of the peracetylated derivative have assisted in the elucidation of the structure of 11-O-galactosylnogiragenin (*1637*). Elucidation of a steroidal C_{28} lactone of the withanolide type has also used the spectrum of an acetylated derivative (*9*).

Simple Lipids. Zeman and Scharmann have written a very comprehensive review of instrumentation, methods, and fragmentations of many types of lipids (three parts, in German, 361 references) (*1642*). Pallotta (*1198*) has reviewed applications of GC–MS in lipid research (53 references). Papers citing newer ionization methods include one on the FI of methyl esters of various types of fatty acid (*1285*) and another on the analysis of alkene mixtures by capillary GC–CIMS (*174*). The latter is a particularly good illustration of the use of combined EI/CI methods and describes the determination of unsaturated isomers of long chain compounds utilizing CI to obtain the molecular weight of an alkene with EI of the TMS derivative of the *vic*-diol to determine double bond position. Hexafluoroacetone ketals have been proposed as alternatives to other types of derivative for the determination of double bond position (*793*). These ketals, however, apparently lack abundant molecular ions and the MS data alone are hardly sufficient for determination of geometry. The interaction of acrylonitrile with unsaturated fatty acids has been investigated and appears to give rather complex mixtures of *bis*-acryloamide derivatives but MS of the products has nevertheless been proposed as a method for determining double bond position (*172, 173*). Identification of monomethyl paraffin chain-branching (close to the methyl terminus) in long chain compounds is not always simple even by GC–MS methods. Karlsson *et al.* (*826*) have proposed conversion of such compounds to alcohols and GC–MS of the methyl ether derivatives. This apparently allows better GC separation and MS differentiation of isomers. To determine the position of cyclopropane rings in fatty acids, methoxylation with BF_3-methanol and MS of the resulting isomer mixture has been proposed as an alternative to catalytic hydrogenation or chromium trioxide oxidation (*1082*).

Much mass spectral information has been recently published on fatty acids and various derivatives including all of the methylepoxyoctadecanoates (*610*), 1,4 and 1,5 epoxides of octadecanoates (*2*), very long chain compounds (*1252*), methylene- and non-methylene-interrupted *cis,cis*-methyloctadecadienoates (as tetra O-TMS derivatives) (*1116*) and various unsaturated and oxygenated methyl esters (*861*). The formation of ions containing two silicon atoms from macrocyclic transition states in long chain α,ω-bis(TMS)ethers is discussed (*1588*).

Dimeric fatty acids formed anaerobically in the reaction between linoleic acid and L-13-hydroperoxy-octadec-*cis*-9-*trans*-11-dienoic acid, catalyzed by soya bean lipoxygenase, have been characterized (*557*). GC–MS has been used in the characterization of mono- and di- acids in the bark of the Douglas fir (*1000*). The cutin layer of plants is a complex polymer of hydroxy fatty acids; GC–MS is a convenient technique for identifying the monomer units as methyl esters–TMS ethers following hydrolysis [see *e.g.* (*689, 723*)]. Walton and Kollattukudy (*1564*) describe a novel technique for characterizing the constituent monomers, using lithium aluminum hydride reduction of the polymer and GC–MS of the resulting polyols as TMS ethers. The method has been applied to various cutins including that of *Vicia faba* (*886, 887*) in which a novel aldehyde monomer was identified. Biosynthetic pathways for cutin and cutin acids have been proposed (*887, 888*). Jacob's group has carried out extensive chemotaxonomic investigations of glandular waxes of different birds using GC–MS (*767–769, 1238, 1641*). Long chain 1,2-diols have been identified in the preen glands of some birds using GC–MS of the isopropylidene derivatives (*1317*). An analysis of waxes from insect cuticular lipids by mass spectrometry has revealed the presence of secondary alcohols with the hydroxyl group near the center of the carbon chain (*171*). More than fifty single- and multi-branched acids have been identified in a GC–MS analysis of human milk lipids (*466*). The constituent acids and alcohols of sperm whale oil have been identified in a similar manner (*1411*). Novel fatty acids from *Solanum tuberosum* have a divinyl ether structure (*552*).

Acholeplasma laidlawii can incorporate deuterated lauric acid and produce hybrid ^2H-^1H fatty acids of longer chain length; these species can be recognized by GC–MS of the methyl esters (*1185*). The free fatty alcohols (primary and secondary) from *E. coli* have been analyzed as the acetates by GC–MS (*1148*). The composition of this fraction depends on the aerobic or anaerobic nature of the culture. Degradation by soil microorganisms of methyl-branched acids has been studied (*630*). Rat liver microsomes catalyze the oxidation of ω- and (ω-1)-hydroxy fatty acids to diacids and (ω-1)-oxo acids (identified by GC–MS) (*162*).

