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Development of an Advanced Spacecraft Tandem Mass Spectrometer

Final Report

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Principal Investigator

SBIR Phase II Contract
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PROJECT SUMMARY

The **purpose** of this research was to apply current advanced technology in electronics and materials to the development of a miniaturized Tandem Mass Spectrometer that would have the potential for future development into a package suitable for spacecraft use. The mass spectrometer to be used as a basis for the tandem instrument would be a magnetic sector instrument, of Nier-Johnson configuration, as used on the Viking Mars Lander mission. This instrument configuration would then be matched with a suitable second stage MS to provide the benefits of tandem MS operation for rapid identification of unknown organic compounds. This tandem instrument is configured with a newly designed GC system to aid in separation of complex mixtures prior to MS analysis.

A number of important **results** were achieved in the course of this project. Among them were the development of a miniaturized GC subsystem, with a unique desorber-injector, fully temperature feedback controlled oven with powered cooling for rapid reset to ambient conditions, a unique combination inlet system to the MS that provides for both membrane sampling and direct capillary column sample transfer, a compact and ruggedized alignment configuration for the MS, an improved ion source design for increased sensitivity, and a simple, rugged tandem MS configuration that is particularly adaptable to spacecraft use because of its low power and low vacuum pumping requirements.

The **potential applications** of this research include use in manned spacecraft like the space station as a real-time detection and warning device for the presence of potentially harmful trace contaminants of the spacecraft atmosphere, use as an analytical device for evaluating samples collected on the Moon or a planetary surface, or even use in connection with monitoring potentially hazardous conditions that may exist in terrestrial locations such as launch pads, environmental test chambers or other sensitive areas. Commercial development of the technology could lead to a new family of environmental test instruments that would be small and portable, yet would give quick analyses of complex samples.

EXECUTIVE SUMMARY

In little more than a decade the field of mass spectrometry has made great progress towards simple, highly reliable and easy to operate systems that maintain the high sensitivity and resolving power necessary to provide accurate and detailed information about the materials being analyzed. Mass spectrometry has for some time been recognized as a very powerful analytical technique, but it carried a well deserved reputation for being difficult to master, with instruments that required almost continuous attention from skilled technicians to keep them operating. In addition, there was the need for Ph.D.-level analytical chemists to be able to process the samples so that they were properly entered into the instrument. Even more expert attention was then required to analyze and interpret the data that the instrument generated. It is no wonder then that use of mass spectrometry was considered to be restricted to the analytical laboratory- and only a very well-equipped one at that.

The demands of the space program played an important role in changing this situation, and coupled with advances in microelectronics, microprocessors, displays, data processing, software developments and a host of other advances too numerous to mention, all combined to cause a rapid, and significant improvement in mass spectrometer technology. Principal among the space program efforts in this regard was the challenge of placing an analytical package on the surface of Mars for an in situ look at that planet's surface and atmosphere. The Viking Mars Lander included a pioneering miniaturized magnetic sector mass spectrometer that was designed to withstand the shock and vibration of launch, the temperature extremes of space, the sterilization heat soak before launch and yet operate remotely and obtain mass spectra from soil and atmospheric samples. The remarkable achievement was that this instrument operated as expected and provided excellent data on both missions to the surface and was only turned off when data requirements were complete. In this project, Viking Instruments Corporation, which holds an exclusive patent licence from NASA for the technology embodied in the Mars Lander, is building upon the legacy of the Viking program as well as drawing upon its know-how in gas chromatography and analytical systems design.

The progress in mass spectrometry in the years following the singular achievement represented by the successful Viking mission has been equally impressive. The mass range that can be achieved has been increased from several hundred amu to well over 10,000, the types of pre-screening analytical techniques that can be interfaced with the MS has been extended from just gas chromatography to include among others liquid chromatography, Fourier Transform InfraRed, Inductively coupled plasma and mass spectrometry itself (for MS/MS analysis). The sample handling approaches have also expanded considerably, including supercritical fluid extraction, fast atom bombardment, laser desorption, and particle beams. At the same time, new approaches to operation of the ion source itself have been developed, including chemical ionization, both positive and negative, glow discharge atmospheric ionization, atmospheric pressure ionization, laser excitation and high gradient electric field ionization. This has been matched by a proliferation of mass spectrometry techniques such as quadrupole mass analyzers, time-of-flight analyzers, three dimensional quadrupoles such as the ion trap, and the ion mobility spectrometer. And each of these has been, at least theoretically, teamed with another to yield a variety of hybrid MS configurations, from the most common--a triple quadrupole analyzer--to such combinations as a magnetic sector instrument followed by two quadrupole analyzer segments, a quadrupole analyzer followed by a time-of-flight segment, an ion mobility spectrometer followed by a quadrupole segment, and so on. Perhaps the most significant improvement was in the supporting electronics and the coupling of computer-operated controls and data handling to make the instruments much more powerful, flexible, and user-friendly.

While mass spectrometer technology was improving, so also was the technology of gas chromatography. This was in large part driven by the demand for better analyses of organic compounds for environmental purposes. As the technology matured, the demand for better analysis of foods and drugs, structural determinations of newly synthesized compounds and analyses of biological materials also drove both GC and MS technologies to higher and higher performance. One of the principal improvements in gas chromatography was the introduction of capillary columns and associated stationary phases that can be bonded and cross-linked to the column support so that they do not "bleed through" and provide a high background for separations requiring high temperature. The capillary GC column also gives sharper, more easily quantifiable peaks and enables shorter analysis times with minimal carrier gas flows, and reduces the vacuum pumping capacity needed in the mass spectrometer.

Thus, a combination of forces were bringing about advances in the necessary supporting technologies that made it appear feasible to propose to NASA that Viking Instruments Corporation undertake development of a compact, power-efficient, light weight, yet sensitive, tandem mass spectrometer system that would be suitable for space use. NASA supported this proposal as a Phase II continuation of an SBIR contract, NAS8-38422.

This report describes the objectives, work performed and results of this contracted effort. It should be stressed that, while the technology base upon which this project has been carried out has been substantial and growing, the successful accomplishment of the end result of the research was by no means assured. Indeed, the project called for a number of future breakthroughs in several key areas to meet the system design goals. For example, in order to successfully carry out the proposed project, it would be necessary to create a new miniaturized gas chromatograph, invent and produce an entirely new inlet system and test and validate new sample handling pathways, connect this with the mass spectrometer in such a way that both atmospheric sampling and gas chromatographic separations can be performed, produce a new, compact, easy-to-assemble magnetic sector MS, integrate a light weight and low power vacuum system into the package, add an interstage fragmentation system that does not require a collision gas to operate, couple this with a second stage mass spectrometer with associated electronics, and operate this instrument system as a single integrated unit.

The relatively independent nature of the multiple new approaches that were required in order to meet the project goals allowed several of the subsystems to be pursued simultaneously, otherwise the limited time available for the project would have made it virtually impossible to complete. As it was, a break in the availability of NASA funds for several months at a critical stage in the contract resulted in a delay in its completion, with recovery from this delay requiring several additional month's work, all of which was provided at no additional cost to the Government. The result of this work has been construction and delivery of a prototype GC/MS/MS system that is well suited to spacecraft use.

The major subsystems of the prototype are: the inlet, including trap/desorber and injector/desorber and associated sample handling components; gas chromatograph oven assembly; transfer line and associated supporting hardware; GC/MS interface including direct atmospheric sampling inlet; first stage MS with associated electronics; vacuum envelope for MS; interstage ionization mechanism for fragmenting parent ions from the first stage MS; second stage MS. Each of these subsystems represented quite different problems, and each was a particularly challenging project on its own. Taken together, they were a more ambitious package than was originally conceived, but the results have been rewarding to Viking in terms of new technology that is now available to the company and in the new insights that have been developed regarding commercial prospects for compact tandem MS systems. Some of the technology has already been utilized in commercial products that Viking is offering.

Briefly, some of the highlights of the subsystems developments that have been produced under this project are listed below:

INLET

- A method has been developed for gold-plating the interior of nickel sample lines that provides a highly inert, yet tough and long-lasting coating that is not damaged by bending the tubing and can be heated to avoid loss of sample on cold tubing walls without degradation or out-gassing that would interfere with MS detections.

- A unique, new design injector/desorber was developed that permits use of interchangeable injector liners for standard split/splitless injections or alternatively, a commonly used adsorber trap can be inserted in the injector and the same assembly can be used to trap sample molecules that are drawn through the assembly and then, using the integral heater, thermally desorb the sample either to a GC column for separation and analysis by the MS or directly to the MS, depending upon the type of analysis being performed.

- A sample handling system was developed that permits multiple sample pathways and permits control of carrier gas for a combination of cycles, without loss of sample, including direct MS sampling, concentration on an adsorbing trap followed by desorption either direct to the MS or via a controlled GC run and then to the MS, and via direct injection to the GC and then to the MS.

GC OVEN

- The GC oven was miniaturized, with use of new, space-age, light weight, super-insulating material to keep heating requirements down, a custom-wound heater assembly, an internal fan to insure good heat transfer and heat distribution over the GC column, a miniaturized column cage for the capillary GC column, a cryofocusing attachment for trapping light volatiles and an automatic door opening and closing mechanism with associated cooling fans for rapid and precise temperature control in the GC oven.

TRANSFER LINE ASSEMBLY

- A heated transfer line assembly was developed that incorporates a separate heater block and temperature sensor, a vacuum tight seal for the GC column, a dual-jacketed line, with an outer stainless steel support tube providing the primary vacuum envelope and an inner, gold-plated copper tube encasing the GC column and providing the uniform heat distribution over the column that is essential for good chromatography of high boiling point samples.

DUAL MEMBRANE/GC CAPILLARY DIRECT INLET SYSTEM

- The need to provide both a direct sample pathway to the MS and a pathway via the GC column was solved by the development of a unique, dual interface assembly that permits both direct sample entry via a membrane system and sample entry via GC column. The membrane assembly and the column connections are part of a single machined stainless steel fitting to which the transfer line assembly is welded. The membrane assembly is a Viking proprietary design that enables efficient sample transfer over a special membrane material, while excluding most of the nitrogen, oxygen and water vapor present in the atmosphere, thus improving the signal-to-noise of direct atmospheric sampling. The membrane is isolated from the MS by an electrically-operated, vacuum-tight valve except during direct membrane sampling, while the GC column is continuously connected to the MS. Entry of sample into the MS is via concentric pathways, with the gold-plated copper tube containing the GC column at the center and the membrane sample flow in the annular region surrounding the heated GC tube.

MS-1

- A special combination alignment fixture and vacuum envelope assembly was created that serves as a primary reference plane for the major components of MS-1, i.e., the ion source, the electric sector, the magnet and magnetic sector and the detector, when a detector is present in MS-1. This configuration was adapted from a patent pending design developed by Viking for a portable MS.

- A new compact ion source was developed to give relatively consistent ion production over a particularly wide range of accelerating potentials, with high extraction efficiency and ion production at both low and high voltages.

MS/MS INTERSTAGE

- An extremely compact, rugged, light weight and power efficient interstage fragmentation system was designed, after consideration of a number of alternative methods of creating daughter ions without need for a collision gas cell.

- A positioning system was designed that permits easy exchange of the interstage ionization device and a detector for the first stage MS, so that the first stage MS can be operated as a primary detector system, and thus provide greater flexibility in the operational modes available to the system operator.

MS-2

- As a second stage MS, after considering a range of alternatives, a uniquely designed energy analyzer sector was utilized for daughter ion detection. Among its special features are a special mounting and alignment system that provides simultaneous positioning and alignment in three dimensions as well as electrical insulation.

While this is an extensive list, there is an even broader array of alternative configurations, experimental set-ups, paper studies and analyses, simulations and design effort that is behind the hardware configuration that is being delivered to NASA as a result of this contracted effort. There were a number of important lessons learned in this process which are discussed in greater detail in the main report.

As a result of the work done in connection with this project, Viking Instruments was able to incorporate a number of the improvements that were made in the technology of GC/MS/MS systems design into commercial products, principally the SpectraTrak 600 series of transportable instruments. In this instrument package, Viking has successfully demonstrated its ability to incorporate a complex, laboratory-level performance system into a rugged, compact, easily transportable system, that is being used now by a number of both government and industrial customers. In this regard, one of the end objectives of the SBIR Program has already been achieved, that of transferring technologies developed in the course of SBIR contracts into the commercial sector.

In completing the work on this SBIR contract, we believe that NASA's objectives of advancing the state-of-the-art in spacecraft GC/MS/MS instrumentation have also been achieved. Both the SpectraTrak 600 and the prototype system produced under this contract have been developed such that, with rather straightforward engineering, they could be the basis of a system that could fly in space. Converting these systems to actual space-qualified hardware would require additional contracted effort, but no fundamental change in the design since the approach taken in developing these systems has been to make system design decisions compatible with a possible future space-qualified package. Thus, the conceptual design of a space qualified GC/MS/MS flight prototype are not significantly different from the prototype system that is being delivered.

Finally, it should be noted that the cooperation and assistance of contracting office representatives in handling contract extensions and the periodic communications with the two technical representatives that were assigned to this project during its lifetime were greatly appreciated and contributed significantly to the project's results.

FINAL REPORT

PART I. PROJECT OBJECTIVES

A. INTRODUCTION

It seems apparent that there will be a need for better analytical information regarding the detailed composition of the atmosphere in manned spacecraft as the length of occupancy of the spacecraft increases and also as the diversity of industrial processing operations increases, some of which can involve hazardous or irritating compounds. While measurements of the basic atmospheric constituents of manned spacecraft have always been important, even in short duration missions such as present shuttle or previous Apollo and Gemini flights, the ability to sense trace contaminants has not been a priority. With the prospect of a long-lived Space Station, however it appears that the option of an improved monitoring capability would be desirable. Several of the Space Station development efforts have included instrumentation packages that contained elements of such an improved monitoring capability.

It is our understanding that there is currently no manned spaceflight qualified instrument that is capable of providing on-orbit analytic data on trace organic constituents of the spacecraft atmosphere. Returned air samples are collected on current shuttle flights and subsequently analyzed after the mission to give snapshots of what atmospheric conditions may have existed in flight, but on-board monitoring is not done. For a system that has been characterized as well as the Space Shuttle and that returns back to earth usually within a week, this procedure should be adequate. As the length of time in orbit increases, however the prospect for a build up of trace contaminants increases. Further, when the range of activity performed in the station expands to include materials processing experiments, commercial materials processing in space, or EVA activity that may involve the risk of introducing leaking rocket fuel into the station via the air lock, early warning of potentially hazardous atmospheric constituents appears to be desirable.

Given the prospective need for sensitive, rapid, and precise information about the trace components of a space station's atmosphere, and possibly early warning of the onset of a hazardous condition, the question is how to acquire this information. Among the various analytical techniques that are available to give sensitive, definitive, and relatively rapid results for air samples collected in situ, that is, from defined points as contrasted with remotely sensed atmospheric analyses, mass spectrometry coupled with gas chromatography has the broadest capability. Recent advances in mass spectrometry have expanded the field tremendously so that there are many choices available in the type of instrument, the performance, mass range, ionization method, vacuum system, data output, degree of automation, and other instrument characteristics.

Beyond the more immediate potential application associated with a manned space station, there is also the prospect that future missions to the surface of Mars or possibly the Moon would also benefit from the availability of an analytical instrument system with the power and broad functional ability of an MS. Although such systems tend to be designed specifically for the particular mission in question and are highly integrated into the spacecraft and its operating and data management system, having a demonstrated system design would reduce the time needed for the development cycle and could reduce the total mission cost as well.

Thus, for several important future applications there is a role for an advanced MS-based system that would be capable of being space-qualified and would incorporate advances in MS and GC technologies and their associated supporting subsystems such as power supplies, microcomputer systems, data storage and processing techniques, vacuum systems and advanced materials.

The space program has utilized mass spectrometry as part of an analytical package in high altitude atmospheric samplers and, most importantly, in the Viking Mars Lander missions. It was the demands of the Viking Mission that brought together some of the best minds in the analytical instrument field in the early 1970s to define the GC/MS instrument package that was eventually to fly on the Mars Lander module and be operated on the surface of the planet for both analyses of soil pyrolysis samples and analyses of the Martian atmosphere.

The constraints that were applied to the design of this GC/MS system were very significant even when viewed in the light of today's technology. When the first designers began to work on the system almost twenty years ago, they required major breakthroughs in design and performance. The system had to be very light weight, yet rugged enough to withstand the vibration of launch and the shock of a possible hard landing on Mars. The system had to spend almost a year in space after launch before it would be operated on the planet's surface. It had to withstand a heat soak and surface treatment to destroy any living organisms that might be transported from Earth to Mars and thereby contaminate Mars with foreign organisms. It needed to be operated remotely via data link from the Earth's surface and report its data to analysts here on Earth, and it had to use relatively little electrical power, since the lander had limited solar panel capacity. The development of this GC/MS system involved hundreds of people, was a major project for the Jet Propulsion Laboratory, took more than 6 years to produce, and reportedly cost more than $40 million to develop.

The end result of this work was a compact GC connected via a membrane separator to a double-focusing, Nier-Johnson configuration, magnetic sector MS, with a permanent magnet and electrically scanned, electron-impact ion source. The design included an innovative dual use for the primary magnet where an extension in the pole faces was used to provide a reduced magnet field for an integral ion pump. This pump was of exceedingly small capacity, 0.5 L/sec, so only very small samples could be handled, and the MS-to-GC interface had to remove nearly all of the carrier gas. This was accomplished by using hydrogen as the carrier gas and a silver palladium membrane system which had the effect of scavenging nearly all of the hydrogen but allowing the sample to pass through to the MS ion source. The system was tightly sealed, with electron beam welded seams and very low outgassing surfaces on the interior of the instrument. Viking Instruments has the exclusive patent license for commercialization of the technology embodied in the instrument developed for the Mars mission.

Building upon this technology base, in this SBIR project Viking proposed to use the basic Mars lander MS technology and incorporate it into a more modern GC/MS system with the additional benefit of a second stage MS, so that the system would be a GC/MS/MS. Such a system would have the potential of operating in several modes, GC/MS, MS/MS, or GC/MS/MS, as needed, to fit the type of sampling environment that may be encountered. In performing the tasks identified in the proposal, it was necessary for Viking to design and develop an entirely new miniaturized GC, a trapping system for concentrating and then thermally desorbing ultra-trace samples, a new inlet system for the entry of samples into the MS, a new ion source that would be easier to fabricate and assemble than the original Viking source, a new vacuum envelope and pumping system since the original system would not provide sufficient capacity for manned spacecraft use, a new interstage fragmentation scheme that would not burden the design with extra pumping capacity and a heavy collision gas cell plus extra gas supply, and a new second stage MS analyzer for the detection of daughter ions. Finally, based upon the work on the prototype system, Viking would need to prepare a conceptual design of a space qualified GC/MS/MS system that would be compatible with possible future Space Station use.

B. TECHNICAL CONSIDERATIONS

1. CHARACTERISTICS OF A GAS CHROMATOGRAPH

In proposing a GC/MS/MS system to NASA, Viking recognized the value of opening up the prospect of using recent advances in mass spectrometry to construct a system that would provide an additional level of information about the sample molecule than is possible with a single-stage MS system. In a typical GC/MS, the sample is introduced into the front-end of the gas chromatographic column in a state such that sample molecules can readily be transported down the column by a carrier gas flow. The GC column is coated with a special formulation of polymeric material into which certain classes of molecules are preferentially adsorbed. The process of adsorption and desorption of the sample molecules proceeds down the column aided by the carrier gas flow and by control of the temperature of the column. The differing rates at which this process occurs has the effect of taking an undifferentiated mixture of molecules and separating this mixture into its various components, with the components emerging from the column after a distance of 20 meters or more in a series of clumps, which when detected show up on data displays as peaks. This is a very brief and over-simplified picture of the process of gas chromatography.

This technique for separation of a sample mixture can be used with relatively simple detectors that respond to the bunches or clumps of sample molecules to comprise a widely used instrument in analytical chemistry, the Gas Chromatograph. By careful control of the carrier gas flow rate, the temperature and the injection process by which the sample enters the GC, it is possible to catalogue the transit times for various compounds through a specific column. These are called retention times. By measuring the retention times very accurately, and using standards for reference, it is possible to come to very good conclusions regarding the identities of the components of an unknown mixture. This technique is not always a reliable method, however because of the possibility that two different compounds might transit a column in very nearly the same time, i.e., have the same retention times. If, based upon other information about the unknown sample, one cannot eliminate one or the other of the two or perhaps more overlapping possibilities, there would be no good way to differentiate between them without performing some other analysis. Thus, a GC measures only one attribute of a sample compound, the retention time. Because of the possibility of overlap and the difficulty of sorting out times for very complex mixtures of 50 or more compounds, Gas Chromatography is not usually considered to be a definitive method for determining the identity of an unknown in a sample mixture. What is needed for more definitive work is a detection system that provides more information than just the presence of the bunched molecules as they exit the column.

Some thirty-five years ago, the technique of Gas Chromatography was first linked with a Mass Spectrometer as a detector, instead of the simpler detectors then in use. The Mass Spectrometer provides a whole new dimension of information about the sample molecules as they exit the GC column. This results from the ability of the MS to discriminate between charged particles of different masses. Thus, the foundation was laid for a revolution in the tools available to the analytical chemist.

2. CHARACTERISTICS OF A BASIC MASS SPECTROMETER

In its simplest form, a typical MS used for environmental analysis consists of an ion source, an analyzer section for discriminating between ions of different masses, a detector for the ions, a method for scanning the analyzer to form a spectrum of the ions that are created, and a data system for collecting and recording the spectra. The most common ion source is one that uses electron impacts with an energy of 70 electron volts to break up the sample molecule into ion fragments that are positively charged. This energy was chosen because it gives good fragmentation patterns, each unique and typical of the molecule being fragmented. By international convention, the major mass spectrometer spectrum libraries are all based upon this electron impact (EI) ionization scheme. Other ionization methods are also employed for special purposes such as negative and positive chemical ionization, laser ionization, fast atom bombardment, various high gradient electric field or electric spark sources, glow discharge, and others.

The source is intended to provide enough ion fragments from sample molecules that may be present in the source so that, when accelerated out of the source, focussed, and analyzed by mass, there will be enough ion current to measure with a sensitive detector and amplifier. The source should also provide a relatively monoenergetic set of ions for any particular set of source potentials.

From the ion source, the ions are passed through an analyzer assembly that separates them by mass. The analyzer that is used by Viking is a double-focusing, magnetic sector type. In this configuration, the ions are first passed through an electric sector and an intermediate slit which serves to narrow the energy spread that may exist in the ion beam. The emerging ion beam from the electric sector is then directed to the magnetic sector which serves to separate the ions by momentum. Since the energy is determined, by suitable shaping of the magnetic field, the relationship between the mass-to-charge ratio of a ion and its trajectory through the magnetic field can easily be determined. Depending upon the specifics of the configuration that are chosen, a mass spectrum can be generated by varying the ion source and electric sector potentials or by varying the trajectory being monitored by the detector in what is called a Mattach-Herzog configuration in which the separated ions emerge on a focal plane.

Detection of the ions is normally with an electron multiplier of some type. In this device, the ion as it emerges from the magnetic field impacts upon a surface coated with a material that emits one or more electrons upon ion impact. These electrons are then accelerated by an electric field established as part of the detector design to impact another point on the surface coating, where each of the electron impacts generates its own set of secondary electrons. The geometry of the detector is such that each successive set of collisions multiplies the number of electrons in an avalanche-type effect, such that an ion collision on the detector results in a much more measurable current at the detector output connector. This output current is then fed to an amplifier where it is used to generate a signal that is synchronized with the values of source voltage that were used to produce the ions. By plotting the output signal from the detector on the Y-axis versus a calibrated mass-to-charge ratio scale along the X-axis for each set of scanning voltages, a mass spectrum can be produced. Since microprocessors have been introduced to the field to process both the operating instructions and the data collected, the output and the input signals have increasingly been handled in digital form, with signals converted to discrete steps rather than a continuous analogue form.

3. CHARACTERISTICS OF A TANDEM MS/MS

Tandem Mass Spectrometry fundamentally deals with the measurement of ion dissociation phenomena, generically characterized by the following expression, where m_p^+ is the mass of the original or parent ion, m_d^+ is the mass of the fragment or daughter ion and m_n

is the mass of the neutral fragment (or fragments) formed in the process:

$$m_p^+ \;->\; m_d^+ \;+\; m_n \qquad \text{(I-1)}$$

This process can occur in the ion source, in field-free regions of the mass spectrometer, in special regions and under special conditions created to observe the phenomena, either following a GC separation or with direct sample input, at high or low energies, either self-excited as in the case of metastable ions or induced, as in the case of a collision cell. A complete description of this process and the related complex and continuously expanding field of tandem mass spectrometry would go well beyond the scope of this report. This brief review is intended to highlight the basic operating principles, point out some of the problems that must be over come and touch on the considerations that enter into trade-offs and system design decisions that were made in the course of carrying out this contract. For a more complete treatment of the subject, the recent book MS/MS: Techniques and Applications of Tandem Mass Spectrometry by Busch, Glish, and McLuckey is a good survey of the current state-of-the-art in the field.

In a typical tandem MS instrument used for environmental analysis, the basic dissociation reaction outlined above is created under controlled conditions when the output of the first stage analyzer is subjected to additional fragmentation, most often in a collision gas cell in which the incident ions go through a series of collisional ion-molecule reactions with a target gas. This is called "collision-induced dissociation" (CID). In the collision gas cell, the nature of the daughter ion production is a function of the choice of target gas as well as the energy of the incident ion beam. The cell must be designed to keep the target gas pressure high enough to provide good fragmentation and not so high that the ion beam will be destroyed and the MS will cease to function. The collision gas cell also involves an additional burden on the vacuum system of the MS, including a pump to keep the collision gas pressure in a range acceptable for interstage MS interactions, and a separate supply of target gas, since the target gas is continually pumped away. Other means of creating the desired fragmentation also exist, including photodissociation, where a laser or other intense light source is focussed on the incident ion beam, and of greatest interest to this project, collision with a solid surface or surface-induced dissociation (SID).

Following the formation of the daughter ions in a tandem MS instrument, in the most common mode of operation, some means of characterizing the daughter ion spectrum is required. This daughter ion spectrum can reveal a great deal of useful information about the parent ion, and ultimately about the composition of the compound that is present in the ion source. There are other modes of operation of a tandem MS instrument also, for example, one in which the mass-to-charge of the daughter ion is fixed and potential parent ions are scanned. This can serve to identify quickly various classes of compounds. Similarly, through a neutral loss scan, compounds that loose a specific neutral fragment can be identified. These latter two methods of operation are not used as often as the simple daughter ion scan.

The daughter ion scan is essentially the mass spectrum of an ion in a mass spectrum. Figure 1 shows this schematically. The first stage of the MS serves to select the particular parent ion to be fragmented and the second stage analyzes the daughter ions that are created in this process. This spectrum reflects the structure of the parent ion, and in analytical applications of the MS/MS technique, is a key discriminator between different compounds. It should be recognized that many families of compounds fragment in such a way that they have one or two ions that are common. If these ions are used as parent ions, then their daughter ion spectra would also look alike and there would be no way to tell the compounds apart. Thus, careful selection of parent ions is required for the MS/MS technique to be used successfully. In general, when compared with GC/MS, this approach is best suited for the analysis of known or targeted compounds in complex mixtures, while GC/MS is better suited to the analysis of unknown mixtures or mixtures of compounds that do not exhibit sufficiently different parent ion structures. A schematic comparison of the two techniques is shown in Figure 2, which is taken from the referenced work on MS/MS techniques.

A variety of configurations of mass spectrometer elements have been experimentally and theoretically evaluated as MS/MS systems. Each has, to some extent, its own advantages and disadvantages. The earliest MS/MS work was done with magnetic sector instruments, both single-focusing and double-focusing. Today, however most magnetic sector instruments that are being sold commercially are of the large, very high resolution type, and are used primarily for research applications that require high mass-high resolution capabilities. For general purpose analytical applications, on the other hand, most commercial GC/MS systems use a quadrupole as the mass analyzer. Since many users were already familiar with quadrupoles, most MS/MS systems that are commercially available make use of an MS/MS configuration that uses three separate quadrupole sectors in tandem, the so-called "triple-quad". These systems are very large and heavy, require large amounts of electric power, and are difficult to operate and tune successfully without the aid of sophisticated tuning software. Building on this technology therefore would not be suitable for the type of space application envisioned in this contract.

Magnetic sector mass spectrometers, particularly the type of instrument that was used in the Mars mission with a fixed magnetic field and a voltage-scanned source and electric sector, can be very low power instruments and if appropriately designed, can be small, lightweight and rugged. Thus, as the point of departure for an advanced spacecraft tandem MS, the Mars Lander MS configuration design as Viking has modified it, is a good starting point since it already reflects some of the key attributes that will be needed in any space qualified design.

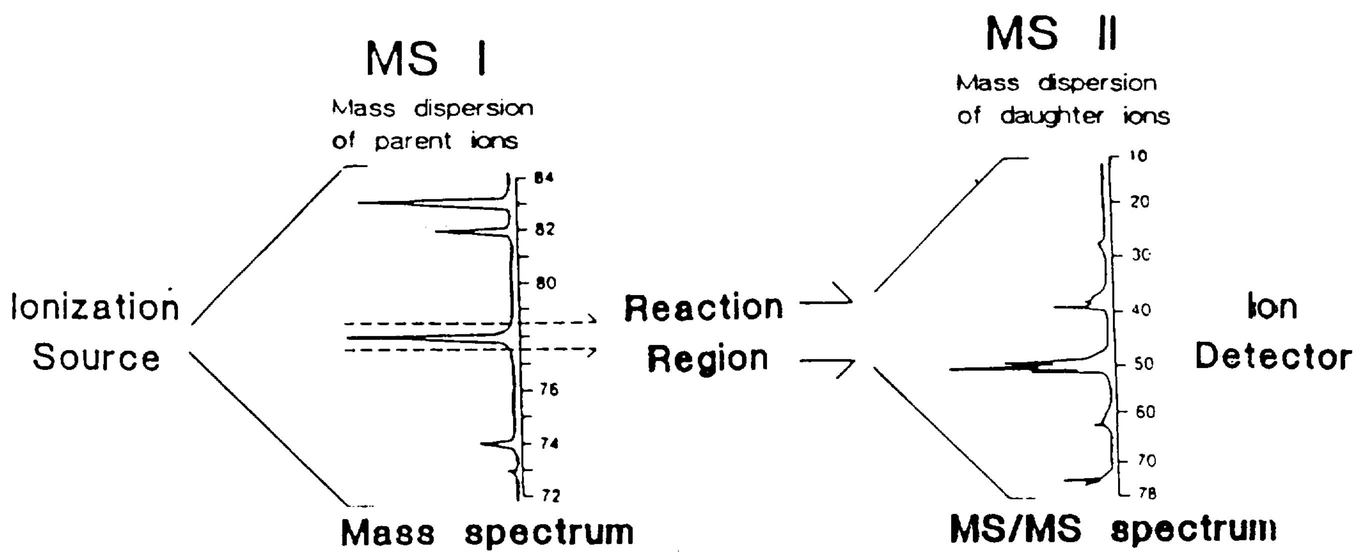


Figure 1

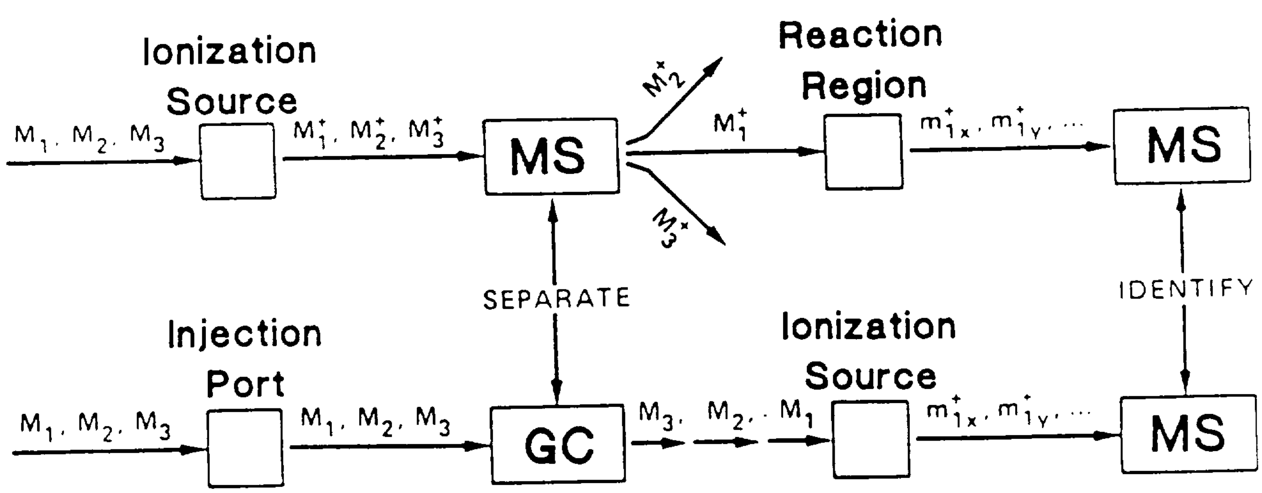


Figure 2

In the commonly used shorthand of the field of mass spectrometry, the Viking instrument, with first an electric sector ("E") followed by a magnetic sector ("B"), would be designated an "EB" machine. There are magnetic analyzers with the BE configuration also. A time-of-flight MS is designated "TOF", a quadrupole, "Q", an ion trap, "ITD", and a wien filter, "W". Given these designations, theory shows that tandem MS instruments could be constructed that consist of EBE, EBB, BEE, BBE, EEE, BBB, EEB, BEB three stage configurations, using just electric and magnetic sectors. In practice, however only the EBE, BEB and BEE configurations have been built, even in an experimental mode. Hybrid instruments also can be constructed, and a BEQQ instrument has been reported as well as an EBQQ and other combinations.

C. SPACEFLIGHT CONSTRAINTS

This knowledge base regarding tandem mass spectrometry has been developed primarily for terrestrial instruments, where the instrument is not constrained by weight, power, size, vibration, shock, temperature, data system capacity, operator training and availability, system outgassing and other characteristics that become important when a system is considered for possible flight on a manned spacecraft. Therefore, while there is a large set of possible configurations that may be used to construct a tandem MS system in a laboratory here on earth, most if not all of them could not be used since they would not be compatible with the spaceflight environment.

One of the key objectives of this project was to go through each of the major subsystems needed to make a tandem MS system function and pick a configuration that would appear to be best suited for spaceflight, design and test this configuration, and then assemble the tested subsystems into an experimental prototype package.

One of the principal issues that must be confronted in any of the MS configurations is the provision of a suitable vacuum pumping system. This is a problem for even a single-stage MS, but it becomes more so for a tandem instrument, since the primary method of interstage fragmentation is via a collision gas cell. As pointed out earlier, such cells require a supply of collision or target gas as well as the extra vacuum pumping capacity to allow the target gas to be held at a higher pressure than the rest of the mass spectrometer, even with openings at each end of the collision cell for entry of the parent ion beam and exit of the daughter ions. The extra burden of the associated equipments to support a collision cell could make the size, weight and power requirements of a space qualified tandem MS impossible to fit into a reasonable allocation for such an instrument. Thus, one of the first considerations that made it possible to consider a tandem MS design for space use was the prospect of using a much simpler method of creating daughter ions. In the proposal, two mechanisms were suggested involving surface collisions, and the objective of this phase of the project was to test and validate one of these methods for actual use in a tandem instrument.

In a surface collision device, the parent ions are directed to a flat conducting surface at an acute angle, with the daughter ions produced by the energy of the collision event (and some parent ions) reflected from the surface typically at an angle of 90 degrees from the incident beam. This process is called surface induced dissociation (SID). The SID process has some significant advantages for a system intended for eventual spaceflight. First, it is very simple and lightweight, involving only a small stainless steel piece about 2 cm square and an appropriate mounting bracket, perhaps with a provision for withdrawing the surface from the ion beam. Second, it does not require any additional power. Third, it does not require additional vacuum pumping capacity. Finally, since it intercepts the ion beam, it ensures there is 100% interaction with the parent ions, and studies of this mechanism have shown that it operates over a range of incident ion energies, without losing its effectiveness. With a mechanism like SID, it became possible to consider seriously the prospect of a tandem MS for space.

The basic MS vacuum system therefore can be used in a tandem MS as long as SID is used. Today, MS systems primarily use diffusion pumps, turbomolecular pumps, cryopumps and ion pumps to maintain a high vacuum inside the system. Turbopumps and diffusion pumps require continuous, or near continuous roughing usually with some sort of mechanical pump. Such pumps are rather heavy and require considerable electrical power. Recent developments in turbopumps have resulted in a model that combines a standard turbopumping stage with a molecular drag pump, the net effect being to reduce the requirements on the mechanical roughing pump. These new generation turbopumps can operate with a small diaphragm pump interface with the atmosphere. This vacuum pumping system configuration makes the best all-around package for use in the tandem MS and would be our recommendation, since there are major drawbacks for each of the others.

For example, the diffusion pump would not work in space, since it depends upon maintaining a vertical position and on gravity to help with flow control of the working fluid in the pump. The ion pump works well once pressures in the pump are below 10^{-3} Torr, and lowering the pressure in the system to the point where the ion pump will begin to function normally requires a mechanical roughing pump. So even though the ion pump does not require an outside pump when it is operating, such a pump is required to start the ion pump. Since every mass spectrometer needs to be opened to atmospheric pressure at some time for source cleaning and other maintenance procedures, any long term use of the system using an ion pump would require some provision for re-starting the pump. This could be done by connecting the MS to the space environment which would be a suitable rough vacuum, but it is our understanding that venting systems to the immediate environment of the space station is highly restricted in order to avoid accumulating excess molecular-level contamination that might affect optical surfaces. So, it might be necessary to have a mechanical vacuum pump present for restarting the ion pump, and thus, any potential weight advantages that an ion pump might have would be lost.

One of the other principal constraints on system design is electric power consumption. In general, not counting the vacuum system discussed above, the MS itself is not a high power consuming device. The major power consuming element in magnetic sector MS instruments is usually the scanning magnet, but the system being used here has a fixed magnetic field and a scanned electric sector and ion source which do not use much power. The largest power consuming items it turns out are the heaters, both for the MS and for GC components and the heated sample lines that would be required for gathering atmospheric samples from locations remote from the instrument. In the design for the system, therefore the size and location of resistance heaters, the insulation provided for heated components, the recognition that in space convection is not operative, and the efficient operation of heated elements will all be important considerations.

Ruggedness is not normally a characteristic that is associated with mass spectrometers, yet the shock and vibration environment of launch must not adversely affect the system. Some designs, such as the normal quadrupole system, where positioning of the four rods supplying the field is critical to the performance of the system, do not survive shocks or vibration very well. Similarly, magnetic sector instruments normally require careful alignment and their independent segments would not withstand the typical launch environment and remain adequately aligned. Viking Instruments fortunately has considerable experience in developing systems that survive rough handling, and in its SpectraTrak Model 600 series transportable GC/MS instruments has demonstrated that such GC/MS systems can be ruggedized and still maintain sensitive, laboratory-quality performance. The heart of this system is a monolithic quadrupole analyzer, where the four pole faces are part of a single extrusion and can never come out of alignment, short of breaking the analyzer. This analyzer is not well-suited to a compact, tandem system but would make an excellent single-stage, space-qualified GC/MS.

In Viking Instrument's redesign of the Mars Lander MS, an entirely new approach to mounting and alignment of the system sectors was developed that also becomes part of the vacuum envelope for the system. This innovation in MS design has been the subject of a previous patent application and was made available to this NASA project in connection with the tandem MS development. In essence, the design approach was to mount each of the system elements on a precision-machined plate that acts as a reference plane for each of the elements and a fixture on which they can be mounted. By constructing the plate of sufficiently rigid material the resulting MS system will be rugged and will withstand considerable shock and vibration without damage or misalignment. Similarly, the design of each of the elements of the MS system needs to be reassessed and modified to improve their resistance to shock and vibration effects.

Overall system weight is another significant constraint as well as the size and shape of the package. The GC/MS/MS needs to be able to fit into available rack space as defined for Space Station Freedom, which means that it would be desirable if the instrument were capable of being mounted in a standard 19 inch rack and not be more than 38 inches deep as a maximum. Since the Viking SpectraTrak 600 series instruments are all 19 inch rack mountable, and are not more than 30 inches deep, Viking has demonstrated that it can package a complex MS-based system that will fit the space station environment. The SpectraTrak system is also designed to minimize system weight as a key parameter, so the understanding of the trade-offs that are needed to meet minimum weight goals are well understood by the Viking design team.

Finally, the instrument must be relatively autonomous, since there will not be much operator time available for this type of function. That means that the instrument should be nearly maintenance-free, with maintenance procedures that are easily performed by minimally trained personnel. The instrument must also be capable of running unattended for long periods, and must have interfaces that are compatible with the on-board data and electric power systems. If operated in an early warning mode, the instrument must be capable of providing an alarm signal or other triggering signal to the on-board data system.

These are the major areas where there are significant constraints on a GC/MS/MS that are imposed by the objective of creating a system design that is compatible with the space flight environment. These constraints plus the nature of the basic technologies of gas chromatography and tandem mass spectrometry set the boundaries within which this project was conducted. They limit the solutions that can be considered and they shaped the specifics of the designs that were developed. Where these constraints have been particularly important to the choices that were made, they will be pointed out in the text.

D. STATEMENT OF WORK

The more formal description of the project objectives is contained in the Statement of Work that was incorporated into the contract terms and conditions. It should be noted that no samples of actual spacecraft atmosphere were made available to Viking or examples of specific contaminants, as envisioned under item 4. of the SOW. In place of this, Viking has selected its own list of typical contaminants for its testing. The SOW is attached as Exhibit A.

III. PHASE II STATEMENT OF WORK

A. STATEMENT OF WORK

The contractor shall design, fabricate, test, and evaluate a demonstration prototype of a spacecraft tandem mass spectrometer including the following experimental development efforts:

1. Perform systems engineering and analysis as needed to prepare detailed design and technical specifications of the proposed spacecraft GC/MS/MS demonstration prototype system based upon the technical results and design effort completed in Phase I. The demonstration prototype shall be designed to industrial grade specifications using standard commercial parts, but, to the extent feasible, the design shall be consistent with anticipated space qualification to NASA specifications.

2. Conduct experimental development, fabrication, and testing of advanced GC/MS/MS components and subassemblies including the following subassemblies designed for optimal Tandem MS operation:

   a. Miniaturized gas chromatorgraph and molecular leak inlet;
   b. Compact MS vacuum envelope and advanced magnet assembly;
   c. Multiple collision surface induced ionization interstage;
   d. Tandem MS ion optics with electro-optical ion detection;
   g. High vacuum ion pumps and turbomolecular pumping system;
   f. Tandem MS power supplies, controls and data processing.

3. Assemble and test a GC/MS/MS demonstration prototype based on the results of the experimental development efforts described above including system integration, precision alignment, adjustments, and refinement.

4. Test and evaluation of selected spacecraft GC/MS/MS analytical and monitoring applications including experimentation with typical spacecraft environmental. industrial process, and medical samples or simulants and alternative sampling methods and operating cycles.

5. Prepare conceptual design of a space qualified GC/MS/MS flight prototype based on the above test and evaluation results including review of applicable NASA specifications and analytical instrumentation requirements for the Space Station.

6. Prepare quarterly progress reports and final reports required under the contract.

Exhibit A

PART II. WORK PERFORMED

The major tasks leading to the deliverable experimental prototype system were organized into three principal efforts: systems engineering leading to an overall system design; subsystems fabrication, assembly and test; system assembly and test. The work performed in each of these areas is described in summary fashion in the following sections. Only the highlights of the various tasks are included here, assuming that trial solutions that did not yield satisfactory results are not of particular relevance, even though they required effort by the project team. Additional detail is available in any of these areas upon request. The quarterly progress reports submitted as part of the project reporting requirements also include additional details of the work.

Based upon the results of the system work, a final step was the conceptual design of a flight prototype which is included as a separate appendix since it is identified as a separate deliverable under the contract. Testing of samples and the sampling methods was carried out as part of the proof-of-concept work for the overall system and is included as part of the "Results" section of this report.

A. REVIEW OF SCIENTIFIC BASE AND SYSTEMS ENGINEERING

The basic configurations of GC/MS/MS, using a magnetic sector instrument as a baseline, have already been discussed in the previous section of this report. Careful review of the scientific literature in the field, consultation with experts and discussions with colleagues, and our experience in designing and developing single stage systems led us in the direction of a simplified design as the most practical solution for a spacecraft-oriented system. We were convinced that the constraints imposed by space compatibility made the EB configuration, with scanned E sector and a fixed magnetic field the best starting point upon which to build the tandem MS system. Previous scientific studies and experiments on instrument configurations led us to conclude that the best choice for a tandem system, given the starting point of an EB system as the first stage, was an EBE configuration. The experimental prototype system that is being delivered to NASA as part of the deliverables of this project is such an EBE system.

1. EQUATIONS OF MOTION FOR IONS IN THE SYSTEM

The motion of the ions in such a system can be characterized, to a first order, through some rather straightforward relationships. In the electric sector, the equation of motion for an ion is:

$$m v^2 / r = z E, \text{ and} \tag{II-1}$$

the equation of motion of an ion in the magnetic sector is

$$m v^2 / r = z v B , \tag{II-2}$$

where z is the charge of the ion (usually assumed to be unity for most analytical mass spectrometry), m is the mass of the ion, r is the radius of curvature of the path of the ion in the respective fields, E is the electric field strength, v is the velocity of the ion as it enters the field, and B is the field strength of the magnetic field. From the second relationship, which can be rearranged as follows:

$$m\,v = B\,r\,, \qquad \text{(II-3)}$$

it can be seen that the magnetic sector acts to disperse ions according to their momentum (for singly charged ions). The kinetic energy of the ion that is accelerated out of the ion source is, ignoring for the moment any initial velocity that the ion may possess before it is accelerated out of the source,

$$m\,v^2 / 2 = z\,V\,, \qquad \text{(II-4)}$$

where m, v, and z are as defined previously and V is the net accelerating voltage in the source. From this relationship and equation (1), it can be seen that the electric sector acts to disperse ions of different energies, as determined by the action of the ion source. In a double focusing instrument, such as the first stage EB configuration used in this project, the first stage electric sector acts to narrow the energy spread of the ions that are accelerated from the ion source. This highly monoenergetic ion beam is then introduced into the magnetic field where, for a constant B field, the trajectory through the field is related to the accelerating potential of the source by the following relationship which is derived by combining equations (1) and (4):

$$m / z = B^2\,r^2 / 2\,V \qquad \text{(II-5)}$$

From this it can be seen that, for a fixed geometry and placement of the detector slit and assuming singly charged ions, a mass spectrum can be generated by sweeping the accelerating voltage. It should also be noted that the product of mass times accelerating voltage for a particular geometry and fixed field is a constant. Thus, the highest accelerating potential is associated with the lightest ions and vise-versa. This has some important implications for the operation of the MS for detection of higher mass ions, since these heavier ions are being accelerated by lower potentials. As the accelerating potential decreases there is a loss of resolution because of the proportionally greater impact of fringing fields and ion-molecule collisions. These effects, for a fixed value of magnetic field intensity, serve to set a practical upper limit to the mass-to-charge values of ions that can be resolved by a particular instrument. For the scanning instrument with the dimensions and configuration of the EB mass spectrometer used in this project, this minimum scanning potential is in the vicinity of 250 Volts. Thus, the stronger the magnetic field, in general, the higher the mass that can be effectively focused in the instrument at this minimum accelerating potential. The dimensions of the ion optics of the first stage MS are shown in Figure 3.

OPTIC AXIS DIAGRAM 90°—90°

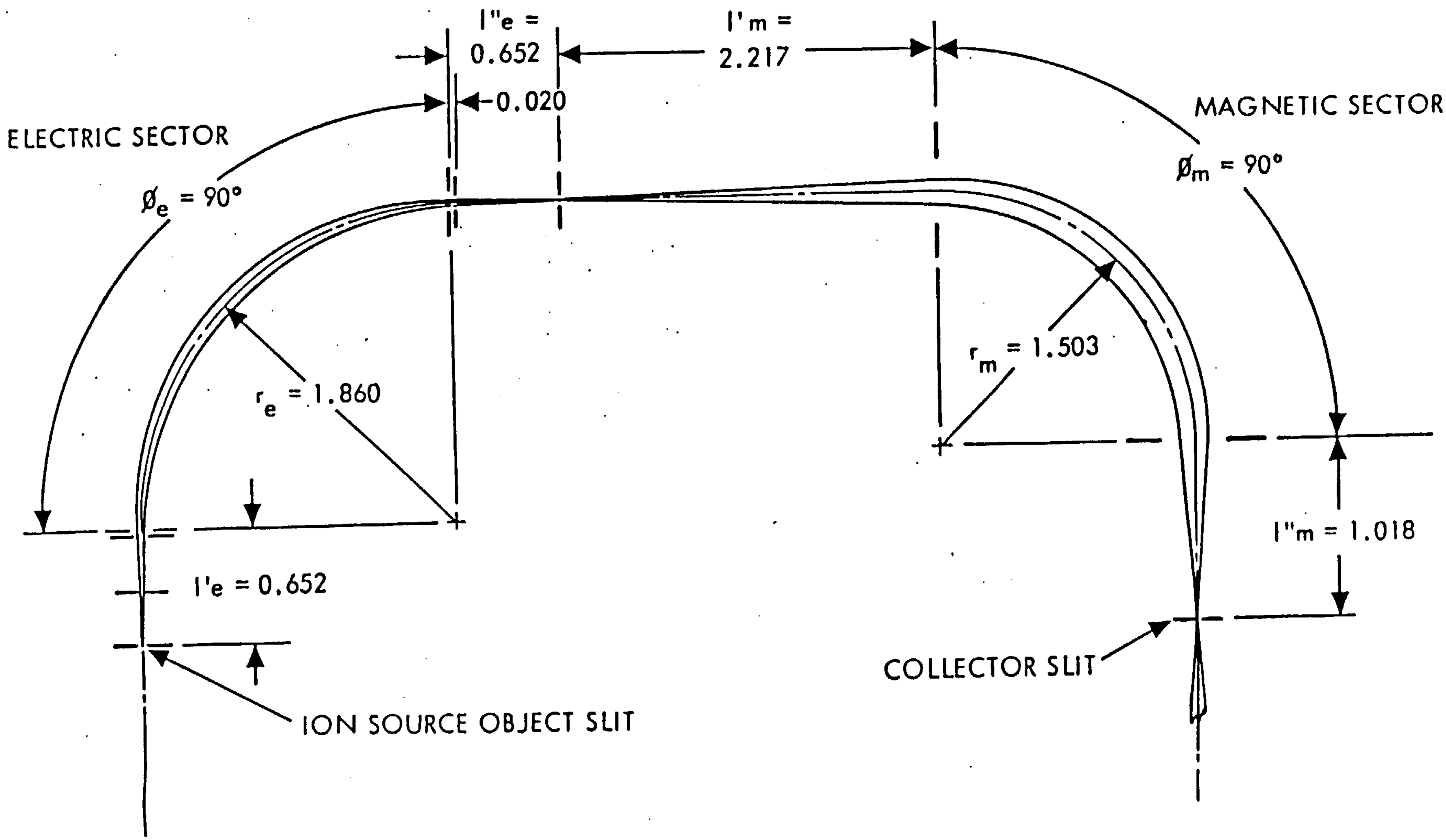


Figure 3

In a tandem MS, the interaction that results in the formation of the daughter ions, shown in equation I-1, is most often created in a field-free region and hence the products of this interaction do not experience accelerations from the effects of either a magnetic or electric field. Thus, the velocities of both the parent ion and the daughter ion will be essentially the same and the energies of the daughter and parent ions are proportional to their masses. In constructing a tandem instrument based upon an EB first stage MS, therefore, the first and simplest choice is to add an electric sector, to have an EBE configuration, where the mass of the daughter ions, in a daughter ion scan is given by:

$$m_d = E_d \ m_p \ / \ E_p \qquad \text{(II-6)}$$

assuming singly charged parent and daughter ions. In this configuration, if the accelerating voltage of the first stage is then set to pass just the parent ion, a scan of the voltages of the second stage electric sector, i.e., an energy scan, will provide a mass spectrum of the daughter ions. This is the configuration that was adopted after much review and analysis and the survey of a wide variety of possible configurations for the second stage MS. This approach has the advantage of simplicity, and a spacecraft system is not a good place to insert extra complexity for a system that is already quite sophisticated. It also is an effective configuration for performing tandem MS validations of compounds of interest, and it has the advantage of being much smaller in size and weight than any other alternative system. Hence, it appeared to be the best choice for this project. Analysis has also shown that the second stage electric sector for an EBE configuration tandem MS should have the same geometry as the first stage electric sector, so in our design we have preserved the first stage electric sector dimensions.

2. MAGNETIC FIELD CONSIDERATIONS

Viking Instruments had several existing Alnico V magnets that were already available at Viking Instruments that could be modified to fit the needs of the project. So, in order to save on project costs, these magnets were used although it was recognized that this would result in a smaller mass range than would be desired for the eventual spacecraft instrument. However, the mass range that can be achieved with the existing magnets is sufficient to demonstrate the principals involved, and for this reason no procurement of magnets of more exotic material was carried out. For the next generation prototype, new magnets, most likely of neodymium-boron-iron would be needed.

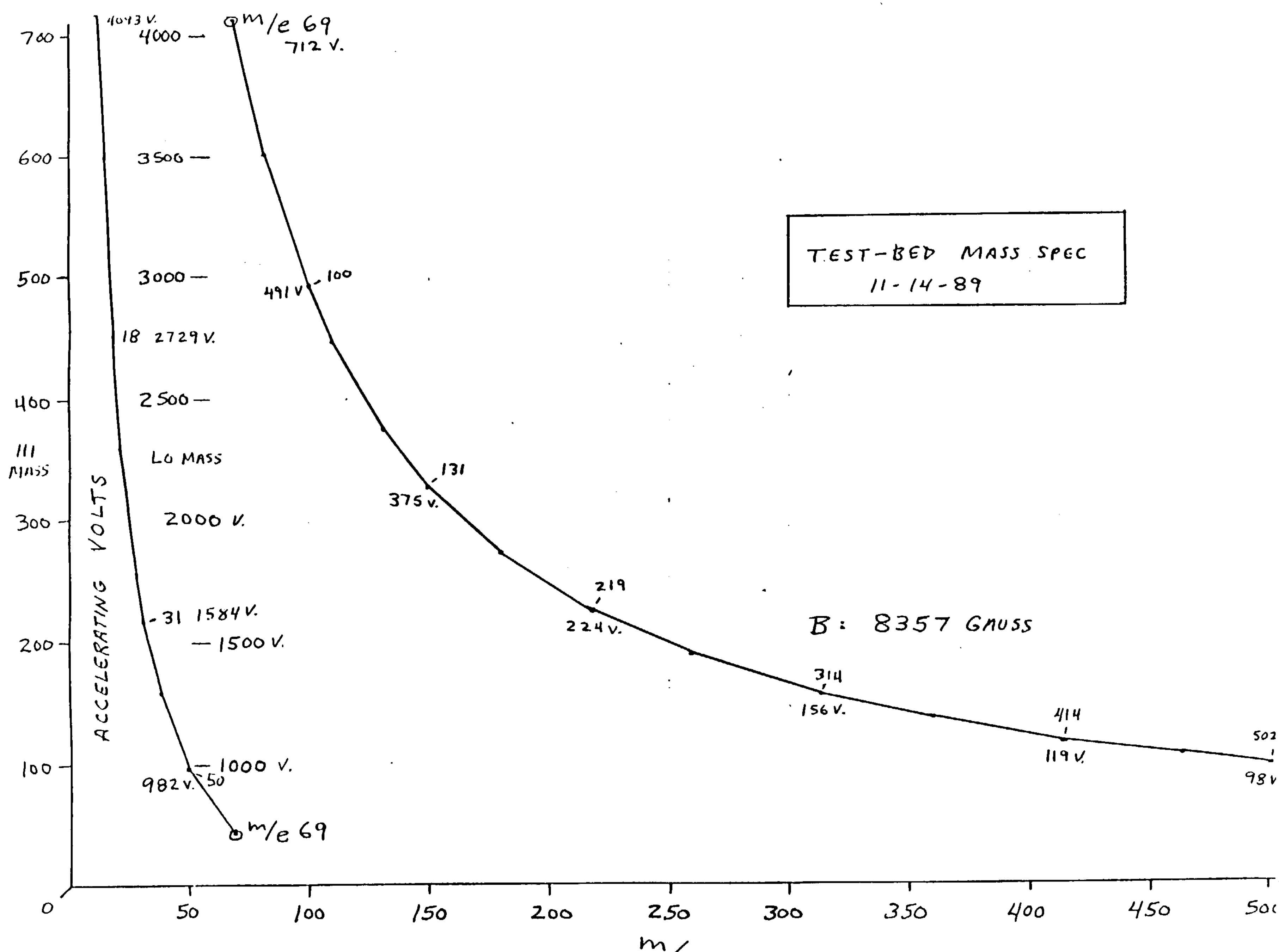
Based upon this theoretical analysis, measurements were made of the magnets that were available to use in the project. These magnets were only partially charged, and before being used in a system had measured fields in the air gap between the magnet pole faces of 5 to 5.5 kilogauss. As will be discussed later in the section on hardware design and development, magnets with both a large, 17 mm gap, and a narrow, 5 mm gap, were used in the project.

The magnets were of Alnico V-7, and their predicted saturation field is indicated as being in the vicinity of 12 kgauss. In practice, for a magnet of this size, fields of 8+ kgauss are about what can be achieved on a continuous basis. Figure 4 shows the relationship between accelerating voltage and mass-to-charge values for one of the initial magnets used in the project, with a field of 8357 gauss. Note that the voltage scale is split, so that values below 700 volts can be shown in greater detail. Note also that for this magnet the accelerating voltage of 250 V that was earlier cited as the approximate lower boundary in order to retain good resolution in the system corresponds to an m/z of slightly over 219 amu. Figure 5 shows how dramatically this practical upper mass limit for the MS changes with increasing magnetic field strengths. This demonstrates that with the latest magnetic materials it will be possible to fabricate a magnet that would have sufficient field strength to yield a mass range for the MS that would cover all of the compounds of interest to NASA.