GC–MS may be a convenient method for the characterization of long chain aldehydes and ketones using the *O*-methyl oxime derivatives (*1071*). MS methods have also been used in the identification of multi-methyl-branched alkanes in the eggs of the tobacco hornworm (*1165*), in the examination of the hydrocarbon constituents of three species of Norwegian lichens (*559*), those of earthworms (*1170*), and in the characterization of plant polyacetylenes (*180, 928, 1526*).

Complex Lipids. The spectra of ester lipids derived from glycerol and other polyhydric alcohols is discussed, with particular reference to the origin of $[M-X]^+$ and $[M-XH]^+$ ions (X = RCOO, RO, OH) (*85*). Triglycerides have been eluted from a short GC column into a mass spectrometer and the spectrum of a C_{56} triglyceride is exhibited (*1115*). Diglycerides have been analyzed by GC–MS as the monoacetyl derivatives (*645*).

β-Hydroxy fatty acids having long side chains at the α-position (nocardomycolic and corynomycolic acids) frequently occur as mixtures and can be conveniently characterized by GC–MS of the intact molecules as TMS ethers (*1628, 1629*). An ornithine-containing lipid of *Thiobacillus thiooxidans* contains hydroxy-*n*-fatty acids and *cis*-11,12-methylene-2-hydroxyoctadecanoic acid (*879*). Mass spectrometry of methyl esters of acid hydrolysis and of methanolysis products served to identify the components.

Procedures for the GC and GC–MS analysis of phospholipids are described (*471*). TMS or isothiocyanate–TMS derivatives have been found to be suitable for the characterization of alkyl- and aminoalkylphosphonates by GC–MS (*644*). Low voltage spectra and metastable scanning have been used in the investigation of spectra of underivatized phosphatidyl amino alcohols (*865*). Certain substances, such as phosphatidyl cholines, produce molecular ions of short lifetime; the formation of these was deduced from the presence of metastable ions corresponding to their fragmentation. MS analyses of the prenol and derivatives thereof have led to the characterization of a mannosyl-1-phosphoryl-octahydroheptaprenol from *Mycobacterium smegmatis* (*1456*).

For characterization of ceramides, mass spectrometry of the intact compounds as TMS derivatives (introducible by GC) can give extensive information on base and fatty acid composition. Hydrolysis to the free bases and fatty acids may be followed by analyses of the bases as per-TMS or *N*-acetyl, *O*-TMS derivatives and of the fatty acids as methyl esters. These methods are more fully described in the following recent papers (*498, 622, 629, 714, 827, 842, 911, 1037, 1297*).

Fragmentations of glycosylglycerides are discussed (*260*). Utilization of the fragmentations of both peracetyl and per-TMS compounds can give extensive information on base, fatty acid, and sugar composition according to studies on homogeneous cerebrosides containing one sugar moiety (*30, 824*). A xylose-containing cerebroside has been identified using these methods in addition to degradative studies (*825*). GC–MS of the per-TMS derivative and degradative studies have been used for characterization of glycolipids (containing one sugar residue) from algal het-

erocysts (*929*). Peracetylation has assisted in identifying mycosides by mass spectrometry (*560*).

Glycolipids containing two or more sugars have been fully characterized although breakdown into smaller units is mandatory for analysis. If of the ceramide-containing type, application of techniques referred to above can give the base and fatty acid content. To obtain the sugar sequence and nature of glycosidic linkages, mass spectral methods discussed in the section on sugars are often employed. The following recent papers deal with glycolipids of this type: (*484, 486, 1038, 1373, 1417, 1427*). Sialic acid-containing glycolipids have also been studied (*823, 882*); CI of gangliosides are reported (*1029*).

Two other elucidations have been those of a macrocyclic lactone from a lichen (*721*) and of ascaroside aglycones (*1460*).

Carbohydrates. FD spectra of such derivatives of stereoisomeric monosaccharides as the 6-bromo-2-naphthyl and *p*-nitrophenyl compounds can be used to differentiate the isomers by consideration of the relative intensities of fragment ions (*954*). The FD technique has also been applied to disodium D-glucose-6-phosphate and certain derivatives, the spectra showing quasi-molecular ions inclusive of metals (*1340*). In elucidating the structure of an anthraquinone glycoside, FD has also been used (*1555*). CI methods using ammonia and methane reagent gases have been applied to some sugars and derivatives (*684*) and give structural information such as the positions of linkages in acetylated disaccharides, in addition to the molecular weights. GC–MS methods are increasingly used for analyses of sugars and derivatives thereof. This is largely because of the bewildering number of structural possibilities for these compounds that either technique on its own would have difficulty in completely resolving. Reports have recently appeared on the GC–MS of aldonitrile acetates of partially methylated pyranoses (*476*), boronated sugars (*1264, 1606*), benzeneboronates of hexopyranoses (*1280*), silylated tetrulose and pentuloses (*649*), silylated partially-methylated sugars (*650*), silylated methoximes (*924*), trifluoroacetates (*893*), silylated sugar phosphates (*643*), and permethylated aldoxyl aldonates (*1590*). GC–MS of the derived alditol acetates is widely used for sequencing polysaccharides (see below). These compounds can also be separated by GC, collected, and analyzed by direct probe (*320*). The fragmentations of glucose (as the pentaacetyl derivative and of glycerol-1-phosphate (as the TMS ether-dimethyl ester) have been explored using ^{18}O-labeling (*284, 285*). The same isotope has been used as a tracer in an elucidation of the reaction mechanisms of fructose-1,6-diphosphate aldolases (*666*). Investigations of the fragmentations of 2-acetamido-1,3,4,6-tetra-*O*-acetyl-2-deoxy-α-D-glucopyranose (*440*), 1,6-anhydro-2,3-*O*-isopropylidene-β-D-talopyranose (*710*) and of some methyl, *O*-methyl-D-xylofuranosides (*900*) have been made using specifically deuterated analogs. Studies have been made of the mass spectra of acetoxymercurated derivatives of an acetylated sugar (*711*), of acetylated 6-deoxy-6-halogeno-α-D-glucopyranoses (*309*), of two methylated pseudoaldobiouronic acids (*913*), of acetylated-methyl ester-methyl glycoside derivatives of sialic acids (*881*) and of syn and antiaromatic aldoximes (*245*). *N*-Salicylidene derivatives of amino sugars may be useful for elucidation (*749*). The spectra of the TMS derivatives of several aldohexopyranoses have been studied and small but reproducible differences between isomers claimed (*1539*). The utility for structure elucidation of the spectra of the TMS derivatives of a series of disaccharides has also been explored (*817*). Some fructose-containing oligosaccharides (2–4 residues) have been permethylated and the fragmentations recorded and discussed (*381*). Trisaccharides have been reduced to diglycosylpolyols, permethylated and analyzed by MS (*310*). Peracetyl derivatives of *N*-arylglycosylamines of tri-, tetra-, and pentasaccharides can give certain structural information (*311*).

From the foregoing, it is apparent that a wealth of techniques exists for saccharide derivatization and elucidation by mass spectrometry. It is difficult to judge which derivatives are best for this purpose but, of the newer types, boronates and silylated oximes appear to be most promising, having greater asymmetry in their structures. For saccharides having more than four or five sugar residues, permethylation (see below) retains its advantage because of the small increase in molecular weight introduced. GC–MS of partially methylated aldonitrile acetates or methoxime-TMS derivatives derived from permethylated oligosaccharides may compete with the commonly-used alditol acetates.

GC–MS of silylated inositols is a convenient method for identification and quantitation; different isomers of inositol occurring in the cockroach have been analyzed in this manner (*673, 674*). A synthesis of 3,6-di-*O*-methyl-D-galactose is described, this compound apparently being identical with a product from methylation analysis of polysaccharides related to ξ-carrageenan (*1221*). 3-Nitro-1-propyl-β-D-glucopyranoside is a constituent of *Astralagus miser* (*1418*), the fragmentations of the peracetylated compound being utilized. Various sugars have been identified in human urine (*1008, 1009*) and in human cerebrospinal fluid (*1232*).

For analysis of oligosaccharides containing perhaps four or more residues, there appears to be agreement as to the most fruitful type of approach, at least as far as current information allows. This approach relies on all or some of the following procedures or minor variations thereof: 1) a spectrum of the permethylated, persilylated, or peracetylated oligosaccharide (if of sufficiently low molecular weight) can give the number of sugar units and some information on type and sequence; 2) complete hydrolysis followed by GC–MS analysis of derivatized monosaccharides and/or GC–MS analysis of acetylated alditols can give the sugar composition; 3) permethylation of the oligosaccharide and acid hydrolysis followed by GC–MS analysis of the acetyl derivatives of the $NaBH_4$- and/or $NaBD_4$-reduced products (partially-methylated alditol acetates) can give valuable information on the nature of the sugar linkages; 4) partial hydrolysis with isolation of a disaccharide fraction may be combined with MS analysis of the derivatized disaccharides, or better, with procedure 3 repeated on the disaccharides. Such procedures can give virtually complete information on the sugar sequence and nature of the linkages.