3. FIRST STAGE MS DESIGN

One of the key requirements for the system was a first stage MS that would have well resolved peaks so that a specific parent ion could be selected for subsequent fragmentation. As pointed out in the phase I work on this project, the EB configuration MS that Viking was developing independently as a potential commercial product appeared to be well-suited as the first stage MS for a tandem system. For this reason, we devoted some effort to understanding the system design parameters of such an EB system and applying them to the tandem design. The work that Viking had already done on a method for mounting and alignment of the various components of he system appeared to be adaptable to a tandem design directly without significant modification. This meant that the configuration of the tandem would start with a rigid mounting plate, machined to provide an accurate reference plane for all components. Figures 6, 7 and 8 show drawings of that plate as it evolved through several stages of development, showing the various feed-throughs for signals and potentials, the different size flight tubes for the ions as they pass through the magnetic sector, corresponding to the two different magnet gaps, the alignment pins for key components, the vacuum envelope for the electric sector, etc.

The challenge of establishing an appropriate mounting for the electric sector resulted in development of one of the new innovations that were produced under this contract. As eventually implemented, the two electric sector plates, after they are machined and polished, are clamped with their desired spacing established (with a machined gauge block) and positioned on a machined flat plate that has an accurately positioned set of locating pins. These pins serve to place the electric sector plates in the proper position with respect to the ion source. With the electric sector elements properly positioned, a series of holes is bored through the elements and the mounting plate to which they are clamped, as shown in Figures 9 and 10.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111 MASS
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3000
18 2729 V.
2500
LO MASS
2000 V.
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1500 V.
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982 V.
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414
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98 V

Figure 4

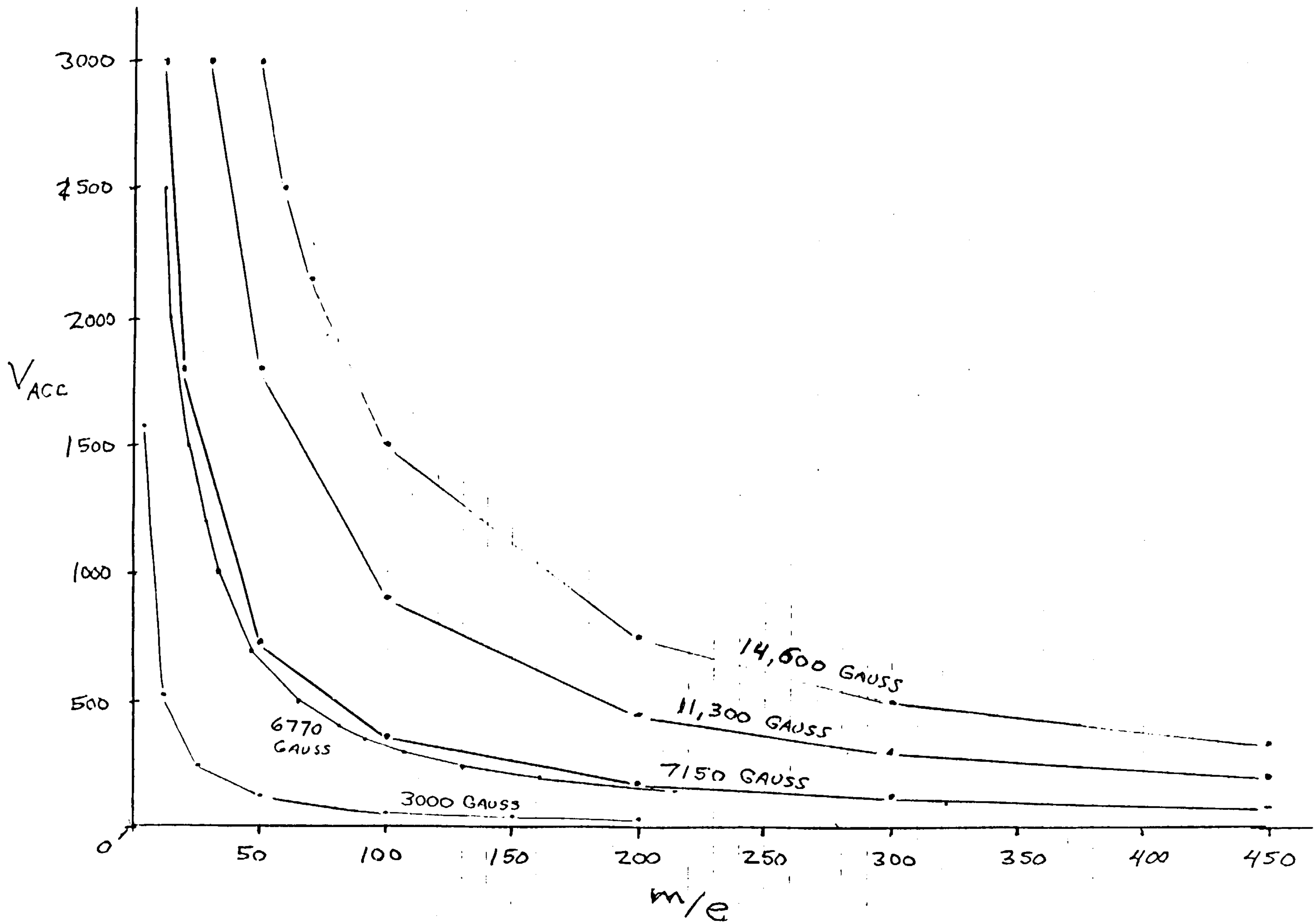

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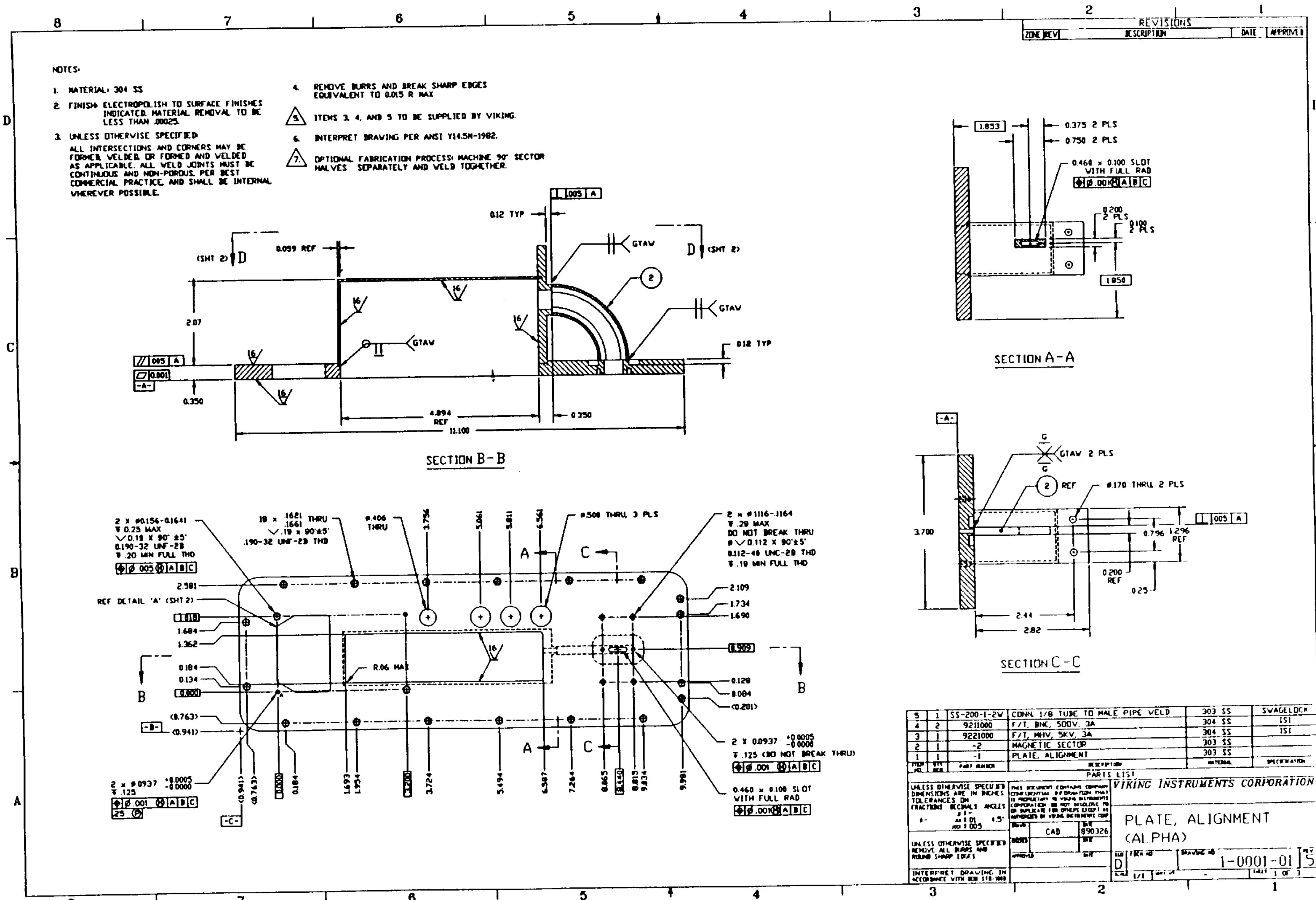
Figure 5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3. UNLESS OTHERWISE SPECIFIED: ALL INTERSECTIONS AND CORNERS MAY BE FORMED, WELDED, OR FORMED AND WELDED AS APPLICABLE. ALL WELD JOINTS MUST BE CONTINUOUS AND NON-POROUS, PER BEST COMMERCIAL PRACTICE AND SHALL BE INTERNAL WHEREVER POSSIBLE.
4. REMOVE BURRS AND BREAK SHARP EDGES EQUIVALENT TO 0.015 R MAX
5. ITEMS 3, 4, AND 5 TO BE SUPPLIED BY VIKING.
6. INTERPRET DRAWING PER ANSI Y14.5M-1982.
7. OPTIONAL FABRICATION PROCESS: MACHINE 90° SECTOR HALVES SEPARATELY AND WELD TOGETHER.
SECTION B-B
SECTION A-A
SECTION C-C
REVISIONS
ZONE REV DESCRIPTION DATE APPROVED
5 1 SS-200-1-2W CONN. 1/8 TUBE TO MALE PIPE WELD 303 SS SWAGELOCK
4 2 9211000 F/T, BNC, 500V, 3A 304 SS ISI
3 1 9221000 F/T, MHV, 5KV, 3A 304 SS ISI
2 1 -2 MAGNETIC SECTOR 303 SS
1 1 -1 PLATE, ALIGNMENT 303 SS
PARTS LIST
VIKING INSTRUMENTS CORPORATION
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1 OF 3

Figure 6

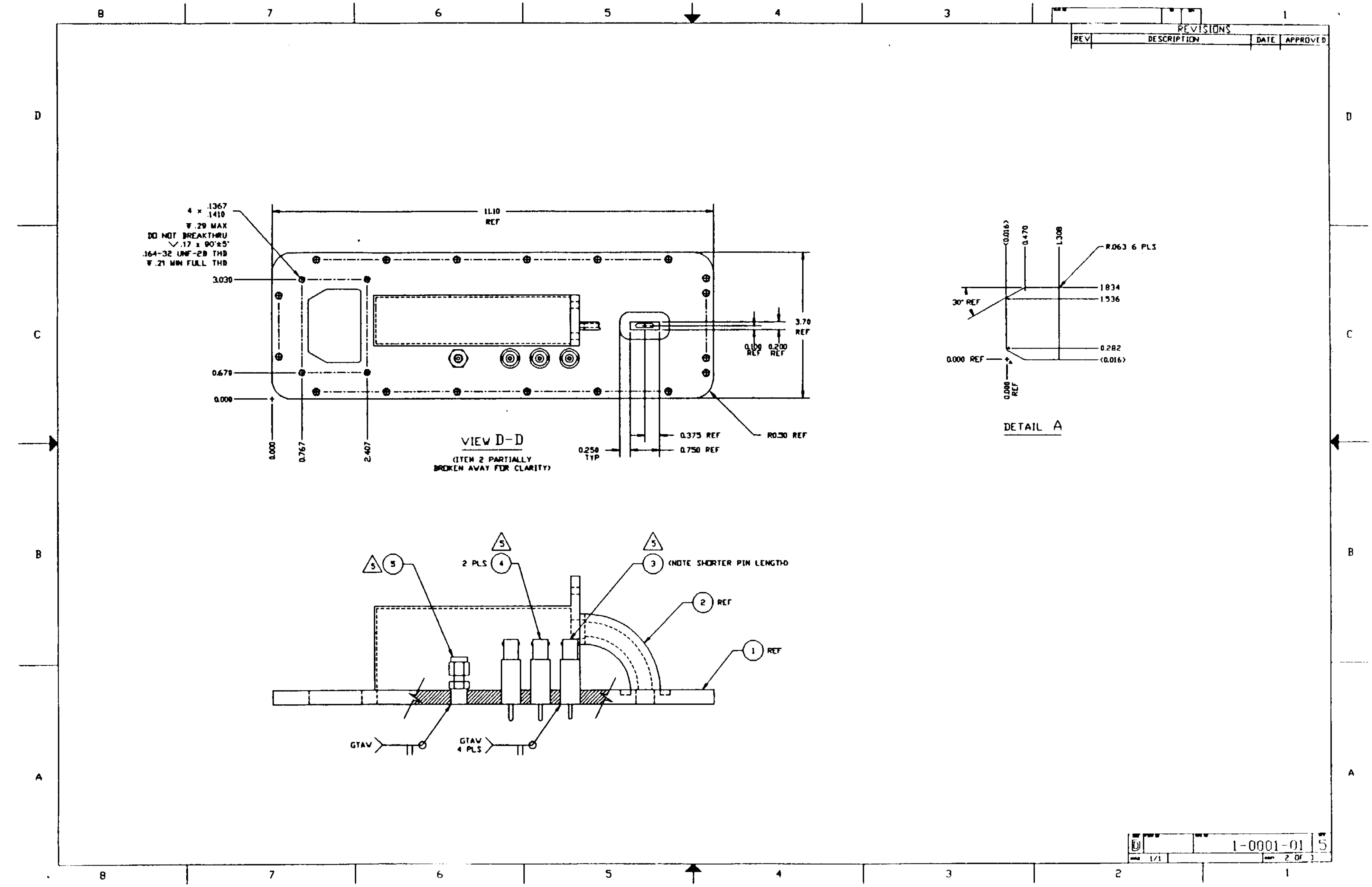

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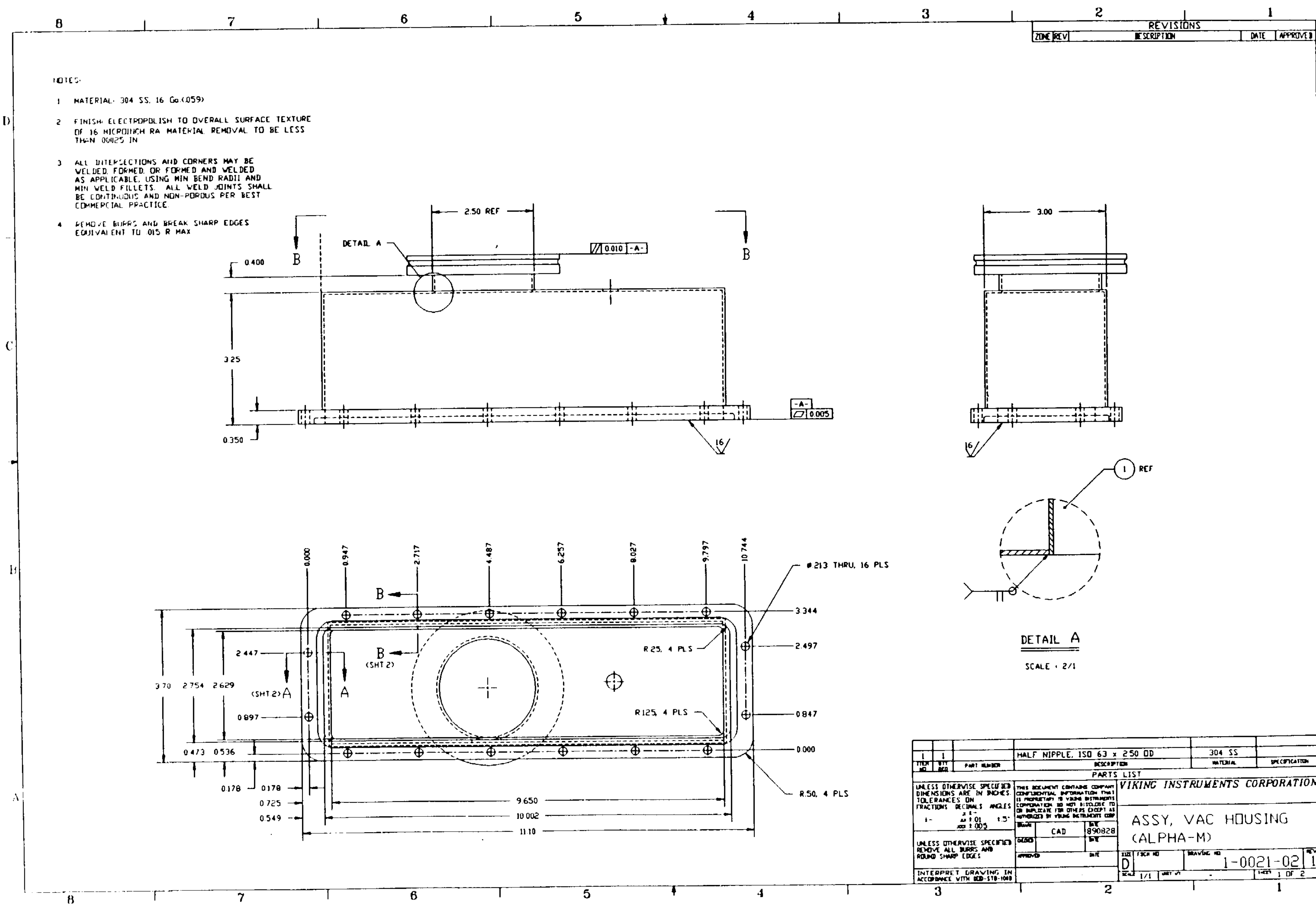
Figure 7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NOTES:
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3 ALL INTERSECTIONS AND CORNERS MAY BE WELDED, FORMED, OR FORMED AND WELDED AS APPLICABLE, USING MIN BEND RADII AND MIN WELD FILLETS. ALL WELD JOINTS SHALL BE CONTINUOUS AND NON-POROUS PER BEST COMMERCIAL PRACTICE.
4 REMOVE BURRS AND BREAK SHARP EDGES EQUIVALENT TO .015 R MAX
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-A-
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DETAIL A
SCALE : 2/1
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R.25, 4 PLS
R.125, 4 PLS
R.50, 4 PLS
(SHT 2)
HALF NIPPLE, ISO 63 x 2.50 OD
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PARTS LIST
VIKING INSTRUMENTS CORPORATION
ASSY, VAC HOUSING
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1 OF 2
UNLESS OTHERWISE SPECIFIED DIMENSIONS ARE IN INCHES. TOLERANCES ON FRACTIONS DECIMALS ANGLES
UNLESS OTHERWISE SPECIFIED REMOVE ALL BURRS AND ROUND SHARP EDGES
INTERPRET DRAWING IN ACCORDANCE WITH DOD-STD-100

Figure 8

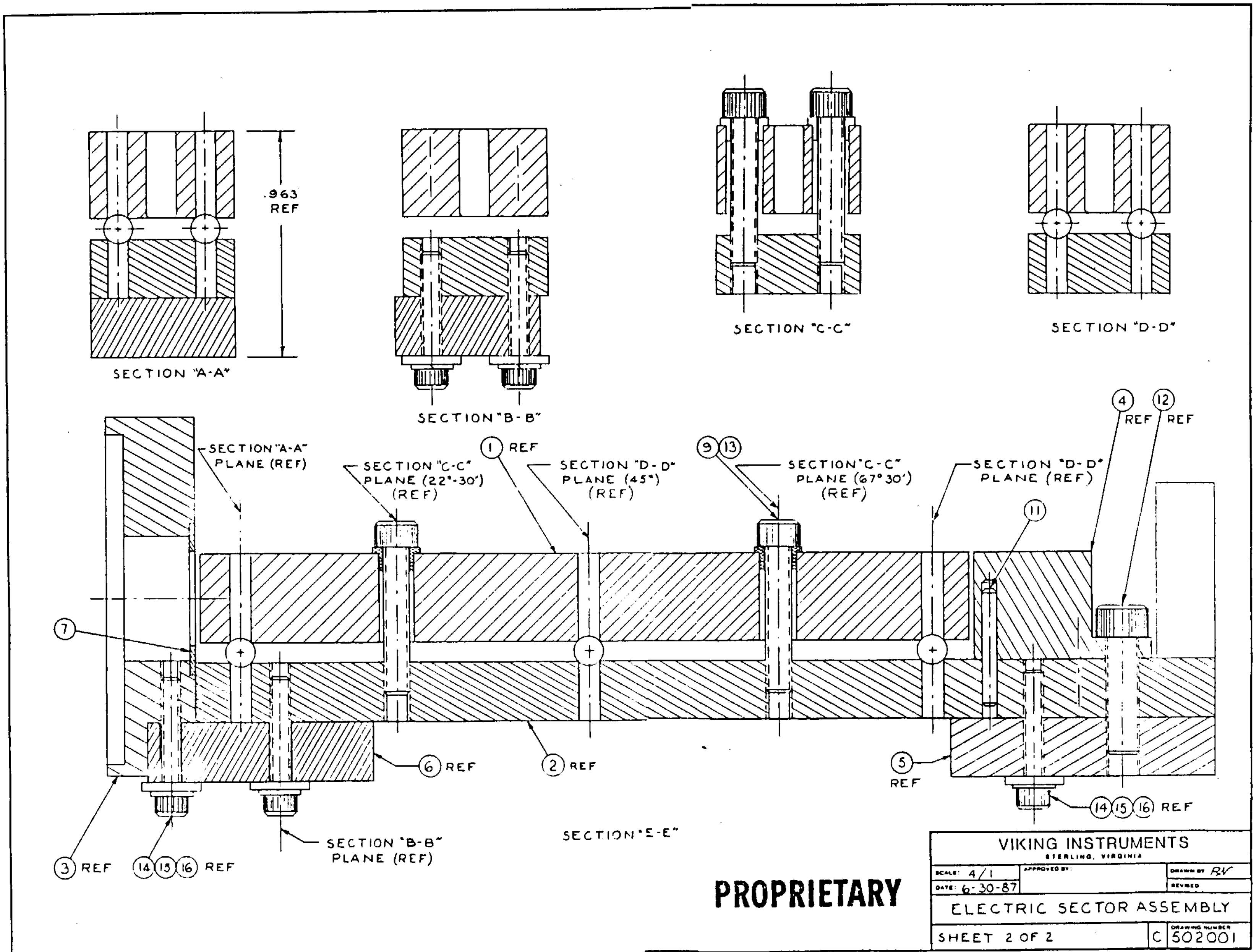
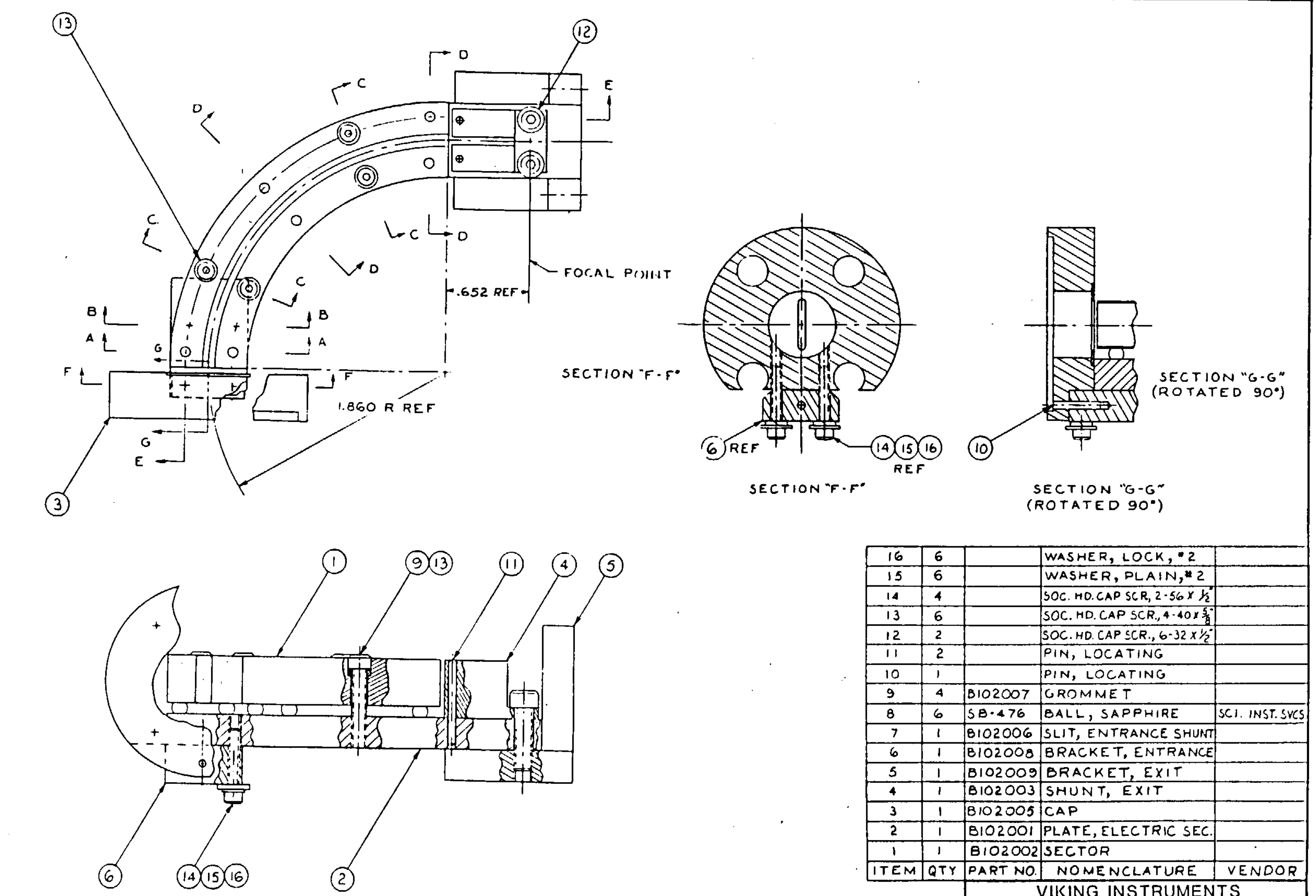

SECTION "A-A"
.963 REF
SECTION "B-B"
SECTION "C-C"
SECTION "D-D"
4 REF
12 REF
SECTION "A-A" PLANE (REF)
SECTION "C-C" PLANE (22°-30') (REF)
1 REF
SECTION "D-D" PLANE (45°) (REF)
9 13
SECTION "C-C" PLANE (67°30') (REF)
SECTION "D-D" PLANE (REF)
11
7
6 REF
2 REF
5 REF
14 15 16 REF
3 REF
14 15 16 REF
SECTION "B-B" PLANE (REF)
SECTION "E-E"
PROPRIETARY
VIKING INSTRUMENTS
STERLING, VIRGINIA
SCALE: 4/1
DATE: 6-30-87
APPROVED BY:
DRAWN BY RV
REVISED
ELECTRIC SECTOR ASSEMBLY
SHEET 2 OF 2
DRAWING NUMBER
C 502001

Figure 9



ITEM	QTY	PART NO.	NOMENCLATURE	VENDOR
16	6		WASHER, LOCK, #2	
15	6		WASHER, PLAIN, #2	
14	4		SOC. HD. CAP SCR, 2-56 X 1/2"	
13	6		SOC. HD. CAP SCR., 4-40 X 5/8"	
12	2		SOC. HD. CAP SCR., 6-32 X 1/2"	
11	2		PIN, LOCATING	
10	1		PIN, LOCATING	
9	4	B102007	GROMMET	
8	6	SB-476	BALL, SAPPHIRE	SCI. INST. SVCS
7	1	B102006	SLIT, ENTRANCE SHUNT	
6	1	B102008	BRACKET, ENTRANCE	
5	1	B102009	BRACKET, EXIT	
4	1	B102003	SHUNT, EXIT	
3	1	B102005	CAP	
2	1	B102001	PLATE, ELECTRIC SEC.	
1	1	B102002	SECTOR	

VIKING INSTRUMENTS
STERLING, VIRGINIA

SCALE: 2/1 | APPROVED BY: | DRAWN BY RN
DATE: 6-30-87 | REVISED

ELECTRIC SECTOR ASSEMBLY

SHEET 1 OF 2 | C | DRAWING NUMBER 502001

PROPRIETARY

Figure 10

The diameter of the holes is chosen so that it is about 25% smaller than the diameter of a set of ruby spheres that are used as spacers in three of the holes positioned so that there is one hole at each end of the electric sector section and one in the middle. Two of the holes in the mounting plate are tapped for screws which pass through the sector and are insulated from it by an insert made of vespel or Macor or some other suitable insulating material that has little or no vapor pressure. By placing a ruby sphere in each of the locating holes and then holding the electric sector segments tightly against the mounting plate with the two screws, the sector segments will automatically be positioned in three dimensions and insulated from each other and the support plate. This mounting method permits rapid assembly yet insures that all elements are properly aligned.

An additional feature of the electric sector design is the incorporation of fringing field corrections, or Herzog shunts, at both the entrance and the exit of the electric sector. Because of space limitations of the geometry of the EB system, the entrance uses a thin shunt and the exit, a thick shunt. These have the effect of reducing the focusing effects of the fringing fields that would otherwise bulge out of the gap between the electric sector plates and thus, counteract the aberrations that would otherwise be incurred at these points.

4. ION SOURCE DESIGN

One of the most important components of the tandem MS system is the ion source. Source design is particularly critical for an instrument with a fixed magnetic field, since the scan of ions with differing mass-to-charge ratios is accomplished by varying the accelerating potential of the ions exiting the source while simultaneously and proportionally varying the strength of the electric field in the electric sector. The control of electric sector potentials is normally accomplished by tying the electric sector to the source voltages through a resistor network. A key aspect of the source is that it be able to take ions of widely differing masses, extract them from the ionizing region and accelerate them while focusing them into a well collimated beam. This beam is then directed through the electric and magnetic sectors to the detector slit and detector where the resolution of the system must be such that ions of about unitary mass difference can be discriminated. The resolution of a mass spectrometer is most often defined as:

$$R = m / \Delta m \qquad \text{(II-7)}$$

where Δm is the closest separation of adjacent mass peaks when they overlap by no more than 10% at the valley between the two peaks. For a magnetic sector instrument, this resolution is a constant over the mass range. Thus, for an instrument to have the ability to discriminate between two adjacent masses at the upper end of the desired mass scale for which it is designed, it must have a resolution equal to, or better than this high mass value. That is, an instrument intended for an upper limit of 300 amu must have a resolution of 300 to be of practical value. From this relationship, it can also be seen that the mass peaks will be better resolved at the lower mass end of the spectrum, with the spacing between adjacent masses gradually decreasing until they begin to overlap significantly beyond the point at which the resolution number equals the mass. A number of factors influence the resolution, among then are slit widths, manufacturing and assembly tolerances, ion source design, effects of fringing fields and any second order or higher order corrections that may have been made, operating vacuum, etc. It was our task as system designers to reduce each of these contributions and still keep the system complexity within practical bounds. The starting point for this process is with the source itself. It must function to give a well-defined ion beam over the mass range of interest and produce enough ion current so that it is possible to detect the daughter ions, which at best are about 1 to 2% of the incident ion beam intensity.

The ion source for this system has gone through many iterations. An example of one of the early model sources is shown in Figures 11 through 14. This source provided a reasonably intense ion beam and was used to verify the alignment of the elements of MS I and determine the operating characteristics of the MS. The source had a dual repeller configuration that allowed a certain amount of "steering" of the ion beam to allow for variability in source elements and internal alignment of the source. Through testing with this source, it was determined that such steering did not result in appreciably better ion currents so it was dropped in later models to avoid excessive complexity. One key approach was followed in assembling these designs- the system should be as simple as possible for ease in fabrication, assembly and maintenance, yet be able to do its job. Following this approach, if it was determined that a single lens properly configured could replace what might normally require two lenses, we would choose the single lens as the preferred solution.

In the process of testing MS I with the early ion sources, it became clear that a more efficient source with better extraction characteristics for a wider set of ion masses would be desirable. We then conducted a more detailed literature search for reports of various lens combinations that had been tried by researchers in the field to determine if a suitable configuration might already have been tried. We were unable to find such a source design but we did uncover work by Matsuda, et. al.[1], that provided additional insight into an approach that would improve the source performance.

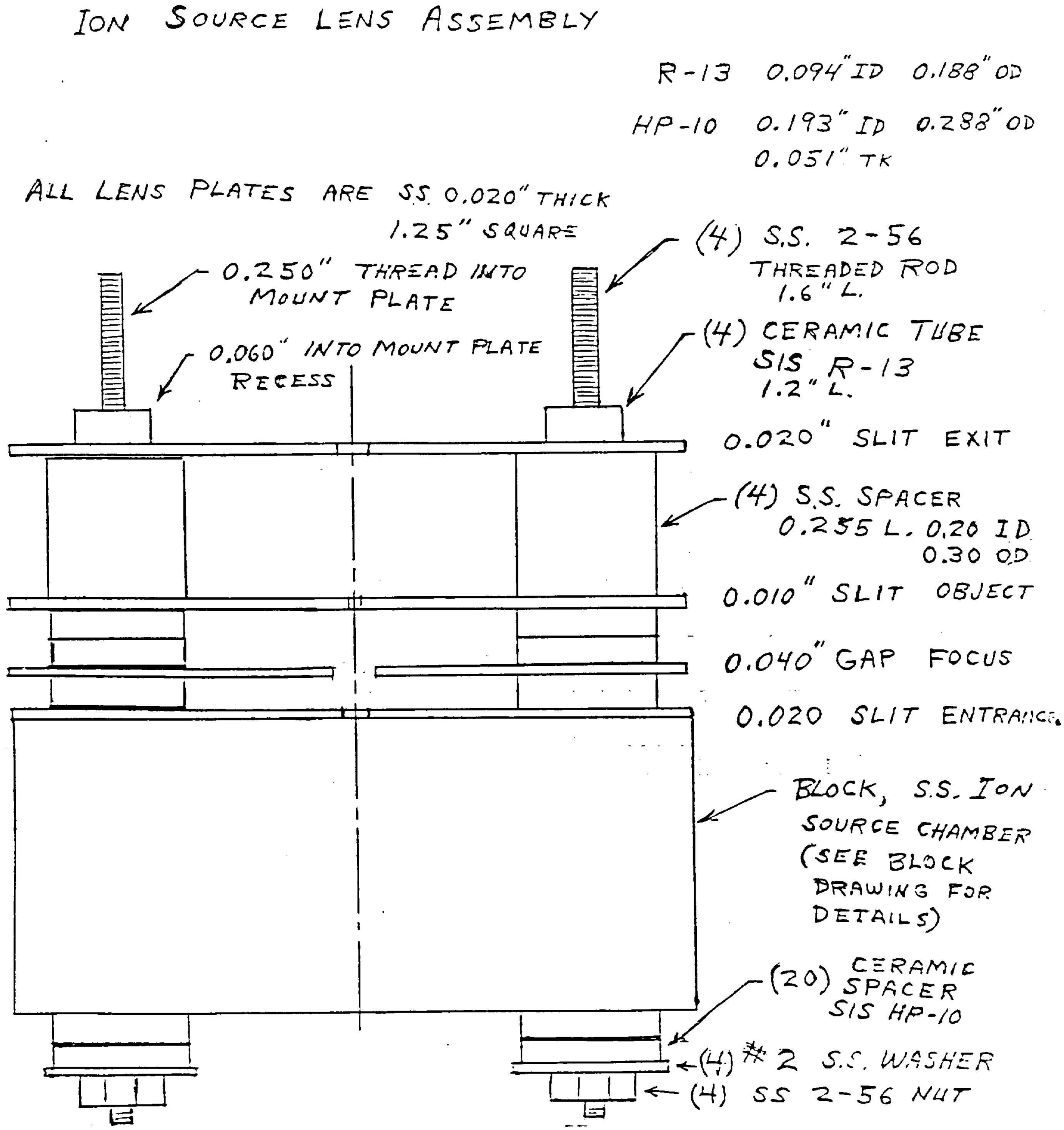
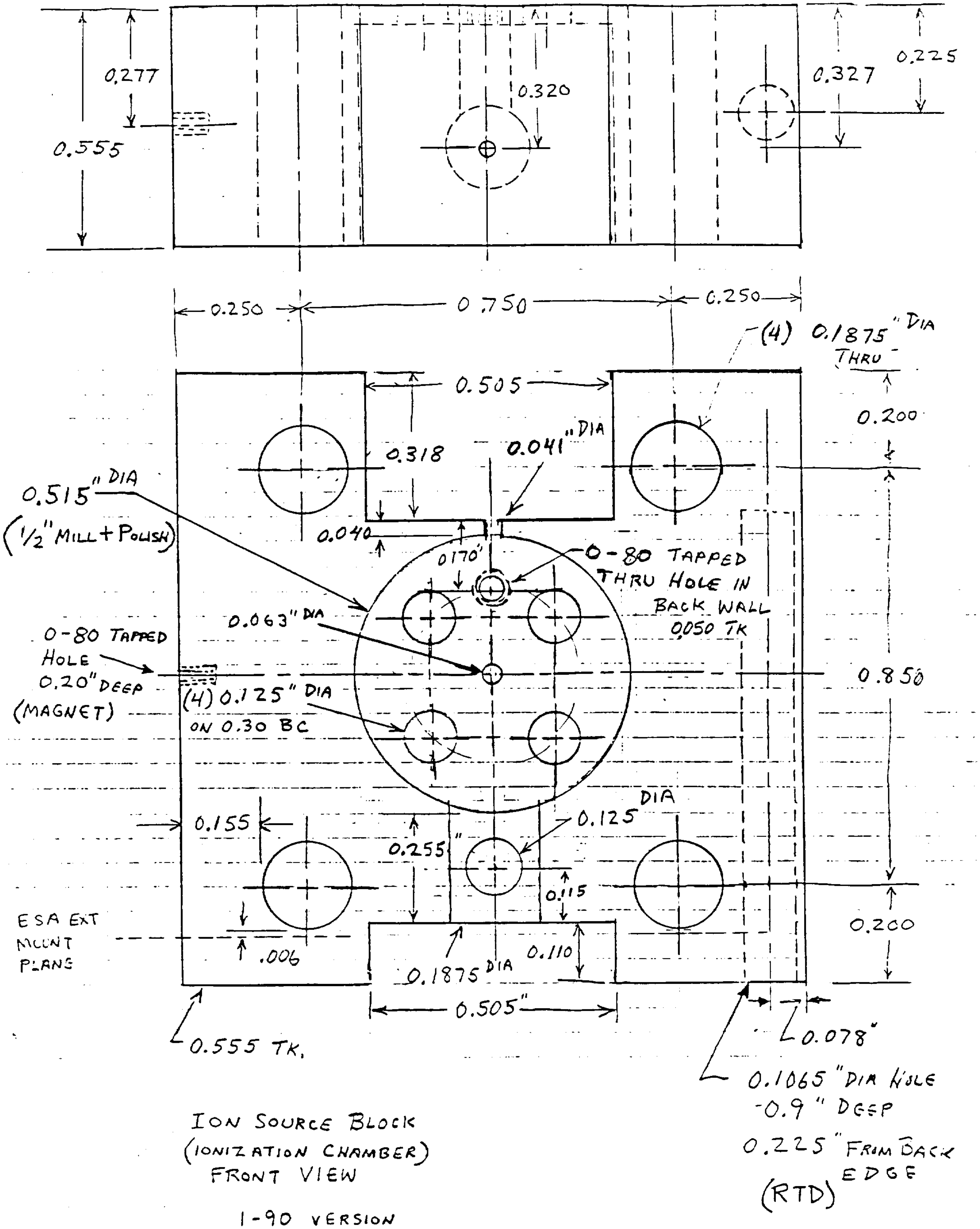

ION SOURCE LENS ASSEMBLY
R-13 0.094" ID 0.188" OD
HP-10 0.193" ID 0.288" OD
0.051" TK
ALL LENS PLATES ARE SS 0.020" THICK
1.25" SQUARE
0.250" THREAD INTO MOUNT PLATE
(4) S.S. 2-56 THREADED ROD 1.6" L.
0.060" INTO MOUNT PLATE RECESS
(4) CERAMIC TUBE SIS R-13 1.2" L.
0.020" SLIT EXIT
(4) S.S. SPACER 0.255 L. 0.20 ID 0.30 OD
0.010" SLIT OBJECT
0.040" GAP FOCUS
0.020 SLIT ENTRANCE
BLOCK, S.S. ION SOURCE CHAMBER (SEE BLOCK DRAWING FOR DETAILS)
(20) CERAMIC SPACER SIS HP-10
(4) #2 S.S. WASHER
(4) SS 2-56 NUT

Figure 11



0.277
0.555
0.320
0.327
0.225
0.250
0.750
0.250
(4) 0.1875" DIA THRU
0.505
0.200
0.318
0.041" DIA
0.515" DIA
(1/2" MILL + POLISH)
0.040
0170'
0-80 TAPPED THRU HOLE IN BACK WALL 0.050 TK
0.063" DIA
0-80 TAPPED HOLE 0.20" DEEP (MAGNET)
(4) 0.125" DIA ON 0.30 BC
0.850
0.155
0.255"
0.125 DIA
0.115
ESA EXT MOUNT PLANE
.006
0.110
0.1875 DIA
0.200
0.505"
0.555 TK.
0.078"
0.1065" DIA HOLE -0.9" DEEP 0.225" FROM BACK EDGE (RTD)
ION SOURCE BLOCK (IONIZATION CHAMBER) FRONT VIEW
1-90 VERSION

Figure 12

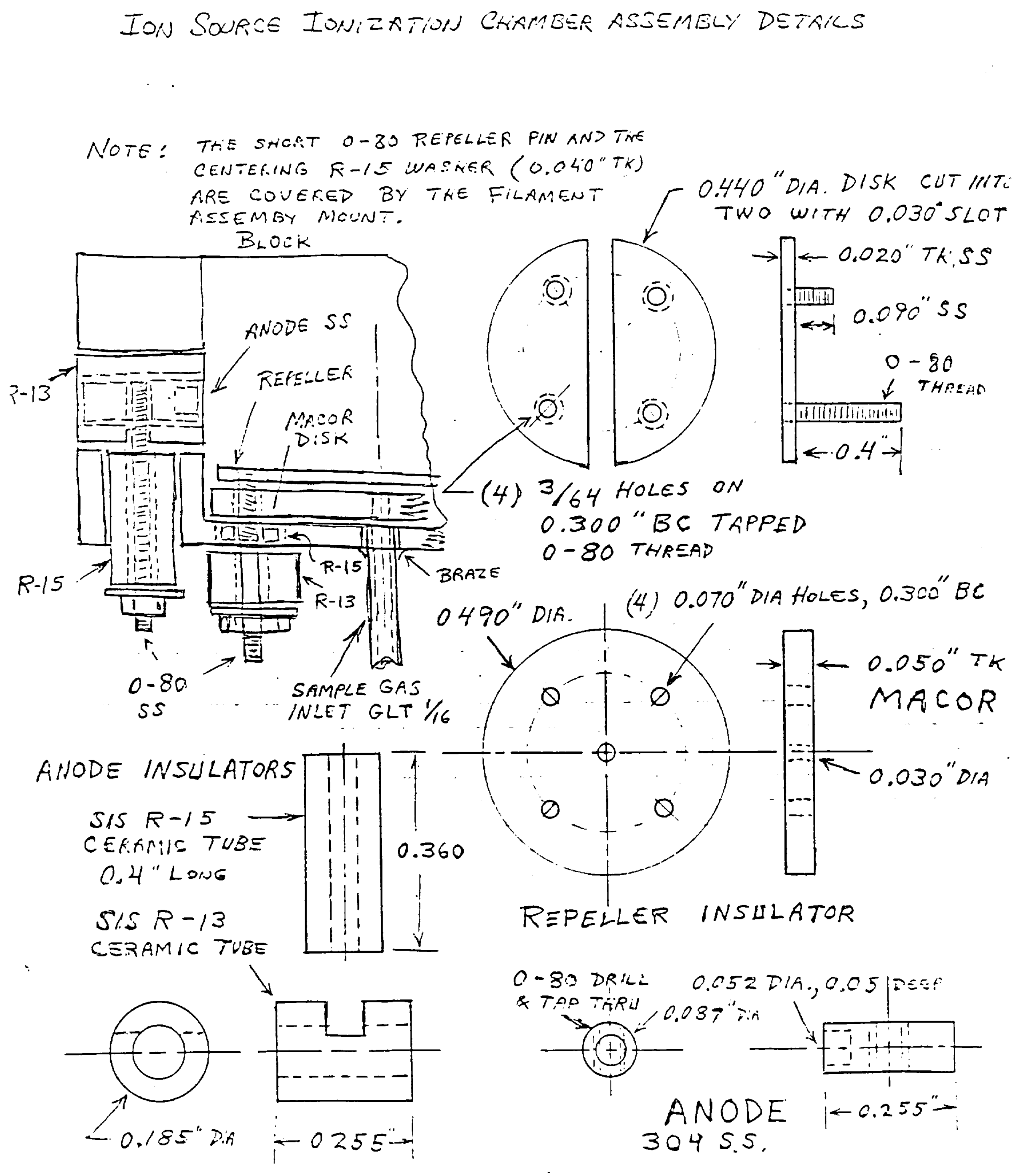

ION SOURCE IONIZATION CHAMBER ASSEMBLY DETAILS
NOTE: THE SHORT 0-80 REPELLER PIN AND THE CENTERING R-15 WASHER (0.040" TK) ARE COVERED BY THE FILAMENT ASSEMBY MOUNT.
BLOCK
ANODE SS
REPELLER
MACOR DISK
R-13
R-15
R-15
R-13
BRAZE
0-80 SS
SAMPLE GAS INLET GLT 1/16
0.440" DIA. DISK CUT INTO TWO WITH 0.030" SLOT
0.020" TK. SS
0.090" SS
0-80 THREAD
0.4"
(4) 3/64 HOLES ON 0.300" BC TAPPED 0-80 THREAD
0490" DIA.
(4) 0.070" DIA HOLES, 0.300" BC
0.050" TK
MACOR
0.030" DIA
REPELLER INSULATOR
ANODE INSULATORS
S/S R-15 CERAMIC TUBE 0.4" LONG
0.360
S/S R-13 CERAMIC TUBE
0.185" DIA
0255
0-80 DRILL & TAP THRU
0.087" DIA
0.052 DIA., 0.05 DEEP
ANODE 304 S.S.
0.255"

Figure 13

MAGNETIC MOUNTING BRACKET

1 MATERIAL .015 CRES

2 MATERIAL .002 CRES

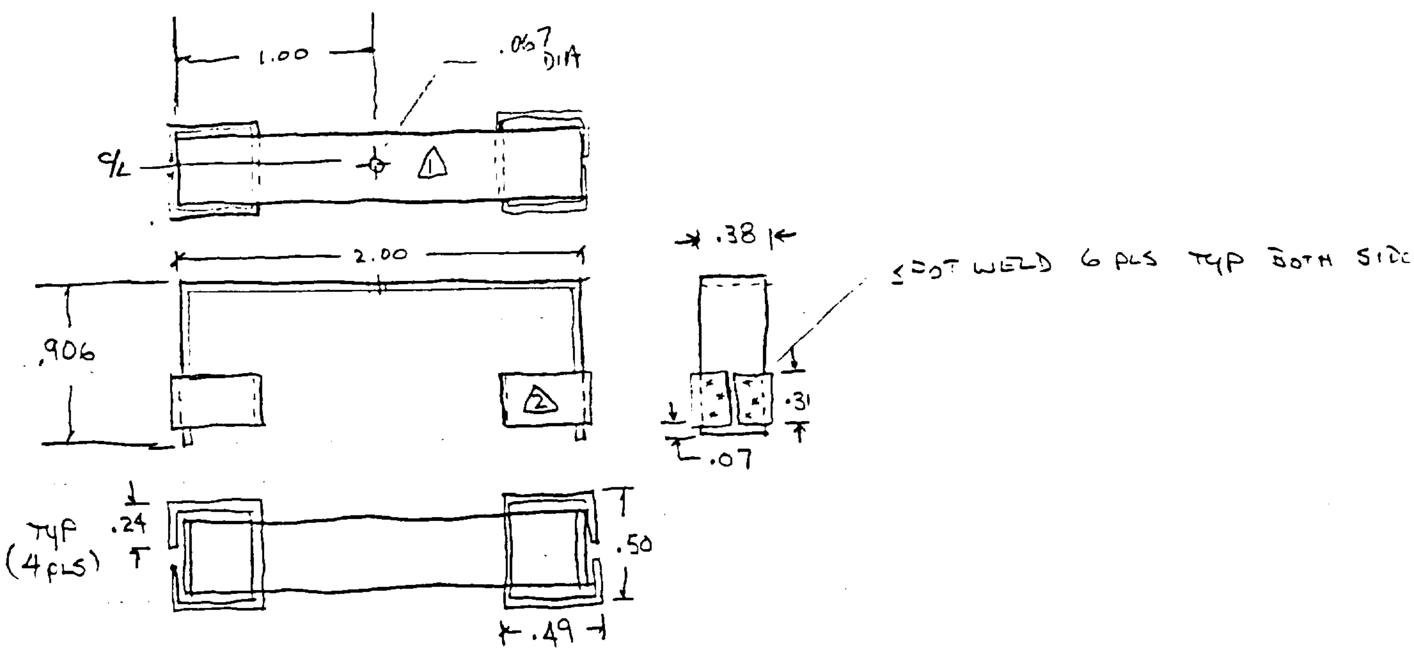


Figure 14

Beginning with the basic source configuration used in the Viking Mars Lander system as a reference point, a set of alternative ion source designs were modeled using the ion optics and trajectory program "SIMION".[2] This program calculates the trajectories of positively or negatively charged ions in electric or magnetic fields based upon the shape of the elements that are used to create the fields or other description of the fields. The program is dynamic, that is, it can account for varying potentials while the ions are traversing the fields and can locate the ions in time at various points, given a start time. The program is also capable of drawing the equipotential lines from a lens configuration, so it is an invaluable tool to the designer of systems that involve charged particles and fields. It permitted us to consider a number of possible configurations and evaluate them quickly rather than depend upon very rough static calculations that would be a much poorer approximation of actual system performance. To illustrate the very powerful, yet highly utilitarian functionality of SIMION, Figures 15 through 18 show ion trajectory plots of ions originating at the ionization region of the Viking source, with the lens combination in its original configuration, for ions of 57, 95, 143 and 382 amu. Note that some of the higher mass ions do not exit the source but are intercepted by the lens array, thereby reducing the total ion current in the resulting ion beam. In this system, the ion source makes use of a shaped repeller which aids in focusing the extracted ions prior to exiting the ionization chamber region. In the final form of the ion source that was developed for this system, the modeling shows improved performance, as illustrated in Figures 19 through 22. Here, we have added a cylindrical lens extension, shown in cross-section. With this addition, it can be seen that the ions formed in the ionization chamber and extracted by the same initial lens system are now all passed through the accelerating and collimating lenses, giving more total ion current for a particular mass. This source was fabricated and is included as part of the experimental prototype system.

5. DETECTOR

For the detector in this system, we felt there was a need to break away from the bulky and easily contaminated discrete dynode electron multiplier and, instead, use a smaller and much more rugged ceramic, continuous dynode detector. We chose a relatively new product from K and M Electronics, Inc., the Model TX-7505, the performance characteristics of which are shown in Figure 23. We incorporated this model detector into the experimental configuration at two places, since it was so compact, so that we could monitor the output from MS I as a conventional double-focusing instrument and also monitor the output of the second electric sector, MS II. The detector was operated with a post-detection acceleration potential to optimize detector performance at the higher masses.

VIKING LENS500D.PA0 57 u 500 V BLOCK

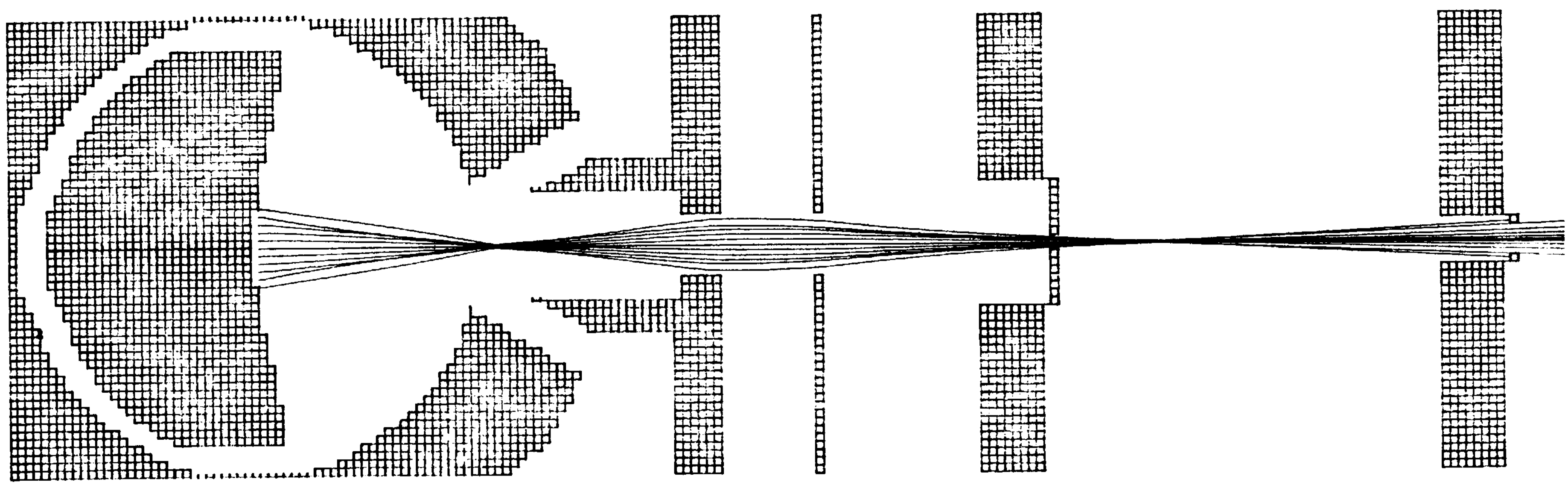


Figure 15

VIKING LENS500D.PA0 95 u 300 V BLOCK

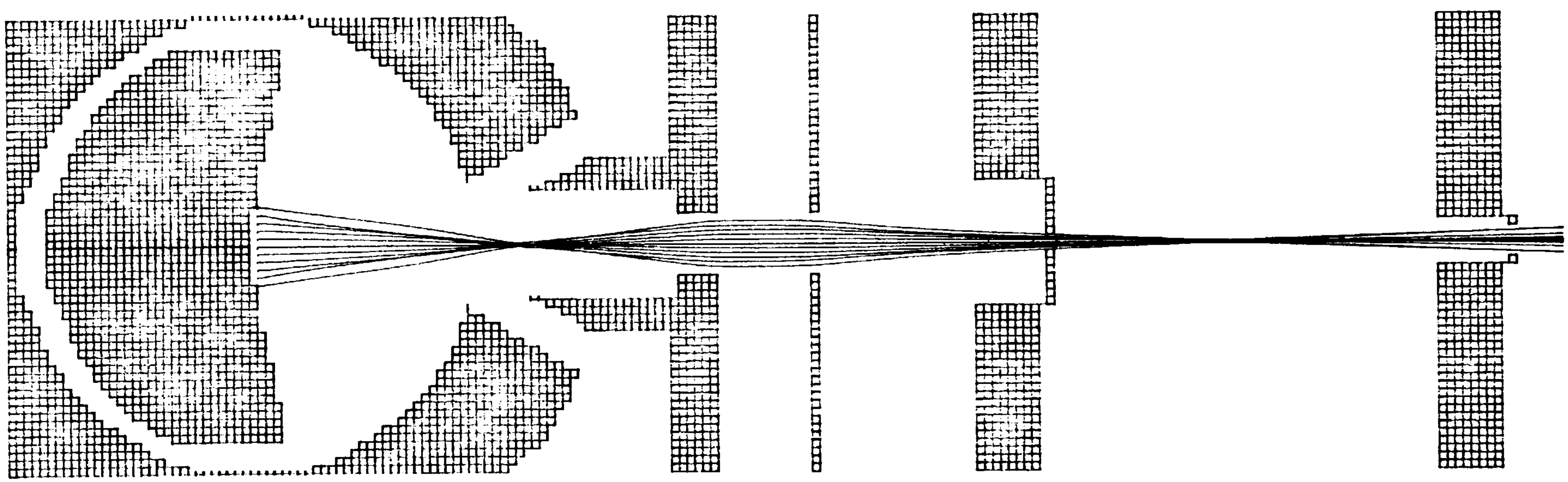


Figure 16

VIKING LENS500D.PA0 143 u 200 V BLOCK

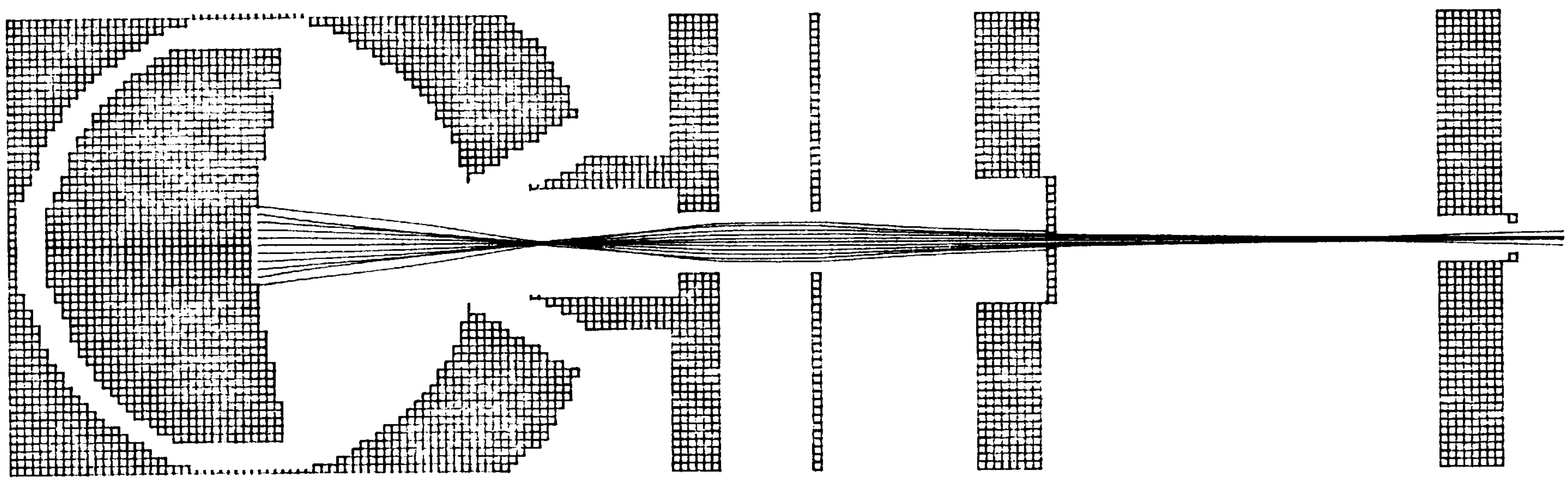


Figure 17

VIKING LENS500D.PA0 382 u 75 V BLOCK

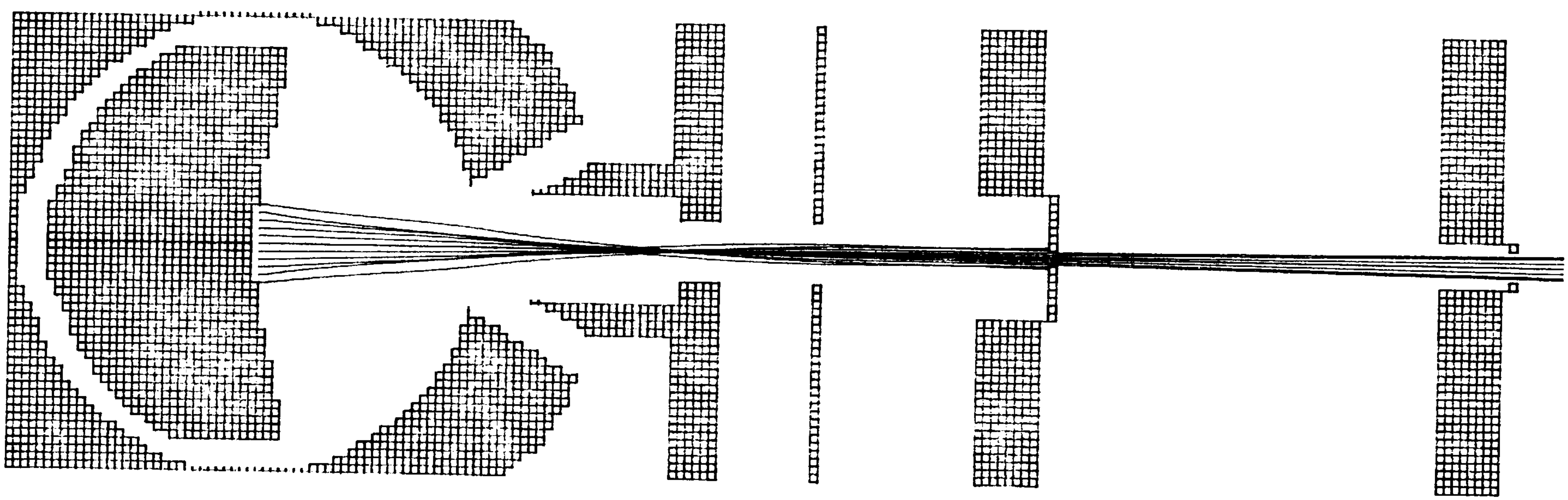


Figure 18

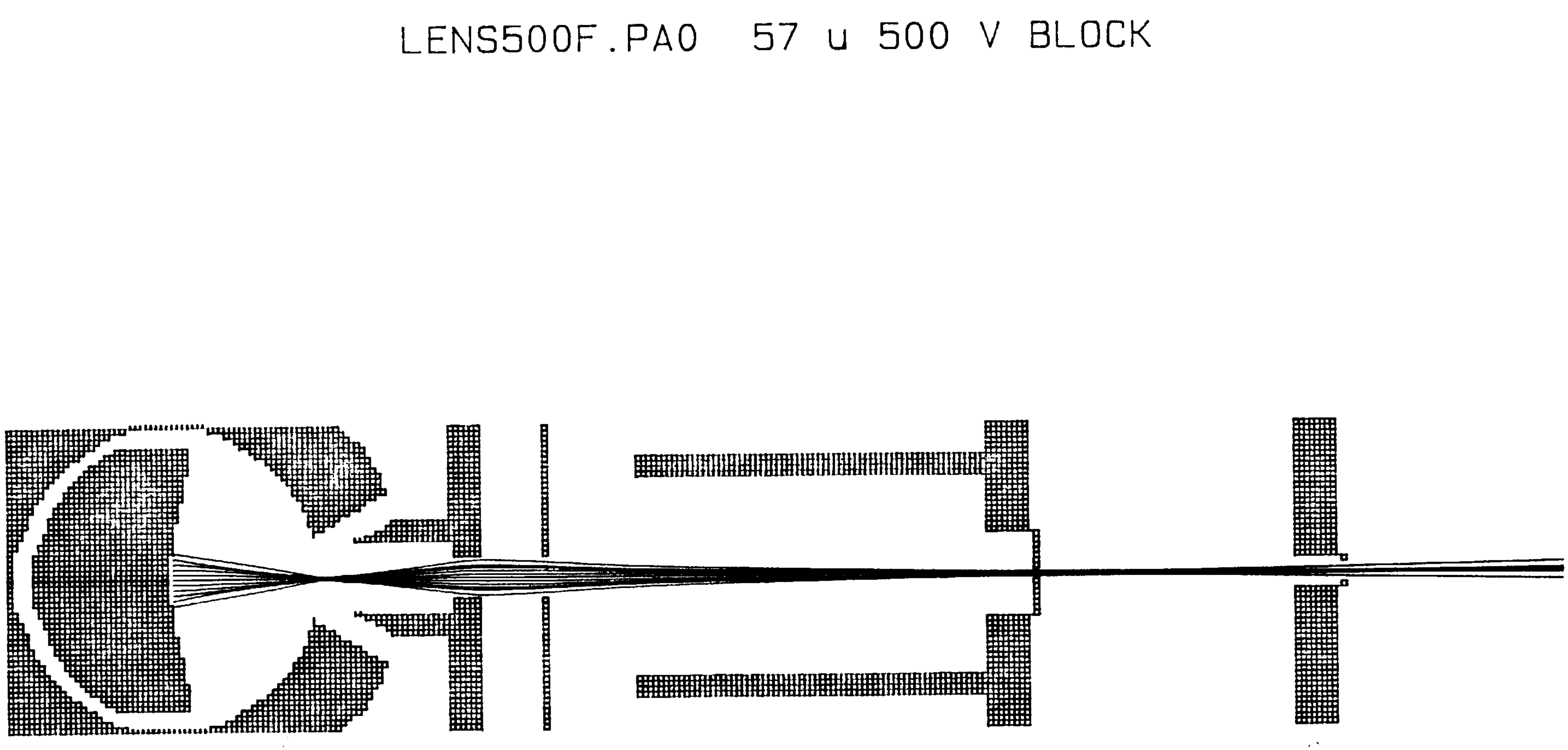


Figure 19

LENS500F.PA0 95 u 300 V BLOCK

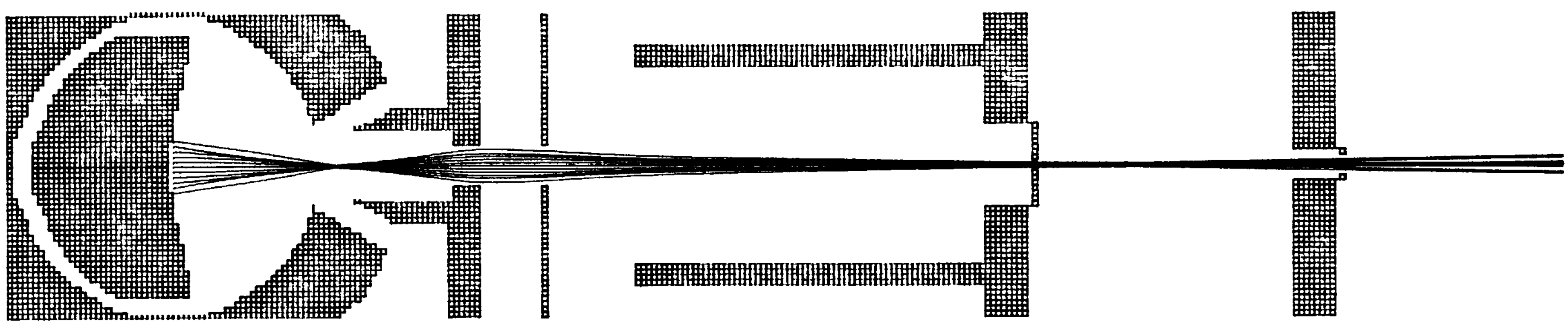


Figure 20

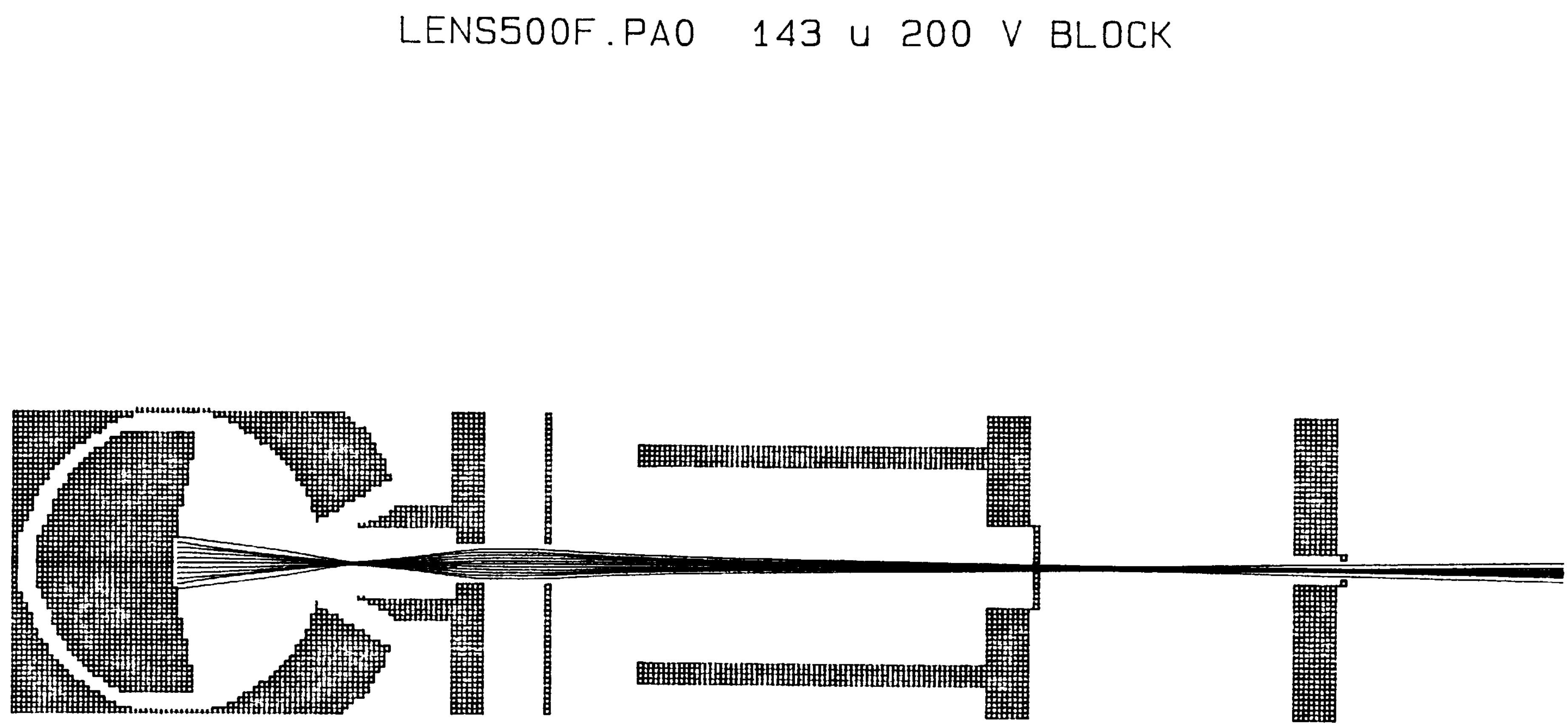


Figure 21

LENS500F.PA0 382 u 75 V BLOCK

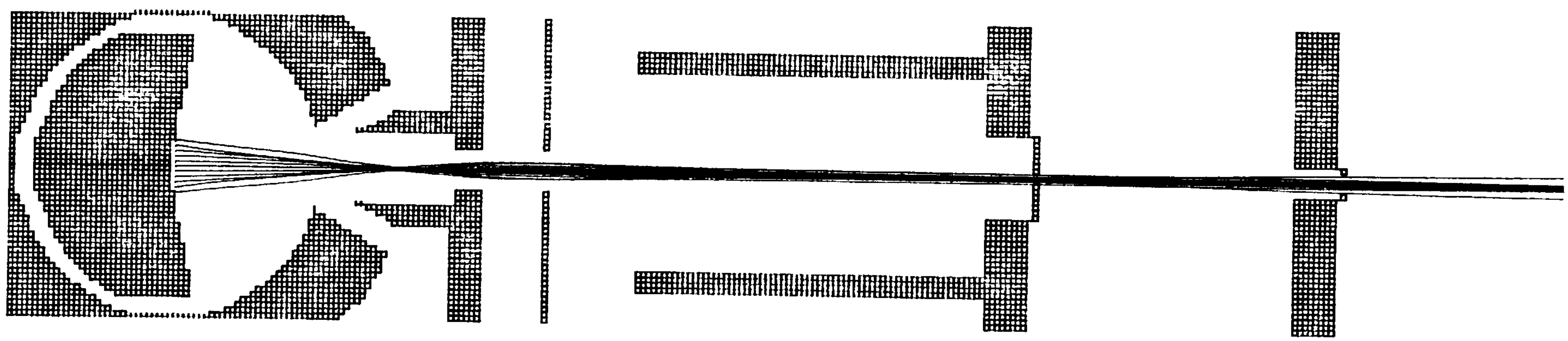


Figure 22

KAND M ELECTRONICS, INC.
1988

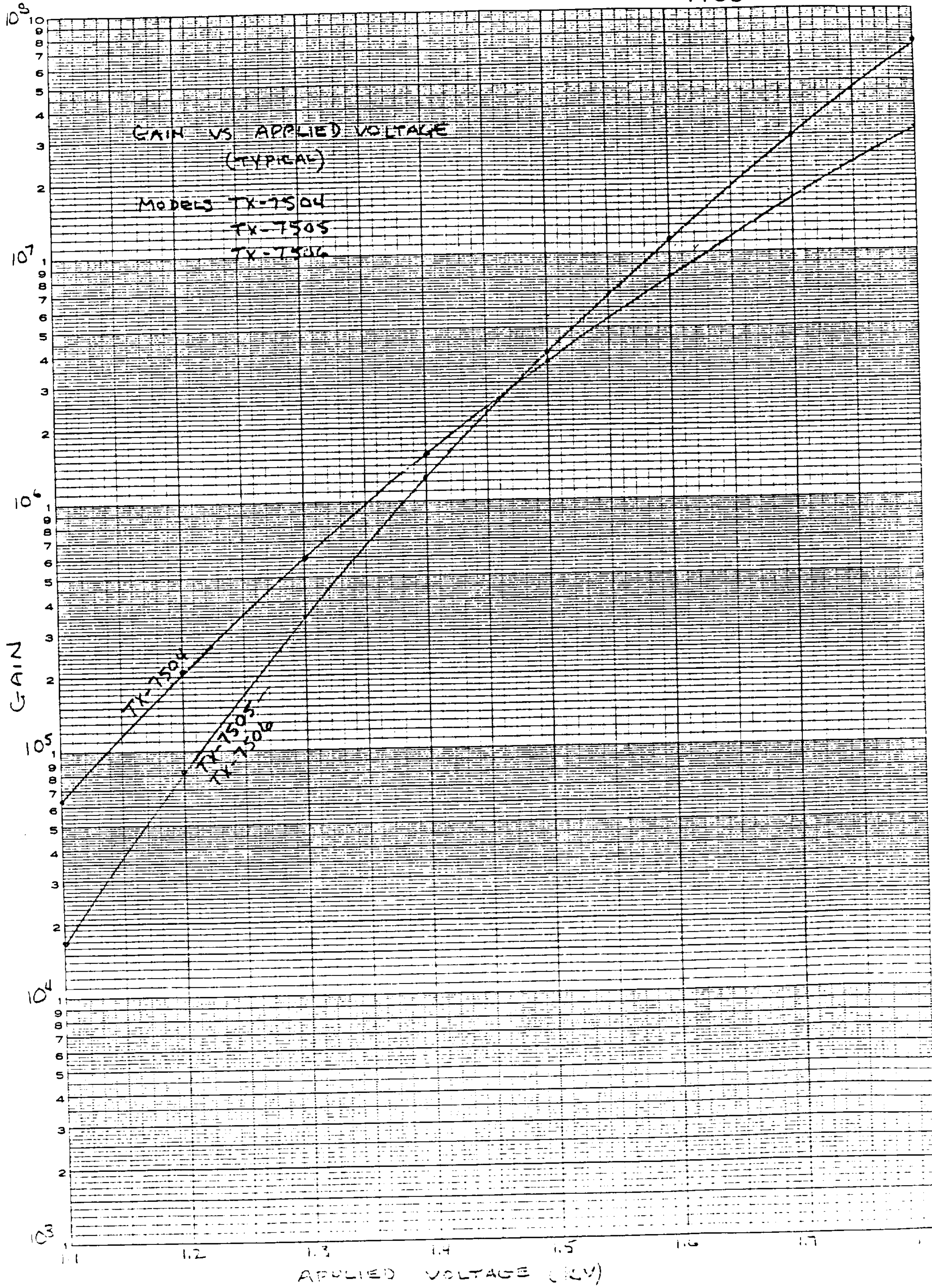


Figure 23

6. THE GC, SAMPLE COLLECTION, AND CONCENTRATION SYSTEM DESIGN

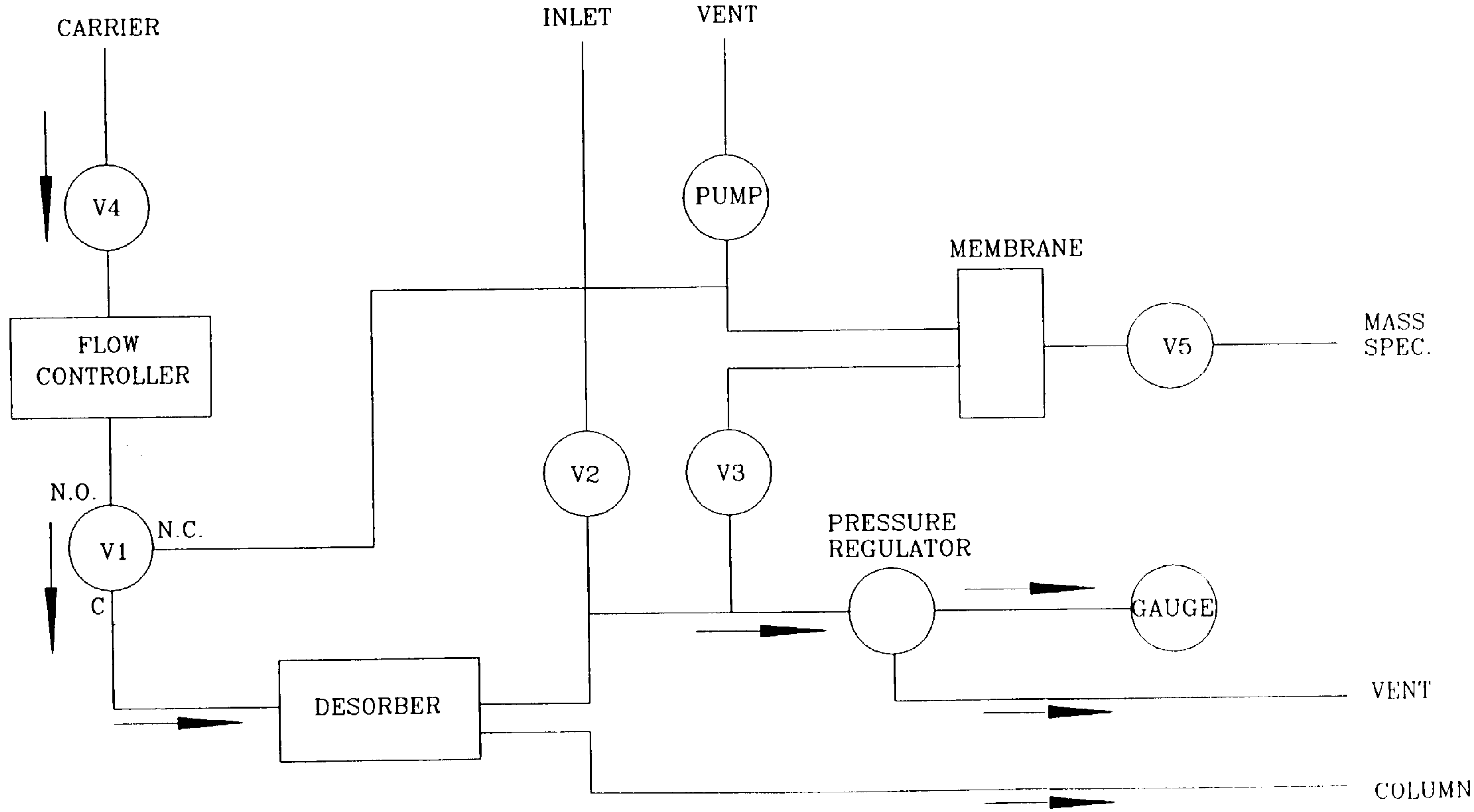
In addition to the work on the MS configuration and the several subsystems within the MS, considerable effort was required to define and, based upon tests and analysis, further refine the elements of the sample concentration and gas chromatograph subsystems. Briefly, the role of these subsystems is to draw a sample of the atmosphere collected from some distant point into the instrument, either route this sample directly to the tandem MS for analysis or concentrate the sample on a trapping medium and then thermally desorb the sample from the trap either to the MS or via the GC column to the MS. These optional pathways are needed because many of the compounds that need to be detected will be sufficiently dilute in the ambient atmosphere that they cannot easily be detected. For these ultra-trace detections, it is possible to draw a large volume of air through the trap, and thereby concentrate the sample on the sorbant material. By rapidly heating the trap, the sample can be desorbed in a relatively tight plug of sample molecules that can either be routed to the MS for analysis or sent through the GC column for separation and then to the MS for analysis.

The diagram of the system that was developed to route the sample properly through the various configurations to give the operator these options is shown in Figure 24. The various pathways can be traced in the following description of the basic operating cycles for this tandem MS:

1. DIRECT MS. In order to draw a sample directly into the MS, first the sample line valve, V2, is opened, V3 is opened and the sample pump is turned on. Opening V5 will then permit the sample to diffuse through the membrane to the MS.

2. SAMPLE CONCENTRATION MS. In order to perform this operation, first the sample is loaded onto the desorber cartridge by opening V2, energizing V1, thereby opening its normally closed pathway to the pump, and turning the sample pump on. After the cartridge is loaded, V2 is closed and V1 is de-energized, V4 is opened and V3 is opened, while the pump is left on. This permits the flow of carrier gas to pass through the desorber and over the membrane. This is normally called "cold flow" and purges the oxygen from the desorber. The MS valve, V5 can be open or closed during this time. After cold flow, the desorber is rapidly heated to a selected temperature with the valves remaining as set, thereby driving the sample off the sorbant medium in the trap and over the membrane where, with V5 open, it will diffuse into the MS.

GC BLOCK DIAGRAM



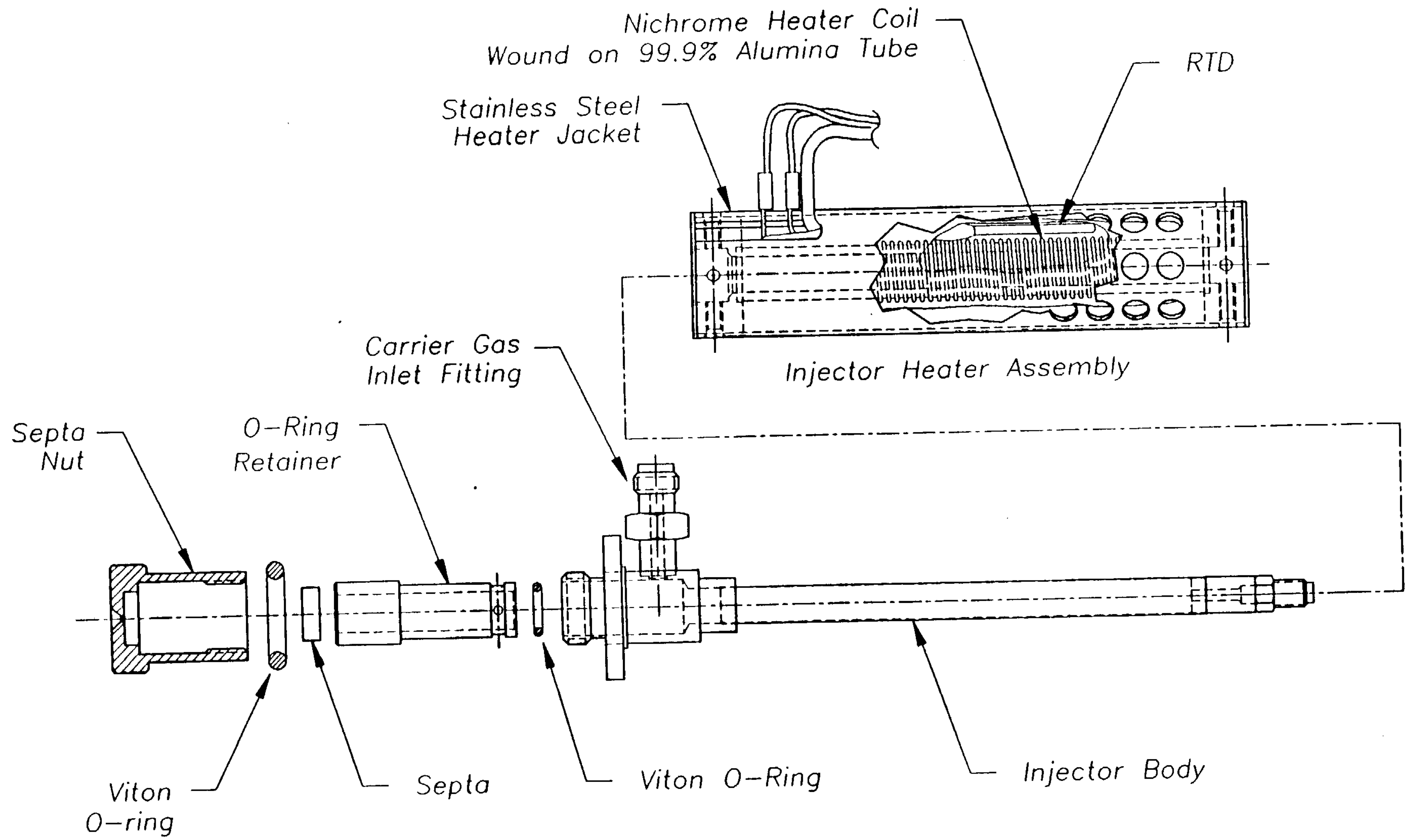
DESORB CARTRIDGE (To Column)

Figure 24

3. SAMPLE CONCENTRATION GC/MS. In order to perform this operation, the cartridge in the desorber is loaded as in cycle 2, above. After cold flow, however V3 will be closed and the pump turned off. With V3 closed, the flow of carrier gas will pressurize the region between V1 and the GC column to the pressure set by the operator on the pressure regulator. This pressure is set to optimize the flow of carrier gas through the GC column in order to obtain the best separation from the column. When the system is pressurized, the desorber is heated rapidly to drive off the sample which flows with the carrier gas into the GC column where normal separation in time takes place. The output of the column is entered directly into the MS for analysis.

The design of the desorber and the dual inlet system, with both membrane and GC column connections, were important steps that made possible the compact, yet efficient sample collection and concentration system. The desorber has gone through a number of iterations before reaching its present form. The current design provides a leak-tight, yet easily removable sealing mechanism, an internal seal between the cartridge and the gas-tight envelope for the desorber that ensures that gas flow is through the cartridge, not around it, a thin-walled envelope that heats with little or no time lag, and a special heater assembly providing rapid ballistic heating, better than 300°C/min. The design of the desorber allows easy replacement of the cartridge, if necessary, and accepts standard 6 mm by 115 mm glass or metal cartridges. A cross-section of the desorber is shown in Figure 25.

The membrane interface to the MS also represents an important milestone that enables this package to perform sensitive direct atmospheric sampling. Although membrane inlets to MS systems are not unknown, they were originally conceived as a method for interfacing the outlet of a packed GC column with its rather heavy carrier gas flow to the MS in a way that reduced the pumping load on MS vacuum system. With the development of small capillary GC columns with their associated lower carrier gas flow rates, the technology of membrane inlets became unnecessary in favor of capillary direct connections. For direct atmospheric sampling, however the membrane offers some distinct advantages over the other option, a direct molecular leak. The membrane, with its selective permeability, reduces the concentration of the background gasses such as nitrogen, oxygen, carbon dioxide and argon, while enhancing the relative concentrations of organics and a variety of other compound classes, the specifics of which depend upon the type of membrane material in use. Viking experimented with several configurations before finding a combination that was not only very effective in passing samples into the MS but also made it easy to replace membranes. The solution was the design shown in Figure 26. In this design, the membrane can be replaced simply by removing the four capscrews and disconnecting the sampling lines, which allows direct access to the membrane, the supporting glass frit, the O-rings and the sample entry and exit ports. Note that the sample is drawn onto the membrane surface at its center and exits the membrane along its outer periphery, thus ensuring utilization of as much of the membrane surface as possible.



Injector/Desorber Assembly

Figure 25

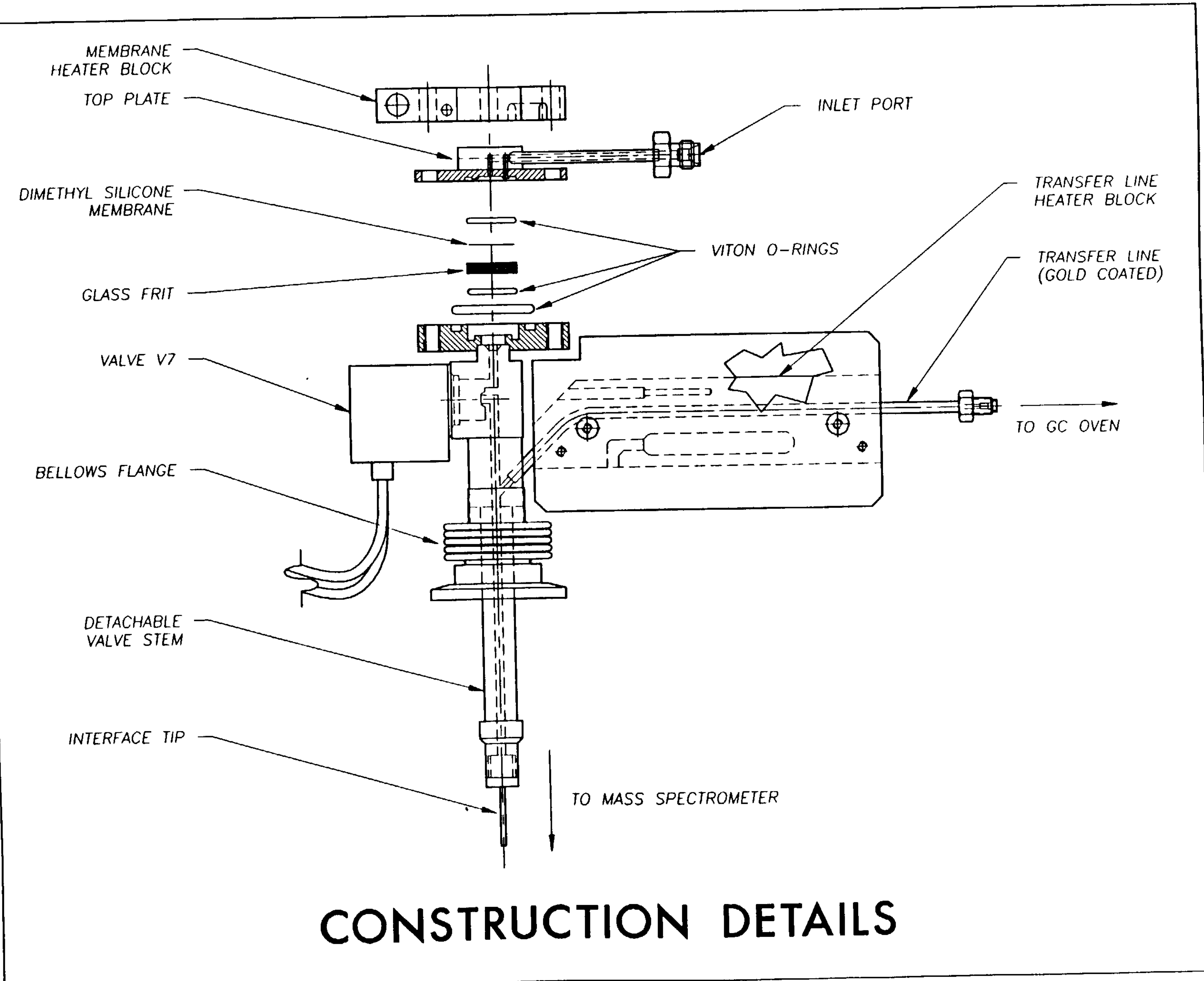

MEMBRANE HEATER BLOCK
TOP PLATE
INLET PORT
DIMETHYL SILICONE MEMBRANE
TRANSFER LINE HEATER BLOCK
VITON O-RINGS
TRANSFER LINE (GOLD COATED)
GLASS FRIT
VALVE V7
TO GC OVEN
BELLOWS FLANGE
DETACHABLE VALVE STEM
INTERFACE TIP
TO MASS SPECTROMETER
CONSTRUCTION DETAILS

Figure 26

The membrane is isolated from the MS by a solenoid valve. This ensures that the MS will not be put out of commission by a leak in the membrane, and permits easy membrane replacement whenever this is necessary. It should be recognized that the membrane material that we have been using is dimethyl silicone, 1 mil, unbacked. It is possible that something that is being sampled may have a deleterious effect upon the membrane, weakening it until a leak develops. Our experience with this material in terrestrial environmental applications has been excellent, but occasional replacement should be considered as part of routine maintenance procedures.

Several other aspects of sampling and then desorbing the sample need to be considered. Our experience has shown that it is important to load a sample onto the cartridge with the gas flow in one direction and then desorb the sample with the carrier gas flowing in the opposite direction. This is because the sample molecules tend to be adsorbed onto the trapping medium in the cartridge preferentially at the first part of the cartridge they encounter. When desorbing this cartridge, if the same direction of flow is maintained, the sample is forced to migrate through the entire cartridge packing, being re-adsorbed and desorbed many times before it emerges, if it emerges at all. This has the effect of degrading the chromatography and making quantitative results less accurate. A second aspect is the use of low-reactivity sample lines in any part of the system seeing sample materials. Viking has developed a technique for gold-plating just the inside of sample lines of nickel-stainless alloy to provide a highly non-reactive surface that has the additional advantage of being able to be heated to high temperatures without outgassing or breaking down and also being able to bend or flex repeatedly without breaking like glass lined tubes. Heating the sample lines is also important to prevent loss of sample on "cold spots" that exist at bends or other constricted flow locations.

B. SUBSYSTEMS FABRICATION, ASSEMBLY AND TEST

The major subsystems of the tandem GC/MS/MS, are: 1) sample acquisition; 2) sample inlet; 3) GC; 4) vacuum envelope; 5) MS-I; 6) MS-II; and 7) supporting electronics and software. Each of these subsystems will be treated separately in the following sections. It should be obvious that a highly integrated system such as a spacecraft instrument with the capabilities of the tandem GC/MS/MS will require careful attention to the interfaces between the subsystems as well as operation of the subsystems themselves. Where these interface questions are particularly significant, they will be included.

1. SAMPLE ACQUISITION

The sampling system must be capable of drawing in a selected amount of the atmosphere or other gaseous material at a sufficient rate to provide adequate sample flow across the membrane interface or through the adsorbing medium in the concentrator cartridge. Experimentally, we determined that standard sampling pumps such as those commonly used for occupational health and safety purposes (SKC or MSA sampling pumps, for example) would not be adequate for the purpose. This was primarily because of the backpressure that is developed when attempting to pull a sample through a packed adsorbant cartridge. Since it was not desirable to reduce the packing density in the cartridge to make it easier for the pump to operate because of the possible loss of sample, we looked into the prospect of using a larger capacity pump. A larger pump would have the advantage that it could handle a wide variation in packing density in various alternative cartridges that may be used, and in addition would be able to draw samples from distant locations via narrow sample lines without augmentation. We settled on a motor driven piston pump with diaphragm valves from KNF Neuberger. This pump has a nominal pumping rate of 5 L/min, and can pump against a backpressure of better than 30 psi. It runs on 24 Volts, as do all of the electrically operated components in the sampling and GC subsystems.

The pump is connected to the sampling subsystem in such a way that the gas flow passes through the pump last. This is for two reasons: 1) if the sample passes through the pump before it is trapped or flows over the membrane certain trace constituents could be lost on the internal surfaces, valves, etc of the pump, and 2) the pump may introduce contamination into the system from pump lubrication and previous sample runs that have adsorbed on valve surfaces. This arrangement also permits the outlet of the pump to be connected to an additional trap such as activated charcoal so that any residual toxic vapors that may be sampled from a contaminated area would not be released into another spacecraft space that was otherwise free of contamination.

The other major component of the sampling subsystem is the desorber unit. This has been described, at least in part, previously. The desorber must fulfill the role of trap and also be capable of rapid heating to drive off adsorbed materials for further analysis. The desorber must contain a sorbant medium for trapping the desired constituents of the gaseous material being sampled. It was determined that it would be most desirable if the trapping medium could be in a removable cartridge, so that various media could be used interchangeably, and so that contaminated media could be replaced when necessary. The cartridge that was chosen after some evaluation of alternatives was a standard glass tube, 6 mm O.D. and 4 mm I.D. , 11.5 cm long, with a glass frit at one end. This cartridge is then housed in a gas-tight envelope that must be capable of easy opening to permit cartridge changes. Considerable experimentation was conducted on various configurations for this component. Early efforts used a special spring-backed O-ring to seal each end of the enclosed cartridge in a double O-ring package with removable cap. This version had a tendency to leak, particularly after a number of cartridge exchanges and desorption runs have been made. Eventually we arrived at the current configuration which permits easy access to the cartridge but keeps a tight seal through many opening and closing cycles. The wall of this assembly is made of very thin stainless which is silver soldered into fittings at each end. The tube is sized such that it is a good fit around the glass cartridge and thus provides good thermal contact with it. The stainless tube assembly is then encased by a ceramic tube chosen for its excellent heat transmission properties, upon which is wound a heater coil with a resistance of about 4 ohms providing about 150 watts when energized. The heater coil is cemented on the ceramic tube with a high temperature ceramic epoxy material together with an RTD temperature sensor. This entire assembly is enclosed by a protective aluminum shield, with about 1/4 inch air gap around the heater coil. The shield is perforated with a series of holes to permit rapid cooling of the system to ambient temperatures after a desorber run so that the cartridge can be used again to adsorb sample.

The remaining components of the sampling system consist of solenoid operated valves to control the various pathways during sampling, sample tubing and fittings, a sample inlet quick-disconnect, and if appropriate for the environment being sampled, a particulate filter. These include relatively standard Swagelock-type fittings and standard 1/8 inch, nickel-stainless, chromatographic grade tubing.

2. SAMPLE INLET

This dual inlet system has also been described previously. In the process of developing this subsystem, considerable difficulty was encountered in maintaining a leaktight interface to the MS because of the difficulty in soldering the various components together and maintaining their tolerances. A technique for producing the membrane support and the valve body plus connecting tubing to the ion source from a single piece of stainless was developed that has proven effective and provides a much improved vacuum seal. The valve used is a high pressure ASCO solenoid valve with demountable plunger and seal. This dual interface assembly also has a transfer line connected to the body of the assembly which allows the capillary column to be inserted and guided to the entrance of the ion source. This transfer line provides a vacuum seal for the column and external heating using an aluminum block in which a 50 watt cartridge heater is embedded together with an RTD temperature sensor.

3. GC SUBASSEMBLY

The GC is designed to accommodate a standard capillary column, preferably one that is no more than 20 meters long, has an I.D. of 0.18 mm, and uses any suitable bonded, general purpose stationary phase. This type of column is readily available from a number of sources and is well-suited to the compact system with limited pumping capacity that we have been developing in this project. This column is economical on carrier gas, running at about 0.5 - 0.7 ml/min for helium. A capillary column operates optimally if the carrier gas pressure at the head of the GC column is controlled, so our system design includes a pressure regulator that is manually settable to the desired operating pressure for the column. To provide better performance of the desorber in the system, we have also included a manually settable flow controller that sets the flow rate of the carrier gas. Excess carrier gas flow beyond what is necessary for the column is vented.

The GC has a miniaturized, Viking-designed, fully temperature controlled oven, with internal resistance heater, a circulating fan to improve internal temperature distribution during heated runs, an RTD temperature sensor, super-insulation to minimize heat losses, and a computer-controlled oven door mechanism that opens the oven door for cooling or inspection of the column, and closes the door during heated runs. The oven is encased in a stainless shell for rigidity and protection of the various components. Cooling fans are provided to assist with cool down to reduce reset times between runs.

4. VACUUM ENVELOPE

The structure that provides the vacuum envelope for the mass spectrometer portion of the instrument should be as light weight and efficient as possible to keep the size and weight of the overall system down. In the case of the Mars Lander MS, this was accomplished by packaging each of the elements as tightly as possible into a stainless jacket that was meticulously cleaned and passivated and then electron-beam welded into position. Certain components were fitted into solid stainless blocks that were machined and laser etched to carve out space that would be just big enough for them. The entire assembly was rigidly welded together after dynamic alignment at two key reference points, and the resultant structure was then bolted down to a support structure to hold it in position and support the external magnet. This degree of effort is very costly, and would just by itself far exceed the total budget for this project, so we looked for alternative means for accomplishing the objective. We based our design on a concept developed here at Viking in connection with an earlier commercial project involving a magnetic sector instrument, which is part of a pending patent application for work outside of this project.

The basic building block for the vacuum envelope is a flange plate that acts as a reference plane and support structure for all of the MS components as well as being part of the vacuum envelope. This mounting plate is bolted to a thin-walled shell that forms the other half of the envelope body. The assembly is rugged, simple, and easy to disassemble for routine maintenance or repair. It has the drawback of being a larger volume for the vacuum system to pump than an envelope that was tighter to the interior elements, but the single chamber with less constrictions and corners, once it is pumped down, performs well for normal sample flows into the MS.

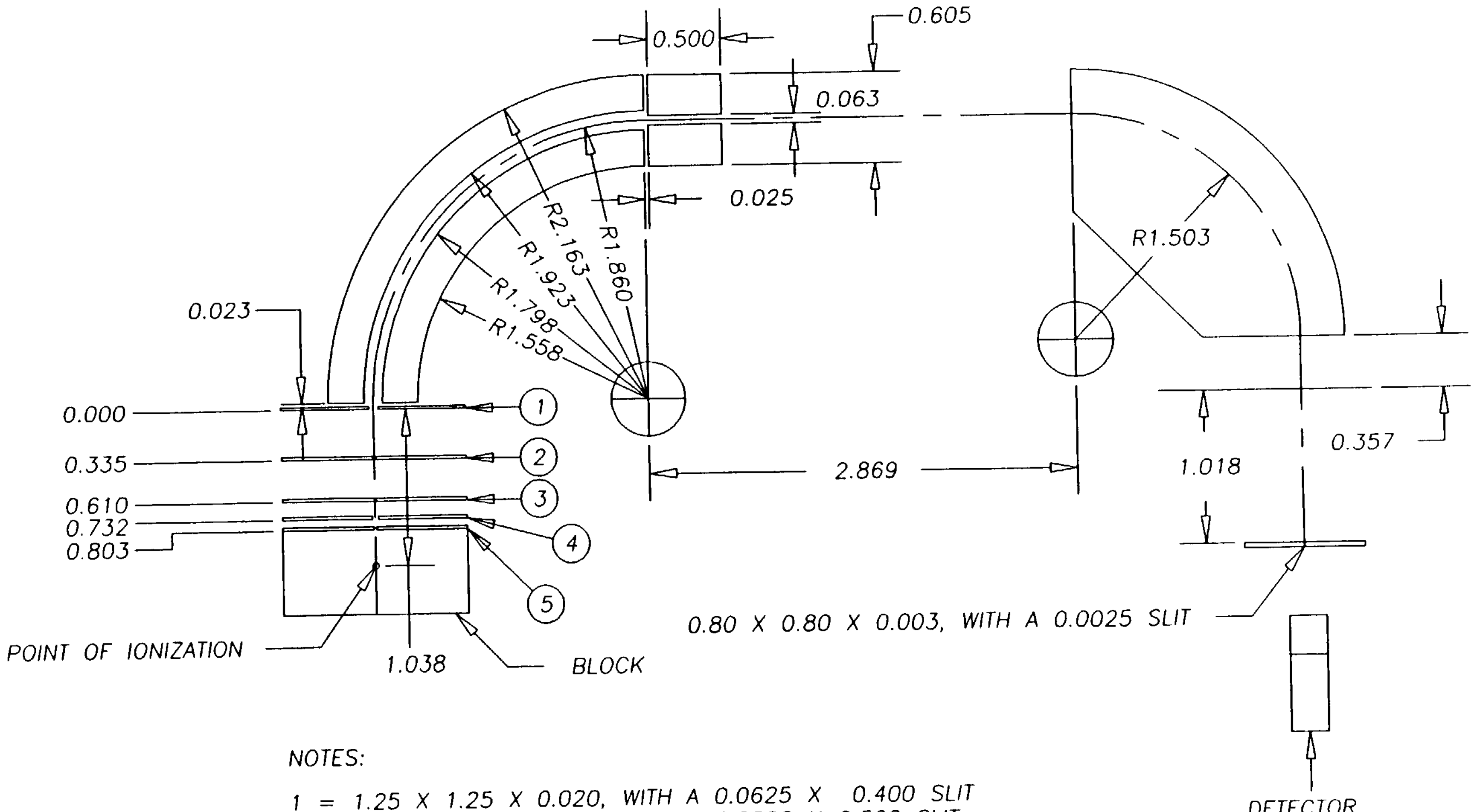
5. MS-I

The first stage MS is the heart of the system and for this reason occupied a major part of the work on subsystems development. In order to package the elements of MS-I for eventual incorporation into a system suitable for space use, each of the components of the system was carefully examined to determine whether re-design or modification would be desirable to better meet the constraints imposed by space-qualification. The resulting work on developing a new mounting and alignment system for the electric sector has been discussed earlier. There were also many alternative configurations of MS considered in relation to the choice of second stage MS. The decision was made to use the EB configuration shown in Figure 27. In addition, following the decision to use the current EB configuration, and based upon early test results, the magnet for MS-I was modified to narrow the gap between the pole faces and to make the walls of the ion beam chamber between the pole faces of a non-magnetic stainless steel. This was done to make the fabrication of the ion beam channel and its incorporation into the vacuum envelope much easier and principally to permit fine tuning the focusing properties of the magnetic sector by allowing the magnet to be moved slightly from its nominal position. This operation is performed by locking the instrument on a peak, and while observing the peak with an oscilloscope, adjusting the position of the magnet to give the best peak intensity and resolution.

Much of the effort on MS-I was connected with the ion source and the power supplies needed to drive the various active elements of the system. As noted previously, the design of the ion source went through a number of iterations, and was subject to a highly detailed set of modeling exercises where a number of variables were introduced and their effects observed on the ion beam intensity exiting the source. The source design is based upon a Nier-type, electron impact configuration, where there is an electron gun or filament that produces a flow of electrons that are accelerated to 70 eV and directed into a ionization chamber or block and are subsequently collected by an anode on the opposite side of the block. In the ionization chamber they collide with an inlet stream of molecules of the sample plus any ambient gasses that might be present in the source.

The electron beam is made more effective as an ionizing mechanism by adding a magnetic field parallel to the filament-anode axis which causes the electrons to follow helical paths through the ionization region in the block. In this region, the collisions produce a number of reactions, one of the principal ones being the creation of positive ions from the molecules in the source. The statistical distribution of the frequency of formation of these positive ions is what is observed in the mass spectrum, so all of the molecules that may be present in the source at a particular time will contribute to the mass spectrum that is observed. In the ionization chamber, a small, usually flat surface called the repeller is located parallel to the electron beam, to which a small positive potential is applied to eject the positive ions from the electron beam and into the region where they can be accelerated and focussed into the electric and magnetic sectors. The remainder of the source serves to give the ions the desired energy and to form the ions into the desired beam shape, with fine tuning of lens potentials to account for physical irregularities or misalignment of elements in the source.

500 E.B. LAYOUT



NOTES:

1 = 1.25 X 1.25 X 0.020, WITH A 0.0625 X 0.400 SLIT
2 = 1.25 X 1.25 X 0.020, WITH A 0.0200 X 0.500 SLIT
3 = 1.25 X 1.25 X 0.020, WITH A 0.0100 X 0.400 SLIT
4 = 1.25 X 1.25 X 0.020, WITH A 0.0400 X 1.25 SLIT
5 = 1.25 X 1.25 X 0.020, WITH A 0.0200 X 0.500 SLIT
BLOCK IS 1.25 X 1.25 X 0.55

Figure 27

In the final version of the source, the electron gun used a conventional wire filament with a curved filament shield connected to one side of the filament leads and a Farraday cup-type of anode. The block was gold plated and the ionization chamber was formed by the inside of a unique cylindrical magnet that had a slit to permit the ions to escape. The lenses are rather straightforward, but the process of locating them with respect to the ion beam was specially devised for use in this source. A special shaped repeller was also used to improve ion beam intensity.

The ion source has a separate heater in the block to avoid trapping sample molecules on cold surfaces in the source. The source includes as part of its structure a mounting flange with precision locating pins to position it accurately with respect to other components and the electric sector is located with respect to the source also with precision locating pins in order to maintain the integrity of the alignment. Low-reactivity gold-plated surfaces and macor (a machineable ceramic) are used extensively in the source to avoid loss of sample. In addition, to make the installation or replacement of sources easier the source and its connections can easily be removed from the mounting plate without affecting the integrity of the vacuum envelope. Figure 28 shows a cross-section of the ion source block and lenses.

A conventional exit slit was used during the development of MS-I, together with the continuous dynode detector that was described earlier. This permitted generation of mass spectra for tuning purposes and to optimize the various electrical and physical parameters to ensure that MS-I was capable of performing its task in the tandem system, that is, the selection of a parent ion for subsequent daughter ion scan. In the process of generating numerous spectra with many different system elements, improvements in these elements were made. For example, it was determined experimentally that a straight exit slit did not function as well as a curved slit and so a curved slit was used. This was explained by analysis of the ion trajectories and the determination that the ion beam actually takes a curved shape when it emerges from the magnet because of second and higher order aberration effects. A number of selected mass spectra taken during various phases of the development process is shown in Figures 29, 30, 31, and 32.

Figure 29 shows a scan of the background constituents made using the original Viking spacecraft MS. This spectrum displays some of the difficulties that the scientists and mass spectrometrists could not overcome with the miniaturized MS design of that time. It is clear that the signal-to-noise ratio is very poor and, without more data, it is difficult to make a quantitative assessment of this ratio. The ion source-electric sector-magnetic sector transmission required great improvement. The resolution at m/z 44 is measured to be 37. This is quite low, indicating that for MS-I to operate as a parent ion selector, the resolution also would have to be improved. It is also clear that there remain some optical aberrations that have an effect on the peak shape. Our research found that this tailing effect is more pronounced for higher masses and may be a result of the fringing magnetic fields. Furthermore, the high mass sensitivity was unknown. Nevertheless, this spectrum represents the starting point of our research and thus provides a model for comparison.

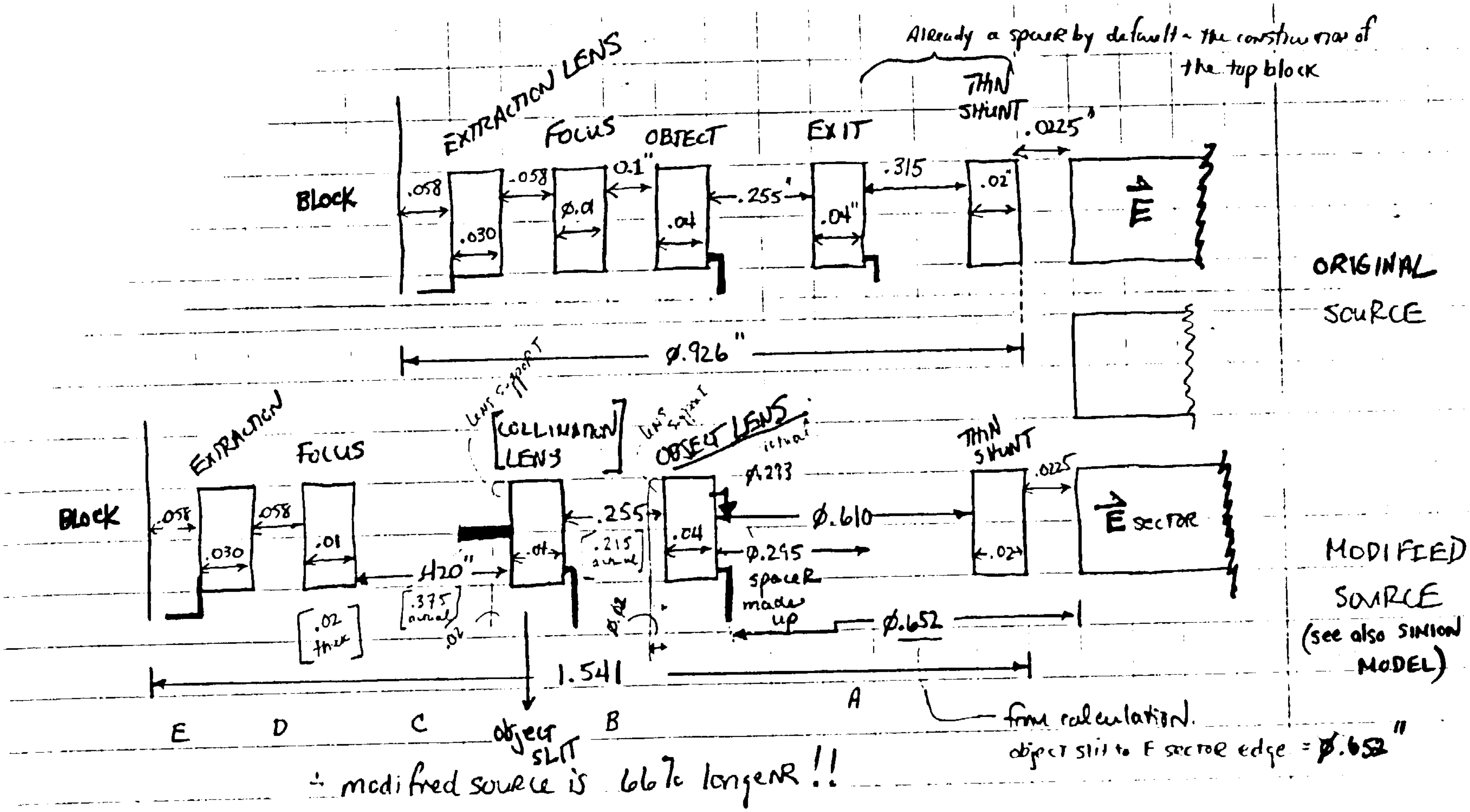

Already a spacer by default - the construction of the top block
BLOCK
EXTRACTION LENS
FOCUS
OBJECT
EXIT
THIN SHUNT
.058
.030
.058
.01
0.1"
.04
.255"
.04"
.315
.02"
.0225"
E
ORIGINAL SOURCE
.926"
EXTRACTION
FOCUS
COLLIMATION LENS
OBJECT LENS
.01
.01
.04
.255
.215 actual
.420"
.375 actual
.02 thick
.610
.295
spacer made up
.652
1.541
.02
E SECTOR
MODIFIED SOURCE
(see also SIMION MODEL)
E
D
C
object SLIT
B
A
from calculation.
object slit to E sector edge = .652"
∴ modified source is 66% longer!!