These procedures are exemplified by the following recent papers. A pentasaccharide of oleanolic acid has been identified in a *Bersama* sp. (*1525*) and nystose (a tetrasaccharide) in horse-chestnut seeds (*816*). Other reports cover a galactan from the bark of the white willow (*1488*), lipopolysaccharides of *E. coli* (*545*), of a *Pasteurella* sp. (*656*), of a *Xanthomonas* sp. (*1542*), of a *Rhodopseudomonas* sp. (*1578*), and of *Klebsiella* strains (*981*). Capsular polysaccharides of other *Klebsiella* types have been examined (*319, 980, 982*). Other reports dealing with compounds containing oligosaccharide units are listed in the sections on complex lipids and flavonoids.

Amino Acids. The CI spectra of some free amino acids and derivatives thereof (amides, methyl esters, *N*-acetylated) have been presented and discussed (*946*). The FD method has also been applied to free amino acids; all show strong molecular or quasi-molecular ions (*1602*). *N*-Dimethylaminomethylene alkyl ester derivatives may be suitable for GC–MS analysis of amino acids (*1472*). These compounds appear to be easily prepared, give single GC peaks for most acids, and generally show molecular ions. Fragmentography of the *N*-trifluoroacetyl,*O*-*n*-butyl ester derivatives has been used for the simultaneous quantitation of ten amino acids in soil extracts (*1222*). *N*,*O*-Isopropyl derivatives have also found application for GC–MS of these compounds (*170*). The Edman degradation of peptides can give thiohydantoin derivatives of amino acids and the mass spectra of these have been discussed (*1441, 1444*). The former report emphasizes use of the abundant metastable ions present in these spectra, some of which are unique to a given compound. Compilations of fragmentation data are given for sulfur-containing amino acids (*1167*) and for the tris-TMS derivatives of certain types (*1083*).

An α-hydroxymethyl-α-amino acid (thermozymocidin) is a novel antifungal compound isolated from a thermophilic mold (*39*). A chloro-amino acid, *trans*-2-amino-5-chloro-4-hexenoic acid has been extracted from a mushroom (*308*), and the unusual *trans*-3-hydroxyproline is a constituent of peptide alkaloids from *Zizyphus amphibia* (*1500*). N^G,N^G- and $N^G,N^{G'}$-dimethylarginine have been

identified as constituents of bovine myelin hydrolysates by GC–MS of the benzamides (*242*). Antibiotics have been the source of novel amino acids including 3-amino-12-methyltetradecanoic and 3-amino-12-methyltridecanoic (from iturin) (*1226*) and β-hydroxy-L-valine and others from YA-56 (*1182*). A sponge has yielded a series of *N*-acyl-2-methylene-β-alanine methyl esters (*832*). In the course of a characterization of toxins from a plant pathogenic *Pseudomonas* sp., a novel amino acid, 3-aminomethyl-6-carboxy-3-hydroxy-2-piperidone has been detected (*1468*).

Peptide Sequencing. Of recent reports dealing with MS sequencing of peptides whose structures were previously unknown, the majority have dealt with peptides containing less than about six amino acid residues and for those of significant length, chemical or enzymic degradations have first been used to produce single amino acids (Edman degradation) or peptides with between two and five amino acids.

Improvements continue to be made in techniques for derivatization of peptides to increase their volatility. A report by Beuhler *et al.* (*136*) has however emphasized the importance of using evaporation from inert surfaces such as PTFE when introducing peptide samples into a spectrometer. Volatility when this material is used, is considerably enhanced over that from metal or glass surfaces. Permethylated derivatives are already widely used for peptides and, with recent improvements in technique, the method will probably find even wider use. Morris *et al.* have employed a much shorter reaction time (60 secs) and demonstrated application of the method to histidine-(*1095*) and methionine-, cysteine- and arginine- (*1096*) containing peptides. An example of the advantages of using both acetylated-permethylated and deuterioacetylated-perdeuteriomethylated derivatives is given (*1284*) in cases where sequence ions of particular formulas cannot unambiguously determine the sequence. Acetylated-permethylated derivatives of dipeptides are conveniently analyzed by GC–MS (*280*). A procedure for quantitative pyrolitic conversion of a peptide trimethylanilinium salt to the corresponding methyl ester on an insertion probe is described (*1322*). *N*-Decanoyl derivatives continue to find some applications, principally to rather small peptides (*1184, 1189, 1294*). A variety of derivatives for the *N*-terminus of test tripeptides have been extensively explored (*384, 1209*). Those such as the 4-(*N,N*-dimethylamino)-naphthylidenes are reported to give volatile compounds whose spectra exhibit intense molecular ions and clearer *N*-terminal fragmentations.