Figure 28

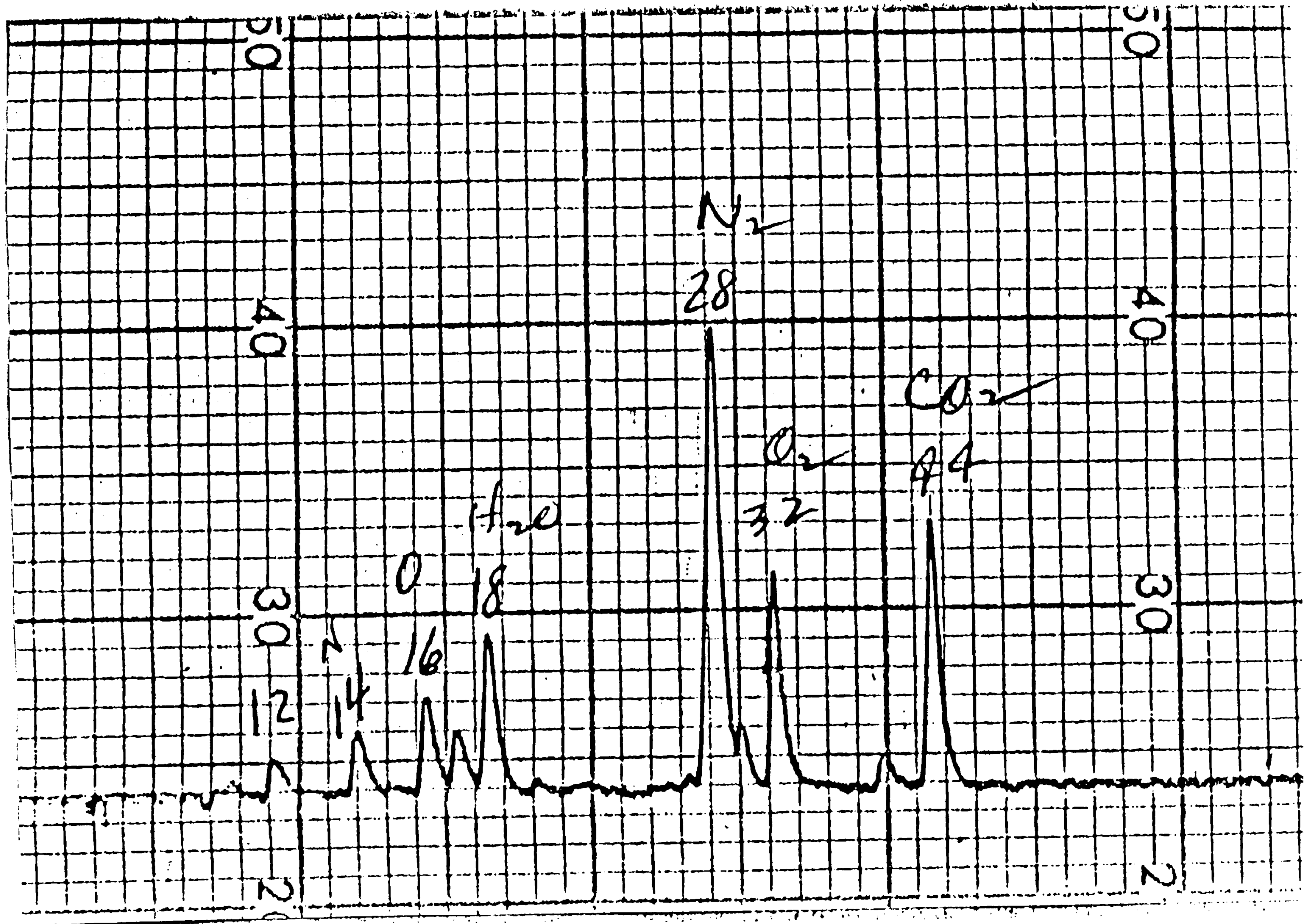


Figure 29

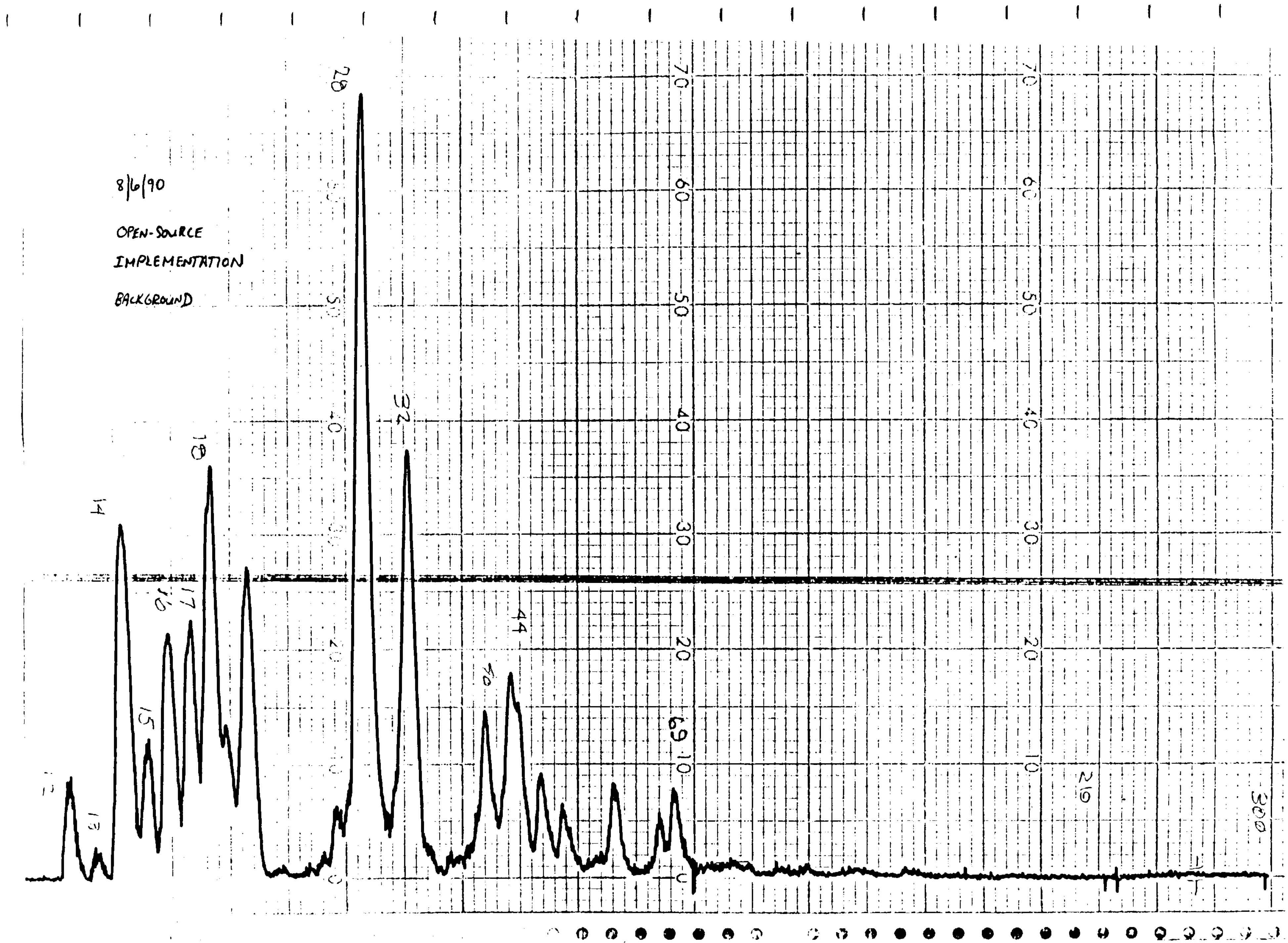

8/6/90
OPEN-SOURCE
IMPLEMENTATION
BACKGROUND
12
13
14
15
16
17
18
28
32
40
44
69
219
300
70
60
50
40
30
20
10
0

Figure 30

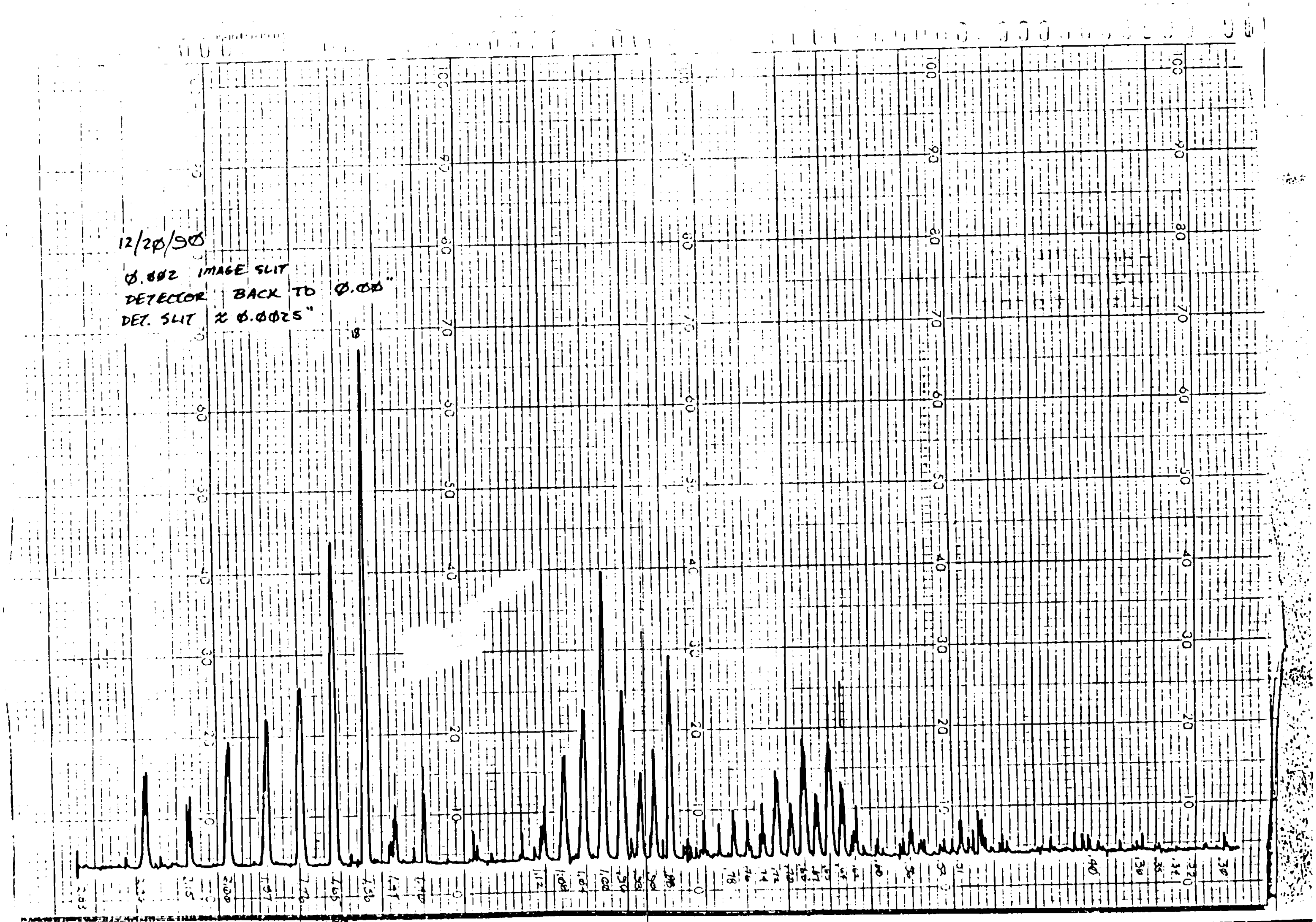


Figure 31

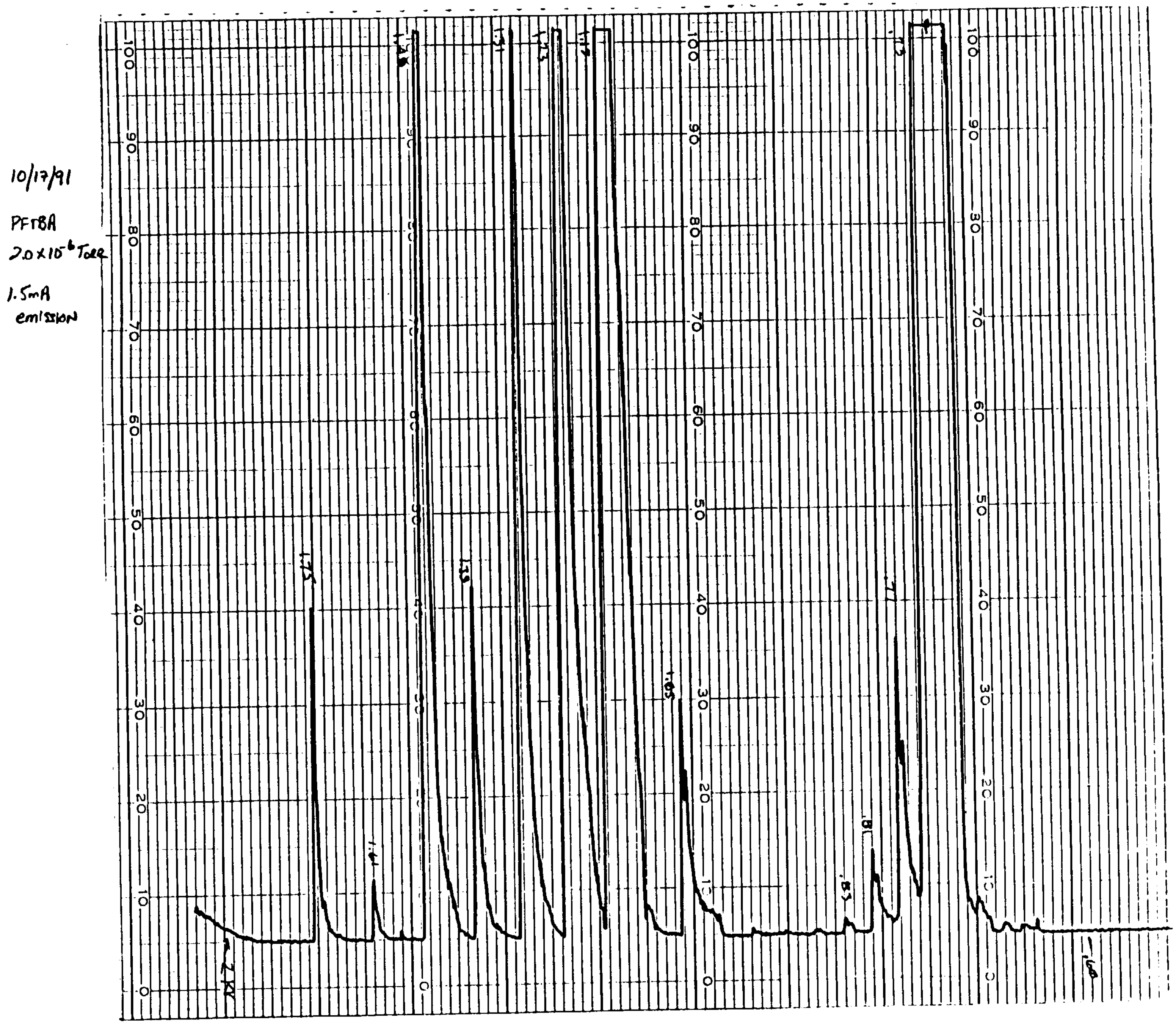

10/17/91
PFTBA
2.0x10^-6 Torr
1.5mA
emission
2 KV
.60
.73
.77
.81
.83
1.05
1.17
1.23
1.31
1.33
1.61
1.75

Figure 32

In August of 1990, we had designed another source that was significantly simpler and had more of an open design. An early spectrum is shown in Figure 30. The signal-to-noise ratio was very poor and the resolution was measured to be 16 at m/z 44. Initially, it seemed as though we had made a giant leap backward. We, therefore, tried many experiments over the following months to improve the spectra. We moved the image slit back a given distance, we adjusted the electron beam housing, and made slight adjustments to the magnet and electric sectors. The power supply was adjusted in several ways. We also decreased the image slit width and, by December of the same year, the resulting spectra was shown in Figure 31. The resolution at m/z 44 was measured to be 88 and represented an improvement of 2.4 over the original spacecraft MS. The high mass response was better than before; however, the sensitivity remained quite poor, even with a low air and water background.

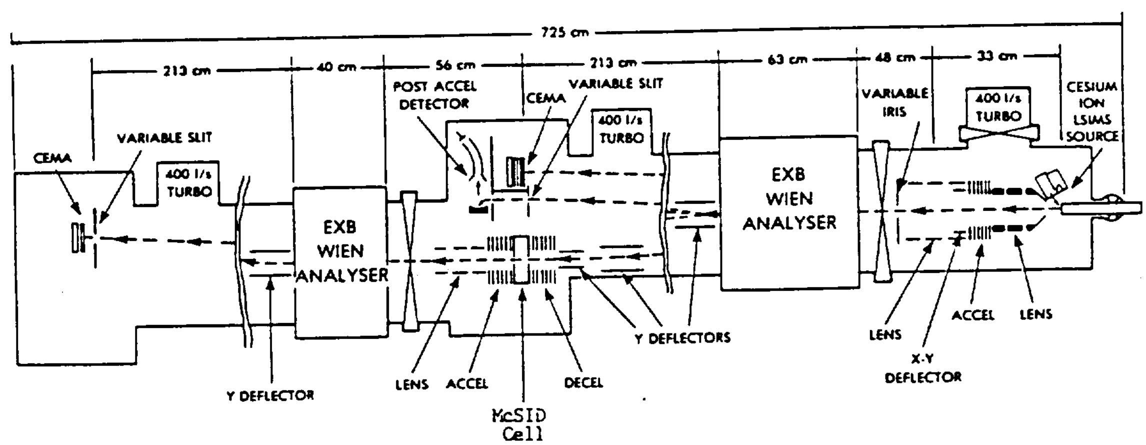
For the first several months in 1991 we embarked on adding a more flexible vacuum housing to provide room for MS-II as well as modifying the ion source for improved ion production and transmission. As explained above, we went back to the original Viking spacecraft source and computer modelled it. A major lens was added and called the collimation lens, as shown in Figure 28. This lens provides an accel-decel to the ions to aid the optics of our accelerating voltage scanned system. This improved the ion transmissions characteristics of the MS and, by the fall of 1991, we had achieved some measure of success, as shown in Figure 32. This is a spectrum of the low mass region of perfluorotributlyamine present at a pressure of 2.0×10^{-6} Torr. This compound has a very distinguishable ion at m/z 69. We clearly had generated more signal and it is estimated to be at least one order of magnitude more sensitive than the original Viking spacecraft MS, but more work was required to improve the resolution. This source proved quite good, as shown later in this report (Figure 57), with a resolution at m/z 44 measured to be 235. This represents a factor of greater than 6 over that of the original Viking spacecraft MS. The background pressure was 7.0×10^{-6} Torr and is mainly water and air. We feel that the high mass response will be much higher if the background water and air are eliminated. However, the time and financial constraints of this project did not permit us to optimize MS-I much further.

6. MS-II.

The definition of MS-II and the interstage fragmentation scheme was an important matter for both analytical and practical reasons. Initially, it was expected that a microchannel plate (MCP) fragmentation device would be the method of choice. Work was done to determine the fragmentation patterns from a selected microchannel plate at Viking. These measurements required a larger experimental vacuum chamber and manipulators than were available at Viking, so we utilized the facilities of the University of Maryland physics department and a consultant to perform more detailed characterization of the performance of the MCP. This data is included in the Appendices.

In connection with this work with the MCP, we also continued consultation with the only researcher who has reported on using this approach, Dr. William Aberth of UCalif(SF). This revealed that the conditions for successful application of the MCP were going to be very difficult to achieve in the standard EB configuration. The apparatus used by Dr. Aberth in performing his MCP experiments was also very bulky and complex, as can be seen by the sketch that he provided, shown in Figure 33. Note that three 400 L/sec turbo pumps are used on his system, among other features that would make such a system completely unsuitable for the type of instrument that could fly in space. we attempted to design around these bulky and power-hungry items, but eventually concluded that the MCP could not be adapted to our system design within the time and dollar constraints that were in existence.

We then looked again at the single collision with a fixed metallic surface, the SID approach to production of daughter ions. This has had considerably more attention and has been successfully used in a number of experimental tandem MS instruments, so the scientific base for SID is better understood, although we are not aware of any commercial instrument that incorporates this approach. Some of its advantages have been discussed earlier. Some of the key advantages are its very light weight, simplicity, ruggedness, ease of fabrication, low cost, similarity of daughter ion spectra to the more conventional CID spectra, and adaptability to the EBE design. An experimental platform was fabricated to carry out SID work, and to evaluate the various aspects of MS-II component configuration. This platform permitted MS-I and the interstage device as well as the electric sector for MS-II to be operated independently or as a system and had ports for vacuum gauges, auxiliary inputs, visual inspection, etc. The reflecting surface used was a polished, gold plated stainless plate about 2 cm x 2 cm and about 1 mm thick. It was mounted at an angle of 45 degrees to the axis of a rod that is moveable from outside the vacuum envelope using a Cajon fitting as a seal. This permitted the surface to be inserted into the ion path or withdrawn, and with detectors mounted both at the normal detection position for MS-I and another mounted to observe the daughter ions as they are reflected from the plate, the operation of the plate can be measured. Figure 34 illustrates the effect of inserting the plate into an ion beam in which the parent ion that has been selected is CO_2. This illustrates the daughter ion intensity as measured at the angle for specular reflection. Other measurements at different angles and for other parent ions are also possible. In addition, by using a retarding potential on the reflected ions, a determination of the components of the daughter ion spectrum can be made. Although such determinations are somewhat noisy because of power supply fluctuations and surface effects, Figure 35 shows the presence of C^+ and O_2^+ as noted on the trace. From this work it was clear that additional lenses to control and shape the ion beam would be desirable.



725 cm
213 cm
40 cm
56 cm
213 cm
63 cm
48 cm
33 cm
CEMA
VARIABLE SLIT
400 l/s TURBO
EXB WIEN ANALYSER
POST ACCEL DETECTOR
CEMA
VARIABLE SLIT
400 l/s TURBO
EXB WIEN ANALYSER
VARIABLE IRIS
400 l/s TURBO
CESIUM ION LSIMS SOURCE
Y DEFLECTOR
LENS
ACCEL
McSID Cell
DECEL
Y DEFLECTORS
LENS
X-Y DEFLECTOR
ACCEL
LENS

Figure 33

Figure 34

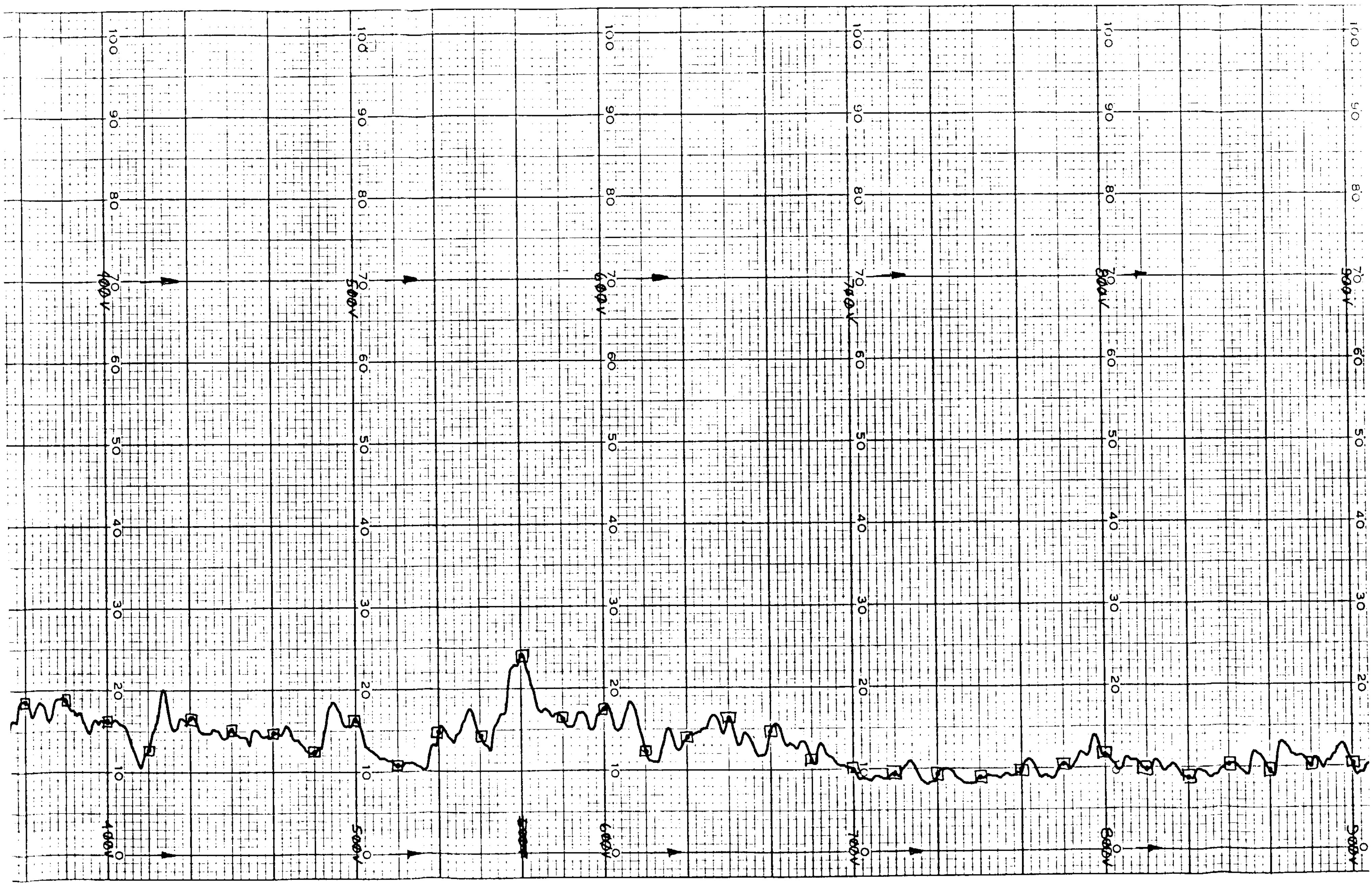


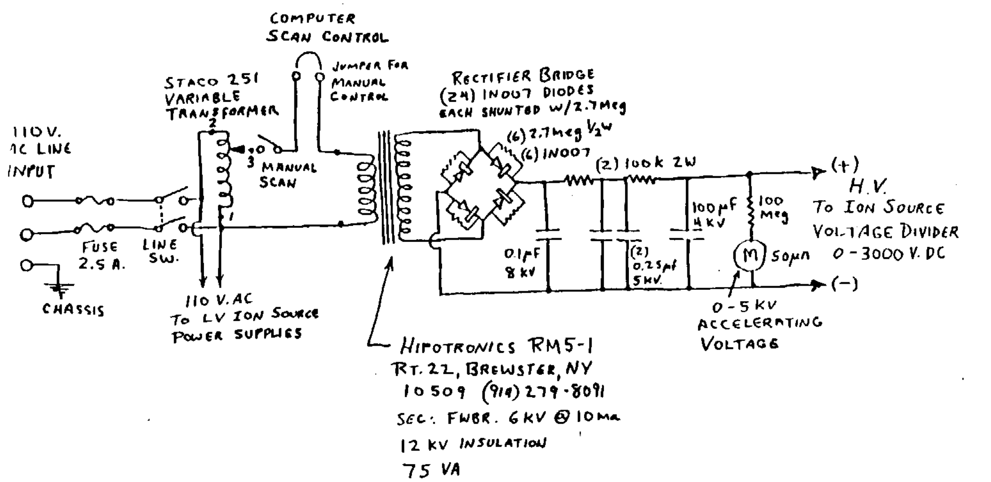
Figure 35

7. ELECTRONICS AND SOFTWARE

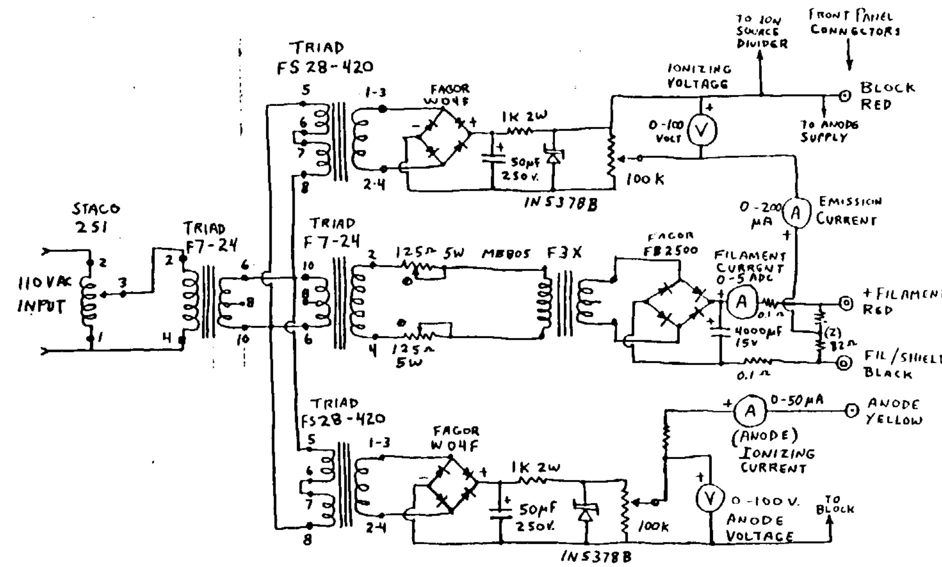
In order to operate the various subsystems, Viking utilized a variety of standard power supplies as well as custom-made supplies with controls and other interfaces provided by our own circuit boards or switch arrays. Our primary interest in this area was to achieve functionality, rather than to be concerned with miniaturization or packaging. These aspects would then be the subject of later work, as the experimental prototype transitioned to a more flight-oriented prototype stage. Thus, in this contract, we concentrated on those hardware components such as the electric sectors, ion source, GC components and the like, where the ability to convert an operating design to a miniaturized package is not obvious and may even be impossible, and we left the construction of miniaturized and more densely packaged power supplies and other electronics for later. Our experience and general practice in the field shows that once a highly specific set of specifications can be established for a circuit, it can be designed and laid out in a highly efficient package, using a variety of computer-aided tools that take the various components and give a very compact end product.

As part of the experimental work that was carried out, starting with very basic subassemblies and components, we felt the need for a simple, bench top power supply that would be capable of handling 3-4 kVolts and could provide an exponential sweep voltage by simply using the decay of the charge on a capacitor in an RC circuit. Such a supply was designed and built, and was used to drive at least part of the MS during all of the project work. It is also being delivered as part of the experimental prototype hardware. A schematic of this supply is shown in Figure 36. The front panel controls are sketched out, together with their functions in Figure 37. For continuing work on the system, however we strongly recommend that one of the next steps be to replace this supply with a smaller and better regulated supply for ion source operation. We have laid out the approach we would favor for this next step and Figure 38 shows the basic components and interconnections of an integrated power supply for the system.

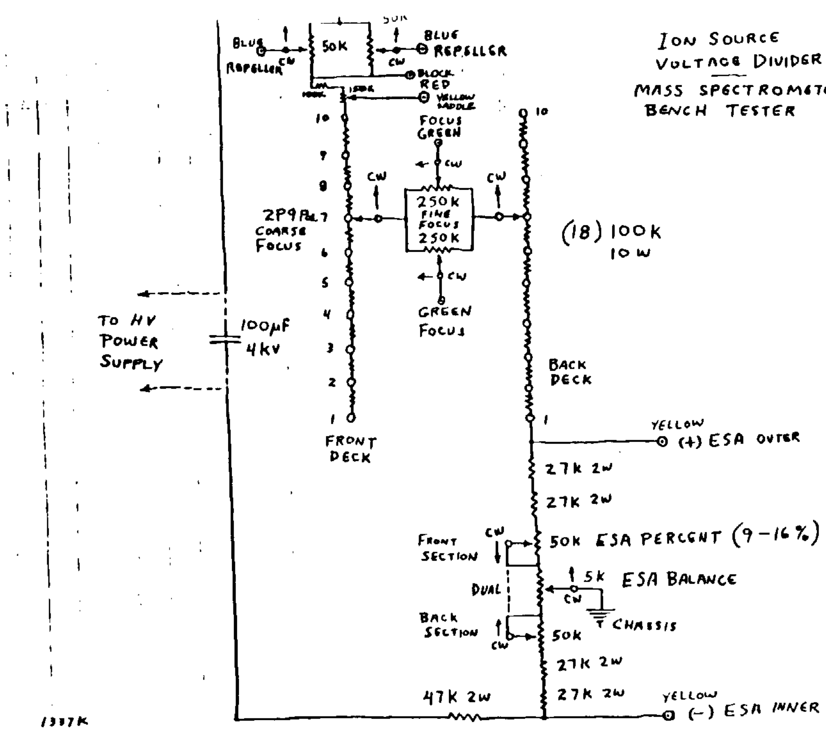
Computer operation of the spaceflight system that would eventually result from this work is obviously what is desired, and Viking has taken the first step in putting together the software approach that would be desirable. To keep within the available budget for the project, we had to work with computer systems that were readily available to us and would have the capacity and flexibility to handle all of the operating and computational tasks that may be required. This meant that we needed IBM-compatible formats, and so we based our system on MS-DOS and WINDOWS, recognizing that this would probably change later.



HV POWER SUPPLY SECTION
MASS SPECTROMETER BENCH TESTER

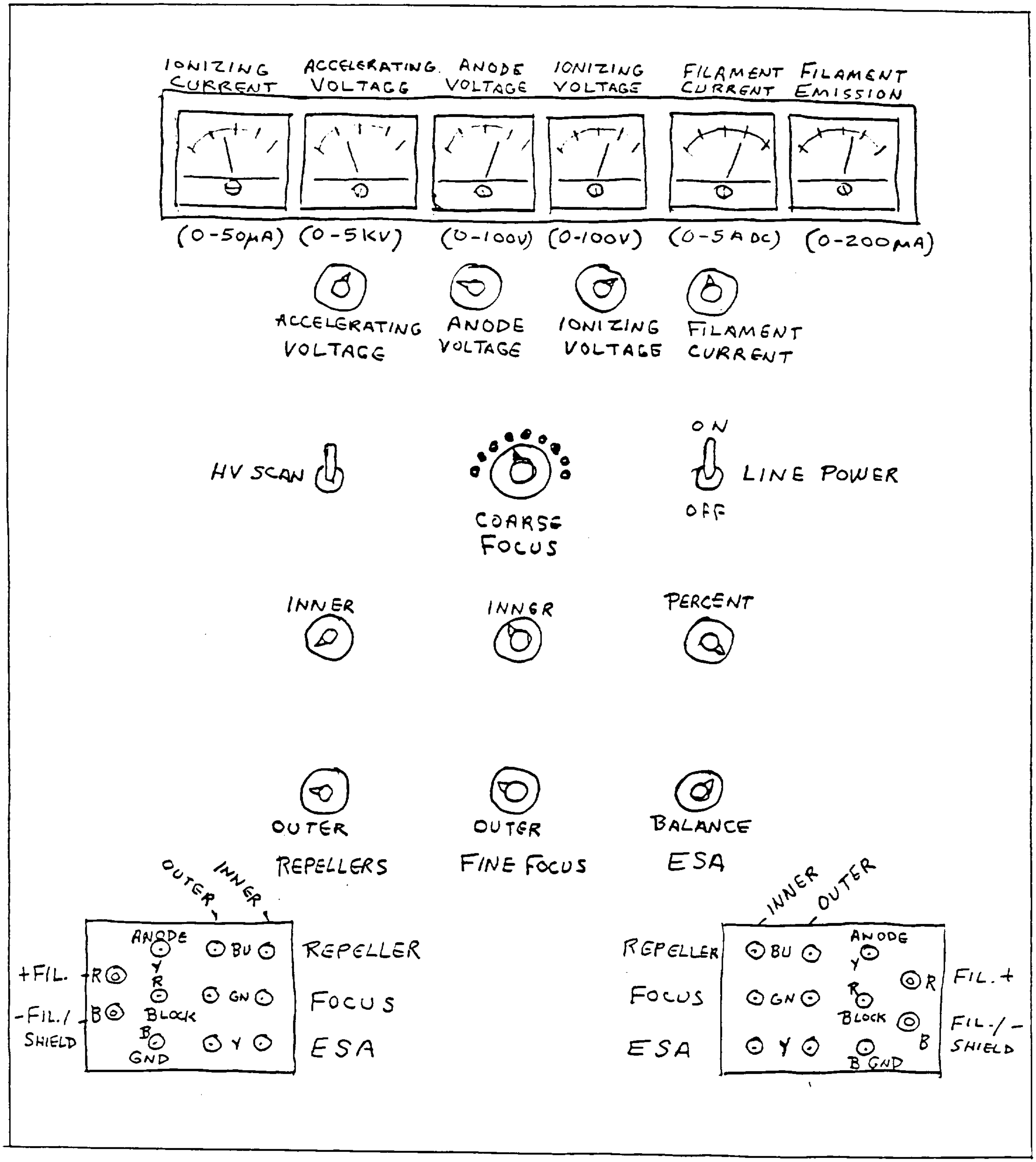


LOW VOLTAGE ION SOURCE POWER SUPPLIES
MASS SPECTROMETER BENCH TESTER



ION SOURCE VOLTAGE DIVIDER
MASS SPECTROMETER BENCH TESTER

Figure 36



MASS SPECTROMETER BENCH TESTING
POWER SUPPLY

1-90

Figure 37

MS / MS POWER SUPPLY OVERVIEW

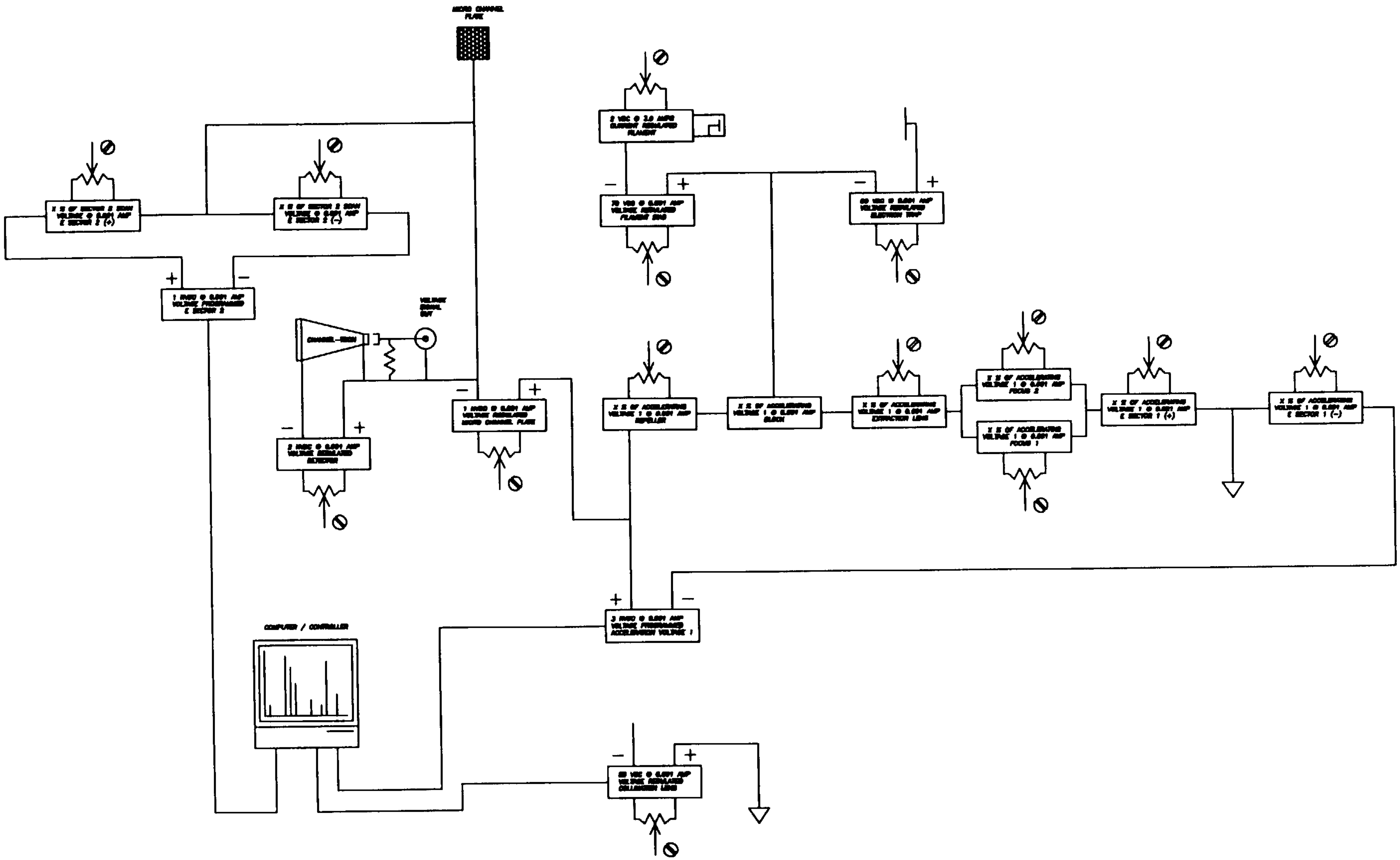


Figure 38

We also considered several bus choices for the embedded system in the instrument, including the STD bus, VMEbus, Multibus II, and PC-bus with passive backplane, and chose to work with the least constraining, that is, a passive backplane that would enable easy connectivity to the PCs in our laboratory and in the software development offices. We did so because it seemed clear that any packaging of this GC/MS/MS system for space would require a CPU and control configuration that would have to be compatible with the platform and whatever interfaces were established by the platform itself. Thus, we decided that we would be as generic and un-specific as possible, and maintain easy compatibility with our own PCs. The system therefore requires an external computer with at least an i386-level microprocessor, a 3.5 inch floppy disk drive, and a VGA display. The interface with the experimental prototype is via a Data Acquisition Processor (DAP) board from Microstar Laboratories, which is provided as part of the prototype package. This board has its own CPU, a 16 bit, 80186 processor with up to 512K RAM, and plugs into a standard expansion slot on any IBM-compatible PC, so it was well suited to our system design approach. It is capable of an array of functions that interface the GC/MS/MS with the PC. Table 1 illustrates the functional versatility of the board, which enabled Viking programmers to generate an operating system in a remarkably short period of time.

Our approach to system control has been to automate as many routine functions as possible, while keeping the operator in the loop for those steps that set variables or operating conditions for which a degree of flexibility is needed at this stage in system development. We recognized that, as the system became more developed and approached an actual space-qualified package, more and more autonomy would need to be incorporated, and that eventually fully automatic operation would be the normal mode, with operator intervention as an option. Each step in the software development is consistent with this future pathway. Initially, we have only certain functions running autonomously, for example, temperature control for heated elements. Currently, the software permits the operator to set temperatures for each of the active elements manually. This value is then used, together with the output signal of a temperature sensor, to control the heater element on and off to maintain the set value within certain tolerances. This level of control is automatic and requires no operator intervention--in fact, the operator cannot interfere with the automatic temperature control loop except to turn off the unit entirely or turn it on to the set value.

Using the WINDOWS format, the system is set up to operate from a window labelled "TOP." The menu bar shows a number of selections that can be made: AutoRUN, Special, Utilities, Help, and Exit. If the user selects AutoRUN, the menu choices shown in Figure 39 appear (this is a printout of the actual screen display). The choices are largely self-explanatory, except for the cycles, which will be covered in the following paragraphs. Selecting "Special" allows a particular set of parameters for a cycle to be stored and given a name that can be recalled under this menu item. The choices here are shown in Figure 40. The "Utilities" selections are shown in Figure 41. The "Help" item deals with WINDOWS features only and is not shown. "Exit" handles the programmed shutdown of the system, safing all active components.

TABLE 1

On-board Software

- Averaging
- Maximum and minimum
- Trigger detection
- Peak extraction
- Time stamping
- Autoranging
- Sensor linearization
- Closed loop process control
- Digital filtering
- Fast Fourier Transform
- Power spectrum
- DAPL™: real-time multitasking operating system for data analysis and compression

Hardware

- On-board 16 bit micro-computer: 80186 processor with 128K-512K RAM
- Single slot board, PC/XT/AT compatible
- 16 analog inputs, 12 bit resolution
- Expansion to 512 analog inputs
- Programmable gain amplifier
- 2 analog outputs
- 16 synchronous digital inputs
- 16 digital outputs
- Expansion to 64 digital inputs and outputs

PC Interface Software

- Command input: text
- Data output: text or binary
- Conversion to engineering units
- Buffering adjusts data flow as required by the PC
- Standard languages supported
- Compatible with Pascal, BASIC, C, Fortran, Lotus 1-2-3, Asyst, ILS, and LabWindows
- DOS driver
- DAPview™ program
- Filter design program
- Disk logging program

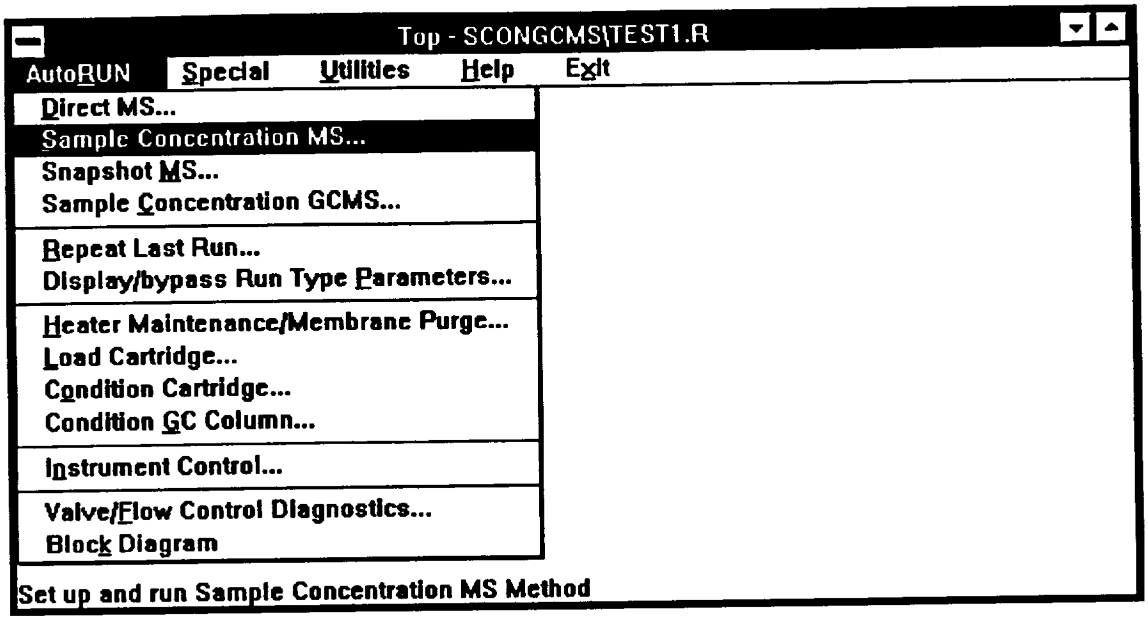


Figure 39

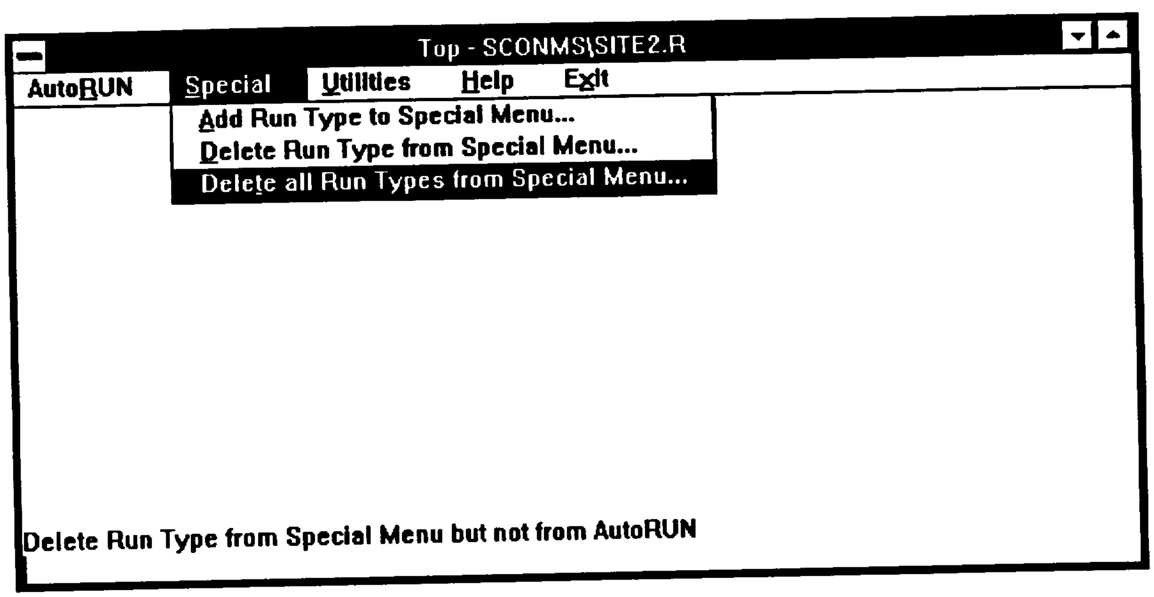


Figure 40

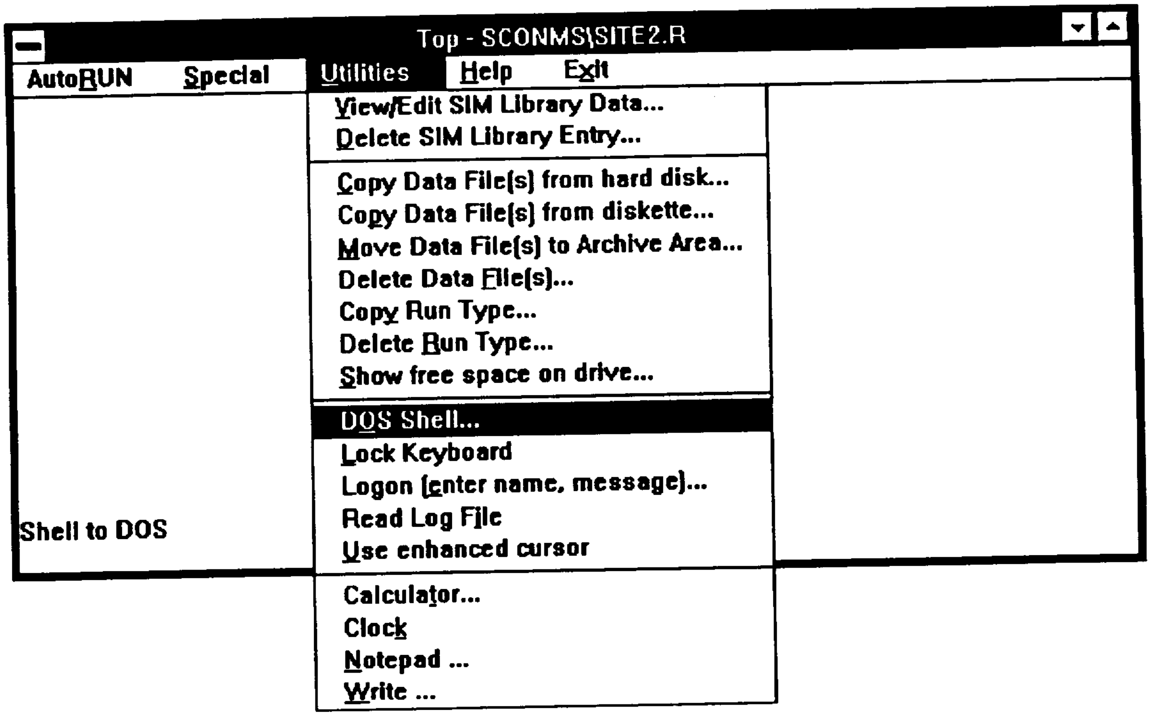


Figure 41

The concept of operation of the system is to provide three basic cycles for analysis of samples, any one of which can be repeated at intervals in accordance with pre-programmed instructions. The controllable parameters for each of these cycles initially are entered by the operator, however once such parameters were established as the most desirable set for a particular situation they would be locked in and could be automatically recalled and used in running the cycle in question. The reason that we established these three cycles is that no single cycle utilizes the capabilities of the instrument optimally. It is our belief that each of these cycles would be needed at one time or another to analyze the atmosphere to the detail that will be needed in the spacecraft over long periods in space. The cycles are: DIRECT MS and SNAPMS (same cycle but different MS operating modes), SAMPLE CONCENTRATION MS (SCONMS), and SAMPLE CONCENTRATION GCMS (SCONGCMS). In a specific cycle, the sequence of events leading to sample entry into the tandem MS is fixed, but the times and temperatures are settable. Each of the cycles will be summarized in the following paragraphs. The settings for various valves and heaters has already been covered in section II.A.6. of this report. The strategy for MS operation after sample entry will be covered elsewhere.

In DIRECT MS or SNAPMS, the sample is drawn into the instrument by the sampling pump, passing over the membrane interface. The sample that permeates the membrane passes into the ion source when the membrane valve is opened. The variables that must be specified are the membrane temperature and the time that the sample pump will be running, and MS operation. The set up window for this cycle is shown in Figure 42. In this cycle, the sample stream consists of the ambient atmosphere with no concentration except that which is supplied by the membrane itself. This generally is the least sensitive cycle, in terms of the instantaneous concentration of sample molecules in the ion source.

In <u>SCON MS</u> (Figure 43), the sample stream is drawn into the instrument by the sample pump and passed through a concentrator cartridge. This cartridge is loaded with a sorbant material chosen for its affinity for molecules of interest in a particular situation. Tenax is often used for general purpose environmental analyses but there are other materials and proprietary products commercially available that are optimized for certain classes of compounds. After the sample has been adsorbed onto the cartridge packing, the cartridge is heated rapidly to desorb the sample into a stream of non-reacting carrier gas such as helium, hydrogen or nitrogen. We use helium, but on the space station another gas may be more readily available and could be used. The carrier gas with sample is then routed to pass over the membrane as in DIRECT MS. The variables that must be set in this cycle are: sampling time, cold flow time, desorption temperature, desorption time, membrane temperature and MS operation. In this cycle, the cartridge acts to concentrate the sample from the background gasses such as oxygen and nitrogen. Assuming helium as a carrier gas, these background gasses are purged from the sample stream before heating and desorption takes place, in a cold flow step. This cycle permits more sensitive analyses to be carried out, for example, if a direct detection can be made at 10 ppb, concentration should permit detection at less than 1 ppb for the same compound.

In <u>SCON GCMS</u> (Figure 44), the sample stream is drawn into the instrument as above and loaded onto the cartridge. A cold flow of carrier is used to purge the air from the cartridge as above and then the cartridge is heated to desorb the sample. The sample pathway however is now into the head of the GC column. The system is equipped with a flow control valve for the carrier gas as well as a pressure regulator and gauge. Capillary columns work best when the carrier gas is pressure regulated, and the gauge permits the operator to set the pressure at the optimum value for a particular column I.D. and length. The flow controller controls the amount of carrier gas that is split, that is, is excess to the amount that can flow through the GC column at the established pressure. This excess carrier gas contains some sample, so by splitting the flow, excess sample is removed from the molecules that reach the MS. By varying the split ratio, the system can accommodate a larger range of sample concentrations than otherwise. Once in the GC column, which is contained in an oven, with the increase of temperature the various components of the sample mixture will be separated and will emerge from the end of the column at well-resolved times. These concentrations of specific components are called "peaks" in view of their appearance on traces of standard GC detector output. The peaks of various sample compounds are introduced directly into the ion source of the MS.

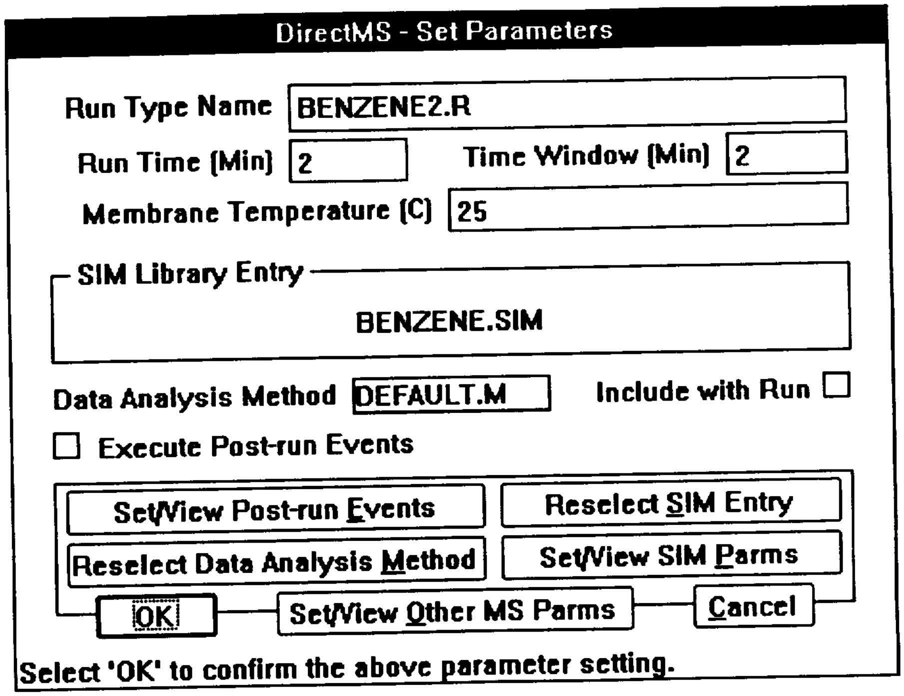


Figure 42 (Part A)

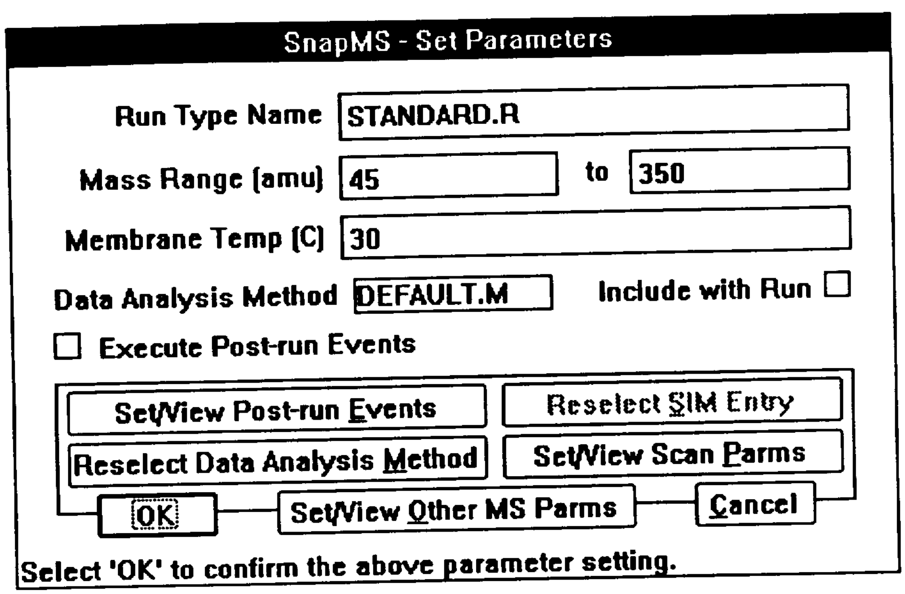


Figure 42 (Part B)

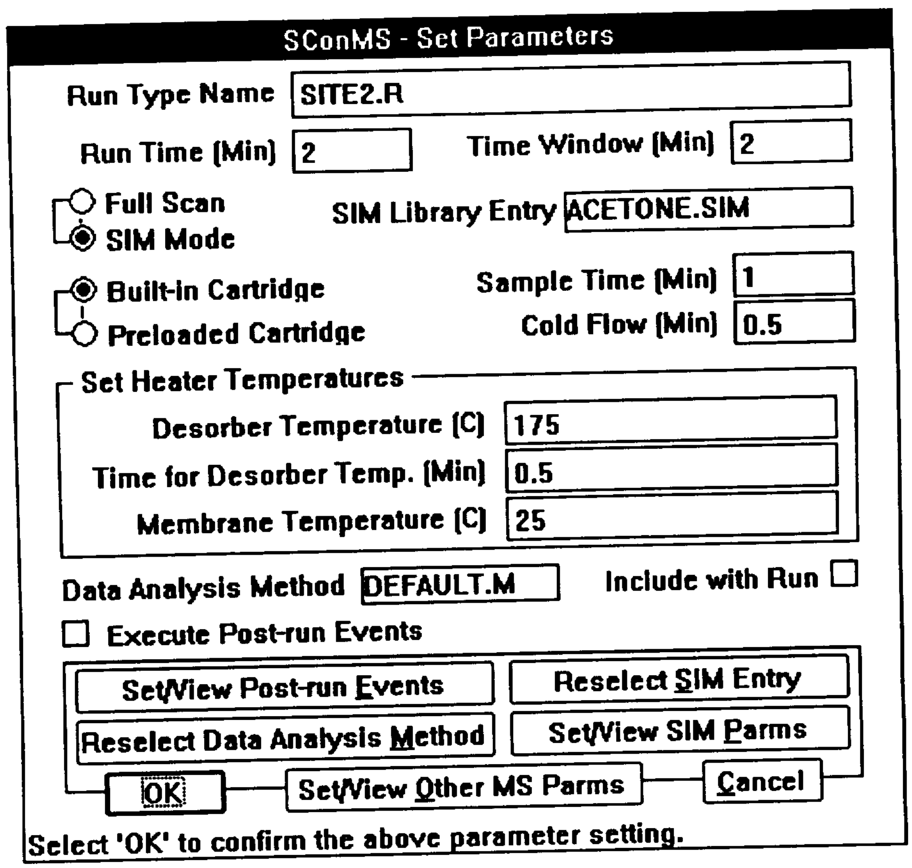

SConMS - Set Parameters
Run Type Name
SITE2.R
Run Time (Min)
2
Time Window (Min)
2
Full Scan
SIM Mode
SIM Library Entry
ACETONE.SIM
Built-in Cartridge
Preloaded Cartridge
Sample Time (Min)
1
Cold Flow (Min)
0.5
Set Heater Temperatures
Desorber Temperature (C)
175
Time for Desorber Temp. (Min)
0.5
Membrane Temperature (C)
25
Data Analysis Method
DEFAULT.M
Include with Run
Execute Post-run Events
Set/View Post-run Events
Reselect SIM Entry
Reselect Data Analysis Method
Set/View SIM Parms
OK
Set/View Other MS Parms
Cancel
Select 'OK' to confirm the above parameter setting.

Figure 43

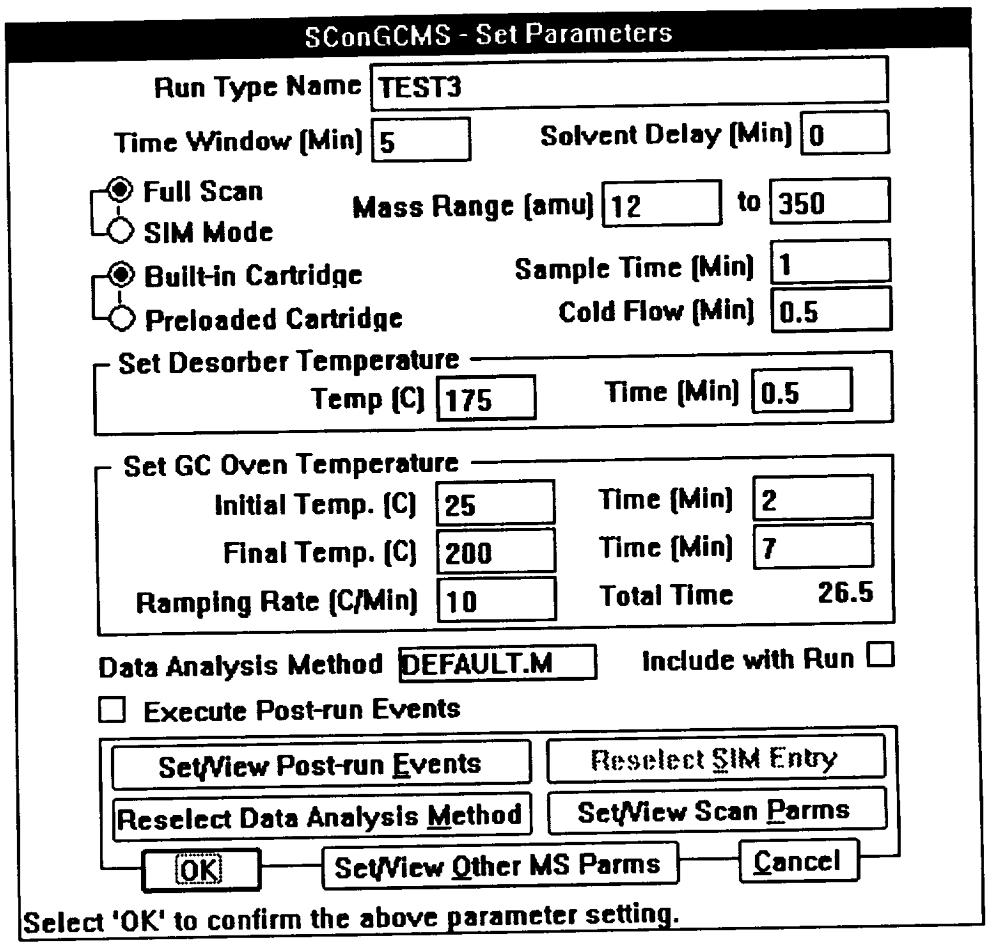

SConGCMS - Set Parameters
Run Type Name TEST3
Time Window (Min) 5
Solvent Delay (Min) 0
Full Scan
SIM Mode
Mass Range (amu) 12 to 350
Built-in Cartridge
Preloaded Cartridge
Sample Time (Min) 1
Cold Flow (Min) 0.5
Set Desorber Temperature
Temp (C) 175
Time (Min) 0.5
Set GC Oven Temperature
Initial Temp. (C) 25
Time (Min) 2
Final Temp. (C) 200
Time (Min) 7
Ramping Rate (C/Min) 10
Total Time 26.5
Data Analysis Method DEFAULT.M
Include with Run
Execute Post-run Events
Set/View Post-run Events
Reselect SIM Entry
Reselect Data Analysis Method
Set/View Scan Parms
OK
Set/View Other MS Parms
Cancel
Select 'OK' to confirm the above parameter setting.

Figure 44

In a typical analysis on a capillary column with 0.18 mm I.D. the peak widths can be as small as 2-3 sec or, with very poor resolution, as long as 20 sec or more. For good MS detection, several samples of the ion current would be desirable over a period of a second or two, so with the use of the GC column in circumstances where there were unknown compounds present, there would not be sufficient time for a tandem MS analysis. In such cases, the MS would typically be operated in the single MS mode. The parameters that need to be specified in this cycle are: sample time, cold flow time, desorption temperature, desorption time, GC oven start temperature and time at this temperature, GC oven heating rate, GC oven final temperature and time at this temperature, and MS scan upper and lower mass values. This cycle provides the extra sensitivity of the concentrator cartridge plus the ability to separate and identify the individual components of a complex mixture. It is particularly useful in two situations: 1) as a means of identifying compounds that are not expected to be present and therefore do not have a pre-determined parent-daughter ion spectrum to observe; and 2) as a check on the operation of the tandem MS, since it separates compounds differently. For example, if two compounds have identical daughter spectra for the most intense parent ions that are available for analysis, it may be necessary to perform a GC separation on them and then use the MS as a detector rather than operate in the MS/MS mode.

The software provided with the prototype hardware is designed so that an operator can select and process samples through the various cycles and then operate the MS manually. As the hardware evolves further, more of the functions that are illustrated in the windows would become operable under software control. Ultimately, the type of control that is available in this generation software would be overlaid by a more autonomous level of control as the system came closer to a spaceflight package. At this higher level of development, certain standard sampling sequences and MS run variables would be pre-set and the system would run unattended, perhaps with certain artificial intelligence features to respond to off-nominal conditions. If, however an operator wanted to perform a particular experiment or wanted to manually select a cycle and run type, the current software could be called up as an option, and the menus that are here would be available to that operator.

C. SYSTEMS ASSEMBLY AND TEST

1. EXTERNAL INTERFACES

Much of the work on the various subsystems flowed directly into larger and larger aggregates of these subsystems and some of the results of this work has already been covered in previous sections. Therefore, this section will primarily treat the interfaces between subsystems and between the instrument as a whole and its external support structure. The external connections to the system are electric power (110 Volts, 60 cycles); a mechanical forepump for the turbopump; a structural framework to support the chassis; a carrier gas supply or supply line; an external sampling system to bring an atmospheric sample from a remote location to the instrument inlet port, if desired; and an external computer system.

2. SAMPLE COLLECTION AND CONCENTRATION

The major challenges in assembling the system are in the interfaces that involve transfer of sample molecules, in matching the timing of various events across the active elements, in synchronizing the start times, and in connecting each of the subsystems to the computer control and data handling system. To highlight the system integration issues and problems, and show the solutions that were adopted by Viking, the following paragraphs will generally follow the order in which a sample molecule passes through the system.

The sample collection process involves transfer of the sample molecule from a larger stream of molecules to the MS in a way that minimizes loss of sample and maximizes the number of sample molecules compared to its ambient surroundings. One of the factors that was involved was the rate of gas flow. Our choice of sample pump was made to ensure that adequate sample flow would occur even with a relatively high back pressure caused by a tightly packed concentrator cartridge. The pump is rated at 5 L/min under no load. With direct sampling cycles, the only restrictions in gas flow are the two valves and the membrane passages, hence nearly full pump capacity is realized. For some purposes this may be too high a flow rate, so depending upon what type of external sampling lines were involved, it may be necessary to restrict the pumping rate for these cycles. When loading the cartridge, it appears from our testing that the sample loading is satisfactory.

3. MEMBRANE INTERFACE

The transfer of sample molecules to the MS via the membrane is an important interface. At the present time, the membrane is a single stage device that has good sample transfer characteristics and increases the relative concentration of sample molecules to the fixed gasses by about 10^3 thus greatly improving the detection sensitivity over a direct molecular leak. When the membrane is open to the source, since it is not a perfect separation device, it also admits some of the fixed gasses so that there is some nitrogen, oxygen and carbon dioxide present in the background. A reasonably high pumping rate is needed to ensure that the MS is not adversely affected by this additional molecular flow into the source, or the source may need to be opened up more to keep increased source pressure down. Alternatively, the membrane may be modified to a two stage system. This would require auxiliary pumping between the stages and the trade-offs would need to be examined. Transfer of the molecules from the membrane to the source is via inert tubing.

4. CONCENTRATOR-TO-COLUMN INTERFACE

There is another interface that required careful attention, that is, between the concentrator cartridge and the GC column. The function of the concentrator is to increase the number of sample molecules available to the detector, while the column serves to separate those molecules by compound. This separation is most effective if the sample is delivered to the column in a tight plug. If this is the case, the GC peaks at the exit of the column will tend to be sharp and well resolved. Otherwise, if the sample is slowly fed into the column, the resulting bunching of the sample molecules will be limited and the peaks, if any, will be very broad and difficult to distinguish from each other. The cartridge is constructed from low reactivity glass with an I.D. typically of 4 mm and is packed with a sorbant material of a particular mesh size range, 60-80 mesh being quite commonly used. This construction allows large volumes of air to be passed through the cartridge, since generally the more air that is sampled the more sample molecules will be captured by the cartridge. During the desorption process, therefore there is a relatively large volume of sorbant material that must be purged in a short time if the sample molecules are to come off in a relatively tight plug. On the other hand, the GC capillary column only flows 0.5-0.7 mL/min of carrier gas for optimum performance. This mismatch takes careful attention, if the system is to maintain high performance.

Initially, the desorber was connected to the GC column by valves and connecting tubing in order to give flexibility to the various sampling cycles. This configuration however resulted in broad, poorly resolved peaks. As a result, we designed a new desorber/injector assembly that brings the entrance to the GC column actually into the mouth of the cartridge. We found that optimum performance was obtained if the column is positioned approximately 1 mm from the surface of the glass frit that is inside the cartridge body. To accommodate the mismatched flow rate, we then provided a split pathway that enabled the cartridge to be rapidly and effectively desorbed. In addition, by holding the front of the column at a low temperature, slower desorptions of the cartridge can be carried out since the cold column acts as an auxiliary trap. The molecules that are desorbed from the cartridge pass into the column entrance which is heated because it is positioned inside the cartridge and then begin to move down the column aided by the carrier gas flow. When these molecules proceed down the column to the point at which the column is no longer in the desorber body they are exposed to a cold surface on which they condense. Later in the run, when the column is heated, they will be released and the analysis proceeds in a normal way. We have determined that even lighter molecules can be trapped this way if provisions are made for cryofocusing on the column. We have demonstrated that, using liquid CO_2 expansion, with column temperature lowered to $-70^{\circ}C$, excellent peak shapes and separations can be obtained. These results are illustrated in the next section of the report.

It is also possible to do the flow matching in two steps, desorbing from a large 4 mm I.D. cartridge into a next step trap with a 2 mm I.D. After this smaller trap is loaded, it can be desorbed with a much smaller flow onto the GC column. The penalty associated with this approach is greater complexity in the plumbing and the extended time required for a single analytical cycle to be accomplished. Since light volatiles are not easily trapped, it would also be desirable to use a cryo-cooling system for this approach, also.

5. GC COLUMN-TO-MS INTERFACE

The outlet of the GC column in many capillary systems is introduced directly into the ion source. During development testing of the GC and concentrator system for this project, using a different MS, such a capillary direct interface was used. For the smaller diameter capillary columns, with their associated lower carrier gas flow rates, most vacuum systems can be conveniently sized to handle the gas load from such an interface without degrading the performance of the MS. The current ion source for the tandem MS is quite sensitive to source pressure increases and it appears that further attention will need to be given to this problem. There are two avenues that are readily available, one is to open the source and allow better conductance between the interior of the source and the pumped volume. Another is to provide a splitter or separator to reduce the flow of carrier gas and sample to the source. There are several possibilities, from a simple open-split interface to a more elaborate jet separator or Watson-Biemann separator that requires a separate vacuum pump. The benefit of a direct capillary inlet is that all of the sample that is transferred to the column is made available to the ion source and this is likely to result in the maximum sensitivity. If one of the separators is used, there is inevitably some sample loss from molecules that are pumped away along with the carrier gas. The better designed versions of these separators tend to capture the sample molecules preferentially and split off the usually lighter carrier gas molecules so that there is an enrichment of the sample-to-carrier gas ratio which can make up somewhat for the sample loss. The net result is that larger column diameters can be used for a given vacuum pumping capacity and source, and this larger diameter column allows larger amounts of sample to be deposited on the column, so better detections can be made. In many cases where the amount of sample is not the limiting factor, better overall performance can be realized with a splitter and larger column.

6. MS-I TO MS-II INTERFACE

As pointed out in the discussion of subsystems design and performance, the issue of interstage fragmentation was the subject of considerable theoretical and experimental work. One of the advantages that was attributed to the McSID approach was enhanced daughter ion intensities for a given parent ion beam. It may be possible to make use of this approach but additional work would need to be carried out on lens systems and avoidance of contamination both of which were problem areas that developed. It seem likely that without appreciable investment McSID could not be readied for a space system. The alternative that we chose, SID is well-suited to a compact system and therefore deserves continued attention.

The experimental housing that was used to perform the MS-I tests was replaced by a larger housing, described earlier, and this developmental platform was used to conduct the integrated system tests for MS-I, the SID interstage, and MS-II. The SID surface was mounted so that it was electrically isolated from the case and could be either grounded to the case or operated at a higher or lower potential to provide information on the possible benefit that might be achieved by operating with a potential on the plate. The SID plate was mounted on a moveable rod that could be moved in and out of the ion beam or rotated slightly when in the beam to seek an optimum signal output. In future work, it would be desirable to have a mechanism that could vary the angle the plate makes with respect to the ion beam in order to fine tune the output daughter ion intensity, also.

The location of the MS-II electric sector was carried out using a flat mounting plate that was fastened to the vacuum envelope. This approach allowed each component to be referenced to specific points that were common to MS-I and the SID interstage. Since the vacuum envelope remains rigid during operation and has a precision sealing surface, it constitutes a highly reproducible setting for the mounting plate and for other components. The experimental chamber for the system had an observation window to ensure that components maintained their proper positioning as an added check. The second stage MS electric sector was first mounted to a support plate as described in an earlier section, using the ruby spheres and this assembly was then positioned on the mounting plate in the experimental chamber. Tests of the system were typically conducted with two detectors, one mounted in the normal detector position for MS-I and one mounted at the outlet of MS-II.

7. COMPUTER-TO-SYSTEM INTERFACE

The first tests with subsystems and the system as a whole were conducted with manual controls and manual adjustments of variables. At the system level, a software approach was established and a conceptual framework developed. We determined that the time and funds available would not support a full new development of system control, operation, data acquisition and data analysis software. To give us the most functionality in the least amount of time, we therefore discarded our early efforts to write an entirely new package based upon a XENIX operating system. Instead, we worked in MS-DOS, although we recognized the limitations of this system, because of the ability to draw upon a number of existing pieces of software that had already been developed for this system. Included in this package are a number of such pieces and particularly a part of Chemstation from Hewlett Packard, which, like MS-DOS is part of the framework upon which our software is built. Our choice of WINDOWS for display and other functions, follows the direction of most present-day analytical instrument systems, and results in a user-friendly interface. Given these basic system decisions, the software was generated to meet a hardware system design that gradually evolved from the early development testing and subsystems work to its current form. Since the GC and the sampling systems matured much quicker than the tandem MS, this portion of the software was completed while the details of MS operation were yet to be established. Like many systems, software development is a continuing task, and the principal object of the current package is to establish the foundation on which we recommend any further development should build.

PART III. RESULTS AND ESTIMATES OF TECHNICAL FEASIBILITY

In reporting on the work performed under this contract, and in explaining the technical paths taken and not taken there has already been considerable discussion of results obtained. This section, then will not dwell on points made previously, but will focus on output data and its relevance to future work. The title of this section includes the phrase "estimates of technical feasibility." This was taken directly from the contractual documents for this project as a requirement for the final report. Where the technical feasibility of converting a particular component into one that is suitable for spaceflight is a potential issue it will be pointed out.

Some results can be illustrated with spectra and traces of total ion current, and where this was possible, typical sample runs are shown. Other results are not so easily presented, since they may be observations of system performance, results of leak checking, temperature, pressure or other transient readings. In this report, we will focus on the former output, but it should be emphasized that many hours of monitoring and testing where such output is not readily available lie behind each of the runs that are shown. In the following sections, the results will be presented in terms of end performance of the system or subsystem.

A. ABILITY TO SAMPLE DIRECTLY FROM THE ATMOSPHERE

The system was designed to take a mixture of air and one or more trace contaminants, collect this sample and then transfer it to the analyzer in a controlled manner for subsequent detection and identification. The classes of compounds that are of interest may be inferred from the listing of compounds that need to be detected by the Trace Contaminant Monitor (TCM) planned for the space station. This listing is included as Figures 45 and 46, which also indicates the concentration range that should be detected. Note that the range of interest for most of the compounds is tens of parts-per-million. The lowest detection requirement applies to only 6 compounds from the list of some 200, and is specified as 20 parts-per-billion. With this in mind, we were quite pleased with the performance of our direct sampling system with membrane inlet when challenged with examples of typical trace contaminants. We conducted two types of validation tests during the development of our membrane system, one with relatively high concentration in the ppm range and another in the low ppb range. For example, Figure 47 shows detection of 10 ppb of the hydrocarbon benzene, which is 5 times better than the lowest level specified for the TCM! Figure 48 is another example of direct MS sampling, in this case for a mixture of benzene, toulene and o-xylene showing the separation possible by looking at specific ions. Finally, a chlorinated hydrocarbon, Trichloroethylene, is shown in Figure 49. Obviously, from this work, it seems clear that the direct air sampling system is functioning in a relatively efficient manner to bring the sample into the MS from an ambient atmospheric sampling stream. Exhaustive testing of compounds on the TCM list was clearly beyond the scope of this contract, but we believe that this sampling system would meet the system requirements.

Chemical	Concentration Range, ppm[a]		
1. Alcohols			
Allyl alcohol	0.3	to	0.5
n-Amyl alcohol	18	to	35
Isobutyl alcohol	20	to	40
n-Butyl alcohol	20	to	40
sec-Butyl alcohol	20	to	40
tert-Butyl alcohol	20	to	40
Cyclohexanol	15	to	30
Ethyl alcohol	25	to	50
Ethylene glycol	25	to	50
2-Hexyl alcohol	20	to	40
Methyl alcohol	20	to	40
Octyl alcohol	20	to	40
Phenol	1	to	2
n-Propyl alcohol	20	to	40
Isopropyl alcohol	20	to	40
2. Aldehydes			
Acetaldehyde	15	to	30
Acrolein	0.02	to	0.05
Benzaldehyde	20	to	40
Butyraldehyde	20	to	40
Crotonaldehyde	0.3	to	0.6
Formaldehyde	0.05	to	0.1
Furfural	1	to	2
Propionaldehyde	20	to	40
Valeraldehyde	15	to	30
3. Aromatic hydrocarbons			
Benzene	0.05	to	0.1
Cumene	7.5	to	15
Decalin	1	to	2
Ethylbenzene	10	to	20
1,2-Ethylmethylbenzene	2	to	5
Indene	1	to	2
Mesitylene	2	to	3
Methyl styrene	15	to	30
Naphthalene	1	to	2
Propylbenzene	5	to	10
Pseudocumene	2	to	3
Styrene	5	to	10
Toluene	10	to	20
m-Xylene	10	to	20
o-Xylene	10	to	20
p-Xylene	10	to	20
4. Esters			
n-Amyl acetate	15	to	30
n-Butyl acetate	20	to	40
Cellosolve acetate	15	to	30
Ethyl acetate	25	to	50
Ethyl formate	15	to	30
Ethyl lactate	20	to	40
Isobutyl acetate	20	to	40
Isopropyl acetate	25	to	50
Methyl acetate	20	to	40

Chemical	Concentration Range, ppm[a]		
Methyl butyrate	10	to	20
Methyl methacrylate	12	to	25
n-Propyl acetate	20	to	40
5. Ethers			
2,5-Dimethylfuran	0.02	to	0.04
m-Dioxane	2	to	5
Ethyl butyl ether	40	to	80
Ethyl ether	40	to	80
Furan	0.02	to	0.04
2-Methylfuran	0.02	to	0.04
Methyl vinyl ether	25	to	50
Isopropyl ether	25	to	50
Tetrahydrofuran	20	to	40
HYDROCARBONS			
6. Chlorocarbons			
Butyl chloride	20	to	40
Carbon tetrachloride	1	to	2
Chloroacetone	0.02	to	0.05
Chlorobenzene	5	to	10
Chloroform	0.5	to	1
o-Dichlorobenzene	2	to	5
Ethyl chloride	50	to	100
Ethylene chloride	5	to	10
Ethylidene chloride	12	to	25
Isopropyl chloride	42	to	85
Methyl chloride	10	to	10
Methyl chloroform	15	to	30
Methylene chloride	12	to	25
Perchloroethylene	2	to	5
n-Propyl chloride	15	to	30
Propylene dichloride	5	to	10
beta-Trichloroethane	0.5	to	1
Trichloroethylene	0.05	to	0.1
Vinyl chloride	0.05	to	0.1
Vinylidene chloride	1	to	2
7. Chlorofluorocarbons			
Chlorofluoromethane	25	to	50
Chlorotrifluoroethane	50	to	100
Chlorotrifluoroethylene	50	to	100
Dichlorodifluoroethylene	12	to	25
Freon 11	50	to	100
Freon 12	50	to	100
Freon 21	2	to	5
Freon 22	50	to	100
Freon 112	50	to	100
Freon 113	25	to	50
Freon 114	50	to	100
Monochlorofluoroethylene	12	to	25
Freon FE 1301 (Halon 1301)	50	to	100
8. Fluorocarbons			
Freon 23	50	to	100
Perfluoroethylene	25	to	50

continued

Figure 45

Chemical	Concentration Range, ppm[a]		
9. Hydrocarbons			
Acetylene	250	to	500
Allene	25	to	50
Isobutane	50	to	100
n-Butane	50	to	100
1-Butene	100	to	200
cis-2-Butene	50	to	100
trans-2-Butene	50	to	100
1,3-Butadiene	50	to	100
Isobutylene	250	to	500
Citrene	50	to	100
Cyclohexane	30	to	60
Cyclohexene	30	to	60
Cyclopentane	30	to	60
Cyclopentene	30	to	60
Cyclopropane	30	to	60
n-Decane	20	to	40
1,1-Dimethylcyclohexane	12	to	25
trans-1,2-Dimethylcyclo-hexane	12	to	25
2,2-Dimethylbutane	12	to	25
n-Dodecane	20	to	40
Ethane	500	to	1,000
Ethylacetylene	40	to	80
trans-1-Methyl-3-ethylcyclo-hexane			
Ethylene	150	to	300
n-Heptane	25	to	50
l-Heptene	25	to	50
l-Hexene	25	to	50
n-Hexane	25	to	50
Isoprene	100	to	200
Methane[a]	1,350	to	2,700
Methylacetylene	125	to	250
2-Methyl-l-butene	250	to	500
Methylcyclohexane	8	to	16
4-Methylcyclohexene	50	to	100
Methylcyclopentane	8	to	15
3-Methylpentane	250	to	500
n-Nonane	30	to	60
1-Nonene	25	to	50
n-Octane	38	to	75
l-Octene	25	to	50
Isopentane	50	to	100
n-Pentane	100	to	200
1-Pentene	32	to	65
2-Pentene	32	to	65
Propane	250	to	500
Propylene	250	to	500
Tetradecane	25	to	50
1,1,3-Trimethylcyclohexane	12	to	25
2,3,4-Trimethylhexane	25	to	50
Undecane	25	to	50
10. Inorganic Acids			
Chlorine	0.2	to	0.3
Hydrogen chloride	0.5	to	1
Hydrogen fluoride	0.05	to	0.1
11. Ketones			
Acetone	150	to	300
Acetylbenzene	25	to	50
Cyclohexanone	8	to	15
Diisobutyl ketone	5	to	10
Mesityl oxide	5	to	10
Methyl butyl ketone	5	to	10
Methyl ethyl ketone	10	to	20
Methyl hexyl ketone	10	to	20
Methyl isobutyl ketone	10	to	20
Methyl isopropyl ketone	10	to	20
Methyl propyl ketone	10	to	20
Phorone	10	to	20
12. Mercaptans and Sulfides			
Carbon Disulfide	2	to	5
Carbon oxysulfide	2	to	5
Ethyl mercaptan	0.05	to	0.1
Ethyl sulfide	0.05	to	0.1
Hydrogen sulfide	1	to	2
Methyl sulfide	0.5	to	1
Methyl mercaptan	0.05	to	0.1
13. Nitrogen Oxides			
Nitric oxide	2	to	5
Nitrogen dioxide	0.2	to	0.5
Nitrogen tetroxide	0.2	to	0.5
Nitrous oxide	250	to	500
14. Organic Acids			
Acetic acid	2	to	3
Butyric acid	2	to	5
Caprylic acid	12	to	25
Propionic acid	2	to	5
Pyruvic acid	0.5	to	1
Valeric acid	12	to	25
15. Organic Nitrogens			
Acetonitrile	2	to	4
Carbodiimide	0.4	to	0.8
1,1-Dimethyl hydrazine	0.05	to	0.1
Indole	0.05	to	0.1
Monomethyl hydrazine	0.02	to	0.04
Skatole	0.05	to	0.1
16. Miscellaneous			
Amonia	12	to	25
Carbon monoxide(a)	12	to	25
Hexamethylcyclotrisiloxane	12	to	25
Hydrogen(a)	1,500	to	3,000
Hydrogen cyanide	0.5	to	1
Sulfur dioxide	0.5	to	1

Figure 46

File: C:\CHEMPC\DATA\DIRECTMS\BENZ.R\BENZ-2.D
Operator: Brian
Date Acquired: 19 Sep 91 12:50 pm
Method File: acqmeth.m
Sample Name: Benzene
Misc Info: 10 ppbv Tedlar bag into sample inlet
ALS vial: 1

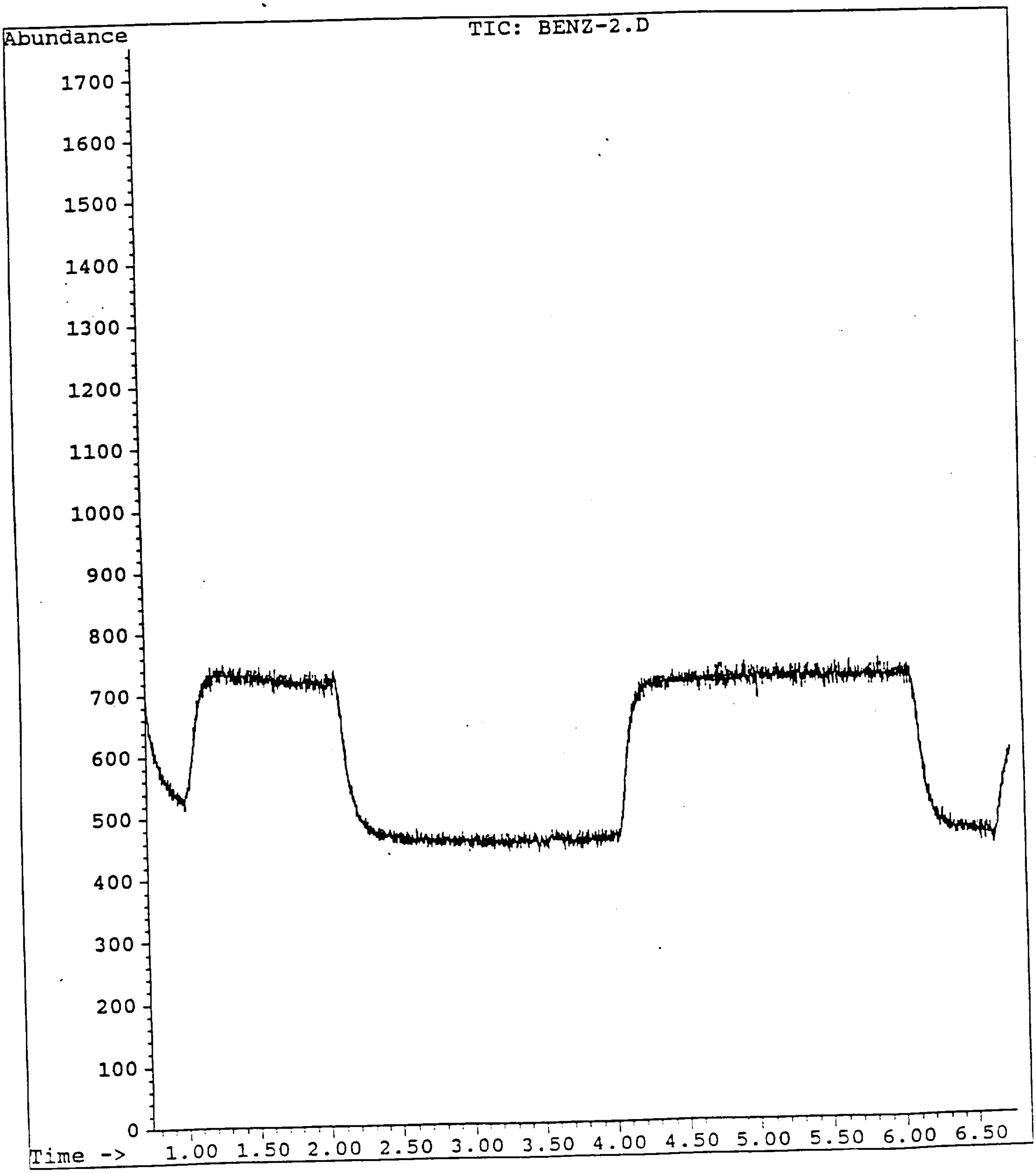


Figure 47

File: C:\CHEMPC\DATA\SNAPMS\BTX.R\BTX-1.D
Operator: Brian
Date Acquired: 19 Sep 91 11:54 am
Method File: acqmeth.m
Sample Name: Benzene, toluene and xylene mix
Misc Info: Headspace vapor sampled for<1 sec
ALS vial: 1

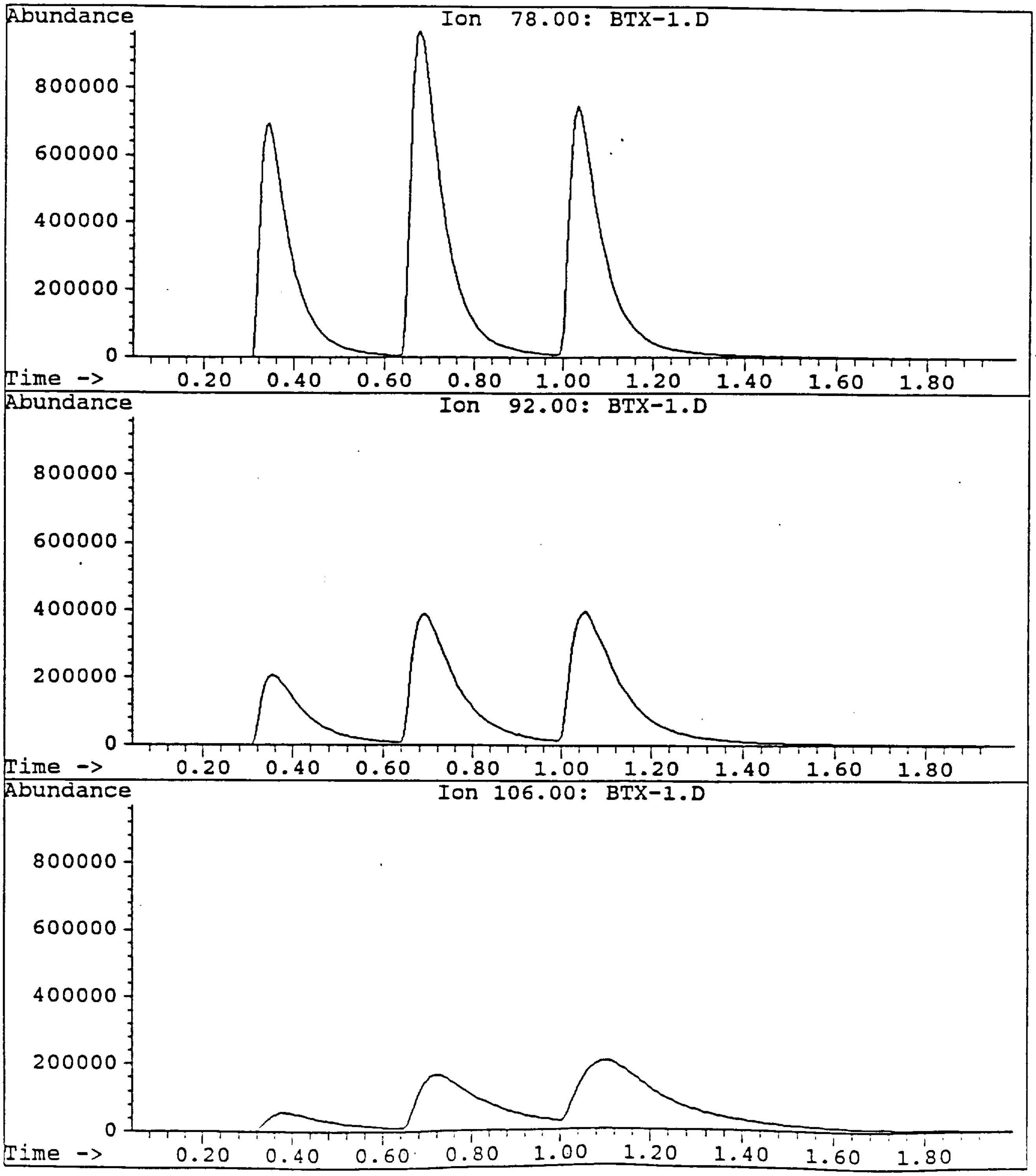
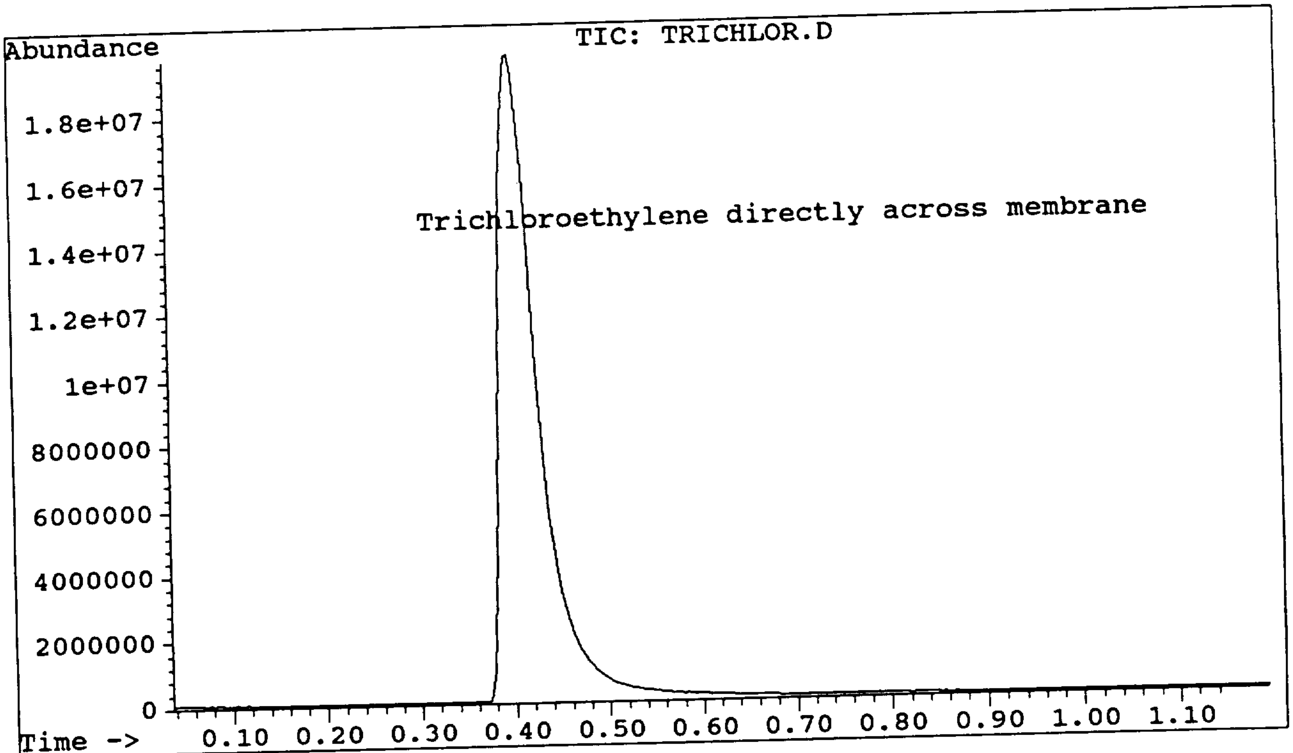


Figure 48

File: C:\CHEMPC\DATA\SNAPMS\STANDARD.R\TRICHLOR.D
Operator:
Date Acquired: 10 Apr 92 9:25 am
Method File: acqmeth.m
Sample Name:
Misc Info:
ALS vial: 1



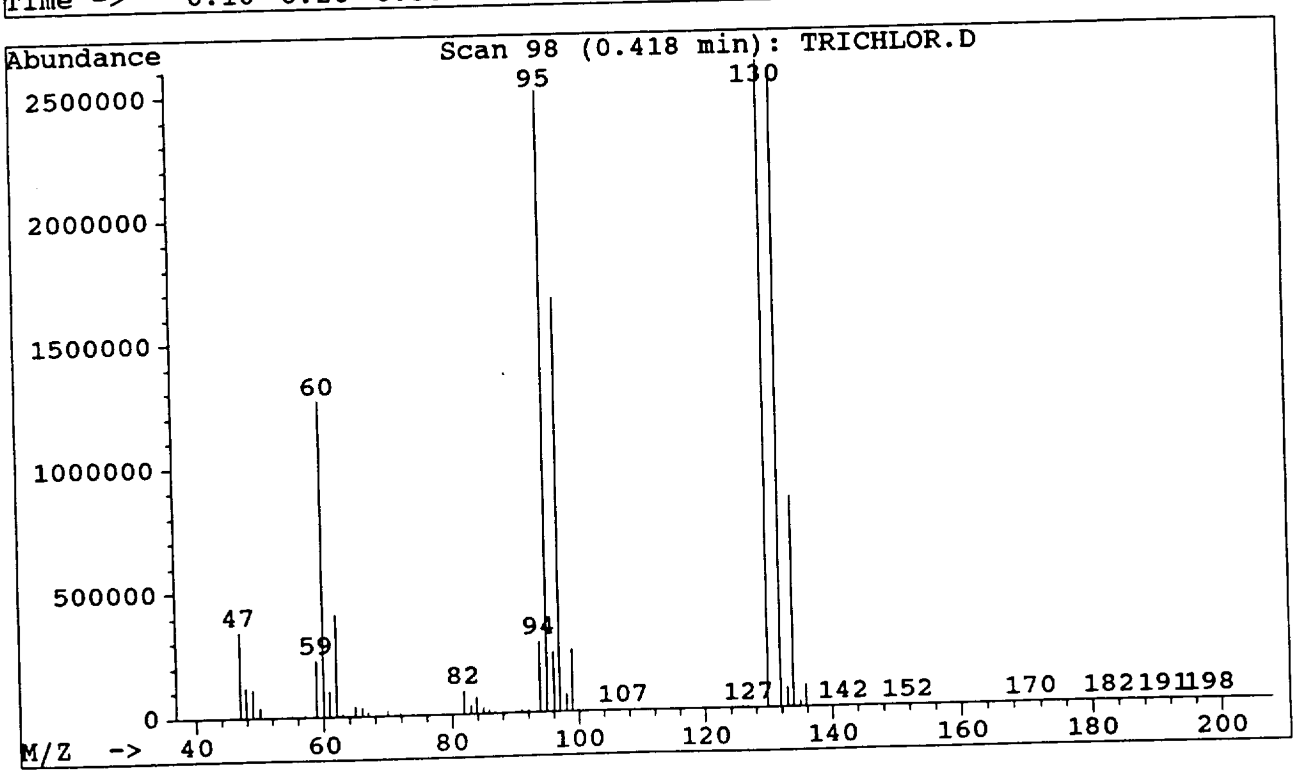


Figure 49

B. SAMPLE CONCENTRATION-TO-MS SAMPLING SYSTEM

The results from operation of the sample concentration cartridge when heated and desorbed to the membrane for direct detection by the MS demonstrate the effectiveness of first trapping and then desorbing samples to improve their detectability. The trapping agent that we used most often was Tenax, which is a good all-purpose sorbant. Other packings can be used depending upon the types of compounds that are principally of concern. The amount of time that a sample is collected can be varied, depending upon the concentration that is present and the minimum detection level that is desired. Figures 50 through 52 show the results of a set of analytical runs where the sample time was held constant at one minute, but the concentration of sample for a mixture of benzene (key ion 78.00 amu), toluene (ion at 92.00 amu), o-xylene (ion at 106 amu), and trichloroethylene (ion at 95.00 amu), in air, was varied from 100 ppb down to 1 ppb, about 10-20 times lower than the lowest limits specified for the TCM. The MS was not operated in its most sensitive mode, but it was still possible to make good detections at 1 ppb for these compounds! The numerical data for the plot of the limits of detection for these sampling conditions is shown in Table 2. These results were also reported in a paper presented at the 1992 Pittsburgh Conference on Analytical Chemistry and Related Topics, the major analytical chemistry conference in the U.S.

C. SAMPLE CONCENTRATION-TO-GC SAMPLING SYSTEM

The concentration and subsequent thermal desorption possible with the cartridge was demonstrated successfully, as illustrated by the sample runs shown in the previous section. Transfer to the GC column for a full GC run with detection by an MS, presents a new set of conditions. The major characteristics of the detected Total Ion Current (TIC) signal that need to be monitored in this run type are the peak widths-- are they relatively sharp and well-defined?--the signal-to-noise-- is the peak clearly identifiable above any noise spectra?-- and the peak shape-- is there excessive tailing or fronting? Figure 53 shows a typical chromatogram, obtained in this case by drawing a sample for 1 min. from the headspace above some contaminated well water and then desorbing the cartridge at 175°C. for 0.5 min. The GC column was held at 30°C. for 1 min. then ramped to 100°C. at 5 degrees per min. This is an example of real-world performance in a sampling situation that might be typical of a case where an on-board water tank in the spacecraft was being monitored for potential contamination. Note the well-resolved peaks with nearly gaussian shape and differentiation from the background, even for a compound present in ultra-trace amounts (below 1 ppb). This data was later confirmed independently. Numerous other examples can be shown to illustrate the performance of the concentration-to-GC-to-MS interface. Figures 54 through 56 are typical of the results of this testing. Our conclusion is that the design of the desorber and the connection to the GC column provides an efficient transfer of sample between these two components with sufficient sensitivity to be suitable for spacecraft use.

File: C:\CHEMPC\DATA\SCONMS\PITT92A.R\25A.D
Operator: hardesty
Date Acquired: 25 Feb 92 2:39 pm
Method File: acqmeth.m
Sample Name: 25 ppb vol
Misc Info: Run 1
ALS vial: 1

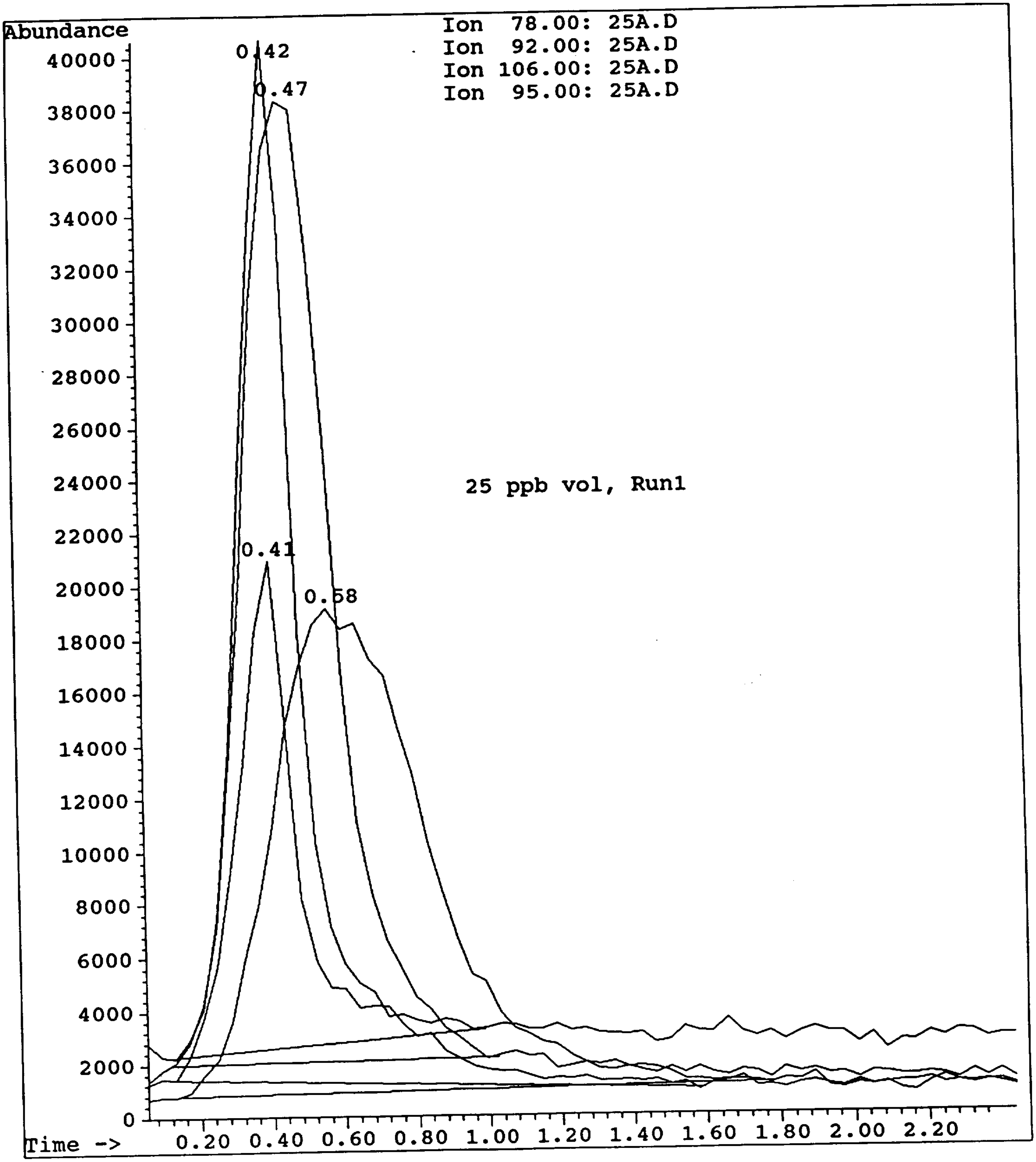


Figure 50

File: C:\CHEMPC\DATA\SCONMS\PITT92A.R\1A.D
Operator: hardesty
Date Acquired: 24 Feb 92 8:11 pm
Method File: acqmeth.m
Sample Name: 1 ppb vol
Misc Info: Run1
ALS vial: 1

0.40 = Benzene
.42 = Toluene
.54 & .71 = o-xylene
TCE

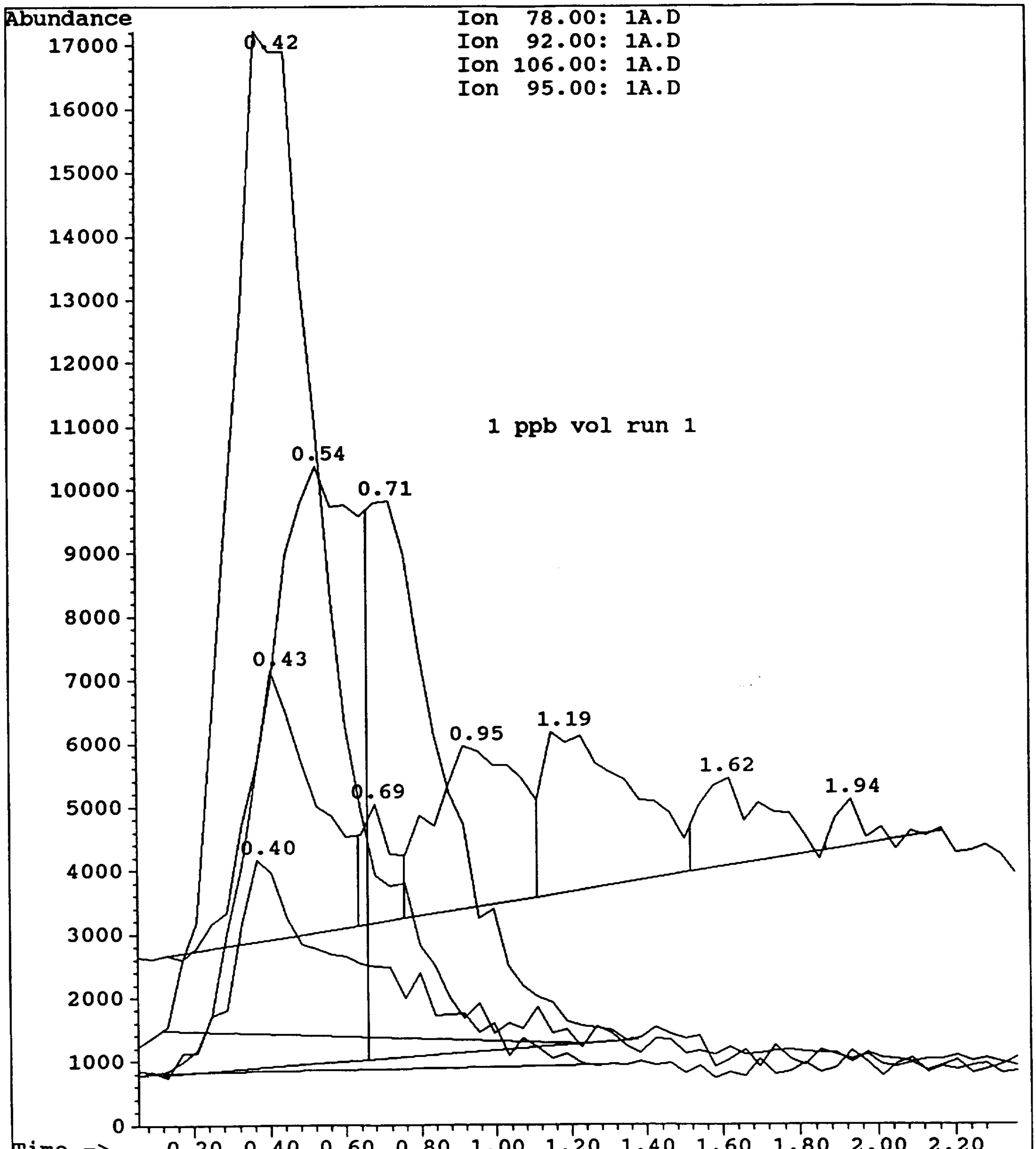


Figure 51

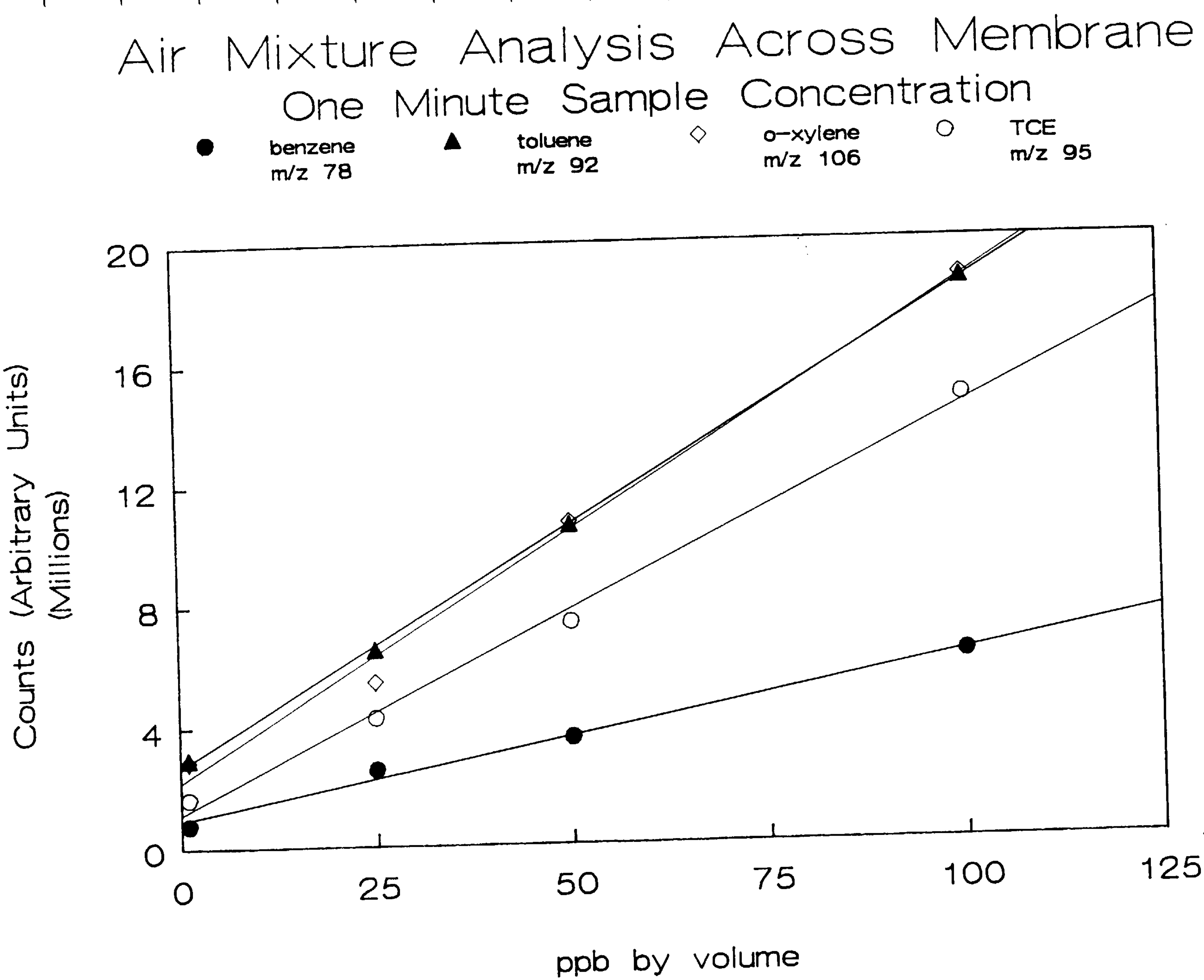
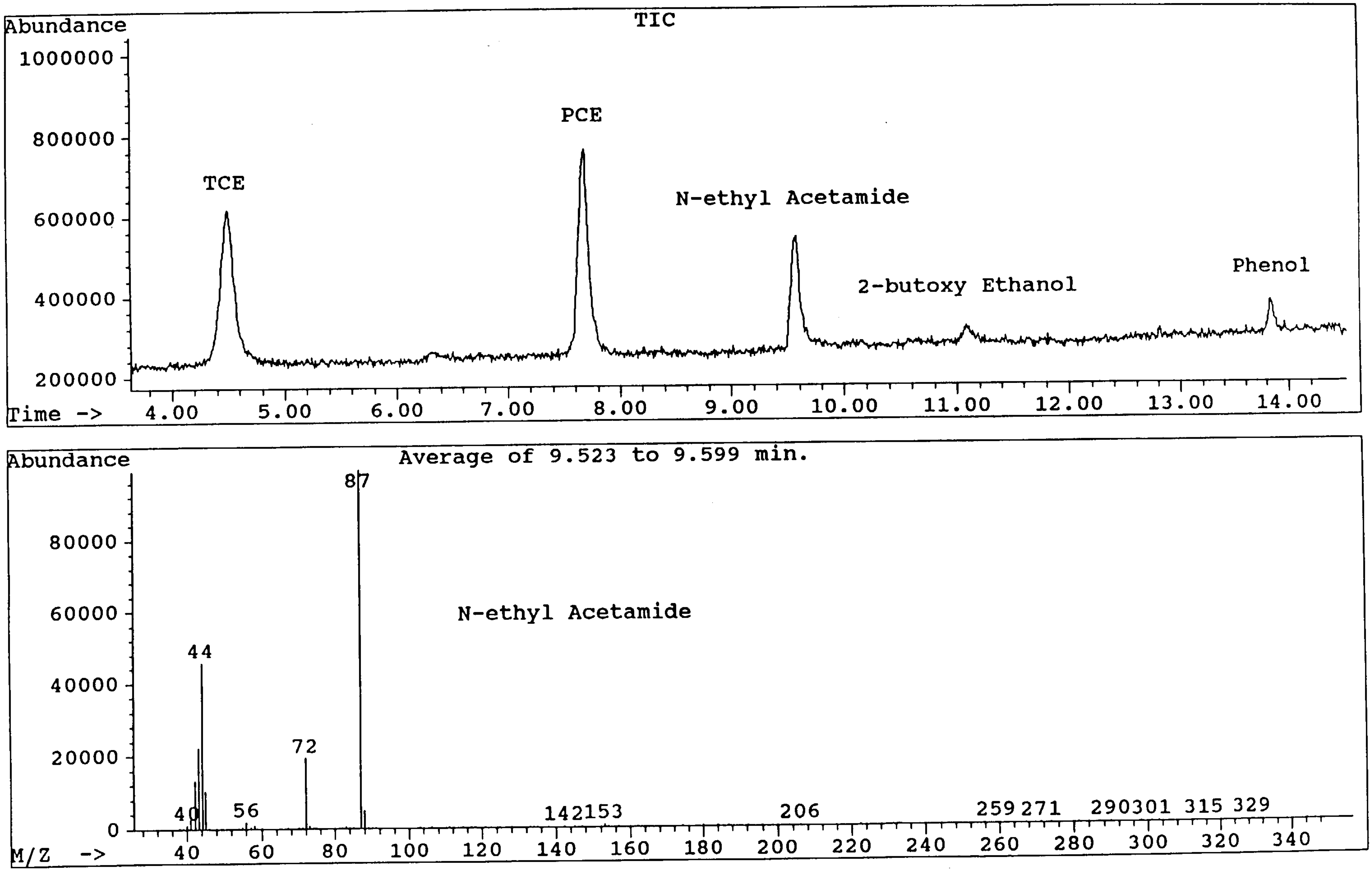