Use of dipeptidases for breakdown of peptides has attracted some interest (*286, 1195, 1296*). The resulting dipeptides may be identified by GC–MS of the *N*-acetyl, permethylated compounds (*280*) or of the *N*-perfluoropropionyl, methyl esters (*286*). Following reaction with the enzyme, the peptide may then be taken through one Edman degradation and the enzyme action repeated with identification of the new set of dipeptides. Enzyme and cyanogen bromide degradation with analysis of permethylated products is well exemplified in a report on a tridecapeptide (*1235*). Enzymic breakdown has been used in other studies (*262, 263, 499, 701, 1184*). The technique of conversion of peptides to polyaminoalcohols has been further improved (*1162*) and may find wider use. The peptide is acid hydrolyzed to lower peptides which are esterified, acetylated, and reduced with $LiAlD_4$ to polyaminoalcohols which may then be analyzed by GC–MS. A computer is useful for assembling the identified fragments into possible structures (*1162*). A combination of some of the above techniques is briefly described (*1605*). Preliminary data on CI (*77*) and FD/FI (*1601*) spectra of underivatized peptides is given. FD spectra exhibit molecular ions but appear to lack significant sequence ions. 10.2-eV PI spectra of some derivatized peptides are reported (*1189*). The relative abundance of the molecular ions and higher mass sequence ions is larger compared to EI spectra.

Lovins *et al.* (*477, 489*) have shown that the *N*-methyl- or *N*-phenylthiourea derivatives of an amino acid (Edman degradation products) on heating in a spectrometer, rearrange to the thiohydantoin derivatives, whose spectra may then be recorded. The same derivatives of the *N*-terminal amino acid of a peptide similarly rearrange to the thiohydantoin derivative of the terminal amino acid, leaving the shortened peptide. Because of possible thermal alteration of the residual peptide, it is unlikely that the procedure can be continued stepwise in this manner for sequencing. A manually-operated interface designed to transfer the pure thiazolinone from Edman degradation into a mass spectrometer is described by this group (*1002, 1003*). The spectra of thiohydantoin derivatives of cysteine are unsuitable for ready identification but conversion to *S*-methylcysteine followed by reaction to the *p*-bromophenylthiohydantoin may be suitable (*1501*). GC–MS analysis of TMS derivatives of thiohydantoins formed by Edman degradation has been used by Burgus *et al.* (*262, 263*).

The mass spectra of some sulfur-containing peptides (*1167*) and of β-lysine-containing types are discussed (*1294*).

The application of many of the above methods is well described in reports of the elucidation of several peptides, *e.g.*, a fluorescent type from iron deficient *Azotobacter vinelandii* (*543*), a crustacean color change hormone (*499*), a glycopeptide from the posterior lobe of pig pituitaries (*701*), human parathyroid hormone (*227*), somatostatin (*263, 986*), ovine hypothalamic luteinizing hormone-releasing factor (*262*), and pyroglutamyl-peptides from snake venoms (*1184*). Cyclic peptides have been elucidated (*181, 336*) but are more conveniently examined by MS methods as linear peptides.

Applications of mass spectrometry to enzyme inhibition studies have been described (*13*) where a spectrum of the hydrolyzed enzyme is used to detect, for example, alkylation of an individual amino acid by the inhibitor. A combination of ^{13}C NMR with mass spectrometry of *N*-trifluoro- and *N*-difluoroacetylated derivatives has been used to determine the composition of a cross-link compound isolated from cow skin collagen (*729*). Use was made of a deuteriomethyl ester derivative and an "equi-isotopic mass shift technique."

Purine, Pyrimidines. Guanosine and adenosine-5′-monophosphate have been ionized by FD and the spectra reported (*1335*). Molecular or quasi-molecular ions are abundant and fragments due to the bases are visible. Herring DNA has been pyrolyzed directly on an FD emitter and molecular ions observed for the five bases present and for larger fragments (*1341*). Ammonia CI spectra of two purine nucleosides show both quasi-molecular and protonated free base ions (*1130*). The fragmentations of both permethylated (*1543*) and pertrifluoroacetylated (*885*) derivatives of nucleosides have been studied in detail, and both types show promise for structural elucidation. TMS derivatives have also been employed, e.g., for cyclonucleosides (*978, 1001, 1503*) and various types of derivatives are compared for pyrimidine cyclonucleosides (*1583, 1584*). Spectra of free pyrimidine nucleosides and their TMS derivatives (introduced by GC) are compared (*1503*). There are good discussions of the spectra (obtained by GC–MS) of TMS derivatives of 33 pyrimidine and purine bases (*1589*) and of the same derivatives of certain pyrimidines and pteridines (*1519*). Also studied have been some 6-substituted ureidopurines and N^6-acyladenines (*652*), purines and substituted dihydropurines (*337*), substituted phenyluracils and phenyl-2-thiouracils (*324*), and chlorinated purines (*102*).