Air Mixture Analysis Across Membrane
One Minute Sample Concentration
benzene m/z 78
toluene m/z 92
o-xylene m/z 106
TCE m/z 95
Counts (Arbitrary Units) (Millions)
20
16
12
8
4
0
0
25
50
75
100
125
ppb by volume

Figure 52

TABLE 2

Sample Concentration MS Cycle

Analyte	Mixture Analysis 1	2	3	Mean	Std. Dev.	RSD	ppbv
Benzene	788,639	780,499	684,175	751,104	58,105	7.7%	1
Toluene	2,907,713	2,925,171	3,052,523	2,961,802	79,049	2.7%	1
O-xylene	2,903,793	2,876,232	2,804,326	2,861,450	51,354	1.8%	1
TCE	1,630,836	(2,026,737)	1,323,944	1,660,505	352,334	21%	1
Benzene	2,776,823	2,425,451	2,397,435	2,533,237	211,415	8.4%	25
Toluene	6,379,009	6,582,894	6,585,701	6,515,868	118,531	1.8%	25
O-xylene	5,521,553	5,378,653	5,431,327	5,443,844	72,267	1.3%	25
TCE	4,181,222	4,663,977	4,018,536	4,287,911	335,686	7.8%	25
Benzene	3,584,969	3,581,418	3,358,298	3,508,228	129,855	3.7%	50
Toluene	10,725,007	10,770,160	10,253,038	10,582,735	286,417	2.7%	50
O-xylene	10,924,165	10,772,574	10,354,171	10,683,636	295,221	2.8%	50
TCE	7,277,051	7,367,901	7,468,506	7,371,152	95,768	1.3%	50
Benzene	6,186,998	5,878,794	6,420,042	6,161,944	271,492	4.4%	100
Toluene	18,793,319	18,136,347	18,955,496	18,628,387	433,766	2.3%	100
O-xylene	19,251,715	18,298,467	18,623,778	18,724,653	484,564	2.6%	100
TCE	14,589,609	14,307,198	15,343,995	14,746,934	536,004	3.6%	100



Abundance
TIC
1000000
800000
600000
400000
200000
TCE
PCE
N-ethyl Acetamide
2-butoxy Ethanol
Phenol
Time ->
4.00
5.00
6.00
7.00
8.00
9.00
10.00
11.00
12.00
13.00
14.00
Abundance
Average of 9.523 to 9.599 min.
80000
60000
40000
20000
0
N-ethyl Acetamide
87
44
72
40
56
142153
206
259 271
290301 315 329
M/Z ->
40
60
80
100
120
140
160
180
200
220
240
260
280
300
320
340

Figure 53

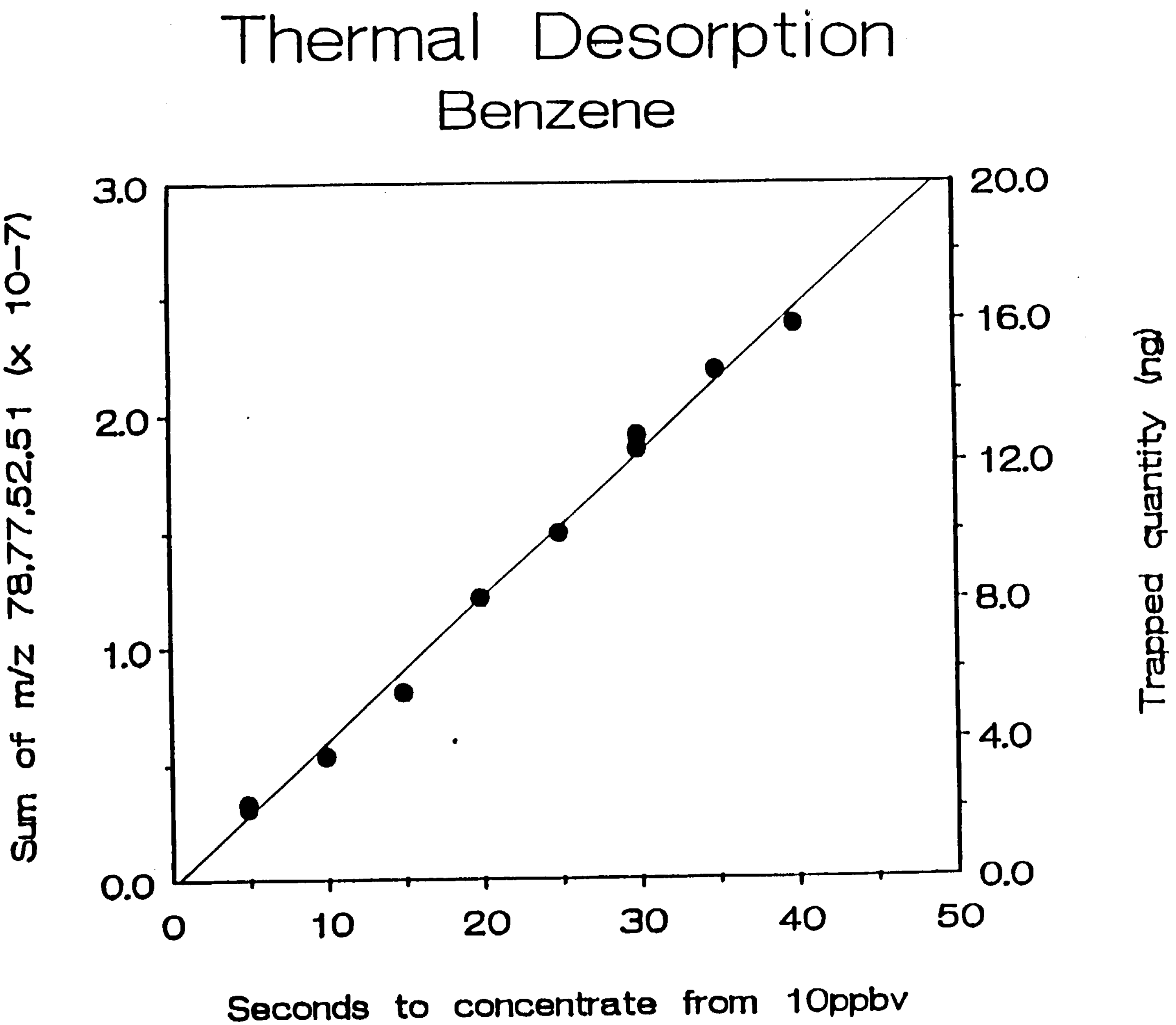
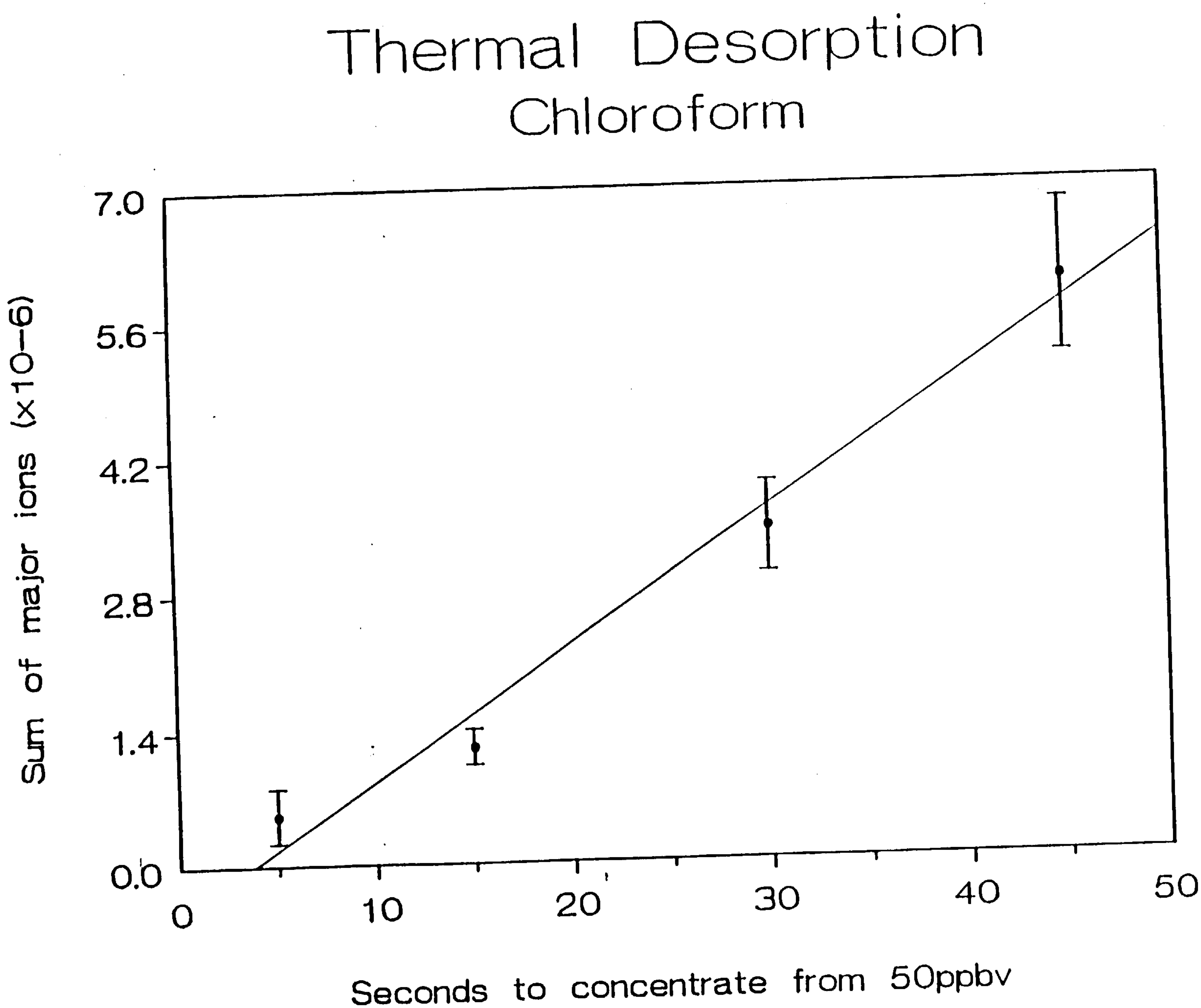

Thermal Desorption
Benzene
3.0
2.0
1.0
0.0
20.0
16.0
12.0
8.0
4.0
0.0
0
10
20
30
40
50
Sum of m/z 78,77,52,51 (x 10−7)
Trapped quantity (ng)
Seconds to concentrate from 10ppbv

Figure 54



Thermal Desorption
Chloroform
Sum of major ions (x10−6)
7.0
5.6
4.2
2.8
1.4
0.0
0
10
20
30
40
50
Seconds to concentrate from 50ppbv

Figure 55

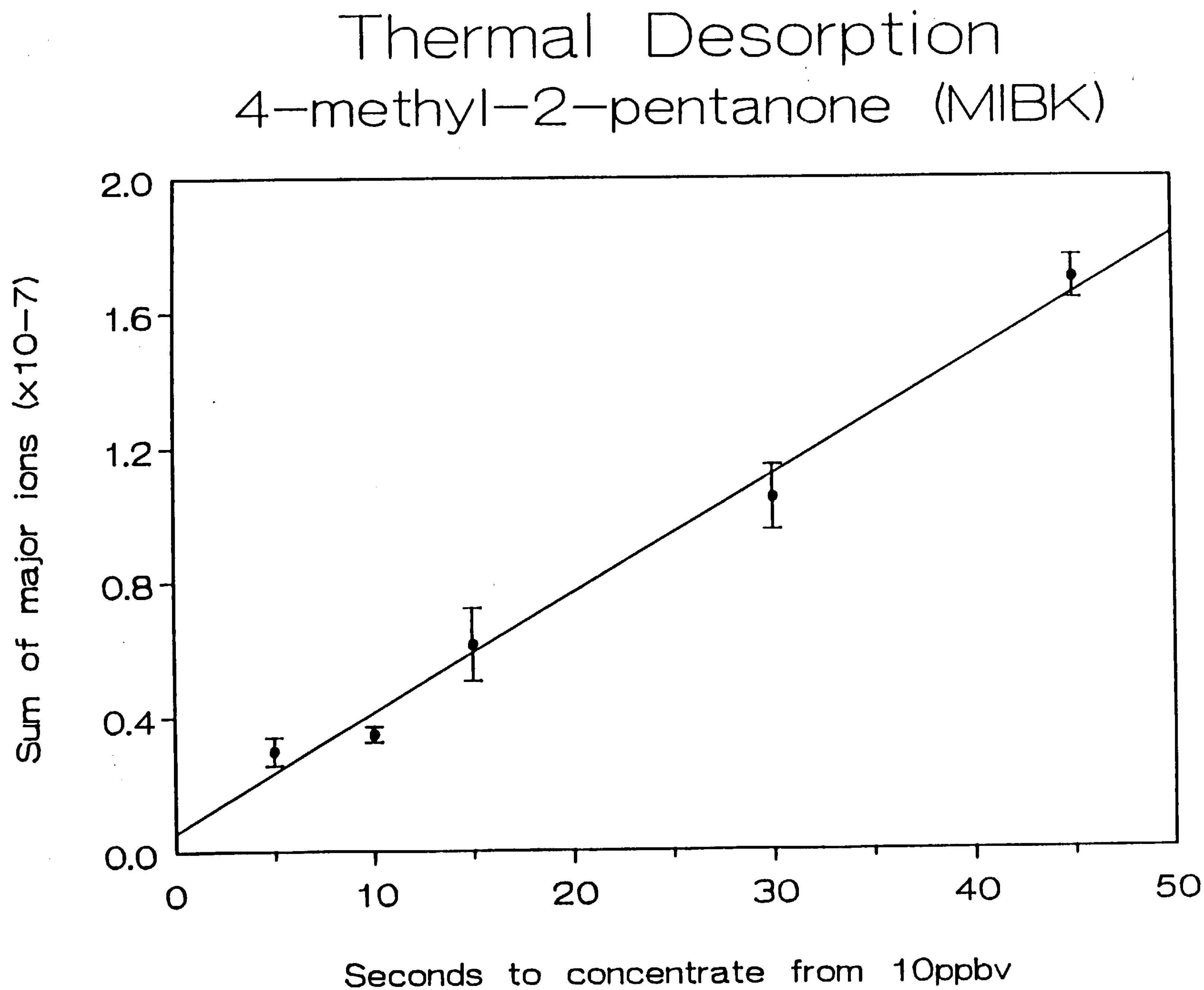

Thermal Desorption
4-methyl-2-pentanone (MIBK)
Sum of major ions (x10-7)
2.0
1.6
1.2
0.8
0.4
0.0
0
10
20
30
40
50
Seconds to concentrate from 10ppbv

Figure 56

As indicated earlier, there are supplemental capabilities that could be added to this interface that would extend the performance, particularly to improve retention and separation of light volatiles. This would involve cooling a portion of the GC column. For experimental purposes, we have tested a system for cooling the column that uses the rapid expansion of a liquified gas such as one of the Freons or preferably CO_2. However, neither of these gasses could be released into the atmosphere of a closed spacecraft such as the space station so it would be necessary to use another cooling means. It is possible that connection with a radiator into the space environment outside the station could be used via a heat pipe to provide such cooling. Alternatively, thermoelectric cooling could be used or a small cryostat. We have tested a small thermoelectric cooling system with two stages that can lower the temperature from ambient by about 40 degrees, given losses between stages and other losses to the atmosphere. This was not enough to give good chromatography, but it did illustrate that such cooling might be technically feasible in a more developed system, with perhaps three stages of cooling or more and better heat transfer characteristics.

D. MS-I AND MS-II

Development of MS-I involved a series of experimental hardware configurations, with different ion sources, different slits, different magnetic sector design and other modifications that were intended to move the system toward better resolution, better signal-to-noise, higher mass detections, and better stability. The full range of potential refinements were not pursued because of the limited funds available for more advanced experimentation. The system has shown that it is capable of excellent definition, as can be seen from the background scan shown in Figure 57. Note that, as shown earlier, the apparent separation between peaks decreases as the mass of the ions increases. In this scan, the basic constituents are nitrogen, oxygen, carbon dioxide, argon, and water vapor, all in trace amounts, since the vacuum in the instrument at this time was about 10^{-7} Torr. In addition to the basic molecular ions for each of these compounds, there are the atomic species of each of the gasses and the isotopes of the atoms present. This trace was taken with a relatively slow response chart recorder, so the actual detail that may be pulled out of this spectrum is not necessarily fully revealed. The higher mass ions that are present are residual amounts of previous samples (benzene) and the calibrant (FC-43). Note that the gain on this trace is quite high, with all of the major peaks truncated by the detection circuitry. In normal operation, the system would be operated with these major peaks set at less than the maximum, with the result that some of the fine structure that is shown here would fade into the background and the spectrum would look more like the normal air background in an MS. Early MS ion profiles did not look as good. Figures 29 through 32 showed typical early stage developmental ion traces, with noise obviously a major contributor. The developmental process for MS-I was not carried to completion in the course of this contract, in view of time and cost limitations, but as is demonstrated, there was adequate resolution and sensitivity for it to be the first stage in a tandem instrument.

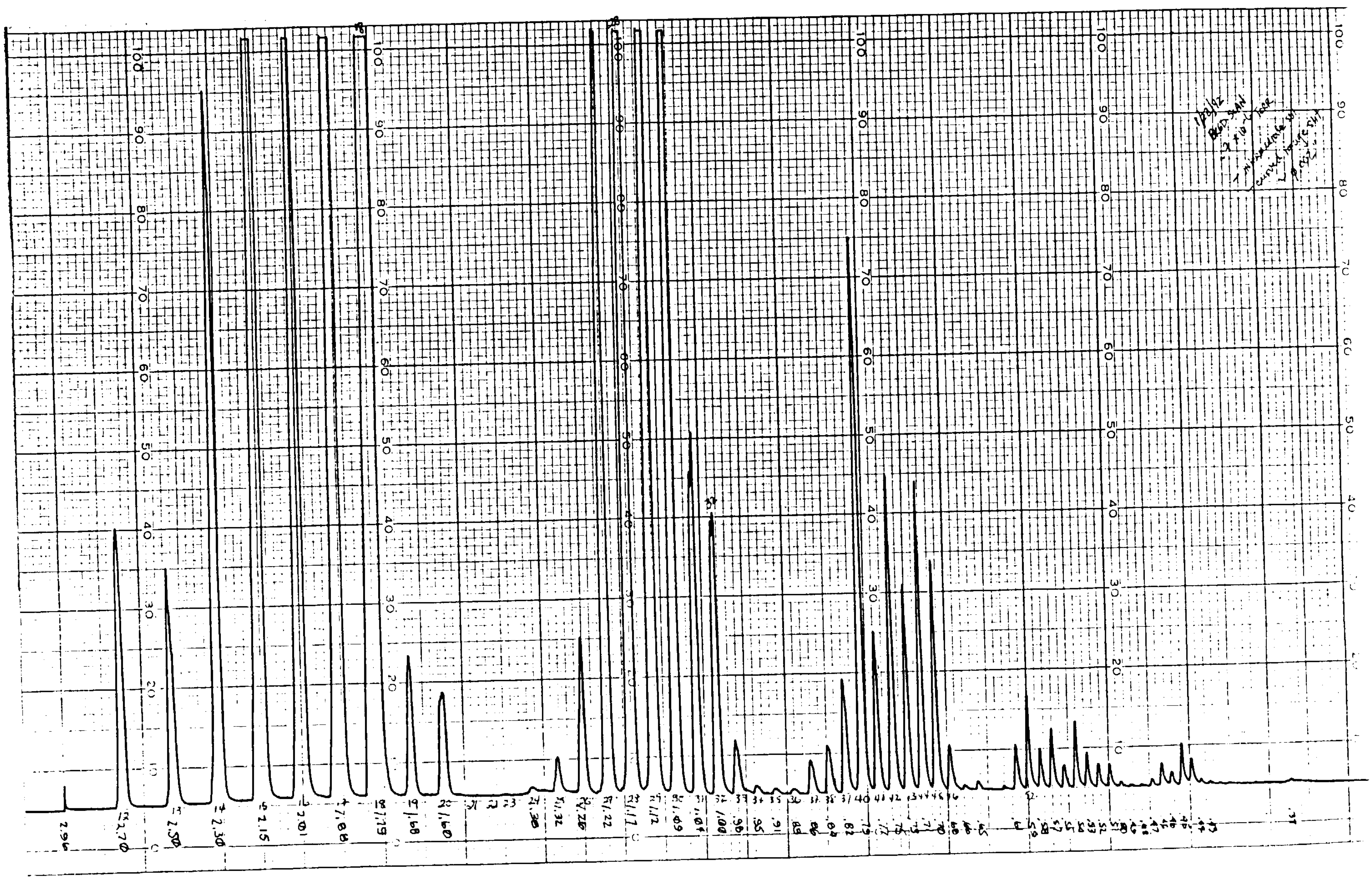


Figure 57

Additional improvements in the resolution of MS-I are possible in the future in connection with follow-on work toward space qualification. One possibility is to reduce slit widths, assuming that there is enough ion current to work with, and another avenue is to increase stability of the power supply for the ion source and electric sector. Other variables are not likely to yield significant changes in the observed performance. However, this level of discrimination between ions of different masses as it is currently demonstrated in MS-I is entirely adequate for tandem MS work, since the principal requirement is that the parent ion be unambiguously selected by MS-I and directed to the surface for fragmentation.

The results from MS-II operations were obtained for a single compound, CO_2, by following a series of steps sequentially through the exit from MS-I to the detector for MS-II. The compound that was chosen, CO_2, was illustrative only and it would be our recommendation that a more complete set of parent-daughter ions should be determined later as the system is more fully evaluated. The first step was to position the reflecting surface at the point of double focus and position the detector behind a modified extra-wide slit that was electrically isolated from other elements of the system. This permitted a potential to be applied to the surface as part of the experimental evaluation of its performance. In this evaluation of the surface performance, no spectrometry could be accomplished in the usual sense, since the detector should capture all of the reflected ions from the surface. The detector signal was monitored first with the surface withdrawn and then with the surface in position, and as expected, the ion current increased with the surface in position. The rotation of the surface about the axis of the rod on which is mounted also clearly indicated an optimal positioning and confirming the formation of daughter ions in a reflected ion beam. With the addition of a negative potential on the reflecting surface, better focusing of the reflected ions was achieved, confirmed by significantly increased ion current at the detector.

MS-II was then installed in place of the detector, leaving the collimating and accelerating slit in place in front of the electric sector, in order to observe the effects of an intermediate potential on MS-II. A number of daughter ion scans were carried out for MS-II, with Figure 58 being a typical example of detector output. The large number of signals present makes the interpretation of this daughter ion spectrum somewhat more difficult than would be expected. This, we believe is caused by surface effects from the reflecting surface of the interstage device. The rather large energies deposited by the incident ion beam cause sputtering of atoms at the surface. This is complicated by surface contamination that is common to such surfaces in a normal vacuum system, where an oil-lubricated forepump is used.

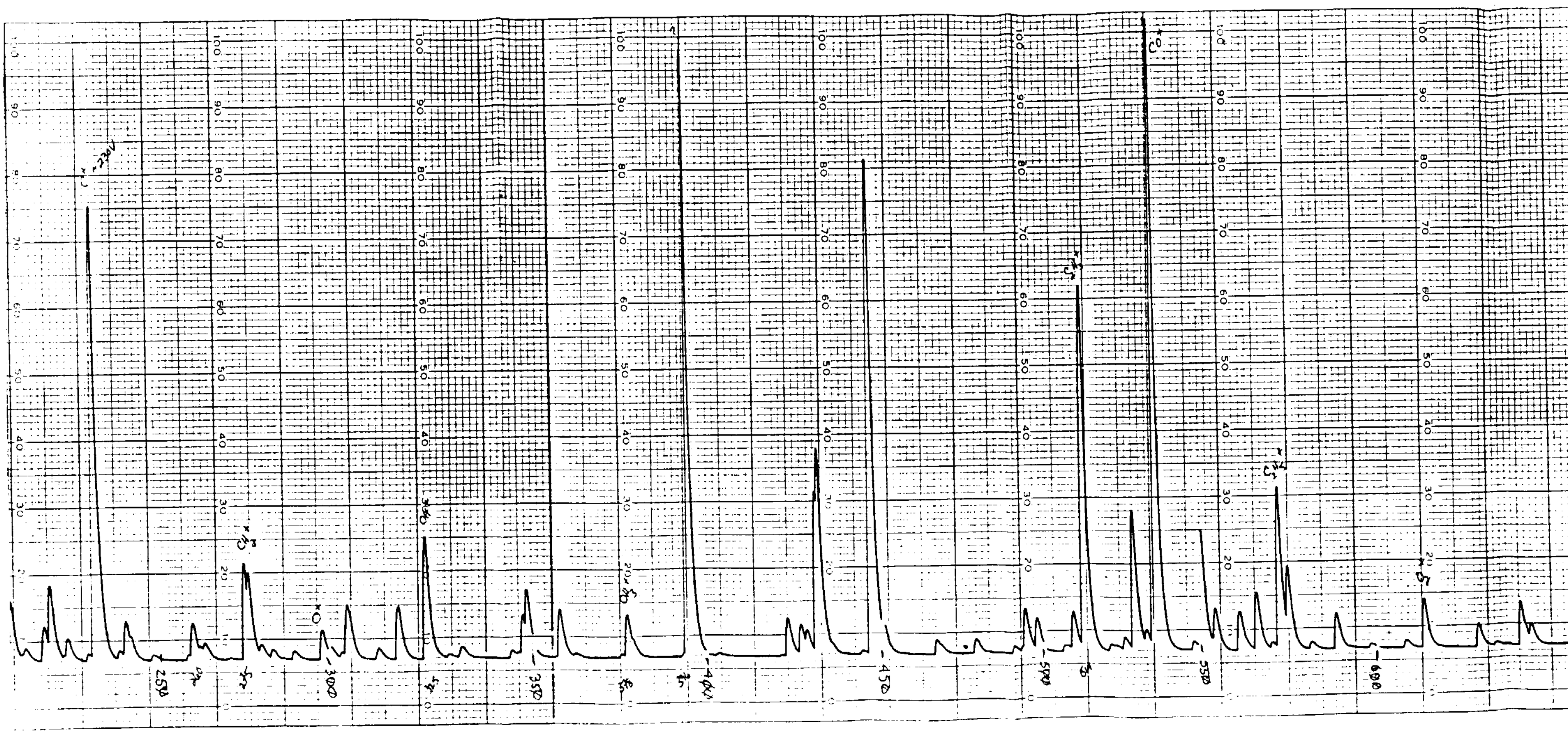


Figure 58

There are two approaches that we recommend be carried out next that should result in much less background signal in the daughter ion spectrum. One is to construct a dynamic lens system to take the parent ions and reduce their incident translational energies as they impact the reflecting surface to the range of 50-100 eV, thus reducing any sputtering effects and also reducing the internal energy transferred to the parent ions, giving better daughter ion patterns. The second step is to use an oil-free pumping system, so that the reflecting surface can be made ultra-clean and stay that way for extended periods in the vacuum system under normal operation. Recent advances in turbopumping systems, using a molecular drag stage in the pump, which allows a small, oil-free diaphragm pump to be used as a forepump, would permit a much cleaner vacuum system to be used. In the conceptual design of a follow-on system, this approach is adopted.

IV. PROJECT OVERVIEW

As the previous sections of this report have shown, Viking Instruments has carried out the tasks identified in this SBIR Phase II contract and, with the delivery of the items specified in the contract, completed its Phase II effort. It has produced an experimental prototype GC/MS/MS system, made a number of significant design improvements in several areas in the process of addressing the project objectives, and developed a conceptual design of a space-qualifiable system.

This project, extending over two years and including a significant period in which work was performed at no cost to the Government, has had a mixed impact upon Viking Instruments Corporation, as the SBIR contract award recipient. There have been a number of spin-offs and results from experimental work carried out under the contract that either influenced commercial designs or found their way into commercial products. In this regard, we see the SBIR work as having already achieved its purpose of stimulating new products and services that enter the marketplace and also serve to meet Government needs. The major product that has benefitted from this project has been the transportable GC/MS that we a currently selling commercially, the SpectraTrak 620. This system utilizes the dual-inlet concept, with membrane interface and capillary direct sample inputs. It is very rugged and compact, easily carried on an aircraft as baggage or in the trunk of a car, and resists rough handling or even being dropped on a hard floor from table top heights. It is capable of analytical laboratory-level performance, and will handle equally well both air samples and samples from water, either purge-and-trap or extracted. Figure 61 shows the SpectraTRak 620 on a roll-around cart for easy mobility in a localized area. The system is shown in its case, which serves as a protective shipping case and when closed, makes the system completely weatherproof. It can be operated equally well outside of the case.

With minimal modifications, it appears that this system could be space-qualified as a GC/MS system that would out-perform any currently planned sensors of which we are aware. The principal changes that we would make are replacement of the current turbopump with a pump that has a molecular drag stage and the addition of a small diaphragm pump. This modification is already being evaluated at Viking. It would serve to make the package even smaller and lighter weight, and would provide the advantages of oil-free operation with the ability to re-establish the vacuum after the system was opened for routine maintenance or repair--something an ion pump cannot do without some form of roughing pump. The second change would be replacement of the microprocessor and auxiliary boards with boards that were either already space-qualified or were assembled with mil-spec components and could be space-qualified easily. With these changes, the SpectraTrak 620 would be well on the way toward space-qualified design. More expert review of the various subsystems would be required as well as confirmation testing, but these do not appear to be major obstacles.

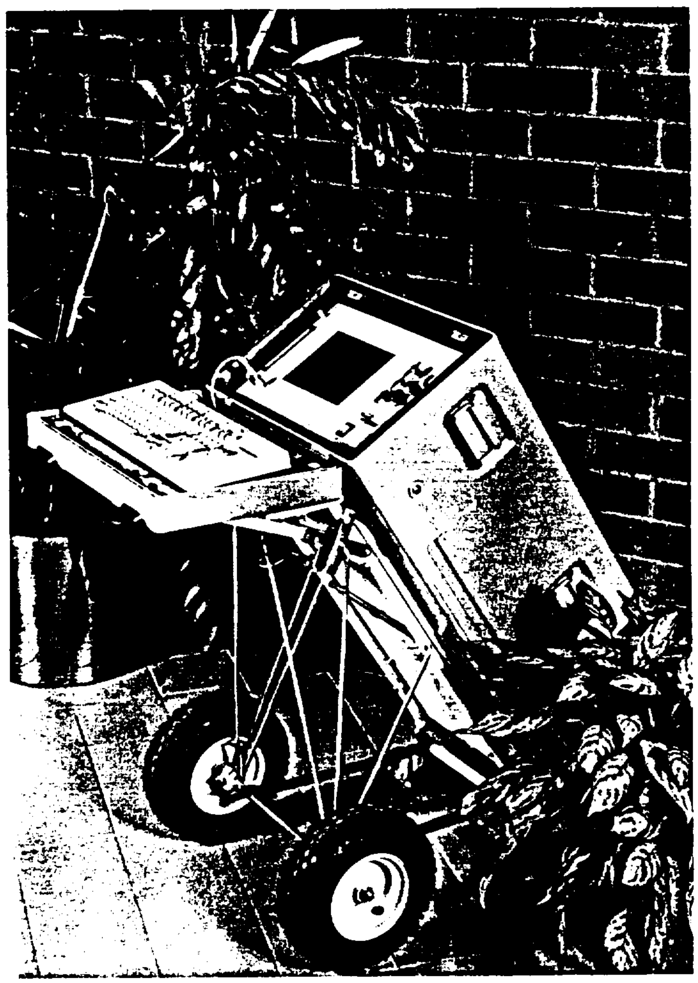


Figure 61

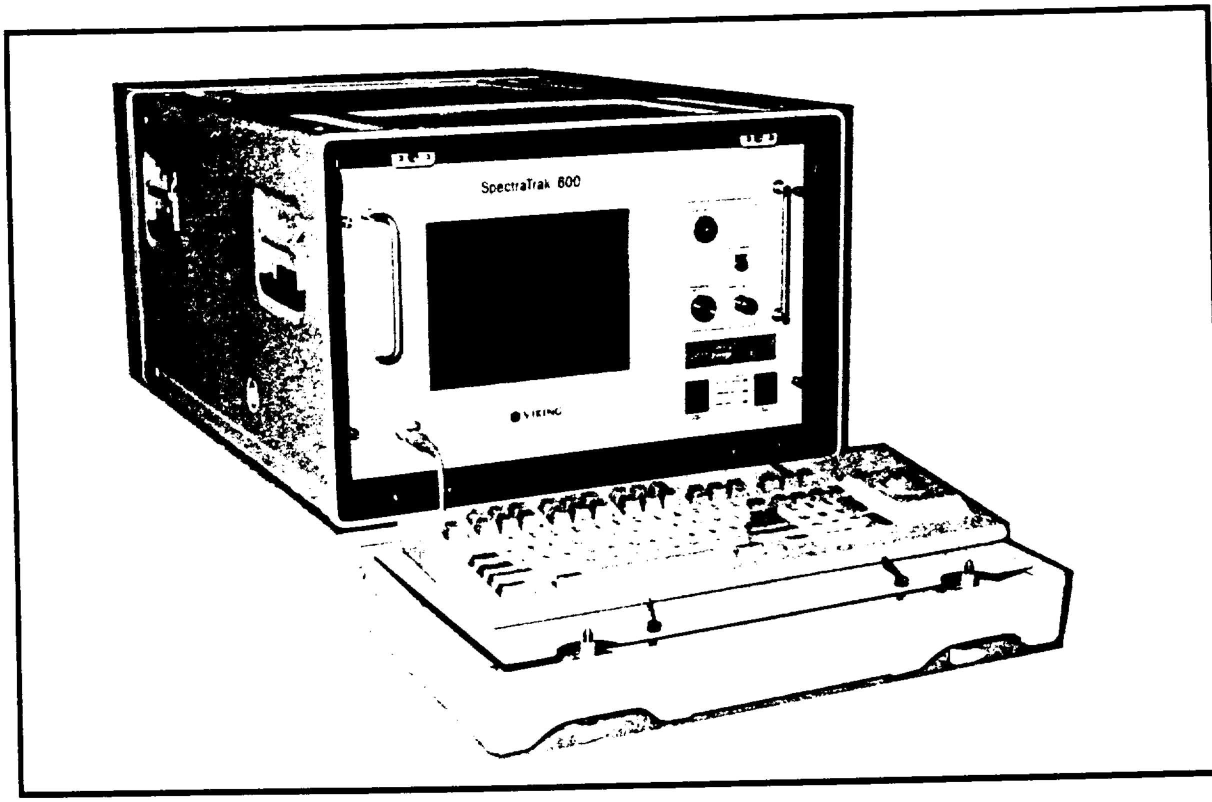
Finally, since the system has its own computer and operating system, it can generate outputs that are configured to match the spacecraft system in which it is mounted, can run either autonomously or via remote control from an external system (this functional capability has already been demonstrated), or can be operated by an astronaut from its front panel. The system is already made to fit into a 19 inch rack, so no change would be needed to fit it into one of the space station rack assemblies. Exhibit B gives a more complete set of system specifications for the SpectraTrak 620.

While the net effect of this SBIR project has been very positive, as illustrated by the SpectraTRak 620 development, one of the disappointing aspects has been the difficulty in identifying Agency interest in follow-on work to take this technology to a more developed stage. The direction of all of our efforts has been to operate within constraints that are consistent with a system intended for eventual space flight. With this in mind, it should be recognized that in carrying out the systems work, we were not completely free to choose the most direct technical solution but rather had to apply the constraints of space-compatibility as we worked out the least expensive or the least complex approach. There are some penalties involved in working on this basis that make the output less attractive as a commercial product. Thus, the obvious customer for a Phase III effort is NASA, while commercial interest in the output is tempered by the recognition that the system will have to be re-engineered, at least from a cost standpoint to be attractive as a commercial product. Therefore, it was very disappointing to receive the information that NASA was not in the practice of supporting follow-on effort--- in effect, Phase III work.

We believe that there are ways that would improve the contacts with program offices and thereby give greater opportunity for their recognition of the value of a particular SBIR project, and greater opportunity for the contractor to shape the project to maximize its utility to NASA. If this happens, it would follow that a certain number of Phase II projects would be picked up by a program office and brought to a greater state of maturity, and perhaps even made flight-ready. It is our recommendation that Phase II SBIR projects that have an obvious connection with a particular flight program office's interests have some sort of provision for communicating the nature of the SBIR work to the program office sometime before the end of the project, perhaps through a formal program review half-way through the project where representatives from the program office were present as well as the COTR and other interested parties. This would serve to bridge the gap between the technology offices and the program office interests for the SBIR contractor, would probably result in a better SBIR product, and would make it more likely that these technologies would be adopted by NASA.

VIKING
INSTRUMENTS CORPORATION

SpectraTrak™ 600 Transportable GC/MS



Field-Transportable GC/MS Opens New Horizons for Environmental and Industrial Users

Viking's analytical-grade SpectraTrak 600 gas chromatograph/mass spectrometer (GC/MS) is designed and built to meet the needs of transportable field operation. It is capable of atmospheric sampling plus direct sample injection and includes a miniaturized sample concentrator and thermal desorber, fully temperature-programmable GC, ruggedized MS, and high-performance microcomputer system adapted for harsh field conditions.

Shock-mounted in a weatherproof Mil-Spec transport enclosure, the SpectraTrak 600 can be readily transported by jeep or aircraft to your field site and set up in minutes for operation. With analytical performance comparable to the best benchtop GC/MS systems, the SpectraTrak 600 is unequaled in versatility and reliability for on-site environmental and industrial applications.

The SpectraTrak 600 is equipped with an internal IBM-AT™ compatible 80386 computer system and Viking's advanced SpectraScan/OS,™ providing integrated GC/MS instrument control, data analysis, and mass spectra matching under the Microsoft Windows graphical environment. Several mass spectra libraries are available, including NIST, Wiley, and Pfleger. The wide range of IBM-AT compatible upgrades and printer options supported by MS-Windows assures you of the computing power and flexibility that your application demands.

The SpectraTrak 600 gives you the freedom to perform definitive and sensitive GC/MS analysis and testing in the field, when and where you need it. Now, you can streamline your operations with cost-efficient sampling and real-time results; no more sampling bottlenecks and weeks of waiting for data. In addition, Viking's Express Service Program and LinkAge Field Area Network™ are available as options to back you up in the field with expert application and service support.

SpectraTrak™ 600 Transportable GC/MS

SPECIAL FEATURES

The SpectraTrak 600 introduces a number of unique innovations in field-transportable analytical instruments (patents pending):

- Complete GC/MS and data system shock-mounted in a weatherproof Mil-Spec transport case
- Genuinely user-friendly software with seamless GC/MS control and library search under MS-Windows environment
- Fully temperature-programmed GC for standard analytical methods and results
- Automated atmosphere sampling inlets for real-time monitoring and trace analysis
- Injection port for prepared soil, water, and solid samples
- Miniaturized and ruggedized components built for reliable field operation and service
- Low-speed rugged turbo-molecular pump for mobile operation, fast relocation, and high reliability.

SPECIFICATIONS

MASS ANALYZER:

Monolithic quadrupole mass filter with hyperbolic pole faces:
Mass Range: 10-650 amu
Scan Rate: 2000 amu/sec
Resolution: Unitary/mass range
Sensitivity: 1 ng of methyl stearate gives S/N >20:1 at m/z 298.3 when scanned at 380 amu/sec; with SIM mode, 10 pg of methyl stearate gives S/N of 10:1 at m/z 298.3 in 50 ms
Vacuum: 80-L/sec turbomolecular low-rpm vacuum pump with external roughing pump

GAS CHROMATOGRAPH:

Fully automatic temp-programmed mini-GC with capillary column:
Max. Temp.: 280 °C
Warmup Time: 10 min
GC Column: Microbore

SAMPLING INLETS:

Automatic atmosphere and injector ports with temperature control, concentrator, and sampling pump:
Air Port: Split capillary molecular leak and capillary direct MS inlets
Injector Port: Split or splitless on-column injection
Concentrator: Front-loaded cartridge and thermal desorber

COMPUTERS:

Internal IBM-AT compatible 80386 microcomputer system with backlit LCD flat panel display; dedicated 80186 and M68000 processors for GC/MS control and data acquisition:
Processor: 80386, 16 MHz (opt 386/25 MHz)
Controllers: 68000 and 80186
Math Coprocessor: 80387 (opt)
Memory: 4 MB RAM
Hard Disk: 80 MB
Floppy Drive: 3.5", 1.44 MB
Display: LCD, 640x480 VGA

SOFTWARE:

SpectraScan/OS data system with AutoRUN™ menu for GC/MS control, applications, and mass spectra library search under MS-Windows graphical user interface

ENVIRONMENTAL:

System shock-mounted and enclosed in weatherproof aluminum Mil-Spec case:
Size: 14"H x 21"W x 32"L
Weight: 130 lbs
Power: 1600 peak watts, 50/60 Hz, 110V or 220V
Operating Range: 5 °C to 40 °C

SERVICES AND OPTIONS

Viking provides customized field support and system integration services, including a wide range of options, accessories, and environmental diagnostic products to support your field operations:

- Express Field Service Program
- Field Area Network System
- Field Sample Preparation Kits
- Field Maintenance Kits
- Mobile Laboratory Vans
- Computer Upgrades
- Mass Spectra Libraries
- Portable Printers
- Transport Case Accessories
- Industrial Rack-Mount Chassis
- Field Generator Sets

In the project that Viking just completed, the hardware that was used in the experimental prototype is being sent to NASA as a deliverable under the contract. Since this is an experimental prototype package, it is not in a form that would make very much sense to anyone besides the developers. In order for Viking to pursue any Phase III effort on its own, therefore it must first reconstruct all of the basic hardware associated with the prototype and then pick up where it left off at the end of the NASA project. This is expensive and may even preclude any additional commercial development. A request by Viking for temporary custody of this hardware during the time that would be needed for further commercial development was denied because of the procurement rules. In these actions, there seems to be an internal inconsistency between what the procurement rules allow and what is needed to carry out the objectives of the SBIR program, which clearly recognize the importance of Phase III commercialization. In this case, NASA has said that it does not as an agency support Phase III work (it might decide later that it was interested in some space application), but it will retain the hardware and not make it available to the contractor, either temporarily or by purchase, to pursue Phase III work outside of NASA. This is a "catch 22" situation, and leads to a second recommendation: NASA should seek authority to permit loan of SBIR Phase II hardware or software to the SBIR contractor, upon their request, in order to support Phase III efforts, at reasonable fees for periods of up to two years. This, it would seem, is more consistent with the intent of the SBIR program and with other agency practices. (Viking Instruments negotiated purchase of certain SBIR Phase II assets from the DOD at the completion of a Phase II contract, at reasonable prices and with minimum administrative burden. NASA should seek a similar capability.)

Finally, as noted in various progress reports, the break in the funding available to support this contract contributed directly to the delays in completion. The contracting office and technical representative were very cooperative and prompt in processing extensions to the period of performance, and this was appreciated. Everyone concerned recognizes the serious disruptions that a break in work on a project can cause and it is unnecessary to reiterate this fact. The most important aspect is to have as much advance notice as possible so that the company can plan alternate work for the personnel involved.

ENDNOTES

1. Takeda, T.; Shebata, S.; Matsuda, H. "An Accelerating Voltage Scanning Mass Spectrometer," Mass Spectroscopy, Vol. 28, No. 3, Sept. 1980.

2. Dahl, D.A. and Delmore, J.E. "SIMION PC/AT," Idaho National Engineering Laboratory, EG&G Idaho, Inc., P.O. Box 1625, Idaho Falls, ID 83415.

APPENDIX A

ION TRAJECTORY MODELING

Viking Instruments Corporation has utilized a program called "SIMION" to aid in design of the ion optics of both the ion source in the prototype instrument and in the layout of system elements. This program was developed by D.A.Dahl and J.E.Delmore from EG&G Idaho, Inc. at the Idaho National Engineering Laboratory under a Department of Energy Contract No. DE-AC07-76IDO1570. Additional copies may be obtained by writing to Mr. Dahl at P.O. Box 1625, Idaho Falls, ID 83415. The following pages include the specific modeling results from the ion source design, and are provided for reference purposes.

To compare the source transmission characteristics of the original Viking spacecraft MS with our modified source, we first set up the SIMION model and optimized the voltages to pass a wide dynamic range of ions for each source. Six ion trajectories were compared at m/z values of: 28, 57, 95, 143, 286, 382, and 572 for each source. The model yields the position and velocity of ions issuing from the object slit for evaluation. A comparison of the off-axis velocity and the deviation in the y axis could then be made with certain limits placed on them for delineation. For example, the number ions of the set that had off-axis velocities in excess of 0.25 mm/microsecond for the modified source was 10. There were 14 ions with off-axis velocities in excess of 0.15 mm/microsecond, and 17 with off-axis velocities in excess of 0.1 mm/microsecond. The total loss can be estimated at 24 to 40%. In contrast, the original Viking source ion loss can be estimated, under optimal conditions, to be 38 to 48%. The loss of ions is for approximately 8 to 14% greater for the original Viking source than for our modified source. The distance off axis from the object slit is approximately 10% greater for the original Viking source than for our modified source. The end result is that our new source should provide or transmit roughly an order of magnitude more ions and also since the beam is "flatter" the resolution should improve at the image slit. We predicted this early in 1991 and realized it later in the same year.

In the following pages are outputs from SIMION that allow the tracking of specific ions in time and space for each mass in the corresponding ion source. The numbers are separated by commas and are titled as follows: number of the ion; x, y, z positions in mm; x, y, and z velocities in mm/microsecond; potential energy in volts; and flight time in microseconds. There are two sets labelled by the type of source tested, either the original Viking spacecraft MS source or our modified source. Both sets have their associated m/z values listed at the top.

The original Viking spacecraft mass spectrometer -- m/z 28

```
  1,   4.0640    , 0.63500    , 0.00000E+00, 0.58699    ,  0.00000E+00,
0.00000E+00,   1003.0    ,  0.00000E+00
  1,   4.1019    , 0.63170    , 0.00000E+00, 0.95654    , -0.13073    ,
0.00000E+00,   1002.8    ,  0.50002E-01
  1,   4.1628    , 0.62206    , 0.00000E+00,  1.4964    , -0.25298    ,
0.00000E+00,   1002.6    ,  0.10000
  1,   4.2511    , 0.60676    , 0.00000E+00,  2.0254    , -0.35612    ,
0.00000E+00,   1002.4    ,  0.15000
  1,   4.3649    , 0.58668    , 0.00000E+00,  2.5277    , -0.44492    ,
0.00000E+00,   1002.0    ,  0.20000
  1,   4.5038    , 0.56241    , 0.00000E+00,  3.0283    , -0.52457    ,
0.00000E+00,   1001.6    ,  0.25000
  1,   4.6679    , 0.53427    , 0.00000E+00,  3.5401    , -0.60122    ,
0.00000E+00,   1001.1    ,  0.30000
  1,   4.8581    , 0.50223    , 0.00000E+00,  4.0727    , -0.68118    ,
0.00000E+00,   1000.5    ,  0.35000
  1,   5.0757    , 0.46599    , 0.00000E+00,  4.6366    , -0.77045    ,
0.00000E+00,   999.78    ,  0.40001
  1,   5.3226    , 0.42491    , 0.00000E+00,  5.2467    , -0.87629    ,
0.00000E+00,   998.88    ,  0.45001
  1,   5.6016    , 0.37793    , 0.00000E+00,  5.9292    ,  -1.0083    ,
0.00000E+00,   997.74    ,  0.50000
  1,   5.9174    , 0.32339    , 0.00000E+00,  6.7313    ,  -1.1826    ,
0.00000E+00,   996.21    ,  0.55000
  1,   6.2783    , 0.25857    , 0.00000E+00,  7.7536    ,  -1.4235    ,
0.00000E+00,   993.97    ,  0.60000
  1,   6.7003    , 0.17937    , 0.00000E+00,  9.2381    ,  -1.7636    ,
0.00000E+00,   990.16    ,  0.65000
  1,   7.2206    , 0.80734E-01, 0.00000E+00,  11.871    ,  -2.1816    ,
0.00000E+00,   981.87    ,  0.70000
  1,   7.9355    ,-0.34012E-01, 0.00000E+00,  17.398    ,  -2.3111    ,
0.00000E+00,   958.31    ,  0.75000
  1,   9.0003    ,-0.15317    , 0.00000E+00,  24.574    ,  -2.6955    ,
0.00000E+00,   914.29    ,  0.80000
  1,   10.288    ,-0.30533    , 0.00000E+00,  26.364    ,  -3.2379    ,
0.00000E+00,   900.62    ,  0.85000
  1,   11.627    ,-0.43302    , 0.00000E+00,  28.420    ,  0.24598    ,
0.00000E+00,   886.06    ,  0.90000
  1,   13.485    ,-0.32563    , 0.00000E+00,  48.698    ,   5.5439    ,
0.00000E+00,   655.00    ,  0.95000
  1,   16.938    ,-0.42734E-01, 0.00000E+00,  82.967    ,   4.9201    ,
0.00000E+00,   1.3276    ,   1.0000
  1,   21.089    , 0.20157    , 0.00000E+00,  83.026    ,   4.8856    ,
0.00000E+00, 0.49944E-02,   1.0500
  2,   4.0640    , 0.50800    , 0.00000E+00, 0.58699    ,  0.00000E+00,
0.00000E+00,   1002.8    ,  0.00000E+00
  2,   4.1026    , 0.50359    , 0.00000E+00, 0.96418    , -0.17189    ,
0.00000E+00,   1002.7    ,  0.50005E-01
  2,   4.1614    , 0.49141    , 0.00000E+00,  1.3960    , -0.30851    ,
0.00000E+00,   1002.5    ,  0.10000
  2,   4.2425    , 0.47338    , 0.00000E+00,  1.8536    , -0.40821    ,
0.00000E+00,   1002.3    ,  0.15000
```

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  2,   4.3471     , 0.45091     , 0.00000E+00,   2.3307     , -0.48755    ,
0.00000E+00,   1002.0     , 0.20000
  2,   4.4759     , 0.42481     , 0.00000E+00,   2.8225     , -0.55495    ,
0.00000E+00,   1001.6     , 0.25000
  2,   4.6296     , 0.39552     , 0.00000E+00,   3.3318     , -0.61603    ,
0.00000E+00,   1001.2     , 0.30000
  2,   4.8094     , 0.36323     , 0.00000E+00,   3.8643     , -0.67592    ,
0.00000E+00,   1000.6     , 0.35000
  2,   5.0166     , 0.32787     , 0.00000E+00,   4.4285     , -0.73897    ,
0.00000E+00,   999.92     , 0.40001
  2,   5.2531     , 0.28920     , 0.00000E+00,   5.0381     , -0.80942    ,
0.00000E+00,   999.06     , 0.45001
  2,   5.5215     , 0.24673     , 0.00000E+00,   5.7163     , -0.89193    ,
0.00000E+00,   997.99     , 0.50001
  2,   5.8265     , 0.19971     , 0.00000E+00,   6.5042     , -0.99284    ,
0.00000E+00,   996.56     , 0.55000
  2,   6.1751     , 0.14702     , 0.00000E+00,   7.4858     ,   -1.1192    ,
0.00000E+00,   994.53     , 0.60000
  2,   6.5813     , 0.87334E-01, 0.00000E+00,   8.8539     ,   -1.2720    ,
0.00000E+00,   991.24     , 0.65000
  2,   7.0749     , 0.19973E-01, 0.00000E+00,   11.116     ,   -1.4096    ,
0.00000E+00,   984.63     , 0.70000
  2,   7.7312     , -0.49816E-01, 0.00000E+00,   15.719     ,   -1.3176    ,
0.00000E+00,   966.76     , 0.75000
  2,   8.7079     , -0.11231    , 0.00000E+00,   23.364     ,   -1.3815    ,
0.00000E+00,   923.35     , 0.80001
  2,   9.9710     , -0.19912    , 0.00000E+00,   26.274     ,   -1.9784    ,
0.00000E+00,   902.13     , 0.85000
  2,   11.306     , -0.29229    , 0.00000E+00,   27.471     ,   -1.1535    ,
0.00000E+00,   893.27     , 0.90000
  2,   12.987     , -0.25240    , 0.00000E+00,   42.141     ,    2.0885    ,
0.00000E+00,   744.72     , 0.95000
  2,   16.045     , -0.61777E-01, 0.00000E+00,   79.957     ,    3.6435    ,
0.00000E+00,   73.569     ,   1.0000
  2,   20.184     , 0.11226     , 0.00000E+00,   83.086     ,    3.4598    ,
0.00000E+00, 0.78230E-02,   1.0500
  2,   24.339     , 0.28526     , 0.00000E+00,   83.086     ,    3.4598    ,
0.00000E+00, 0.67080E-06,   1.1000
  3,   4.0640     , 0.38100     , 0.00000E+00, 0.58699     ,  0.00000E+00,
0.00000E+00,   1002.7     , 0.00000E+00
  3,   4.1034     , 0.37922     , 0.00000E+00, 0.99248     , -0.70953E-01,
0.00000E+00,   1002.6     , 0.50004E-01
  3,   4.1636     , 0.37393     , 0.00000E+00,   1.4190     , -0.14017    ,
0.00000E+00,   1002.5     , 0.10000
  3,   4.2457     , 0.36525     , 0.00000E+00,   1.8666     , -0.20620    ,
0.00000E+00,   1002.3     , 0.15000
  3,   4.3506     , 0.35343     , 0.00000E+00,   2.3362     , -0.26551    ,
0.00000E+00,   1002.0     , 0.20000
  3,   4.4796     , 0.33880     , 0.00000E+00,   2.8255     , -0.31908    ,
0.00000E+00,   1001.6     , 0.25000
  3,   4.6335     , 0.32157     , 0.00000E+00,   3.3355     , -0.36944    ,
0.00000E+00,   1001.1     , 0.30000
  3,   4.8136     , 0.30185     , 0.00000E+00,   3.8704     , -0.41979    ,
0.00000E+00,   1000.6     , 0.35000
```

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  3,   5.0211    , 0.27954    , 0.00000E+00,   4.4380     , -0.47365    ,
0.00000E+00,   999.89    ,  0.40000
  3,   5.2582    , 0.25436    , 0.00000E+00,   5.0519     , -0.53523    ,
0.00000E+00,   999.03    ,  0.45001
  3,   5.5274    , 0.22580    , 0.00000E+00,   5.7344     , -0.61003    ,
0.00000E+00,   997.95    ,  0.50000
  3,   5.8334    , 0.19300    , 0.00000E+00,   6.5269     , -0.70602    ,
0.00000E+00,   996.52    ,  0.55000
  3,   6.1833    , 0.15465    , 0.00000E+00,   7.5136     , -0.83470    ,
0.00000E+00,   994.48    ,  0.60000
  3,   6.5911    , 0.10875    , 0.00000E+00,   8.8905     ,  -1.0103    ,
0.00000E+00,   991.17    ,  0.65000
  3,   7.0870    , 0.52839E-01, 0.00000E+00,   11.176     ,  -1.2285    ,
0.00000E+00,   984.44    ,  0.70001
  3,   7.7477    , -0.12262E-01, 0.00000E+00,   15.848     ,  -1.3270    ,
0.00000E+00,   966.10    ,  0.75000
  3,   8.7309    , -0.77847E-01, 0.00000E+00,   23.454     ,  -1.4103    ,
0.00000E+00,   922.67    ,  0.80000
  3,   9.9961    , -0.16113    , 0.00000E+00,   26.288     ,  -1.8453    ,
0.00000E+00,   902.04    ,  0.85000
  3,   11.334    , -0.24740    , 0.00000E+00,   27.686     ,  -1.0613    ,
0.00000E+00,   891.50    ,  0.90001
  3,   13.035    , -0.21963    , 0.00000E+00,   42.732     ,   1.7548    ,
0.00000E+00,   737.42    ,  0.95000
  3,   16.139    , -0.62228E-01, 0.00000E+00,   80.438     ,   2.8943    ,
0.00000E+00,   62.641    ,   1.0000
  3,   20.281    , 0.73604E-01, 0.00000E+00,   83.083     ,   2.6923    ,
0.00000E+00, 0.74779E-02,   1.0500
  3,   24.435    , 0.20822    , 0.00000E+00,   83.083     ,   2.6923    ,
0.00000E+00, 0.61368E-06,   1.1000
  4,   4.0640    , 0.25400    , 0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1002.7    ,  0.00000E+00
  4,   4.1040    , 0.25321    , 0.00000E+00,   1.0138     , -0.32203E-01,
0.00000E+00,   1002.6    ,  0.50006E-01
  4,   4.1655    , 0.25073    , 0.00000E+00,   1.4503     , -0.67611E-01,
0.00000E+00,   1002.4    ,  0.10000
  4,   4.2493    , 0.24639    , 0.00000E+00,   1.9014     , -0.10613    ,
0.00000E+00,   1002.2    ,  0.15000
  4,   4.3560    , 0.24012    , 0.00000E+00,   2.3705     , -0.14417    ,
0.00000E+00,   1001.9    ,  0.20000
  4,   4.4866    , 0.23200    , 0.00000E+00,   2.8596     , -0.18054    ,
0.00000E+00,   1001.6    ,  0.25000
  4,   4.6423    , 0.22209    , 0.00000E+00,   3.3713     , -0.21563    ,
0.00000E+00,   1001.1    ,  0.30000
  4,   4.8242    , 0.21043    , 0.00000E+00,   3.9099     , -0.25115    ,
0.00000E+00,   1000.5    ,  0.35000
  4,   5.0339    , 0.19693    , 0.00000E+00,   4.4830     , -0.28975    ,
0.00000E+00,   999.82    ,  0.40000
  4,   5.2734    , 0.18135    , 0.00000E+00,   5.1044     , -0.33460    ,
0.00000E+00,   998.95    ,  0.45001
  4,   5.5455    , 0.16329    , 0.00000E+00,   5.7972     , -0.38997    ,
0.00000E+00,   997.85    ,  0.50000
  4,   5.8550    , 0.14207    , 0.00000E+00,   6.6061     , -0.46231    ,
0.00000E+00,   996.38    ,  0.55001
```

```
   4,   6.2095    ,  0.11661    ,  0.00000E+00,   7.6198    , -0.56191    ,
0.00000E+00,   994.28    ,  0.60000
   4,   6.6236    ,  0.85183E-01,  0.00000E+00,   9.0435    , -0.70360    ,
0.00000E+00,   990.82    ,  0.65000
   4,   7.1295    ,  0.45412E-01,  0.00000E+00,   11.441    , -0.89172    ,
0.00000E+00,   983.65    ,  0.70001
   4,   7.8095    , -0.28436E-02,  0.00000E+00,   16.388    ,  -1.0026    ,
0.00000E+00,   963.64    ,  0.75000
   4,   8.8224    , -0.53316E-01,  0.00000E+00,   23.897    ,  -1.0927    ,
0.00000E+00,   919.66    ,  0.80001
   4,   10.098    , -0.11599    ,  0.00000E+00,   26.368    ,  -1.3608    ,
0.00000E+00,   901.55    ,  0.85000
   4,   11.445    , -0.17657    ,  0.00000E+00,   28.329    , -0.55702    ,
0.00000E+00,   886.27    ,  0.90001
   4,   13.216    , -0.15217    ,  0.00000E+00,   45.155    ,   1.6352    ,
0.00000E+00,   706.67    ,  0.95000
   4,   16.478    , -0.41584E-01,  0.00000E+00,   81.825    ,   1.9031    ,
0.00000E+00,   30.464    ,   1.0000
   4,   20.630    ,  0.48408E-01,  0.00000E+00,   83.102    ,   1.7901    ,
0.00000E+00,  0.63260E-02,   1.0500
   4,   24.785    ,  0.13791    ,  0.00000E+00,   83.103    ,   1.7901    ,
0.00000E+00,  0.41783E-06,   1.1000
   5,   4.0640    ,  0.12700    ,  0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1002.7    ,  0.00000E+00
   5,   4.1043    ,  0.12668    ,  0.00000E+00,   1.0259    , -0.13165E-01,
0.00000E+00,   1002.6    ,  0.50000E-01
   5,   4.1667    ,  0.12565    ,  0.00000E+00,   1.4706    , -0.28527E-01,
0.00000E+00,   1002.4    ,  0.10000
   5,   4.2516    ,  0.12378    ,  0.00000E+00,   1.9262    , -0.46251E-01,
0.00000E+00,   1002.2    ,  0.15000
   5,   4.3596    ,  0.12101    ,  0.00000E+00,   2.3968    , -0.64652E-01,
0.00000E+00,   1001.9    ,  0.20000
   5,   4.4915    ,  0.11732    ,  0.00000E+00,   2.8867    , -0.82775E-01,
0.00000E+00,   1001.5    ,  0.25000
   5,   4.6486    ,  0.11274    ,  0.00000E+00,   3.3999    , -0.10055    ,
0.00000E+00,   1001.1    ,  0.30000
   5,   4.8320    ,  0.10726    ,  0.00000E+00,   3.9413    , -0.11863    ,
0.00000E+00,   1000.5    ,  0.35000
   5,   5.0433    ,  0.10085    ,  0.00000E+00,   4.5188    , -0.13843    ,
0.00000E+00,   999.77    ,  0.40000
   5,   5.2847    ,  0.93366E-01,  0.00000E+00,   5.1461    , -0.16161    ,
0.00000E+00,   998.89    ,  0.45000
   5,   5.5592    ,  0.84592E-01,  0.00000E+00,   5.8477    , -0.19057    ,
0.00000E+00,   997.77    ,  0.50000
   5,   5.8715    ,  0.74153E-01,  0.00000E+00,   6.6691    , -0.22900    ,
0.00000E+00,   996.27    ,  0.55000
   5,   6.2296    ,  0.61432E-01,  0.00000E+00,   7.7024    , -0.28306    ,
0.00000E+00,   994.11    ,  0.60001
   5,   6.6487    ,  0.45440E-01,  0.00000E+00,   9.1658    , -0.36153    ,
0.00000E+00,   990.52    ,  0.65000
   5,   7.1627    ,  0.24788E-01,  0.00000E+00,   11.660    , -0.46744    ,
0.00000E+00,   982.99    ,  0.70001
   5,   7.8587    , -0.69322E-03,  0.00000E+00,   16.828    , -0.53207    ,
0.00000E+00,   961.59    ,  0.75000
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```
  5,   8.8944    , -0.27713E-01,  0.00000E+00,   24.211     , -0.58835    ,
0.00000E+00,   917.52    ,  0.80001
  5,   10.177    , -0.60960E-01,  0.00000E+00,   26.434     , -0.71353    ,
0.00000E+00,   901.19    ,  0.85000
  5,   11.534    , -0.91190E-01,  0.00000E+00,   28.980     , -0.19408    ,
0.00000E+00,   880.83    ,  0.90000
  5,   13.364    , -0.75840E-01,  0.00000E+00,   47.465     ,  0.98970    ,
0.00000E+00,   675.58    ,  0.95000
  5,   16.745    , -0.19830E-01,  0.00000E+00,   82.666     ,  0.93686    ,
0.00000E+00,   10.947    ,   1.0000
  5,   20.901    ,  0.24757E-01,  0.00000E+00,   83.128     ,  0.88984    ,
0.00000E+00, 0.55249E-02,   1.0500
  5,   25.057    ,  0.69248E-01,  0.00000E+00,   83.128     ,  0.88985    ,
0.00000E+00, 0.30373E-06,   1.1000
  6,   4.0640    ,  0.00000E+00,  0.00000E+00,  0.58699     ,  0.00000E+00,
0.00000E+00,   1002.7    ,  0.00000E+00
  6,   4.1044    ,  0.00000E+00,  0.00000E+00,   1.0299     ,  0.00000E+00,
0.00000E+00,   1002.6    ,  0.50005E-01
  6,   4.1671    ,  0.00000E+00,  0.00000E+00,   1.4775     ,  0.00000E+00,
0.00000E+00,   1002.4    ,  0.10000
  6,   4.2523    ,  0.00000E+00,  0.00000E+00,   1.9348     ,  0.00000E+00,
0.00000E+00,   1002.2    ,  0.15000
  6,   4.3608    ,  0.00000E+00,  0.00000E+00,   2.4060     ,  0.00000E+00,
0.00000E+00,   1001.9    ,  0.20000
  6,   4.4932    ,  0.00000E+00,  0.00000E+00,   2.8963     ,  0.00000E+00,
0.00000E+00,   1001.5    ,  0.25000
  6,   4.6508    ,  0.00000E+00,  0.00000E+00,   3.4100     ,  0.00000E+00,
0.00000E+00,   1001.0    ,  0.30001
  6,   4.8347    ,  0.00000E+00,  0.00000E+00,   3.9525     ,  0.00000E+00,
0.00000E+00,   1000.5    ,  0.35001
  6,   5.0466    ,  0.00000E+00,  0.00000E+00,   4.5316     ,  0.00000E+00,
0.00000E+00,   999.75    ,  0.40000
  6,   5.2887    ,  0.00000E+00,  0.00000E+00,   5.1615     ,  0.00000E+00,
0.00000E+00,   998.86    ,  0.45000
  6,   5.5641    ,  0.00000E+00,  0.00000E+00,   5.8670     ,  0.00000E+00,
0.00000E+00,   997.74    ,  0.50001
  6,   5.8774    ,  0.00000E+00,  0.00000E+00,   6.6946     ,  0.00000E+00,
0.00000E+00,   996.23    ,  0.55000
  6,   6.2370    ,  0.00000E+00,  0.00000E+00,   7.7386     ,  0.00000E+00,
0.00000E+00,   994.05    ,  0.60000
  6,   6.6584    ,  0.00000E+00,  0.00000E+00,   9.2228     ,  0.00000E+00,
0.00000E+00,   990.41    ,  0.65000
  6,   7.1764    ,  0.00000E+00,  0.00000E+00,   11.763     ,  0.00000E+00,
0.00000E+00,   982.70    ,  0.70001
  6,   7.8798    ,  0.00000E+00,  0.00000E+00,   17.028     ,  0.00000E+00,
0.00000E+00,   960.70    ,  0.75001
  6,   8.9252    ,  0.00000E+00,  0.00000E+00,   24.340     ,  0.00000E+00,
0.00000E+00,   916.70    ,  0.80001
  6,   10.211    ,  0.00000E+00,  0.00000E+00,   26.472     ,  0.00000E+00,
0.00000E+00,   901.03    ,  0.85000
  6,   11.573    ,  0.00000E+00,  0.00000E+00,   29.318     ,  0.00000E+00,
0.00000E+00,   878.15    ,  0.90000
  6,   13.433    ,  0.00000E+00,  0.00000E+00,   48.592     ,  0.00000E+00,
0.00000E+00,   660.27    ,  0.95001
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  6,   16.863    , 0.00000E+00, 0.00000E+00,   82.943    , 0.00000E+00,
0.00000E+00,   4.0062    ,   1.0000
  6,   21.019    , 0.00000E+00, 0.00000E+00,   83.123    , 0.00000E+00,
0.00000E+00, 0.51934E-02,   1.0500
  6,   25.176    , 0.00000E+00, 0.00000E+00,   83.124    , 0.00000E+00,
0.00000E+00, 0.28212E-06,   1.1000
```

The original Viking spacecraft mass spectrometer -- m/z 57

```
  1,   4.0640     , 0.63500     , 0.00000E+00,  0.41141     ,  0.00000E+00,
0.00000E+00,   502.98     ,  0.00000E+00
  1,   4.1170     , 0.63076     , 0.00000E+00,  0.67393     , -0.83508E-01,
0.00000E+00,   502.86     ,  0.10000
  1,   4.2026     , 0.61866     , 0.00000E+00,   1.0363     , -0.15550     ,
0.00000E+00,   502.68     ,  0.20001
  1,   4.3232     , 0.60012     , 0.00000E+00,   1.3712     , -0.21326     ,
0.00000E+00,   502.44     ,  0.30000
  1,   4.4766     , 0.57635     , 0.00000E+00,   1.6977     , -0.26082     ,
0.00000E+00,   502.14     ,  0.40000
  1,   4.6629     , 0.54812     , 0.00000E+00,   2.0285     , -0.30341     ,
0.00000E+00,   501.77     ,  0.50000
  1,   4.8827     , 0.51569     , 0.00000E+00,   2.3703     , -0.34533     ,
0.00000E+00,   501.31     ,  0.60000
  1,   5.1375     , 0.47892     , 0.00000E+00,   2.7296     , -0.39113     ,
0.00000E+00,   500.76     ,  0.70001
  1,   5.4295     , 0.43714     , 0.00000E+00,   3.1152     , -0.44684     ,
0.00000E+00,   500.08     ,  0.80000
  1,   5.7620     , 0.38893     , 0.00000E+00,   3.5448     , -0.52157     ,
0.00000E+00,   499.22     ,  0.90000
  1,   6.1411     , 0.33166     , 0.00000E+00,   4.0559     , -0.63183     ,
0.00000E+00,   498.03     ,   1.0000
  1,   6.5788     , 0.26039     , 0.00000E+00,   4.7420     , -0.80776     ,
0.00000E+00,   496.17     ,   1.1000
  1,   7.1041     , 0.16654     , 0.00000E+00,   5.8820     ,   -1.0880    ,
0.00000E+00,   492.45     ,   1.2000
  1,   7.7968     , 0.42482E-01, 0.00000E+00,   8.2878     ,   -1.3566    ,
0.00000E+00,   482.19     ,   1.3000
  1,   8.8161     ,-0.95812E-01, 0.00000E+00,   11.993     ,   -1.4524    ,
0.00000E+00,   459.88     ,   1.4000
  1,   10.094     ,-0.25678     , 0.00000E+00,   13.192     ,   -1.7206    ,
0.00000E+00,   450.73     ,   1.5000
  1,   11.432     ,-0.41476     , 0.00000E+00,   13.698     , -0.88655     ,
0.00000E+00,   447.46     ,   1.6000
  1,   13.163     ,-0.36843     , 0.00000E+00,   21.610     ,    1.5936    ,
0.00000E+00,   364.78     ,   1.7000
  1,   16.338     ,-0.10904     , 0.00000E+00,   40.344     ,    2.2498    ,
0.00000E+00,   21.063     ,   1.8000
  1,   20.455     , 0.10419     , 0.00000E+00,   41.226     ,    2.1188    ,
0.00000E+00, 0.34409E-02,   1.9000
  2,   4.0640     , 0.50800     , 0.00000E+00,  0.41141     ,  0.00000E+00,
0.00000E+00,   502.87     ,  0.00000E+00
  2,   4.1173     , 0.50237     , 0.00000E+00,  0.66321     , -0.10835     ,
0.00000E+00,   502.78     ,  0.10000
  2,   4.1980     , 0.48735     , 0.00000E+00,  0.95292     , -0.18651     ,
0.00000E+00,   502.63     ,  0.20000
  2,   4.3085     , 0.46583     , 0.00000E+00,   1.2590     , -0.24135     ,
0.00000E+00,   502.43     ,  0.30000
  2,   4.4502     , 0.43951     , 0.00000E+00,   1.5758     , -0.28346     ,
0.00000E+00,   502.15     ,  0.40001
  2,   4.6240     , 0.40937     , 0.00000E+00,   1.9028     , -0.31860     ,
0.00000E+00,   501.81     ,  0.50000
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  2,   4.8311     ,  0.37589     ,  0.00000E+00,   2.2431     , -0.35085     ,
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  2,   5.0732     ,  0.33918     ,  0.00000E+00,   2.6016     , -0.38377     ,
0.00000E+00,   500.87     ,  0.70000
  2,   5.3523     ,  0.29899     ,  0.00000E+00,   2.9865     , -0.42108     ,
0.00000E+00,   500.22     ,  0.80000
  2,   5.6719     ,  0.25466     ,  0.00000E+00,   3.4137     , -0.46750     ,
0.00000E+00,   499.41     ,  0.90001
  2,   6.0375     ,  0.20495     ,  0.00000E+00,   3.9154     , -0.53016     ,
0.00000E+00,   498.30     ,   1.0000
  2,   6.4599     ,  0.14774     ,  0.00000E+00,   4.5682     , -0.61954     ,
0.00000E+00,   496.64     ,   1.1000
  2,   6.9629     ,  0.79927E-01,  0.00000E+00,   5.5844     , -0.74089     ,
0.00000E+00,   493.54     ,   1.2000
  2,   7.6088     ,  0.43732E-03,  0.00000E+00,   7.5928     , -0.82767     ,
0.00000E+00,   485.68     ,   1.3000
  2,   8.5454     , -0.80827E-01,  0.00000E+00,   11.301     , -0.83085     ,
0.00000E+00,   464.98     ,   1.4000
  2,   9.7933     , -0.17928     ,  0.00000E+00,   13.131     ,  -1.1147     ,
0.00000E+00,   451.63     ,   1.5000
  2,   11.128     , -0.29057     ,  0.00000E+00,   13.596     , -0.93175     ,
0.00000E+00,   448.09     ,   1.6000
  2,   12.721     , -0.28406     ,  0.00000E+00,   19.726     ,  0.68829     ,
0.00000E+00,   387.88     ,   1.7000
  2,   15.511     , -0.10940     ,  0.00000E+00,   37.845     ,   1.9007     ,
0.00000E+00,   78.627     ,   1.8000
  2,   19.586     ,  0.55859E-01,  0.00000E+00,   41.226     ,   1.6021     ,
0.00000E+00,  0.52115E-02,   1.9000
  2,   23.709     ,  0.21606     ,  0.00000E+00,   41.226     ,   1.6021     ,
0.00000E+00,  0.16737E-04,   2.0000
  3,   4.0640     ,  0.38100     ,  0.00000E+00,  0.41141     ,  0.00000E+00,
0.00000E+00,   502.82     ,  0.00000E+00
  3,   4.1183     ,  0.37873     ,  0.00000E+00,  0.67676     , -0.45261E-01,
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  3,   4.1999     ,  0.37201     ,  0.00000E+00,  0.95877     , -0.88625E-01,
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  3,   4.3106     ,  0.36116     ,  0.00000E+00,   1.2572     , -0.12742     ,
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  3,   4.4518     ,  0.34673     ,  0.00000E+00,   1.5699     , -0.16031     ,
0.00000E+00,   502.13     ,  0.40000
  3,   4.6250     ,  0.32924     ,  0.00000E+00,   1.8959     , -0.18895     ,
0.00000E+00,   501.80     ,  0.50000
  3,   4.8315     ,  0.30899     ,  0.00000E+00,   2.2367     , -0.21583     ,
0.00000E+00,   501.38     ,  0.60001
  3,   5.0730     ,  0.28604     ,  0.00000E+00,   2.5964     , -0.24366     ,
0.00000E+00,   500.86     ,  0.70001
  3,   5.3517     ,  0.26012     ,  0.00000E+00,   2.9829     , -0.27580     ,
0.00000E+00,   500.22     ,  0.80000
  3,   5.6709     ,  0.23058     ,  0.00000E+00,   3.4118     , -0.31714     ,
0.00000E+00,   499.40     ,  0.90000
  3,   6.0364     ,  0.19613     ,  0.00000E+00,   3.9145     , -0.37561     ,
0.00000E+00,   498.30     ,   1.0000
  3,   6.4587     ,  0.15444     ,  0.00000E+00,   4.5667     , -0.46478     ,
0.00000E+00,   496.65     ,   1.1000
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  3,   6.9614    ,  0.10153     ,  0.00000E+00,   5.5789    , -0.60251    ,
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  3,   7.6064    ,  0.33117E-01,  0.00000E+00,   7.5795    , -0.75515    ,
0.00000E+00,   485.74    ,   1.3000
  3,   8.5410    , -0.44144E-01,  0.00000E+00,   11.275    , -0.78836    ,
0.00000E+00,   465.11    ,   1.4000
  3,   9.7872    , -0.13272     ,  0.00000E+00,   13.126    , -0.97644    ,
0.00000E+00,   451.69    ,   1.5000
  3,   11.122    , -0.23006     ,  0.00000E+00,   13.638    , -0.82706    ,
0.00000E+00,   447.73    ,   1.6000
  3,   12.720    , -0.23420     ,  0.00000E+00,   19.747    ,  0.46914    ,
0.00000E+00,   387.58    ,   1.7000
  3,   15.516    , -0.10026     ,  0.00000E+00,   37.886    ,   1.4528    ,
0.00000E+00,   78.169    ,   1.8000
  3,   19.593    ,  0.20699E-01,  0.00000E+00,   41.239    ,   1.1574    ,
0.00000E+00, 0.51945E-02,   1.9000
  3,   23.717    ,  0.13644     ,  0.00000E+00,   41.240    ,   1.1574    ,
0.00000E+00, 0.21732E-04,   2.0000
  4,   4.0640    ,  0.25400     ,  0.00000E+00,  0.41141    ,  0.00000E+00,
0.00000E+00,   502.80    ,  0.00000E+00
  4,   4.1190    ,  0.25299     ,  0.00000E+00,  0.68869    , -0.20569E-01,
0.00000E+00,   502.71    ,  0.10000
  4,   4.2020    ,  0.24980     ,  0.00000E+00,  0.97447    , -0.43607E-01,
0.00000E+00,   502.57    ,  0.20000
  4,   4.3143    ,  0.24425     ,  0.00000E+00,   1.2723    , -0.67182E-01,
0.00000E+00,   502.37    ,  0.30000
  4,   4.4569    ,  0.23642     ,  0.00000E+00,   1.5835    , -0.89090E-01,
0.00000E+00,   502.11    ,  0.40001
  4,   4.6314    ,  0.22651     ,  0.00000E+00,   1.9091    , -0.10893    ,
0.00000E+00,   501.77    ,  0.50000
  4,   4.8393    ,  0.21467     ,  0.00000E+00,   2.2509    , -0.12779    ,
0.00000E+00,   501.35    ,  0.60000
  4,   5.0823    ,  0.20092     ,  0.00000E+00,   2.6129    , -0.14760    ,
0.00000E+00,   500.83    ,  0.70001
  4,   5.3628    ,  0.18503     ,  0.00000E+00,   3.0029    , -0.17088    ,
0.00000E+00,   500.18    ,  0.80000
  4,   5.6843    ,  0.16650     ,  0.00000E+00,   3.4368    , -0.20136    ,
0.00000E+00,   499.35    ,  0.90000
  4,   6.0527    ,  0.14432     ,  0.00000E+00,   3.9480    , -0.24526    ,
0.00000E+00,   498.23    ,   1.0000
  4,   6.4790    ,  0.11664     ,  0.00000E+00,   4.6165    , -0.31385    ,
0.00000E+00,   496.53    ,   1.1000
  4,   6.9880    ,  0.80135E-01,  0.00000E+00,   5.6596    , -0.42444    ,
0.00000E+00,   493.35    ,   1.2000
  4,   7.6445    ,  0.30821E-01,  0.00000E+00,   7.7391    , -0.55475    ,
0.00000E+00,   485.08    ,   1.3000
  4,   8.5988    , -0.26532E-01,  0.00000E+00,   11.459    , -0.58704    ,
0.00000E+00,   463.92    ,   1.4000
  4,   9.8547    , -0.91355E-01,  0.00000E+00,   13.164    , -0.70382    ,
0.00000E+00,   451.48    ,   1.5000
  4,   11.194    , -0.16039     ,  0.00000E+00,   13.772    , -0.55397    ,
0.00000E+00,   446.73    ,   1.6000
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0.00000E+00,   380.74    ,   1.7000
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0.00000E+00, 501.75 , 0.50000
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0.00000E+00, 501.33 , 0.60000
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0.00000E+00, 500.80 , 0.70000
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0.00000E+00, 500.15 , 0.80000
5, 5.6952 , 0.86279E-01, 0.00000E+00, 3.4585 , -0.98005E-01,
0.00000E+00, 499.31 , 0.90001
5, 6.0661 , 0.75394E-01, 0.00000E+00, 3.9768 , -0.12136 ,
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5, 6.4958 , 0.61551E-01, 0.00000E+00, 4.6572 , -0.15858 ,
0.00000E+00, 496.43 , 1.1000
5, 7.0100 , 0.42878E-01, 0.00000E+00, 5.7281 , -0.21952 ,
0.00000E+00, 493.14 , 1.2000
5, 7.6764 , 0.17122E-01, 0.00000E+00, 7.8759 , -0.29165 ,
0.00000E+00, 484.50 , 1.3000
5, 8.6470 , -0.13081E-01, 0.00000E+00, 11.606 , -0.30957 ,
0.00000E+00, 462.97 , 1.4000
5, 9.9106 , -0.47016E-01, 0.00000E+00, 13.196 , -0.36552 ,
0.00000E+00, 451.31 , 1.5000
5, 11.255 , -0.82307E-01, 0.00000E+00, 13.899 , -0.26585 ,
0.00000E+00, 445.71 , 1.6000
5, 12.927 , -0.81990E-01, 0.00000E+00, 20.848 , 0.20187 ,
0.00000E+00, 374.40 , 1.7000
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0.00000E+00, 502.79 , 0.00000E+00
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0.00000E+00, 502.69 , 0.10000
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0.00000E+00, 502.55 , 0.20000

```
  6,   4.3175    , 0.00000E+00, 0.00000E+00,   1.2885    , 0.00000E+00,
0.00000E+00,   502.35    , 0.30000
  6,   4.4618    , 0.00000E+00, 0.00000E+00,   1.5996    , 0.00000E+00,
0.00000E+00,   502.08    , 0.40000
  6,   4.6379    , 0.00000E+00, 0.00000E+00,   1.9252    , 0.00000E+00,
0.00000E+00,   501.74    , 0.50000
  6,   4.8475    , 0.00000E+00, 0.00000E+00,   2.2682    , 0.00000E+00,
0.00000E+00,   501.32    , 0.60000
  6,   5.0923    , 0.00000E+00, 0.00000E+00,   2.6326    , 0.00000E+00,
0.00000E+00,   500.79    , 0.70001
  6,   5.3750    , 0.00000E+00, 0.00000E+00,   3.0266    , 0.00000E+00,
0.00000E+00,   500.13    , 0.80000
  6,   5.6991    , 0.00000E+00, 0.00000E+00,   3.4669    , 0.00000E+00,
0.00000E+00,   499.29    , 0.90000
  6,   6.0710    , 0.00000E+00, 0.00000E+00,   3.9888    , 0.00000E+00,
0.00000E+00,   498.14    ,   1.0000
  6,   6.5023    , 0.00000E+00, 0.00000E+00,   4.6763    , 0.00000E+00,
0.00000E+00,   496.39    ,   1.1000
  6,   7.0191    , 0.00000E+00, 0.00000E+00,   5.7626    , 0.00000E+00,
0.00000E+00,   493.04    ,   1.2000
  6,   7.6903    , 0.00000E+00, 0.00000E+00,   7.9420    , 0.00000E+00,
0.00000E+00,   484.23    ,   1.3000
  6,   8.6686    , 0.00000E+00, 0.00000E+00,   11.672    , 0.00000E+00,
0.00000E+00,   462.57    ,   1.4000
  6,   9.9357    , 0.00000E+00, 0.00000E+00,   13.215    , 0.00000E+00,
0.00000E+00,   451.24    ,   1.5000
  6,   11.283    , 0.00000E+00, 0.00000E+00,   13.977    , 0.00000E+00,
0.00000E+00,   445.19    ,   1.6000
  6,   12.972    , 0.00000E+00, 0.00000E+00,   21.121    , 0.00000E+00,
0.00000E+00,   371.16    ,   1.7000
  6,   16.010    , 0.00000E+00, 0.00000E+00,   39.615    , 0.00000E+00,
0.00000E+00,   39.111    ,   1.8000
  6,   20.119    , 0.00000E+00, 0.00000E+00,   41.257    , 0.00000E+00,
0.00000E+00, 0.40383E-02,   1.9000
  6,   24.245    , 0.00000E+00, 0.00000E+00,   41.257    , 0.00000E+00,
0.00000E+00, 0.27326E-05,   2.0000
```

The original Viking spacecraft mass spectrometer -- m/z 95

```
  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.99    ,  0.00000E+00
  1,   4.1530    ,  0.62708    ,  0.00000E+00,  0.60497    , -0.76799E-01,
0.00000E+00,   302.83    ,  0.20001
  1,   4.3077    ,  0.60572    ,  0.00000E+00,  0.93549    , -0.13361    ,
0.00000E+00,   302.58    ,  0.40000
  1,   4.5261    ,  0.57472    ,  0.00000E+00,   1.2487    , -0.17455    ,
0.00000E+00,   302.24    ,  0.60000
  1,   4.8076    ,  0.53641    ,  0.00000E+00,   1.5673    , -0.20786    ,
0.00000E+00,   301.79    ,  0.80000
  1,   5.1540    ,  0.49163    ,  0.00000E+00,   1.9004    , -0.24043    ,
0.00000E+00,   301.21    ,   1.0000
  1,   5.5693    ,  0.43969    ,  0.00000E+00,   2.2578    , -0.28158    ,
0.00000E+00,   300.47    ,   1.2000
  1,   6.0604    ,  0.37730    ,  0.00000E+00,   2.6659    , -0.34905    ,
0.00000E+00,   299.46    ,   1.4000
  1,   6.6443    ,  0.29566    ,  0.00000E+00,   3.2109    , -0.48459    ,
0.00000E+00,   297.83    ,   1.6000
  1,   7.3762    ,  0.17363    ,  0.00000E+00,   4.2602    , -0.76087    ,
0.00000E+00,   293.80    ,   1.8000
  1,   8.4520    , -0.91841E-03,  0.00000E+00,   6.7336    , -0.91428    ,
0.00000E+00,   280.28    ,   2.0000
  1,   9.9731    , -0.19447    ,  0.00000E+00,   8.0428    ,  -1.0328    ,
0.00000E+00,   270.64    ,   2.2000
  1,   11.618    , -0.37620    ,  0.00000E+00,   8.7783    , -0.23325    ,
0.00000E+00,   265.12    ,   2.4000
  1,   14.031    , -0.27949    ,  0.00000E+00,   17.328    ,   1.4305    ,
0.00000E+00,   154.23    ,   2.6000
  1,   18.603    , -0.49736E-01,  0.00000E+00,   24.797    ,  0.95635    ,
0.00000E+00, 0.54306E-02,   2.8000
  1,   23.563    ,  0.14153    ,  0.00000E+00,   24.797    ,  0.95635    ,
0.00000E+00, 0.23860E-04,   3.0000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.90    ,  0.00000E+00
  2,   4.1518    ,  0.49770    ,  0.00000E+00,  0.57028    , -0.96422E-01,
0.00000E+00,   302.78    ,  0.20000
  2,   4.2943    ,  0.47221    ,  0.00000E+00,  0.85829    , -0.15368    ,
0.00000E+00,   302.57    ,  0.40000
  2,   4.4961    ,  0.43756    ,  0.00000E+00,   1.1611    , -0.19061    ,
0.00000E+00,   302.26    ,  0.60001
  2,   4.7596    ,  0.39660    ,  0.00000E+00,   1.4761    , -0.21799    ,
0.00000E+00,   301.84    ,  0.80000
  2,   5.0876    ,  0.35057    ,  0.00000E+00,   1.8075    , -0.24232    ,
0.00000E+00,   301.30    ,   1.0000
  2,   5.4842    ,  0.29946    ,  0.00000E+00,   2.1642    , -0.26999    ,
0.00000E+00,   300.60    ,   1.2000
  2,   5.9565    ,  0.24175    ,  0.00000E+00,   2.5697    , -0.31035    ,
0.00000E+00,   299.64    ,   1.4000
  2,   6.5198    ,  0.17332    ,  0.00000E+00,   3.0963    , -0.38119    ,
0.00000E+00,   298.15    ,   1.6000
  2,   7.2201    ,  0.85583E-01,  0.00000E+00,   4.0234    , -0.50436    ,
0.00000E+00,   294.85    ,   1.8000
```

```
 2,  8.2170    , -0.24565E-01,  0.00000E+00,   6.2379    , -0.56690    ,
0.00000E+00,   283.62    ,   2.0000
 2,  9.6880    , -0.14939    ,  0.00000E+00,   7.9940    , -0.70360    ,
0.00000E+00,   271.23    ,   2.2000
 2,  11.321    , -0.28737    ,  0.00000E+00,   8.4347    , -0.47510    ,
0.00000E+00,   267.84    ,   2.4000
 2,  13.494    , -0.24536    ,  0.00000E+00,   14.767    ,   1.0404    ,
0.00000E+00,   195.07    ,   2.6000
 2,  17.773    , -0.43477E-01,  0.00000E+00,   24.792    ,  0.80970    ,
0.00000E+00,  0.11708E-01,   2.8000
 2,  22.731    ,  0.11846    ,  0.00000E+00,   24.793    ,  0.80969    ,
0.00000E+00,  0.35883E-03,   3.0000
 3,  4.0640    ,  0.38100    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.86    ,  0.00000E+00
 3,  4.1531    ,  0.37674    ,  0.00000E+00,  0.57576    , -0.42199E-01,
0.00000E+00,   302.74    ,  0.20000
 3,  4.2958    ,  0.36441    ,  0.00000E+00,  0.85506    , -0.79735E-01,
0.00000E+00,   302.54    ,  0.40000
 3,  4.4963    ,  0.34544    ,  0.00000E+00,   1.1531    , -0.10856    ,
0.00000E+00,   302.25    ,  0.60000
 3,  4.7580    ,  0.32141    ,  0.00000E+00,   1.4669    , -0.13106    ,
0.00000E+00,   301.84    ,  0.80000
 3,  5.0843    ,  0.29316    ,  0.00000E+00,   1.7986    , -0.15150    ,
0.00000E+00,   301.30    ,   1.0000
 3,  5.4792    ,  0.26060    ,  0.00000E+00,   2.1563    , -0.17521    ,
0.00000E+00,   300.60    ,   1.2000
 3,  5.9499    ,  0.22227    ,  0.00000E+00,   2.5625    , -0.21122    ,
0.00000E+00,   299.65    ,   1.4000
 3,  6.5118    ,  0.17406    ,  0.00000E+00,   3.0875    , -0.27868    ,
0.00000E+00,   298.17    ,   1.6000
 3,  7.2094    ,  0.10628    ,  0.00000E+00,   4.0033    , -0.41254    ,
0.00000E+00,   294.94    ,   1.8000
 3,  8.2000    ,  0.97803E-02,  0.00000E+00,   6.1972    , -0.51998    ,
0.00000E+00,   283.87    ,   2.0000
 3,  9.6656    , -0.99334E-01,  0.00000E+00,   7.9860    , -0.59165    ,
0.00000E+00,   271.32    ,   2.2000
 3,  11.300    , -0.21579    ,  0.00000E+00,   8.4637    , -0.42810    ,
0.00000E+00,   267.55    ,   2.4000
 3,  13.466    , -0.19826    ,  0.00000E+00,   14.670    ,  0.73303    ,
0.00000E+00,   196.68    ,   2.6000
 3,  17.728    , -0.54784E-01,  0.00000E+00,   24.797    ,  0.53287    ,
0.00000E+00,  0.12432E-01,   2.8000
 3,  22.688    ,  0.51781E-01,  0.00000E+00,   24.797    ,  0.53283    ,
0.00000E+00,  0.38611E-03,   3.0000
 4,  4.0640    ,  0.25400    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.84    ,  0.00000E+00
 4,  4.1541    ,  0.25208    ,  0.00000E+00,  0.58439    , -0.19648E-01,
0.00000E+00,   302.72    ,  0.20001
 4,  4.2987    ,  0.24597    ,  0.00000E+00,  0.86362    , -0.41308E-01,
0.00000E+00,   302.52    ,  0.40000
 4,  4.5007    ,  0.23574    ,  0.00000E+00,   1.1596    , -0.60439E-01,
0.00000E+00,   302.23    ,  0.60001
 4,  4.7636    ,  0.22204    ,  0.00000E+00,   1.4727    , -0.76106E-01,
0.00000E+00,   301.82    ,  0.80001
```

```
  4,   5.0911     ,  0.20538    ,  0.00000E+00,   1.8053     , -0.90566E-01,
0.00000E+00,   301.28    ,   1.0000
  4,   5.4875     ,  0.18564    ,  0.00000E+00,   2.1652     , -0.10772    ,
0.00000E+00,   300.58    ,   1.2000
  4,   5.9604     ,  0.16167    ,  0.00000E+00,   2.5756     , -0.13439    ,
0.00000E+00,   299.62    ,   1.4000
  4,   6.5257     ,  0.13029    ,  0.00000E+00,   3.1104     , -0.18550    ,
0.00000E+00,   298.11    ,   1.6000
  4,   7.2299     ,  0.83778E-01,  0.00000E+00,   4.0493     , -0.29106    ,
0.00000E+00,   294.78    ,   1.8000
  4,   8.2343     ,  0.14092E-01,  0.00000E+00,   6.2860     , -0.37963    ,
0.00000E+00,   283.37    ,   2.0000
  4,   9.7111     , -0.64312E-01,  0.00000E+00,   8.0087     , -0.41806    ,
0.00000E+00,   271.21    ,   2.2000
  4,   11.352     , -0.14554    ,  0.00000E+00,   8.5649     , -0.28361    ,
0.00000E+00,   266.77    ,   2.4000
  4,   13.567     , -0.13345    ,  0.00000E+00,   15.192     ,  0.50340    ,
0.00000E+00,   189.15    ,   2.6000
  4,   17.898     , -0.43307E-01,  0.00000E+00,   24.800     ,  0.31416    ,
0.00000E+00,  0.10005E-01,   2.8000
  4,   22.858     ,  0.19521E-01,  0.00000E+00,   24.800     ,  0.31415    ,
0.00000E+00,  0.28493E-03,   3.0000
  5,   4.0640     ,  0.12700    ,  0.00000E+00,  0.31868     ,  0.00000E+00,
0.00000E+00,   302.83    ,  0.00000E+00
  5,   4.1548     ,  0.12623    ,  0.00000E+00,  0.58998     , -0.80669E-02,
0.00000E+00,   302.71    ,  0.20000
  5,   4.3006     ,  0.12364    ,  0.00000E+00,  0.87066     , -0.17925E-01,
0.00000E+00,   302.51    ,  0.40000
  5,   4.5040     ,  0.11909    ,  0.00000E+00,   1.1660     , -0.27323E-01,
0.00000E+00,   302.21    ,  0.60001
  5,   4.7682     ,  0.11281    ,  0.00000E+00,   1.4788     , -0.35260E-01,
0.00000E+00,   301.81    ,  0.80000
  5,   5.0969     ,  0.10502    ,  0.00000E+00,   1.8121     , -0.42646E-01,
0.00000E+00,   301.27    ,   1.0000
  5,   5.4949     ,  0.95657E-01,  0.00000E+00,   2.1739     , -0.51493E-01,
0.00000E+00,   300.56    ,   1.2000
  5,   5.9699     ,  0.84092E-01,  0.00000E+00,   2.5883     , -0.65492E-01,
0.00000E+00,   299.58    ,   1.4000
  5,   6.5384     ,  0.68584E-01,  0.00000E+00,   3.1309     , -0.92969E-01,
0.00000E+00,   298.05    ,   1.6000
  5,   7.2484     ,  0.44857E-01,  0.00000E+00,   4.0907     , -0.15057    ,
0.00000E+00,   294.64    ,   1.8000
  5,   8.2651     ,  0.85275E-02,  0.00000E+00,   6.3628     , -0.19811    ,
0.00000E+00,   282.92    ,   2.0000
  5,   9.7512     , -0.32113E-01,  0.00000E+00,   8.0262     , -0.21510    ,
0.00000E+00,   271.12    ,   2.2000
  5,   11.397     , -0.73371E-01,  0.00000E+00,   8.6446     , -0.13566    ,
0.00000E+00,   266.06    ,   2.4000
  5,   13.652     , -0.66359E-01,  0.00000E+00,   15.612     ,  0.25551    ,
0.00000E+00,   182.85    ,   2.6000
  5,   18.035     , -0.23091E-01,  0.00000E+00,   24.803     ,  0.14773    ,
0.00000E+00,  0.86309E-02,   2.8000
  5,   22.996     ,  0.64537E-02,  0.00000E+00,   24.803     ,  0.14772    ,
0.00000E+00,  0.20838E-03,   3.0000
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    6,    4.0640     ,  0.00000E+00,  0.00000E+00,  0.31868     ,  0.00000E+00,
 0.00000E+00,    302.83     ,  0.00000E+00
    6,    4.1550     ,  0.00000E+00,  0.00000E+00,  0.59185     ,  0.00000E+00,
 0.00000E+00,    302.71     ,  0.20000
    6,    4.3013     ,  0.00000E+00,  0.00000E+00,  0.87316     ,  0.00000E+00,
 0.00000E+00,    302.51     ,  0.40000
    6,    4.5052     ,  0.00000E+00,  0.00000E+00,   1.1683     ,  0.00000E+00,
 0.00000E+00,    302.21     ,  0.60000
    6,    4.7698     ,  0.00000E+00,  0.00000E+00,   1.4811     ,  0.00000E+00,
 0.00000E+00,    301.80     ,  0.80000
    6,    5.0990     ,  0.00000E+00,  0.00000E+00,   1.8147     ,  0.00000E+00,
 0.00000E+00,    301.26     ,   1.0000
    6,    5.4976     ,  0.00000E+00,  0.00000E+00,   2.1773     ,  0.00000E+00,
 0.00000E+00,    300.55     ,   1.2000
    6,    5.9734     ,  0.00000E+00,  0.00000E+00,   2.5934     ,  0.00000E+00,
 0.00000E+00,    299.57     ,   1.4000
    6,    6.5433     ,  0.00000E+00,  0.00000E+00,   3.1406     ,  0.00000E+00,
 0.00000E+00,    298.03     ,   1.6000
    6,    7.2562     ,  0.00000E+00,  0.00000E+00,   4.1124     ,  0.00000E+00,
 0.00000E+00,    294.57     ,   1.8000
    6,    8.2791     ,  0.00000E+00,  0.00000E+00,   6.3990     ,  0.00000E+00,
 0.00000E+00,    282.72     ,   2.0000
    6,    9.7696     ,  0.00000E+00,  0.00000E+00,   8.0363     ,  0.00000E+00,
 0.00000E+00,    271.08     ,   2.2000
    6,    11.418     ,  0.00000E+00,  0.00000E+00,   8.6941     ,  0.00000E+00,
 0.00000E+00,    265.72     ,   2.4000
    6,    13.695     ,  0.00000E+00,  0.00000E+00,   15.825     ,  0.00000E+00,
 0.00000E+00,    179.62     ,   2.6000
    6,    18.104     ,  0.00000E+00,  0.00000E+00,   24.803     ,  0.00000E+00,
 0.00000E+00,  0.80865E-02,   2.8000
    6,    23.064     ,  0.00000E+00,  0.00000E+00,   24.803     ,  0.00000E+00,
 0.00000E+00,  0.17362E-03,   3.0000
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The original Viking spacecraft mass spectrometer -- m/z 143

```
 1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.99    ,  0.00000E+00
 1,   4.1298    ,  0.63038    ,  0.00000E+00,  0.41615    , -0.45150E-01,
0.00000E+00,   202.89    ,  0.20000
 1,   4.2334    ,  0.61756    ,  0.00000E+00,  0.61612    , -0.81054E-01,
0.00000E+00,   202.74    ,  0.40001
 1,   4.3751    ,  0.59853    ,  0.00000E+00,  0.80043    , -0.10792    ,
0.00000E+00,   202.54    ,  0.60000
 1,   4.5534    ,  0.57482    ,  0.00000E+00,  0.98190    , -0.12832    ,
0.00000E+00,   202.30    ,  0.80000
 1,   4.7681    ,  0.54746    ,  0.00000E+00,   1.1656    , -0.14471    ,
0.00000E+00,   202.00    ,   1.0000
 1,   5.0199    ,  0.51707    ,  0.00000E+00,   1.3537    , -0.15908    ,
0.00000E+00,   201.65    ,   1.2000
 1,   5.3099    ,  0.48382    ,  0.00000E+00,   1.5475    , -0.17370    ,
0.00000E+00,   201.22    ,   1.4000
 1,   5.6395    ,  0.44734    ,  0.00000E+00,   1.7501    , -0.19209    ,
0.00000E+00,   200.72    ,   1.6000
 1,   6.0110    ,  0.40633    ,  0.00000E+00,   1.9683    , -0.22039    ,
0.00000E+00,   200.11    ,   1.8000
 1,   6.4290    ,  0.35778    ,  0.00000E+00,   2.2204    , -0.27017    ,
0.00000E+00,   199.31    ,   2.0000
 1,   6.9046    ,  0.29527    ,  0.00000E+00,   2.5583    , -0.36538    ,
0.00000E+00,   198.07    ,   2.2000
 1,   7.4684    ,  0.20672    ,  0.00000E+00,   3.1451    , -0.52982    ,
0.00000E+00,   195.49    ,   2.4000
 1,   8.1995    ,  0.86503E-01,  0.00000E+00,   4.2572    , -0.64107    ,
0.00000E+00,   189.29    ,   2.6000
 1,   9.1658    , -0.39858E-01,  0.00000E+00,   5.2585    , -0.63201    ,
0.00000E+00,   182.23    ,   2.8000
 1,   10.250    , -0.16978    ,  0.00000E+00,   5.5136    , -0.66272    ,
0.00000E+00,   180.17    ,   3.0000
 1,   11.368    , -0.29430    ,  0.00000E+00,   5.7521    , -0.47026    ,
0.00000E+00,   178.37    ,   3.2000
 1,   12.715    , -0.32161    ,  0.00000E+00,   8.0194    ,  0.39723E-01,
0.00000E+00,   155.38    ,   3.4000
 1,   14.808    , -0.21932    ,  0.00000E+00,   13.734    ,  0.68573    ,
0.00000E+00,   62.867    ,   3.6000
 2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.91    ,  0.00000E+00
 2,   4.1297    ,  0.50190    ,  0.00000E+00,  0.40223    , -0.58144E-01,
0.00000E+00,   202.83    ,  0.20000
 2,   4.2263    ,  0.48608    ,  0.00000E+00,  0.56529    , -0.96873E-01,
0.00000E+00,   202.71    ,  0.40001
 2,   4.3564    ,  0.46397    ,  0.00000E+00,  0.73702    , -0.12264    ,
0.00000E+00,   202.54    ,  0.60001
 2,   4.5214    ,  0.43750    ,  0.00000E+00,  0.91353    , -0.14103    ,
0.00000E+00,   202.32    ,  0.80000
 2,   4.7221    ,  0.40786    ,  0.00000E+00,   1.0946    , -0.15488    ,
0.00000E+00,   202.05    ,   1.0000
 2,   4.9596    ,  0.37572    ,  0.00000E+00,   1.2811    , -0.16625    ,
0.00000E+00,   201.72    ,   1.2000
```

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2,   5.2350    ,  0.34140    ,  0.00000E+00,   1.4742    , -0.17696    ,
0.00000E+00,   201.32    ,   1.4000
2,   5.5499    ,  0.30483    ,  0.00000E+00,   1.6764    , -0.18925    ,
0.00000E+00,   200.84    ,   1.6000
2,   5.9066    ,  0.26539    ,  0.00000E+00,   1.8943    , -0.20631    ,
0.00000E+00,   200.26    ,   1.8000
2,   6.3096    ,  0.22163    ,  0.00000E+00,   2.1433    , -0.23361    ,
0.00000E+00,   199.51    ,   2.0000
2,   6.7686    ,  0.17064    ,  0.00000E+00,   2.4649    , -0.28060    ,
0.00000E+00,   198.39    ,   2.2000
2,   7.3080    ,  0.10746    ,  0.00000E+00,   2.9795    , -0.35516    ,
0.00000E+00,   196.29    ,   2.4000
2,   7.9911    ,  0.29507E-01,  0.00000E+00,   3.9481    , -0.41257    ,
0.00000E+00,   191.28    ,   2.6000
2,   8.9052    , -0.53965E-01,  0.00000E+00,   5.1085    , -0.43121    ,
0.00000E+00,   183.47    ,   2.8000
2,   9.9752    , -0.14584    ,  0.00000E+00,   5.4900    , -0.48147    ,
0.00000E+00,   180.44    ,   3.0000
2,   11.086    , -0.24094    ,  0.00000E+00,   5.6439    , -0.42577    ,
0.00000E+00,   179.21    ,   3.2000
2,   12.339    , -0.26948    ,  0.00000E+00,   7.3456    ,  0.68461E-01,
0.00000E+00,   162.97    ,   3.4000
2,   14.181    , -0.19628    ,  0.00000E+00,   12.054    ,  0.66504    ,
0.00000E+00,   94.976    ,   3.6000
2,   17.167    , -0.85469E-01,  0.00000E+00,   16.545    ,  0.41525    ,
0.00000E+00,  0.30023E-01,   3.8000
2,   20.476    , -0.25985E-02,  0.00000E+00,   16.546    ,  0.41431    ,
0.00000E+00,  0.13634E-02,   4.0000
2,   23.785    ,  0.80265E-01,  0.00000E+00,   16.546    ,  0.41432    ,
0.00000E+00,  0.73477E-05,   4.2000
3,   4.0640    ,  0.38100    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.88    ,  0.00000E+00
3,   4.1305    ,  0.37854    ,  0.00000E+00,  0.40713    , -0.24363E-01,
0.00000E+00,   202.80    ,  0.20000
3,   4.2275    ,  0.37137    ,  0.00000E+00,  0.56466    , -0.46994E-01,
0.00000E+00,   202.69    ,  0.40000
3,   4.3570    ,  0.36002    ,  0.00000E+00,  0.73149    , -0.65754E-01,
0.00000E+00,   202.52    ,  0.60000
3,   4.5206    ,  0.34534    ,  0.00000E+00,  0.90546    , -0.80329E-01,
0.00000E+00,   202.31    ,  0.80001
3,   4.7196    ,  0.32810    ,  0.00000E+00,   1.0855    , -0.91710E-01,
0.00000E+00,   202.04    ,   1.0000
3,   4.9552    ,  0.30878    ,  0.00000E+00,   1.2716    , -0.10123    ,
0.00000E+00,   201.72    ,   1.2000
3,   5.2287    ,  0.28763    ,  0.00000E+00,   1.4647    , -0.11030    ,
0.00000E+00,   201.33    ,   1.4000
3,   5.5417    ,  0.26457    ,  0.00000E+00,   1.6674    , -0.12083    ,
0.00000E+00,   200.85    ,   1.6000
3,   5.8967    ,  0.23901    ,  0.00000E+00,   1.8856    , -0.13581    ,
0.00000E+00,   200.28    ,   1.8000
3,   6.2979    ,  0.20959    ,  0.00000E+00,   2.1341    , -0.16071    ,
0.00000E+00,   199.53    ,   2.0000
3,   6.7549    ,  0.17339    ,  0.00000E+00,   2.4531    , -0.20588    ,
0.00000E+00,   198.43    ,   2.2000
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  3,   7.2912    ,  0.12492    ,  0.00000E+00,   2.9583    , -0.28482    ,
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  3,   7.9684    ,  0.59210E-01,  0.00000E+00,   3.9113    , -0.36208    ,
0.00000E+00,   191.49    ,   2.6000
  3,   8.8759    , -0.13712E-01,  0.00000E+00,   5.0867    , -0.36410    ,
0.00000E+00,   183.65    ,   2.8000
  3,   9.9441    , -0.89039E-01,  0.00000E+00,   5.4889    , -0.38907    ,
0.00000E+00,   180.48    ,   3.0000
  3,   11.056    , -0.16624    ,  0.00000E+00,   5.6528    , -0.35454    ,
0.00000E+00,   179.16    ,   3.2000
  3,   12.305    , -0.19884    ,  0.00000E+00,   7.2889    , -0.66773E-02,
0.00000E+00,   163.55    ,   3.4000
  3,   14.130    , -0.15671    ,  0.00000E+00,   11.911    ,  0.44338    ,
0.00000E+00,   97.617    ,   3.6000
  3,   17.097    , -0.85883E-01,  0.00000E+00,   16.543    ,  0.22585    ,
0.00000E+00,  0.39739E-01,   3.8000
  3,   20.406    , -0.41066E-01,  0.00000E+00,   16.545    ,  0.22402    ,
0.00000E+00,  0.14099E-02,   4.0000
  3,   23.715    ,  0.37377E-02,  0.00000E+00,   16.545    ,  0.22402    ,
0.00000E+00,  0.10370E-04,   4.2000
  4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.86    ,  0.00000E+00
  4,   4.1312    ,  0.25292    ,  0.00000E+00,  0.41262    , -0.10990E-01,
0.00000E+00,   202.79    ,  0.20000
  4,   4.2294    ,  0.24952    ,  0.00000E+00,  0.57097    , -0.23181E-01,
0.00000E+00,   202.67    ,  0.40000
  4,   4.3600    ,  0.24370    ,  0.00000E+00,  0.73632    , -0.34795E-01,
0.00000E+00,   202.51    ,  0.60001
  4,   4.5244    ,  0.23572    ,  0.00000E+00,  0.90878    , -0.44614E-01,
0.00000E+00,   202.30    ,  0.80001
  4,   4.7240    ,  0.22598    ,  0.00000E+00,   1.0880    , -0.52538E-01,
0.00000E+00,   202.03    ,   1.0000
  4,   4.9601    ,  0.21479    ,  0.00000E+00,   1.2740    , -0.59238E-01,
0.00000E+00,   201.71    ,   1.2000
  4,   5.2341    ,  0.20230    ,  0.00000E+00,   1.4676    , -0.65706E-01,
0.00000E+00,   201.31    ,   1.4000
  4,   5.5478    ,  0.18843    ,  0.00000E+00,   1.6712    , -0.73352E-01,
0.00000E+00,   200.84    ,   1.6000
  4,   5.9036    ,  0.17274    ,  0.00000E+00,   1.8910    , -0.84412E-01,
0.00000E+00,   200.26    ,   1.8000
  4,   6.3062    ,  0.15417    ,  0.00000E+00,   2.1426    , -0.10306    ,
0.00000E+00,   199.50    ,   2.0000
  4,   6.7654    ,  0.13049    ,  0.00000E+00,   2.4677    , -0.13736    ,
0.00000E+00,   198.39    ,   2.2000
  4,   7.3056    ,  0.97357E-01,  0.00000E+00,   2.9834    , -0.19889    ,
0.00000E+00,   196.29    ,   2.4000
  4,   7.9893    ,  0.50630E-01,  0.00000E+00,   3.9508    , -0.26040    ,
0.00000E+00,   191.30    ,   2.6000
  4,   8.9043    , -0.15439E-02,  0.00000E+00,   5.1137    , -0.25701    ,
0.00000E+00,   183.48    ,   2.8000
  4,   9.9757    , -0.54044E-01,  0.00000E+00,   5.4992    , -0.26901    ,
0.00000E+00,   180.45    ,   3.0000
  4,   11.090    , -0.10721    ,  0.00000E+00,   5.6778    , -0.24249    ,
0.00000E+00,   178.99    ,   3.2000
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   4,   12.353     , -0.13060    ,  0.00000E+00,   7.3805     , -0.19658E-01,
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   4,   14.214     , -0.10423    ,  0.00000E+00,   12.157     ,  0.27654     ,
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   4,   17.211     , -0.62678E-01,  0.00000E+00,   16.544     ,  0.11075     ,
0.00000E+00,  0.28717E-01,    3.8000
   4,   20.520     , -0.40645E-01,  0.00000E+00,   16.545     ,  0.11014     ,
0.00000E+00,  0.13343E-02,    4.0000
   4,   23.829     , -0.18617E-01,  0.00000E+00,   16.545     ,  0.11014     ,
0.00000E+00,  0.64531E-05,    4.2000
   5,   4.0640     ,  0.12700    ,  0.00000E+00,  0.25974     ,  0.00000E+00,
0.00000E+00,   202.86     ,  0.00000E+00
   5,   4.1315     ,  0.12657    ,  0.00000E+00,  0.41597     , -0.44244E-02,
0.00000E+00,   202.78     ,  0.20001
   5,   4.2306     ,  0.12517    ,  0.00000E+00,  0.57571     , -0.97663E-02,
0.00000E+00,   202.66     ,  0.40000
   5,   4.3622     ,  0.12266    ,  0.00000E+00,  0.74090     , -0.15243E-01,
0.00000E+00,   202.50     ,  0.60000
   5,   4.5274     ,  0.11911    ,  0.00000E+00,  0.91270     , -0.20109E-01,
0.00000E+00,   202.29     ,  0.80001
   5,   4.7277     ,  0.11467    ,  0.00000E+00,   1.0915     , -0.24125E-01,
0.00000E+00,   202.02     ,    1.0000
   5,   4.9645     ,  0.10950    ,  0.00000E+00,   1.2774     , -0.27542E-01,
0.00000E+00,   201.70     ,    1.2000
   5,   5.2392     ,  0.10366    ,  0.00000E+00,   1.4714     , -0.30858E-01,
0.00000E+00,   201.30     ,    1.4000
   5,   5.5537     ,  0.97117E-01,  0.00000E+00,   1.6758     , -0.34806E-01,
0.00000E+00,   200.82     ,    1.6000
   5,   5.9107     ,  0.89622E-01,  0.00000E+00,   1.8972     , -0.40592E-01,
0.00000E+00,   200.24     ,    1.8000
   5,   6.3148     ,  0.80610E-01,  0.00000E+00,   2.1516     , -0.50504E-01,
0.00000E+00,   199.47     ,    2.0000
   5,   6.7762     ,  0.68858E-01,  0.00000E+00,   2.4816     , -0.68985E-01,
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   5,   7.3200     ,  0.51997E-01,  0.00000E+00,   3.0068     , -0.10227     ,
0.00000E+00,   196.20     ,    2.4000
   5,   8.0098     ,  0.27817E-01,  0.00000E+00,   3.9879     , -0.13513     ,
0.00000E+00,   191.11     ,    2.6000
   5,   8.9315     ,  0.87325E-03,  0.00000E+00,   5.1363     , -0.13185     ,
0.00000E+00,   183.33     ,    2.8000
   5,   10.005     , -0.25918E-01,  0.00000E+00,   5.5065     , -0.13677     ,
0.00000E+00,   180.42     ,    3.0000
   5,   11.122     , -0.52845E-01,  0.00000E+00,   5.6975     , -0.12148     ,
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   5,   12.396     , -0.64790E-01,  0.00000E+00,   7.4624     , -0.13422E-01,
0.00000E+00,   161.64     ,    3.4000
   5,   14.287     , -0.51774E-01,  0.00000E+00,   12.369     ,  0.13252     ,
0.00000E+00,   89.511     ,    3.6000
   5,   17.311     , -0.32824E-01,  0.00000E+00,   16.548     ,  0.46256E-01,
0.00000E+00,  0.21165E-01,    3.8000
   5,   20.620     , -0.23599E-01,  0.00000E+00,   16.549     ,  0.46118E-01,
0.00000E+00,  0.12712E-02,    4.0000
   5,   23.930     , -0.14375E-01,  0.00000E+00,   16.549     ,  0.46118E-01,
0.00000E+00,  0.42803E-05,    4.2000
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    6,   4.0640     ,  0.00000E+00,  0.00000E+00,  0.25974      ,  0.00000E+00,
 0.00000E+00,    202.85     ,  0.00000E+00
    6,   4.1317     ,  0.00000E+00,  0.00000E+00,  0.41707      ,  0.00000E+00,
 0.00000E+00,    202.78     ,  0.20001
    6,   4.2310     ,  0.00000E+00,  0.00000E+00,  0.57737      ,  0.00000E+00,
 0.00000E+00,    202.66     ,  0.40001
    6,   4.3629     ,  0.00000E+00,  0.00000E+00,  0.74257      ,  0.00000E+00,
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    6,   4.5285     ,  0.00000E+00,  0.00000E+00,  0.91418      ,  0.00000E+00,
 0.00000E+00,    202.29     ,  0.80001
    6,   4.7291     ,  0.00000E+00,  0.00000E+00,   1.0928      ,  0.00000E+00,
 0.00000E+00,    202.02     ,   1.0000
    6,   4.9661     ,  0.00000E+00,  0.00000E+00,   1.2787      ,  0.00000E+00,
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    6,   5.2411     ,  0.00000E+00,  0.00000E+00,   1.4728      ,  0.00000E+00,
 0.00000E+00,    201.30     ,   1.4000
    6,   5.5559     ,  0.00000E+00,  0.00000E+00,   1.6776      ,  0.00000E+00,
 0.00000E+00,    200.82     ,   1.6000
    6,   5.9133     ,  0.00000E+00,  0.00000E+00,   1.8997      ,  0.00000E+00,
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    6,   6.3180     ,  0.00000E+00,  0.00000E+00,   2.1556      ,  0.00000E+00,
 0.00000E+00,    199.46     ,   2.0000
    6,   6.7805     ,  0.00000E+00,  0.00000E+00,   2.4885      ,  0.00000E+00,
 0.00000E+00,    198.32     ,   2.2000
    6,   7.3262     ,  0.00000E+00,  0.00000E+00,   3.0196      ,  0.00000E+00,
 0.00000E+00,    196.15     ,   2.4000
    6,   8.0193     ,  0.00000E+00,  0.00000E+00,   4.0063      ,  0.00000E+00,
 0.00000E+00,    191.01     ,   2.6000
    6,   8.9441     ,  0.00000E+00,  0.00000E+00,   5.1465      ,  0.00000E+00,
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    6,   10.019     ,  0.00000E+00,  0.00000E+00,   5.5099      ,  0.00000E+00,
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    6,   11.136     ,  0.00000E+00,  0.00000E+00,   5.7096      ,  0.00000E+00,
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 0.00000E+00,    161.20     ,   3.4000
    6,   14.323     ,  0.00000E+00,  0.00000E+00,   12.471      ,  0.00000E+00,
 0.00000E+00,    87.651     ,   3.6000
    6,   17.358     ,  0.00000E+00,  0.00000E+00,   16.546      ,  0.00000E+00,
 0.00000E+00,  0.18599E-01,   3.8000
    6,   20.668     ,  0.00000E+00,  0.00000E+00,   16.547      ,  0.00000E+00,
 0.00000E+00,  0.12422E-02,   4.0000
    6,   23.977     ,  0.00000E+00,  0.00000E+00,   16.547      ,  0.00000E+00,
 0.00000E+00,  0.35704E-05,   4.2000
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The original Viking mass spectrometer -- m/z 286