A new pyrimidine base, 5-(4′,5′-dihydroxypentyl)-uracil has been isolated from *Bacillus subtilis* phage SP-15 nucleic acid (*212*) and synthesized (*651*). The spectra of the antibiotic pyrazomycin (a nucleoside) and of its TMS derivative are discussed (*356*). Pyrimidines constitute part of other antibiotics and the spectra of some of these are reported (*376, 760*). The mechanism of the base-catalyzed conversion of 1-methyladenosine to N^6-methyladenosine has been studied by means of MS investigation of compounds produced from ^{15}N- and D-labeled substrates (*1600*). Products of methylation of uric acid have been investigated by GC–MS (*932*). MS methods are useful in characterizing phytohormones of the zeatin type (*1206*).

The fragmentations of biopterin and sepiapterin (*764*) and of several pteridines and reduced analogs (*1596*) are discussed. A yellow pteridine from a *Drosophila* sp. has been characterized using the high resolution spectrum (*1438*).

Antibiotics. These compounds are frequently poly-functional molecules of high molecular weight and while EI spectra of appropriate derivatives can often give a molecular ion, both CI and FD methods will often give much more intense molecular ions. CI has been applied to both carbohydrate-containing types such as celesticetin (*712*) and to macrolide structures (*1084, 1085*). Fragmentations easily related to the structures are often observed. FD has been applied to a variety of antibiotics, including neomycin, erythromycin, streptovaricins, filipins, and dermostatins by Rinehart *et al.* (*1272*). Strong molecular ions were obtained for each type.

The structure of vancomycin, a complex antibiotic known for some years, is being slowly but steadily revealed (*792, 1276, 1582*). The structural units described in the latter report account for almost 75% of the molecular weight of the antibiotic. Structures recently described include herqueichrysin, a phenalenone type from *Penicillium herquei* (*1158*), LL-Z1220, containing a cyclohexenediepoxide ring (*190*), maleimycin (a bicyclic maleimide) from *Streptomyces showdoensis* (*478*) and LL-S490β, a novel benzodiazepinedione from an *Aspergillus* sp. (*475*). YA-56 of the phleomycin-bleomycin group has been shown to contain certain sugars and amino acids by MS methods (*1182, 1183*). Fragmentations of a C-nucleoside antibiotic, pyrazomycin, and of its TMS derivative have been considered in detail (*356*). Hikizimycin, isolated from a *Streptomyces* sp. has a molecular formula of $C_{21}H_{37}N_5O_{14}$ and contains 3-amino-3-deoxy-D-glucose and cytosine (*376*). In this study, molecular ions were obtained for peracetyl, permethyl, and perdeuteriomethyl derivatives. *Streptomyces cacaoi* can incorporate 5-fluorouracil, an unnatural precursor into polyoxins which exhibit antibacterial activity (*760*); GC-MS of the TMS derivative was used for characterization. Chetomin, a metabolite of *Chaetomium cochliodes* and *C. globosum*, contains an indole, an indoline, and two epidithiodioxopeperazine systems (*1314*). Inouye (*750*) has described the fragmentations of the *N*-salicylidene derivatives of some aminoglycosidic antibiotics. Spectra of kanamycin A, an aminocyclitol antibiotic, and some of its derivatives (*e.g.*, *N*-acetyl, *N,O*-methyl) have been produced by both EI and CI methods (*389*). The information given by the two methods was found to be conveniently complementary.

Peptide antibiotics described include the kikumycins (*1454*), a tripeptide from *Keratinophyton terreum* (*894*), staphylomycin S, a cyclodepsipeptide type (*336*) negamycin (a hydrazide type) from *Streptomyces purpeofuscus* (*892*), and hydroxypepstatin from a *Streptomyces* sp. (*1515*). Methods used with these compounds include some of those described in more detail in the section on peptides. 3-Amino-12-methyltetradecanoic and 3-amino-12-methyltridecanoic acids are constituents of the peptide iturin (*1226*).

Kagan and Grostic (*810*) have shown that compounds of the lincomycin type can be conveniently characterized by MS methods. Mutants of *Streptomyces caelestis* produce derivatives of celesticetin including 7-*O*-demethylcelesticetin (*41*) and *N*-dimethylcelesticetin and *N*-demethyl-7-*O*-demethylcelesticetin (*42*). Spectra of the TMS derivatives of this type of molecule (introducible by GC) can give structural information such as the nature of the acid moiety (*231*).

Suzuki has discussed the application of mass spectrometry in structure elucidation of macrolide antibiotics (*1329*). Fragmentations of the macrolide megalomycins have been described (*779*). Macrolides recently elucidated are flavofungin from a *Streptomyces* sp. (*178*), YC-17 from *S. venezuelae* (*857*), chlorothricin from *S. antibioticus* (*1113*), the venturicidines from *S. aureofaciens* (*254*), chainin from a *Chainia* sp. (*1200*), angolamycin from *S. eurythermus* (*831*), and antileukemic ansamacrolides from *Maytenus* spp. (*917, 918*). It is of interest to note that another *Maytenus* sp. has yielded a quinonoid triterpene also with antitumor activity (*392*). Two antileukemic simaroubolides, bruceantin and bruceantarin from *Brucea antidysenterica* have been identified (*915*).

Scytalidin, a new fungitoxic metabolite produced by a *Scytalidium* sp. has been described (*1432*). Several 6-alkylpenicillins and 7-alkylcephalosporins have been prepared and the structure of a novel cephalosporin elucidated (*185*). A penta-TMS derivative of tetracycline has been prepared and the structure confirmed by GC-MS (*1506*).

Semiochemicals. Semiochemicals include intraspecific communicants (pheromones) and chemicals that act as attractants and repellants between different species. Although many such compounds can be biosynthetically considered as polyketides or isoprenoids, some papers concerned with this field are gathered here because of their general interest. Regnier (*1259*) has given a general account of the mass spectrometry of semiochemicals.

The volatility of semiochemicals is usually such that GC-MS may be applied directly without prior derivatization. In demonstrating the occurrence of 3-octanone and 3-octanol in a *Cremastogaster* sp. by GC-MS (*1324*), Schlunegger and Leuthdold found that normal solvent peaks interfered with the analysis of these volatile compounds and used a high boiling solvent for injection. This eluted after the compounds of interest.

Other examples of structure elucidation of semiochemicals include two novel norsesquiterpenes, gyrinidal and gyrinidone, from the pygidial glands of gyrinid beetles (*1050, 1587*), alkylpyrazine alarm pheromones from ponerine ants (*1585*), a novel nitrogen heterocycle as a pheromone from Pharaoh's ants (*1457*), *cis*-9- and *cis*-11-tetradecenyl acetate as sex pheromones of the moth *Adoxophyes orana* (*1049*), γ-dodecalactone from the pygidial glands of rove beetles (*1586*), oct-2-en-1-al and 4-oxo-oct-2-en-1-al and other compounds from the scent glands of milkweed bugs (*555*), and new macrocyclic compounds from the odiferous glands of civet cats and muskrats (*1523*), and (2 Z, 6 E)-7-methyl-3-propyl-2,6-decadien-1-ol from the codling moth (*1089*).

Flavors, Odors, and Food Contaminants. GC-MS is a method ideally suited to the analysis of the complex mixtures of volatiles which frequently constitute flavors and odors. Recent examples of its application include: the steam volatile aroma from Ceylon tea (*1621*), the aroma from roasted green tea (*1622*), vinegar volatiles (*811*), passionfruit volatiles (*1119*), capsicum flavor (*1110*), volatile constituents of *Liatris* spp. (*828*), the smell of roasted filberts (*856*), neutral volatile constituents of Greek tobacco (*855*), and the aroma of strawberries (*445*). Certain C_{19} steroids apparently contribute to the "sex odor" in pork and these have been investigated by GC-MS (*1474*). Phenolic components of wood smoke have been studied using TMS ether derivatives (*898*). The mass spectral fragmentations of isohumulones and related compounds, constituents of hops, are discussed (*1363*). Major acids in fruit juices have been isolated by lead precipitation and analyzed by GC-MS of the TMS derivatives (*1302*). 2-*trans*,4-*cis*,7-*cis*-Decatrienal is a constituent of the "fishy off-flavor" of certain strongly autoxidized oils (*1048*). Geosmin is an odorous metabolite of an *Actinomyces* sp. (*850*).

Highly carcinogenic nitrosoamines may be present in certain foodstuffs and GC-MS methods have been described for their identification and quantitation (*257, 581*). The methods use fragmentography in a high resolution mode, adding a high degree of specificity in the determination of these low molecular weight compounds. MS evidence has assisted in the structural elucidation of a reactive aflatoxin B_1 metabolite (*556*).

ENVIRONMENTAL APPLICATIONS (PESTICIDE AND POLLUTANT ANALYSIS)

Extensive use has been made of MS methods in detecting various kinds of pollutants in the geosphere: pesticides, herbicides, and polychlorinated biphenyl (PCB) residues have attracted particular attention. Damico (*373*) has given a comprehensive review of the mass spectrometry of compounds of this type. The fragmentations of some pesticides have been studied using metastable analysis (*1301*). The spectra of some polycyclic chlorinated pesticides obtained by CI with methane are reported (*159*). Quasi-molecular ions are readily observed, but fragmentations are also observed.

GC-MS is particularly suitable for detection of pollutants in, for example, extracts of soils and natural waters. A review by Sherma (*1367*) discusses chromatographic analysis of pesticides. The sensitivity of GC-MS does not compare favorably with that of the electron capture detector for polychlorinated compounds, although quantitation

of known compounds can be readily made by operation in the fragmentographic mode, with comparable sensitivity and greater specificity (*187, 1358, 1467*). Thermal and adsorptive effects in GC–MS interfaces may be encountered with certain compounds. For example, samples of heptachlor and 1-hydroxychlordene have been introduced *via* GC and direct probe and the respective spectra show very noticeable differences (*395*). Residues have been separated by GC, trapped, and introduced by direct probe into a spectrometer scanning repetitively over narrow mass ranges (*1362*).

MS methods, including GC–MS, have been used in the following studies: the metabolism of PCB's in animals and plants (*739, 1105, 1636*), the action of UV light on PCB's (*737*) and on triazin-5(4*H*)-ones (*1201*), detection of DDT-type residues in plants (*1644*), and the detection of a cyanide derived from *p,p'*-DDT in anaerobic sewage sludge (*17*).

GC–MS has been used in analytical studies of preparations of BHC (*1114*) and chlorophenols (*512*). Highly toxic chlorinated dibenzofurans have been found in PCB preparations, and attempts have been made to link these compounds with elevated levels of embryonic death in wildlife populations of certain areas (*200*). Analyses have been made of insecticide and pesticide residues in human adipose tissue (*160, 363*).

A GC–MS study of contaminants in air has resulted in the identification of more than seventy polynuclear aromatic hydrocarbons (*935*). A similar study of organic compounds in diesel exhaust has permitted the identification of 31 hydrocarbons and 6 oxygenated compounds (*822*). Levels of bis-(chloromethyl)ether in air may be determined by fragmentography (*1358*).

The analysis of contaminants in water may also use GC–MS techniques (*188, 272, 676, 677, 1388*). Alkanes, aromatic hydrocarbons, and phthalate esters are common constituents of the organic fraction. Warren and Malec (*1570*) have described a GC technique for the determination of nitriloacetic acid and related aminopolycarboxylic acids in inland waters; the fragmentations of the *N*-trifluoroacetyl, *n*-butyl ester derivatives used are reported. An interesting technique for the identification of oil spills uses fingerprinting by the FI spectrum instead of GC methods (*1350*).

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Mössbauer Spectrometry

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This is the fifth biennial review on Mössbauer spectrometry to appear in *Analytical Chemistry*. The fourth came out in 1972 by Stevens, Travis, and DeVoe (*726*). From a phenomenal growth period in the 60's, a leveling-off was beginning to appear in the fourth review. It is clear now that the publication rate has stabilized at about 800–1000 articles per year. Five new Mössbauer transitions have been reported in the present review period: (*247, 279, 507, 798, 799*), making an even 100 total. However, chemical interest is still concentrated in a relatively few of these. The transitions in ^{57}Fe and ^{119}Sn accounted for most of the papers published over the 1972–73 review period, a percentage apparently increasing in spite of the demonstrated utility of a number of the other 98 transitions (representing less than 15% of the 1972–73 papers) in chemical investigations. The current Mössbauer periodic table is shown as Figure 1. Perhaps the most important recent chemical development in this table has been the demonstration of enormous isomer shifts in the extremely precise ^{181}Ta resonance (*387*).

The maturing of this field of spectrometry has resulted in fewer papers dealing with measurements on large numbers of compounds and more emphasis on detailed investigation of a single compound or small group of related substances. The study of single crystals and the use of backscattering geometry are becoming more common (although spectra of powders in transmission geometry are still by far in the majority). Papers dealing primarily with use of the Mössbauer effect in determining nuclear properties seem to be on the decline. One interesting geographical phenomenon is an increase in publications in Mössbauer spectrometry from the Eastern European nations.

Since the fourth review, several important books on Mössbauer spectroscopy have appeared. The 659-page text by Greenwood and Gibb (*288*) has an essential place in