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  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.18367    ,  0.00000E+00,
0.00000E+00,   102.99    ,  0.00000E+00
  1,   4.1634    ,  0.62731    ,  0.00000E+00,  0.32991    , -0.36866E-01,
0.00000E+00,   102.86    ,  0.40000
  1,   4.3287    ,  0.60719    ,  0.00000E+00,  0.49329    , -0.61940E-01,
0.00000E+00,   102.66    ,  0.80000
  1,   4.5571    ,  0.57898    ,  0.00000E+00,  0.64859    , -0.77916E-01,
0.00000E+00,   102.39    ,   1.2000
  1,   4.8477    ,  0.54565    ,  0.00000E+00,  0.80491    , -0.87934E-01,
0.00000E+00,   102.05    ,   1.6000
  1,   5.2013    ,  0.50913    ,  0.00000E+00,  0.96368    , -0.94249E-01,
0.00000E+00,   101.64    ,   2.0000
  1,   5.6190    ,  0.47035    ,  0.00000E+00,   1.1249    , -0.99847E-01,
0.00000E+00,   101.14    ,   2.4000
  1,   6.1019    ,  0.42860    ,  0.00000E+00,   1.2912    , -0.11053    ,
0.00000E+00,   100.54    ,   2.8000
  1,   6.6542    ,  0.37964    ,  0.00000E+00,   1.4761    , -0.13906    ,
0.00000E+00,   99.768    ,   3.2000
  1,   7.2924    ,  0.31095    ,  0.00000E+00,   1.7381    , -0.21577    ,
0.00000E+00,   98.480    ,   3.6000
  1,   8.0802    ,  0.20198    ,  0.00000E+00,   2.2598    , -0.31688    ,
0.00000E+00,   95.309    ,   4.0000
  1,   9.1085    ,  0.81248E-01,  0.00000E+00,   2.8066    , -0.27549    ,
0.00000E+00,   91.236    ,   4.4000
  1,   10.266    , -0.25984E-01,  0.00000E+00,   2.9432    , -0.26637    ,
0.00000E+00,   90.081    ,   4.8000
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0.00000E+00,   88.460    ,   5.2000
  1,   12.931    , -0.18930    ,  0.00000E+00,   4.3477    , -0.91861E-01,
0.00000E+00,   74.998    ,   5.6000
  1,   15.244    , -0.17232    ,  0.00000E+00,   7.4303    ,  0.48479E-01,
0.00000E+00,   21.193    ,   6.0000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.18367    ,  0.00000E+00,
0.00000E+00,   102.92    ,  0.00000E+00
  2,   4.1616    ,  0.49801    ,  0.00000E+00,  0.30960    , -0.46274E-01,
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  2,   4.3138    ,  0.47388    ,  0.00000E+00,  0.45313    , -0.71980E-01,
0.00000E+00,   102.66    ,  0.80000
  2,   4.5248    ,  0.44185    ,  0.00000E+00,  0.60283    , -0.86911E-01,
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  2,   4.7966    ,  0.40516    ,  0.00000E+00,  0.75645    , -0.95788E-01,
0.00000E+00,   102.11    ,   1.6000
  2,   5.1305    ,  0.36569    ,  0.00000E+00,  0.91376    , -0.10115    ,
0.00000E+00,   101.72    ,   2.0000
  2,   5.5281    ,  0.32440    ,  0.00000E+00,   1.0747    , -0.10534    ,
0.00000E+00,   101.24    ,   2.4000
  2,   5.9910    ,  0.28113    ,  0.00000E+00,   1.2416    , -0.11178    ,
0.00000E+00,   100.66    ,   2.8000
  2,   6.5236    ,  0.23386    ,  0.00000E+00,   1.4261    , -0.12679    ,
0.00000E+00,   99.930    ,   3.2000
  2,   7.1398    ,  0.17685    ,  0.00000E+00,   1.6734    , -0.16318    ,
0.00000E+00,   98.778    ,   3.6000
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2,   7.8896    , 0.10042    , 0.00000E+00,  2.1266    , -0.21641    ,
0.00000E+00,  96.196    ,  4.0000
2,   8.8676    , 0.12743E-01, 0.00000E+00,  2.7282    , -0.21419    ,
0.00000E+00,  91.867    ,  4.4000
2,   10.010    , -0.73630E-01, 0.00000E+00,  2.9261    , -0.21960    ,
0.00000E+00,  90.207    ,  4.8000
2,   11.195    , -0.15985    , 0.00000E+00,  3.0267    , -0.19199    ,
0.00000E+00,  89.344    ,  5.2000
2,   12.561    , -0.19900    , 0.00000E+00,  4.0069    , -0.36294E-01,
0.00000E+00,  79.175    ,  5.6000
2,   14.614    , -0.15885    , 0.00000E+00,  6.7021    ,  0.17533    ,
0.00000E+00,  36.350    ,  6.0000
2,   17.762    , -0.11813    , 0.00000E+00,  8.3352    ,  0.51329E-01,
0.00000E+00, 0.38684E-02,  6.4000
2,   21.096    , -0.97603E-01, 0.00000E+00,  8.3353    ,  0.51305E-01,
0.00000E+00, 0.49830E-03,  6.8000
2,   24.430    , -0.77081E-01, 0.00000E+00,  8.3353    ,  0.51304E-01,
0.00000E+00, 0.18339E-06,  7.2000
3,   4.0640    , 0.38100    , 0.00000E+00, 0.18367    ,  0.00000E+00,
0.00000E+00,  102.89    , 0.00000E+00
3,   4.1625    , 0.37689    , 0.00000E+00, 0.31091    , -0.20223E-01,
0.00000E+00,  102.80    , 0.40001
3,   4.3142    , 0.36522    , 0.00000E+00, 0.44931    , -0.37292E-01,
0.00000E+00,  102.64    , 0.80000
3,   4.5230    , 0.34779    , 0.00000E+00, 0.59603    , -0.49017E-01,
0.00000E+00,  102.41    ,  1.2000
3,   4.7918    , 0.32659    , 0.00000E+00, 0.74840    , -0.56366E-01,
0.00000E+00,  102.11    ,  1.6000
3,   5.1224    , 0.30307    , 0.00000E+00, 0.90525    , -0.60937E-01,
0.00000E+00,  101.72    ,  2.0000
3,   5.5165    , 0.27797    , 0.00000E+00,  1.0662    , -0.64553E-01,
0.00000E+00,  101.25    ,  2.4000
3,   5.9761    , 0.25117    , 0.00000E+00,  1.2332    , -0.70122E-01,
0.00000E+00,  100.68    ,  2.8000
3,   6.5053    , 0.22086    , 0.00000E+00,  1.4174    , -0.83580E-01,
0.00000E+00,  99.955    ,  3.2000
3,   7.1175    , 0.18151    , 0.00000E+00,  1.6614    , -0.11829    ,
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3,   7.8606    , 0.12243    , 0.00000E+00,  2.1045    , -0.17647    ,
0.00000E+00,  96.332    ,  4.0000
3,   8.8301    , 0.50213E-01, 0.00000E+00,  2.7140    , -0.17054    ,
0.00000E+00,  91.978    ,  4.4000
3,   9.9693    , -0.15416E-01, 0.00000E+00,  2.9239    , -0.16250    ,
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3,   11.154    , -0.79758E-01, 0.00000E+00,  3.0227    , -0.15084    ,
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3,   12.510    , -0.12009    , 0.00000E+00,  3.9615    , -0.64558E-01,
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3,   14.531    , -0.11248    , 0.00000E+00,  6.5940    ,  0.71855E-01,
0.00000E+00,  38.476    ,  6.0000
3,   17.657    , -0.10558    , 0.00000E+00,  8.3329    , -0.28237E-01,
0.00000E+00, 0.45022E-02,  6.4000
3,   20.990    , -0.11689    , 0.00000E+00,  8.3331    , -0.28268E-01,
0.00000E+00, 0.52708E-03,  6.8000
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3,   24.324     , -0.12820     ,  0.00000E+00,   8.3331      , -0.28269E-01,
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4,   4.0640     ,  0.25400     ,  0.00000E+00,  0.18367     ,  0.00000E+00,
0.00000E+00,   102.88    ,  0.00000E+00
4,   4.1634     ,  0.25218     ,  0.00000E+00,  0.31442     , -0.93105E-02,
0.00000E+00,   102.79    ,  0.40000
4,   4.3165     ,  0.24645     ,  0.00000E+00,  0.45197     , -0.19137E-01,
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4,   4.5260     ,  0.23715     ,  0.00000E+00,  0.59697     , -0.26912E-01,
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4,   4.7949     ,  0.22528     ,  0.00000E+00,  0.74831     , -0.32040E-01,
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4,   5.1253     ,  0.21177     ,  0.00000E+00,  0.90477     , -0.35281E-01,
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4,   5.5193     ,  0.19714     ,  0.00000E+00,   1.0658     , -0.37910E-01,
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4,   5.9788     ,  0.18125     ,  0.00000E+00,   1.2335     , -0.42051E-01,
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4,   6.5084     ,  0.16273     ,  0.00000E+00,   1.4192     , -0.52138E-01,
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4,   7.1220     ,  0.13742     ,  0.00000E+00,   1.6668     , -0.78394E-01,
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4,   7.8681     ,  0.97021E-01,  0.00000E+00,   2.1135     , -0.12324     ,
0.00000E+00,   96.292    ,   4.0000
4,   8.8410     ,  0.46674E-01,  0.00000E+00,   2.7203     , -0.11675     ,
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4,   9.9818     ,  0.26941E-02,  0.00000E+00,   2.9265     , -0.10747     ,
0.00000E+00,   90.225    ,   4.8000
4,   11.168     , -0.39927E-01,  0.00000E+00,   3.0289     , -0.10150     ,
0.00000E+00,   89.328    ,   5.2000
4,   12.529     , -0.70003E-01,  0.00000E+00,   3.9805     , -0.55215E-01,
0.00000E+00,   79.450    ,   5.6000
4,   14.565     , -0.71853E-01,  0.00000E+00,   6.6384     ,  0.25859E-01,
0.00000E+00,   37.619    ,   6.0000
4,   17.700     , -0.76957E-01,  0.00000E+00,   8.3332     , -0.47720E-01,
0.00000E+00,  0.42911E-02,   6.4000
4,   21.033     , -0.96052E-01,  0.00000E+00,   8.3334     , -0.47741E-01,
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4,   24.366     , -0.11515     ,  0.00000E+00,   8.3334     , -0.47742E-01,
0.00000E+00,  0.23450E-06,   7.2000
5,   4.0640     ,  0.12700     ,  0.00000E+00,  0.18367     ,  0.00000E+00,
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5,   4.5285     ,  0.11980     ,  0.00000E+00,  0.59878     , -0.12021E-01,
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5,   4.7979     ,  0.11443     ,  0.00000E+00,  0.74949     , -0.14626E-01,
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5,   5.1288     ,  0.10822     ,  0.00000E+00,  0.90569     , -0.16285E-01,
0.00000E+00,   101.71    ,   2.0000
5,   5.5231     ,  0.10144     ,  0.00000E+00,   1.0669     , -0.17642E-01,
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 5,   6.5137     ,  0.85184E-01,  0.00000E+00,   1.4225     , -0.25164E-01,
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 5,   8.8554     ,  0.26679E-01,  0.00000E+00,   2.7264     , -0.58593E-01,
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 5,   12.552     , -0.31956E-01,  0.00000E+00,   4.0013     , -0.30683E-01,
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 5,   14.604     , -0.34729E-01,  0.00000E+00,   6.6878     ,  0.65586E-02,
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 5,   17.748     , -0.40084E-01,  0.00000E+00,   8.3336     , -0.31618E-01,
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 6,   4.0640     ,  0.00000E+00,  0.00000E+00,  0.18367     ,  0.00000E+00,
0.00000E+00,   102.88     ,  0.00000E+00
 6,   4.1642     ,  0.00000E+00,  0.00000E+00,  0.31757     ,  0.00000E+00,
0.00000E+00,   102.78     ,  0.40001
 6,   4.3186     ,  0.00000E+00,  0.00000E+00,  0.45549     ,  0.00000E+00,
0.00000E+00,   102.62     ,  0.80001
 6,   4.5294     ,  0.00000E+00,  0.00000E+00,  0.59950     ,  0.00000E+00,
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 6,   4.7991     ,  0.00000E+00,  0.00000E+00,  0.74998     ,  0.00000E+00,
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 6,   5.1301     ,  0.00000E+00,  0.00000E+00,  0.90610     ,  0.00000E+00,
0.00000E+00,   101.71     ,   2.0000
 6,   5.5246     ,  0.00000E+00,  0.00000E+00,   1.0673     ,  0.00000E+00,
0.00000E+00,   101.24     ,   2.4000
 6,   5.9849     ,  0.00000E+00,  0.00000E+00,   1.2360     ,  0.00000E+00,
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 6,   6.5158     ,  0.00000E+00,  0.00000E+00,   1.4240     ,  0.00000E+00,
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 6,   7.1324     ,  0.00000E+00,  0.00000E+00,   1.6769     ,  0.00000E+00,
0.00000E+00,   98.761     ,   3.6000
 6,   7.8839     ,  0.00000E+00,  0.00000E+00,   2.1295     ,  0.00000E+00,
0.00000E+00,   96.209     ,   4.0000
 6,   8.8620     ,  0.00000E+00,  0.00000E+00,   2.7283     ,  0.00000E+00,
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 6,   10.005     ,  0.00000E+00,  0.00000E+00,   2.9286     ,  0.00000E+00,
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 6,   12.561     ,  0.00000E+00,  0.00000E+00,   4.0097     ,  0.00000E+00,
0.00000E+00,   79.099     ,   5.6000
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  6,   14.620    , 0.00000E+00, 0.00000E+00,   6.7077    , 0.00000E+00,
0.00000E+00,   36.232    ,   6.0000
  6,   17.768    , 0.00000E+00, 0.00000E+00,   8.3331    , 0.00000E+00,
0.00000E+00,  0.39551E-02,   6.4000
  6,   21.101    , 0.00000E+00, 0.00000E+00,   8.3332    , 0.00000E+00,
0.00000E+00,  0.49727E-03,   6.8000
  6,   24.434    , 0.00000E+00, 0.00000E+00,   8.3332    , 0.00000E+00,
0.00000E+00,  0.20038E-06,   7.2000
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  1,   4.0640    , 0.63500    , 0.00000E+00,  0.15892    ,  0.00000E+00,
0.00000E+00,   77.991    ,  0.00000E+00
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0.00000E+00,   77.855    ,  0.50000
  1,   4.3559    , 0.60450    , 0.00000E+00,  0.43702    , -0.53646E-01,
0.00000E+00,   77.643    ,   1.0000
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0.00000E+00,   77.362    ,   1.5000
  1,   4.9322    , 0.53915    , 0.00000E+00,  0.71614    , -0.73227E-01,
0.00000E+00,   77.001    ,   2.0000
  1,   5.3256    , 0.50162    , 0.00000E+00,  0.85754    , -0.76499E-01,
0.00000E+00,   76.560    ,   2.5000
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  1,   7.6510    , 0.29583    , 0.00000E+00,   1.5746    , -0.19402    ,
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  1,   8.5497    , 0.18587    , 0.00000E+00,   2.0331    , -0.21707    ,
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0.00000E+00,   67.856    ,   5.5000
  1,   10.782    , 0.51569E-02, 0.00000E+00,   2.3153    , -0.17121    ,
0.00000E+00,   67.358    ,   6.0000
  1,   12.002    ,-0.76138E-01, 0.00000E+00,   2.7099    , -0.14475    ,
0.00000E+00,   63.454    ,   6.5000
  1,   13.619    ,-0.13310    , 0.00000E+00,   3.9986    , -0.43683E-01,
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  1,   16.199    ,-0.15895    , 0.00000E+00,   6.1083    , -0.10924    ,
0.00000E+00,   4.1241    ,   7.5000
  2,   4.0640    , 0.50800    , 0.00000E+00,  0.15892    ,  0.00000E+00,
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0.00000E+00,   77.822    ,  0.50001
  2,   4.3389    , 0.47075    , 0.00000E+00,  0.40192    , -0.62075E-01,
0.00000E+00,   77.644    ,   1.0000
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  2,   5.6908    , 0.31467    , 0.00000E+00,  0.95665    , -0.85300E-01,
0.00000E+00,   76.145    ,   3.0000
  2,   6.2053    , 0.27107    , 0.00000E+00,   1.1027    , -0.90008E-01,
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  2,   8.3369    , 0.83531E-01,  0.00000E+00,   1.9309     , -0.16534    ,
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  3,   4.0640    ,  0.38100    ,  0.00000E+00,  0.15892     ,  0.00000E+00,
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  3,   4.5707    ,  0.34474    ,  0.00000E+00,  0.53003     , -0.41974E-01,
0.00000E+00,   77.388   ,   1.5000
  3,   4.8697    ,  0.32230    ,  0.00000E+00,  0.66677     , -0.47240E-01,
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  3,   5.2380    ,  0.29794    ,  0.00000E+00,  0.80668     , -0.49880E-01,
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  3,   5.6768    ,  0.27256    ,  0.00000E+00,  0.94879     , -0.51686E-01,
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  3,   6.7745    ,  0.21533    ,  0.00000E+00,   1.2584     , -0.68982E-01,
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  3,   7.4573    ,  0.17305    ,  0.00000E+00,   1.4945     , -0.10467    ,
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  3,   8.3017    ,  0.11089    ,  0.00000E+00,   1.9130     , -0.13378    ,
0.00000E+00,   70.663   ,   5.0000
  3,   9.3517    , 0.50569E-01,  0.00000E+00,   2.2256     , -0.10929    ,
0.00000E+00,   68.112   ,   5.5000
  3,   10.486    , -0.28786E-02,  0.00000E+00,   2.2959     , -0.10624    ,
0.00000E+00,   67.486   ,   6.0000
  3,   11.664    , -0.53730E-01,  0.00000E+00,   2.5100     , -0.87145E-01,
0.00000E+00,   65.458   ,   6.5000
  3,   13.134    , -0.89083E-01,  0.00000E+00,   3.4802     , -0.41060E-01,
0.00000E+00,   53.971   ,   7.0000
  3,   15.422    , -0.92424E-01,  0.00000E+00,   5.7213     , -0.15667E-01,
0.00000E+00,   13.136   ,   7.5000
  3,   18.506    , -0.11940    ,  0.00000E+00,   6.2740     , -0.66867E-01,
0.00000E+00,  0.14466E-02,   8.0000
  3,   21.643    , -0.15284    ,  0.00000E+00,   6.2741     , -0.66871E-01,
0.00000E+00,  0.27019E-03,   8.5000
  3,   24.780    , -0.18628    ,  0.00000E+00,   6.2741     , -0.66873E-01,
0.00000E+00,  0.27924E-07,   9.0000
  4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.888   ,  0.00000E+00
  4,   4.1725    ,  0.25197    ,  0.00000E+00,  0.27610     , -0.83074E-02,
0.00000E+00,   77.787   ,  0.50001
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   4,   4.3412    , 0.24562    , 0.00000E+00,  0.39978     , -0.16851E-01,
0.00000E+00,   77.621    ,    1.0000
   4,   4.5735    , 0.23551    , 0.00000E+00,  0.53028     , -0.23151E-01,
0.00000E+00,   77.380    ,    1.5000
   4,   4.8724    , 0.22291    , 0.00000E+00,  0.66612     , -0.26847E-01,
0.00000E+00,   77.058    ,    2.0000
   4,   5.2402    , 0.20896    , 0.00000E+00,  0.80566     , -0.28737E-01,
0.00000E+00,   76.651    ,    2.5000
   4,   5.6785    , 0.19427    , 0.00000E+00,  0.94786     , -0.30088E-01,
0.00000E+00,   76.157    ,    3.0000
   4,   6.1888    , 0.17860    , 0.00000E+00,   1.0946     , -0.33162E-01,
0.00000E+00,   75.563    ,    3.5000
   4,   6.7759    , 0.16000    , 0.00000E+00,   1.2596     , -0.43094E-01,
0.00000E+00,   74.793    ,    4.0000
   4,   7.4601    , 0.13258    , 0.00000E+00,   1.4983     , -0.70148E-01,
0.00000E+00,   73.484    ,    4.5000
   4,   8.3064    , 0.89941E-01, 0.00000E+00,   1.9166     , -0.92437E-01,
0.00000E+00,   70.647    ,    5.0000
   4,   9.3577    , 0.49294E-01, 0.00000E+00,   2.2272     , -0.71305E-01,
0.00000E+00,   68.105    ,    5.5000
   4,   10.492    , 0.14913E-01, 0.00000E+00,   2.2969     , -0.67986E-01,
0.00000E+00,   67.483    ,    6.0000
   4,   11.672    , -0.18822E-01, 0.00000E+00,   2.5156     , -0.63656E-01,
0.00000E+00,   65.412    ,    6.5000
   4,   13.146    , -0.47128E-01, 0.00000E+00,   3.4932     , -0.41263E-01,
0.00000E+00,   53.789    ,    7.0000
   4,   15.442    , -0.58888E-01, 0.00000E+00,   5.7333     , -0.30035E-01,
0.00000E+00,   12.867    ,    7.5000
   4,   18.527    , -0.87773E-01, 0.00000E+00,   6.2746     , -0.68784E-01,
0.00000E+00,  0.14289E-02,    8.0000
   4,   21.664    , -0.12217    , 0.00000E+00,   6.2746     , -0.68787E-01,
0.00000E+00,  0.26646E-03,    8.5000
   4,   24.802    , -0.15656    , 0.00000E+00,   6.2747     , -0.68787E-01,
0.00000E+00,  0.29160E-07,    9.0000
   5,   4.0640    , 0.12700    , 0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.883    ,  0.00000E+00
   5,   4.1731    , 0.12620    , 0.00000E+00,  0.27809     , -0.33678E-02,
0.00000E+00,   77.780    ,  0.50000
   5,   4.3429    , 0.12353    , 0.00000E+00,  0.40177     , -0.72548E-02,
0.00000E+00,   77.613    ,    1.0000
   5,   4.5759    , 0.11908    , 0.00000E+00,  0.53148     , -0.10365E-01,
0.00000E+00,   77.374    ,    1.5000
   5,   4.8753    , 0.11337    , 0.00000E+00,  0.66674     , -0.12249E-01,
0.00000E+00,   77.053    ,    2.0000
   5,   5.2433    , 0.10698    , 0.00000E+00,  0.80605     , -0.13220E-01,
0.00000E+00,   76.646    ,    2.5000
   5,   5.6818    , 0.10020    , 0.00000E+00,  0.94833     , -0.13922E-01,
0.00000E+00,   76.152    ,    3.0000
   5,   6.1925    , 0.92912E-01, 0.00000E+00,   1.0957     , -0.15542E-01,
0.00000E+00,   75.556    ,    3.5000
   5,   6.7805    , 0.84069E-01, 0.00000E+00,   1.2622     , -0.20833E-01,
0.00000E+00,   74.779    ,    4.0000
   5,   7.4666    , 0.70517E-01, 0.00000E+00,   1.5037     , -0.35227E-01,
0.00000E+00,   73.454    ,    4.5000
```

```
  5,   8.3159    , 0.48966E-01,  0.00000E+00,    1.9222    , -0.46659E-01,
0.00000E+00,   70.614    ,   5.0000
  5,   9.3689    , 0.28744E-01,  0.00000E+00,    2.2290    , -0.34853E-01,
0.00000E+00,   68.094    ,   5.5000
  5,   10.504    , 0.12065E-01,  0.00000E+00,    2.2979    , -0.32900E-01,
0.00000E+00,   67.479    ,   6.0000
  5,   11.685    , -0.46227E-02,  0.00000E+00,    2.5230    , -0.33141E-01,
0.00000E+00,   65.343    ,   6.5000
  5,   13.164    , -0.19987E-01,  0.00000E+00,    3.5116    , -0.24242E-01,
0.00000E+00,   53.536    ,   7.0000
  5,   15.472    , -0.28489E-01,  0.00000E+00,    5.7525    , -0.20594E-01,
0.00000E+00,   12.418    ,   7.5000
  5,   18.560    , -0.45773E-01,  0.00000E+00,    6.2741    , -0.40243E-01,
0.00000E+00,  0.13999E-02,   8.0000
  5,   21.697    , -0.65895E-01,  0.00000E+00,    6.2741    , -0.40245E-01,
0.00000E+00,  0.26069E-03,   8.5000
  5,   24.834    , -0.86018E-01,  0.00000E+00,    6.2741    , -0.40245E-01,
0.00000E+00,  0.30698E-07,   9.0000
  6,   4.0640    ,  0.00000E+00,  0.00000E+00,  0.15892    ,   0.00000E+00,
0.00000E+00,   77.882    ,  0.00000E+00
  6,   4.1733    ,  0.00000E+00,  0.00000E+00,  0.27876    ,   0.00000E+00,
0.00000E+00,   77.778    ,  0.50000
  6,   4.3434    ,  0.00000E+00,  0.00000E+00,  0.40251    ,   0.00000E+00,
0.00000E+00,   77.611    ,   1.0000
  6,   4.5768    ,  0.00000E+00,  0.00000E+00,  0.53198    ,   0.00000E+00,
0.00000E+00,   77.372    ,   1.5000
  6,   4.8763    ,  0.00000E+00,  0.00000E+00,  0.66703    ,   0.00000E+00,
0.00000E+00,   77.051    ,   2.0000
  6,   5.2445    ,  0.00000E+00,  0.00000E+00,  0.80625    ,   0.00000E+00,
0.00000E+00,   76.645    ,   2.5000
  6,   5.6831    ,  0.00000E+00,  0.00000E+00,  0.94857    ,   0.00000E+00,
0.00000E+00,   76.150    ,   3.0000
  6,   6.1939    ,  0.00000E+00,  0.00000E+00,    1.0962    ,   0.00000E+00,
0.00000E+00,   75.553    ,   3.5000
  6,   6.7824    ,  0.00000E+00,  0.00000E+00,    1.2635    ,   0.00000E+00,
0.00000E+00,   74.772    ,   4.0000
  6,   7.4695    ,  0.00000E+00,  0.00000E+00,    1.5067    ,   0.00000E+00,
0.00000E+00,   73.441    ,   4.5000
  6,   8.3204    ,  0.00000E+00,  0.00000E+00,    1.9243    ,   0.00000E+00,
0.00000E+00,   70.599    ,   5.0000
  6,   9.3738    ,  0.00000E+00,  0.00000E+00,    2.2291    ,   0.00000E+00,
0.00000E+00,   68.091    ,   5.5000
  6,   10.509    ,  0.00000E+00,  0.00000E+00,    2.2979    ,   0.00000E+00,
0.00000E+00,   67.477    ,   6.0000
  6,   11.691    ,  0.00000E+00,  0.00000E+00,    2.5259    ,   0.00000E+00,
0.00000E+00,   65.313    ,   6.5000
  6,   13.172    ,  0.00000E+00,  0.00000E+00,    3.5196    ,   0.00000E+00,
0.00000E+00,   53.429    ,   7.0000
  6,   15.485    ,  0.00000E+00,  0.00000E+00,    5.7595    ,   0.00000E+00,
0.00000E+00,   12.243    ,   7.5000
  6,   18.573    ,  0.00000E+00,  0.00000E+00,    6.2740    ,   0.00000E+00,
0.00000E+00,  0.13891E-02,   8.0000
  6,   21.710    ,  0.00000E+00,  0.00000E+00,    6.2740    ,   0.00000E+00,
0.00000E+00,  0.25838E-03,   8.5000
```

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  6,   24.847    ,  0.00000E+00,  0.00000E+00,   6.2740    ,  0.00000E+00,
0.00000E+00,  0.31605E-07,   9.0000
```

Modified source -- m/z 28

ion #, x,y,z, velocity in x,y and z, potential energy, time

```
  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1003.0    ,  0.00000E+00
  1,   4.1045    ,  0.63068    ,  0.00000E+00,   1.0737    , -0.17179    ,
0.00000E+00,   1002.8    ,  0.50006E-01
  1,   4.1756    ,  0.61798    ,  0.00000E+00,   1.7815    , -0.33243    ,
0.00000E+00,   1002.5    ,  0.10000
  1,   4.2818    ,  0.59793    ,  0.00000E+00,   2.4581    , -0.46679    ,
0.00000E+00,   1002.1    ,  0.15001
  1,   4.4210    ,  0.57165    ,  0.00000E+00,   3.1096    , -0.58238    ,
0.00000E+00,   1001.5    ,  0.20000
  1,   4.5929    ,  0.53985    ,  0.00000E+00,   3.7695    , -0.68932    ,
0.00000E+00,   1000.8    ,  0.25000
  1,   4.7985    ,  0.50266    ,  0.00000E+00,   4.4573    , -0.79952    ,
0.00000E+00,   999.99    ,  0.30000
  1,   5.0395    ,  0.45967    ,  0.00000E+00,   5.1921    , -0.92329    ,
0.00000E+00,   998.93    ,  0.35000
  1,   5.3189    ,  0.40991    ,  0.00000E+00,   6.0015    ,  -1.0725    ,
0.00000E+00,   997.57    ,  0.40001
  1,   5.6417    ,  0.35173    ,  0.00000E+00,   6.9353    ,  -1.2631    ,
0.00000E+00,   995.76    ,  0.45001
  1,   6.0161    ,  0.28246    ,  0.00000E+00,   8.0938    ,  -1.5219    ,
0.00000E+00,   993.13    ,  0.50000
  1,   6.4587    ,  0.19780    ,  0.00000E+00,   9.7252    ,  -1.8864    ,
0.00000E+00,   988.73    ,  0.55000
  1,   7.0079    ,  0.91735E-01,  0.00000E+00,   12.566    ,  -2.3662    ,
0.00000E+00,   979.26    ,  0.60000
  1,   7.7745    , -0.34454E-01,  0.00000E+00,   19.077    ,  -2.5476    ,
0.00000E+00,   949.24    ,  0.65000
  1,   9.0045    , -0.16318    ,  0.00000E+00,   29.485    ,  -3.0010    ,
0.00000E+00,   875.47    ,  0.70000
  1,   10.556    , -0.33686    ,  0.00000E+00,   31.781    ,  -3.6502    ,
0.00000E+00,   854.47    ,  0.75001
  1,   12.280    , -0.39019    ,  0.00000E+00,   43.080    ,   2.3721    ,
0.00000E+00,   733.00    ,  0.80000
  1,   15.149    , -0.24130    ,  0.00000E+00,   73.010    ,   2.9651    ,
0.00000E+00,   228.39    ,  0.85000
  1,   19.215    , -0.13270    ,  0.00000E+00,   85.374    ,   1.7619    ,
0.00000E+00,  -54.942    ,  0.90000
  1,   23.518    , -0.47080E-01,  0.00000E+00,   86.342    ,   1.6963    ,
0.00000E+00,  -79.012    ,  0.95000
  1,   27.815    ,  0.37407E-01,  0.00000E+00,   84.967    ,   1.6860    ,
0.00000E+00,  -44.817    ,   1.0000
  1,   32.010    ,  0.12128    ,  0.00000E+00,   83.136    ,   1.6324    ,
0.00000E+00, -0.13396    ,   1.0500
  1,   36.167    ,  0.20275    ,  0.00000E+00,   83.130    ,   1.6292    ,
0.00000E+00, -0.37409E-03,   1.1000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1002.7    ,  0.00000E+00
  2,   4.1054    ,  0.50223    ,  0.00000E+00,   1.0818    , -0.22406    ,
0.00000E+00,   1002.6    ,  0.50006E-01
```

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  2,   4.1735    ,  0.48647    ,  0.00000E+00,   1.6508    , -0.39670    ,
0.00000E+00,   1002.4    ,  0.10000
  2,   4.2710    ,  0.46340    ,  0.00000E+00,   2.2553    , -0.52098    ,
0.00000E+00,   1002.0    ,  0.15000
  2,   4.3995    ,  0.43478    ,  0.00000E+00,   2.8855    , -0.62078    ,
0.00000E+00,   1001.5    ,  0.20000
  2,   4.5600    ,  0.40154    ,  0.00000E+00,   3.5403    , -0.70773    ,
0.00000E+00,   1000.9    ,  0.25000
  2,   4.7540    ,  0.36407    ,  0.00000E+00,   4.2286    , -0.79111    ,
0.00000E+00,   1000.1    ,  0.30000
  2,   4.9836    ,  0.32236    ,  0.00000E+00,   4.9648    , -0.87871    ,
0.00000E+00,   999.09    ,  0.35000
  2,   5.2517    ,  0.27601    ,  0.00000E+00,   5.7738    , -0.97738    ,
0.00000E+00,   997.80    ,  0.40000
  2,   5.5630    ,  0.22431    ,  0.00000E+00,   6.6997    ,  -1.0944    ,
0.00000E+00,   996.09    ,  0.45000
  2,   5.9250    ,  0.16612    ,  0.00000E+00,   7.8294    ,  -1.2385    ,
0.00000E+00,   993.66    ,  0.50000
  2,   6.3525    ,  0.99944E-01,  0.00000E+00,   9.3678    ,  -1.4132    ,
0.00000E+00,   989.77    ,  0.55000
  2,   6.8774    ,  0.24817E-01,  0.00000E+00,   11.877    ,  -1.5799    ,
0.00000E+00,   981.96    ,  0.60000
  2,   7.5866    , -0.53409E-01,  0.00000E+00,   17.283    ,  -1.4509    ,
0.00000E+00,   959.15    ,  0.65001
  2,   8.7107    , -0.11778    ,  0.00000E+00,   28.004    ,  -1.4312    ,
0.00000E+00,   888.66    ,  0.70001
  2,   10.236    , -0.21380    ,  0.00000E+00,   31.709    ,  -2.1954    ,
0.00000E+00,   856.18    ,  0.75000
  2,   11.895    , -0.27547    ,  0.00000E+00,   38.465    ,   1.3308    ,
0.00000E+00,   787.96    ,  0.80000
  2,   14.491    , -0.17642    ,  0.00000E+00,   67.355    ,   2.3228    ,
0.00000E+00,   343.79    ,  0.85000
  2,   18.418    , -0.88238E-01,  0.00000E+00,   84.678    ,   1.3891    ,
0.00000E+00,  -37.847    ,  0.90000
  2,   22.709    , -0.21470E-01,  0.00000E+00,   86.289    ,   1.3187    ,
0.00000E+00,  -77.777    ,  0.95000
  2,   27.015    ,  0.44620E-01,  0.00000E+00,   85.374    ,   1.3259    ,
0.00000E+00,  -55.001    ,   1.0000
  2,   31.230    ,  0.11083    ,  0.00000E+00,   83.247    ,   1.3102    ,
0.00000E+00,  -2.9347    ,   1.0500
  2,   35.386    ,  0.17433    ,  0.00000E+00,   83.125    ,   1.2664    ,
0.00000E+00, -0.42192E-03,   1.1000
  3,   4.0640    ,  0.38100    ,  0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1002.6    ,  0.00000E+00
  3,   4.1065    ,  0.37866    ,  0.00000E+00,   1.1187    , -0.93313E-01,
0.00000E+00,   1002.5    ,  0.50004E-01
  3,   4.1764    ,  0.37171    ,  0.00000E+00,   1.6805    , -0.18432    ,
0.00000E+00,   1002.3    ,  0.10000
  3,   4.2751    ,  0.36031    ,  0.00000E+00,   2.2740    , -0.27019    ,
0.00000E+00,   1001.9    ,  0.15001
  3,   4.4043    ,  0.34484    ,  0.00000E+00,   2.8985    , -0.34713    ,
0.00000E+00,   1001.5    ,  0.20000
  3,   4.5655    ,  0.32570    ,  0.00000E+00,   3.5538    , -0.41814    ,
0.00000E+00,   1000.8    ,  0.25000
```

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  3,   4.7603    , 0.30304    , 0.00000E+00,   4.2455     , -0.48837    ,
0.00000E+00,   1000.0    , 0.30000
  3,   4.9909    , 0.27678    , 0.00000E+00,   4.9872     , -0.56366    ,
0.00000E+00,   999.04    , 0.35000
  3,   5.2602    , 0.24647    , 0.00000E+00,   5.8029     , -0.65113    ,
0.00000E+00,   997.74    , 0.40001
  3,   5.5731    , 0.21131    , 0.00000E+00,   6.7358     , -0.76002    ,
0.00000E+00,   996.03    , 0.45000
  3,   5.9372    , 0.16989    , 0.00000E+00,   7.8744     , -0.90365    ,
0.00000E+00,   993.58    , 0.50001
  3,   6.3672    , 0.12008    , 0.00000E+00,   9.4275     ,  -1.0995    ,
0.00000E+00,   989.62    , 0.55000
  3,   6.8959    , 0.58900E-01, 0.00000E+00,   11.977     ,  -1.3541    ,
0.00000E+00,   981.62    , 0.60001
  3,   7.6129    ,-0.13623E-01, 0.00000E+00,   17.528     ,  -1.4833    ,
0.00000E+00,   957.83    , 0.65001
  3,   8.7520    ,-0.85254E-01, 0.00000E+00,   28.228     ,  -1.5649    ,
0.00000E+00,   886.72    , 0.70001
  3,   10.282    ,-0.18144    , 0.00000E+00,   31.742     ,  -2.1257    ,
0.00000E+00,   855.91    , 0.75001
  3,   11.955    ,-0.24134    , 0.00000E+00,   39.256     ,   1.0005    ,
0.00000E+00,   779.03    , 0.80001
  3,   14.597    ,-0.16462    , 0.00000E+00,   68.360     ,   1.7848    ,
0.00000E+00,   324.20    , 0.85000
  3,   18.550    ,-0.10319    , 0.00000E+00,   84.823     ,  0.85572    ,
0.00000E+00,  -41.342    , 0.90000
  3,   22.843    ,-0.63555E-01, 0.00000E+00,   86.301     ,  0.76977    ,
0.00000E+00,  -78.024    , 0.95000
  3,   27.149    ,-0.25747E-01, 0.00000E+00,   85.308     ,  0.74363    ,
0.00000E+00,  -53.285    ,  1.0000
  3,   31.360    , 0.11437E-01, 0.00000E+00,   83.210     ,  0.74183    ,
0.00000E+00,  -1.9506    ,  1.0500
  3,   35.517    , 0.48343E-01, 0.00000E+00,   83.128     ,  0.73779    ,
0.00000E+00,-0.41231E-03,  1.1000
  4,   4.0640    , 0.25400    , 0.00000E+00,  0.58699     ,  0.00000E+00,
0.00000E+00,   1002.6    , 0.00000E+00
  4,   4.1073    , 0.25295    , 0.00000E+00,   1.1470     , -0.42508E-01,
0.00000E+00,   1002.5    , 0.50004E-01
  4,   4.1789    , 0.24967    , 0.00000E+00,   1.7216     , -0.89989E-01,
0.00000E+00,   1002.2    , 0.10000
  4,   4.2798    , 0.24388    , 0.00000E+00,   2.3188     , -0.14148    ,
0.00000E+00,   1001.9    , 0.15000
  4,   4.4113    , 0.23553    , 0.00000E+00,   2.9439     , -0.19234    ,
0.00000E+00,   1001.4    , 0.20000
  4,   4.5748    , 0.22468    , 0.00000E+00,   3.6014     , -0.24154    ,
0.00000E+00,   1000.8    , 0.25000
  4,   4.7721    , 0.21137    , 0.00000E+00,   4.2983     , -0.29118    ,
0.00000E+00,   999.96    , 0.30001
  4,   5.0055    , 0.19548    , 0.00000E+00,   5.0480     , -0.34531    ,
0.00000E+00,   998.94    , 0.35000
  4,   5.2782    , 0.17667    , 0.00000E+00,   5.8750     , -0.40944    ,
0.00000E+00,   997.62    , 0.40000
  4,   5.5950    , 0.15425    , 0.00000E+00,   6.8251     , -0.49088    ,
0.00000E+00,   995.86    , 0.45001
```

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  4,   5.9642    ,  0.12711    ,  0.00000E+00,   7.9926    , -0.60102    ,
0.00000E+00,   993.33    ,  0.50000
  4,   6.4014    ,  0.93375E-01,  0.00000E+00,   9.5977    , -0.75791    ,
0.00000E+00,   989.21    ,  0.55000
  4,   6.9411    ,  0.50226E-01,  0.00000E+00,   12.272    , -0.97736    ,
0.00000E+00,   980.67    ,  0.60000
  4,   7.6810    , -0.35356E-02,  0.00000E+00,   18.215    ,  -1.1278    ,
0.00000E+00,   954.35    ,  0.65001
  4,   8.8612    , -0.59709E-01,  0.00000E+00,   28.835    ,  -1.2466    ,
0.00000E+00,   881.76    ,  0.70001
  4,   10.404    , -0.13315    ,  0.00000E+00,   31.844    ,  -1.5791    ,
0.00000E+00,   855.14    ,  0.75001
  4,   12.116    , -0.17072    ,  0.00000E+00,   41.259    ,  0.71746    ,
0.00000E+00,   755.62    ,  0.80000
  4,   14.876    , -0.11857    ,  0.00000E+00,   70.811    ,   1.1221    ,
0.00000E+00,   274.81    ,  0.85000
  4,   18.891    , -0.83275E-01,  0.00000E+00,   85.127    ,  0.45215    ,
0.00000E+00,  -48.980    ,  0.90000
  4,   23.189    , -0.62772E-01,  0.00000E+00,   86.317    ,  0.39404    ,
0.00000E+00,  -78.580    ,  0.95001
  4,   27.490    , -0.43984E-01,  0.00000E+00,   85.125    ,  0.36313    ,
0.00000E+00,  -48.936    ,   1.0000
  4,   31.693    , -0.25750E-01,  0.00000E+00,   83.144    ,  0.37522    ,
0.00000E+00, -0.54099    ,   1.0500
  4,   35.849    , -0.68803E-02,  0.00000E+00,   83.121    ,  0.37751    ,
0.00000E+00, -0.39042E-03,   1.1000
  5,   4.0640    ,  0.12700    ,  0.00000E+00,  0.58699    ,  0.00000E+00,
0.00000E+00,   1002.6    ,  0.00000E+00
  5,   4.1077    ,  0.12658    ,  0.00000E+00,   1.1630    , -0.17277E-01,
0.00000E+00,   1002.4    ,  0.50000E-01
  5,   4.1805    ,  0.12522    ,  0.00000E+00,   1.7484    , -0.37910E-01,
0.00000E+00,   1002.2    ,  0.10001
  5,   4.2829    ,  0.12273    ,  0.00000E+00,   2.3509    , -0.61797E-01,
0.00000E+00,   1001.8    ,  0.15000
  5,   4.4160    ,  0.11902    ,  0.00000E+00,   2.9783    , -0.86786E-01,
0.00000E+00,   1001.3    ,  0.20000
  5,   4.5812    ,  0.11405    ,  0.00000E+00,   3.6380    , -0.11172    ,
0.00000E+00,   1000.7    ,  0.25000
  5,   4.7805    ,  0.10784    ,  0.00000E+00,   4.3389    , -0.13718    ,
0.00000E+00,   999.90    ,  0.30000
  5,   5.0160    ,  0.10029    ,  0.00000E+00,   5.0950    , -0.16509    ,
0.00000E+00,   998.87    ,  0.35000
  5,   5.2912    ,  0.91238E-01,  0.00000E+00,   5.9311    , -0.19843    ,
0.00000E+00,   997.53    ,  0.40000
  5,   5.6113    ,  0.80292E-01,  0.00000E+00,   6.8949    , -0.24146    ,
0.00000E+00,   995.73    ,  0.45000
  5,   5.9844    ,  0.66821E-01,  0.00000E+00,   8.0838    , -0.30087    ,
0.00000E+00,   993.14    ,  0.50000
  5,   6.4270    ,  0.49752E-01,  0.00000E+00,   9.7297    , -0.38757    ,
0.00000E+00,   988.88    ,  0.55000
  5,   6.9756    ,  0.27411E-01,  0.00000E+00,   12.513    , -0.51176    ,
0.00000E+00,   979.89    ,  0.60001
  5,   7.7341    , -0.10247E-02,  0.00000E+00,   18.770    , -0.60113    ,
0.00000E+00,   951.47    ,  0.65000
```

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  5,   8.9454     , -0.31404E-01,  0.00000E+00,   29.247     , -0.68099    ,
0.00000E+00,   878.33     ,  0.70001
  5,   10.497     , -0.70632E-01,  0.00000E+00,   31.931     , -0.82814    ,
0.00000E+00,   854.49     ,  0.75000
  5,   12.243     , -0.87440E-01,  0.00000E+00,   42.789     ,  0.37192    ,
0.00000E+00,   736.83     ,  0.80000
  5,   15.094     , -0.61170E-01,  0.00000E+00,   72.557     ,  0.52531    ,
0.00000E+00,   238.57     ,  0.85000
  5,   19.150     , -0.45603E-01,  0.00000E+00,   85.319     ,  0.18929    ,
0.00000E+00,  -53.767     ,  0.90001
  5,   23.451     , -0.37127E-01,  0.00000E+00,   86.329     ,  0.16187    ,
0.00000E+00,  -78.931     ,  0.95000
  5,   27.748     , -0.29647E-01,  0.00000E+00,   84.991     ,  0.14290    ,
0.00000E+00,  -45.663     ,   1.0000
  5,   31.945     , -0.22408E-01,  0.00000E+00,   83.127     ,  0.15446    ,
0.00000E+00, -0.19659     ,   1.0500
  5,   36.101     , -0.14649E-01,  0.00000E+00,   83.119     ,  0.15522    ,
0.00000E+00, -0.37753E-03,   1.1000
  6,   4.0640     ,  0.00000E+00,  0.00000E+00,  0.58699     ,  0.00000E+00,
0.00000E+00,   1002.6     ,  0.00000E+00
  6,   4.1079     ,  0.00000E+00,  0.00000E+00,   1.1682     ,  0.00000E+00,
0.00000E+00,   1002.4     ,  0.50003E-01
  6,   4.1810     ,  0.00000E+00,  0.00000E+00,   1.7573     ,  0.00000E+00,
0.00000E+00,   1002.2     ,  0.10001
  6,   4.2838     ,  0.00000E+00,  0.00000E+00,   2.3620     ,  0.00000E+00,
0.00000E+00,   1001.8     ,  0.15001
  6,   4.4175     ,  0.00000E+00,  0.00000E+00,   2.9904     ,  0.00000E+00,
0.00000E+00,   1001.3     ,  0.20000
  6,   4.5834     ,  0.00000E+00,  0.00000E+00,   3.6510     ,  0.00000E+00,
0.00000E+00,   1000.7     ,  0.25000
  6,   4.7833     ,  0.00000E+00,  0.00000E+00,   4.3533     ,  0.00000E+00,
0.00000E+00,   999.88     ,  0.30000
  6,   5.0197     ,  0.00000E+00,  0.00000E+00,   5.1118     ,  0.00000E+00,
0.00000E+00,   998.84     ,  0.35000
  6,   5.2959     ,  0.00000E+00,  0.00000E+00,   5.9521     ,  0.00000E+00,
0.00000E+00,   997.49     ,  0.40001
  6,   5.6170     ,  0.00000E+00,  0.00000E+00,   6.9220     ,  0.00000E+00,
0.00000E+00,   995.68     ,  0.45000
  6,   5.9918     ,  0.00000E+00,  0.00000E+00,   8.1217     ,  0.00000E+00,
0.00000E+00,   993.07     ,  0.50000
  6,   6.4368     ,  0.00000E+00,  0.00000E+00,   9.7891     ,  0.00000E+00,
0.00000E+00,   988.74     ,  0.55000
  6,   6.9894     ,  0.00000E+00,  0.00000E+00,   12.624     ,  0.00000E+00,
0.00000E+00,   979.56     ,  0.60000
  6,   7.7564     ,  0.00000E+00,  0.00000E+00,   19.017     ,  0.00000E+00,
0.00000E+00,   950.23     ,  0.65000
  6,   8.9806     ,  0.00000E+00,  0.00000E+00,   29.407     ,  0.00000E+00,
0.00000E+00,   877.07     ,  0.70000
  6,   10.536     ,  0.00000E+00,  0.00000E+00,   31.986     ,  0.00000E+00,
0.00000E+00,   854.19     ,  0.75001
  6,   12.300     ,  0.00000E+00,  0.00000E+00,   43.472     ,  0.00000E+00,
0.00000E+00,   728.45     ,  0.80000
  6,   15.191     ,  0.00000E+00,  0.00000E+00,   73.285     ,  0.00000E+00,
0.00000E+00,   223.23     ,  0.85000
```

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  6,   19.263     , 0.00000E+00, 0.00000E+00,   85.397     , 0.00000E+00,
0.00000E+00,  -55.615     , 0.90000
  6,   23.566     , 0.00000E+00, 0.00000E+00,   86.339     , 0.00000E+00,
0.00000E+00,  -79.066     , 0.95000
  6,   27.861     , 0.00000E+00, 0.00000E+00,   84.938     , 0.00000E+00,
0.00000E+00,  -44.234     ,  1.0000
  6,   32.055     , 0.00000E+00, 0.00000E+00,   83.129     , 0.00000E+00,
0.00000E+00, -0.12722     ,  1.0500
  6,   36.212     , 0.00000E+00, 0.00000E+00,   83.124     , 0.00000E+00,
0.00000E+00, -0.37271E-03,  1.1000
```

Modified source -- m/z 57

```
  1,    4.0640     ,  0.63500     ,  0.00000E+00,  0.41141      ,  0.00000E+00,
0.00000E+00,    502.98     ,  0.00000E+00
  1,    4.1197     ,  0.62978     ,  0.00000E+00,  0.73533      , -0.10299     ,
0.00000E+00,    502.82     ,  0.10001
  1,    4.2155     ,  0.61486     ,  0.00000E+00,   1.1757      , -0.19169     ,
0.00000E+00,    502.58     ,  0.20000
  1,    4.3535     ,  0.59199     ,  0.00000E+00,   1.5814      , -0.26302     ,
0.00000E+00,    502.24     ,  0.30000
  1,    4.5316     ,  0.56260     ,  0.00000E+00,   1.9815      , -0.32347     ,
0.00000E+00,    501.81     ,  0.40001
  1,    4.7502     ,  0.52740     ,  0.00000E+00,   2.3926      , -0.38060     ,
0.00000E+00,    501.27     ,  0.50001
  1,    5.0109     ,  0.48635     ,  0.00000E+00,   2.8260      , -0.44179     ,
0.00000E+00,    500.58     ,  0.60000
  1,    5.3166     ,  0.43864     ,  0.00000E+00,   3.2952      , -0.51519     ,
0.00000E+00,    499.71     ,  0.70001
  1,    5.6720     ,  0.38252     ,  0.00000E+00,   3.8261      , -0.61268     ,
0.00000E+00,    498.56     ,  0.80001
  1,    6.0857     ,  0.31462     ,  0.00000E+00,   4.4755      , -0.75561     ,
0.00000E+00,    496.91     ,  0.90001
  1,    6.5758     ,  0.22862     ,  0.00000E+00,   5.3970      , -0.98248     ,
0.00000E+00,    494.11     ,   1.0000
  1,    7.1899     ,  0.11389     ,  0.00000E+00,   7.1040      ,   -1.3274    ,
0.00000E+00,    487.58     ,   1.1000
  1,    8.0759     , -0.31244E-01,  0.00000E+00,   11.185      ,   -1.4925    ,
0.00000E+00,    465.39     ,   1.2000
  1,    9.4446     , -0.19321     ,  0.00000E+00,   15.326      ,   -1.8673    ,
0.00000E+00,    432.59     ,   1.3000
  1,    11.016     , -0.38867     ,  0.00000E+00,   15.969      ,   -1.7851    ,
0.00000E+00,    426.75     ,   1.4000
  1,    12.947     , -0.37059     ,  0.00000E+00,   25.203      ,    1.1748    ,
0.00000E+00,    315.00     ,   1.5000
  1,    16.293     , -0.21156     ,  0.00000E+00,   40.839      ,    1.2322    ,
0.00000E+00,    9.9187     ,   1.6000
  1,    20.613     , -0.11436     ,  0.00000E+00,   44.205      ,  0.87066     ,
0.00000E+00,   -74.408     ,   1.7000
  1,    25.048     , -0.28200E-01,  0.00000E+00,   44.412      ,  0.85572     ,
0.00000E+00,   -79.831     ,   1.8000
  1,    29.383     ,  0.56308E-01,  0.00000E+00,   42.275      ,  0.84449     ,
0.00000E+00,   -25.096     ,   1.9000
  1,    33.535     ,  0.13823     ,  0.00000E+00,   41.259      ,  0.79505     ,
0.00000E+00, -0.95105E-03,   2.0000
  1,    37.660     ,  0.21773     ,  0.00000E+00,   41.259      ,  0.79504     ,
0.00000E+00, -0.34161E-03,   2.1000
  2,    4.0640     ,  0.50800     ,  0.00000E+00,  0.41141      ,  0.00000E+00,
0.00000E+00,    502.84     ,  0.00000E+00
  2,    4.1201     ,  0.50109     ,  0.00000E+00,  0.72116      , -0.13266     ,
0.00000E+00,    502.73     ,  0.10000
  2,    4.2099     ,  0.48281     ,  0.00000E+00,   1.0781      , -0.22615     ,
0.00000E+00,    502.52     ,  0.20000
  2,    4.3365     ,  0.45675     ,  0.00000E+00,   1.4558      , -0.29182     ,
0.00000E+00,    502.23     ,  0.30000
```

```
 2,  4.5015    , 0.42490   , 0.00000E+00,  1.8480   , -0.34354   ,
0.00000E+00,  501.84   , 0.40000
 2,  4.7066    , 0.38825   , 0.00000E+00,  2.2570   , -0.38880   ,
0.00000E+00,  501.33   , 0.50000
 2,  4.9537    , 0.34715   , 0.00000E+00,  2.6899   , -0.43365   ,
0.00000E+00,  500.69   , 0.60000
 2,  5.2458    , 0.30135   , 0.00000E+00,  3.1587   , -0.48358   ,
0.00000E+00,  499.86   , 0.70001
 2,  5.5874    , 0.25006   , 0.00000E+00,  3.6866   , -0.54475   ,
0.00000E+00,  498.78   , 0.80000
 2,  5.9867    , 0.19173   , 0.00000E+00,  4.3229   , -0.62612   ,
0.00000E+00,  497.25   , 0.90000
 2,  6.4596    , 0.12378   , 0.00000E+00,  5.1932   , -0.73883   ,
0.00000E+00,  494.76   ,  1.0000
 2,  7.0451    , 0.43072E-01, 0.00000E+00,  6.6857   , -0.87372   ,
0.00000E+00,  489.46   ,  1.1000
 2,  7.8599    ,-0.46104E-01, 0.00000E+00,  10.126   , -0.85827   ,
0.00000E+00,  472.39   ,  1.2000
 2,  9.1423    ,-0.13551   , 0.00000E+00,  14.997   ,  -1.0870   ,
0.00000E+00,  436.11   ,  1.3000
 2,  10.704    ,-0.25866   , 0.00000E+00,  15.964   ,  -1.2529   ,
0.00000E+00,  427.17   ,  1.4000
 2,  12.504    ,-0.27631   , 0.00000E+00,  22.816   ,  0.84486   ,
0.00000E+00,  348.93   ,  1.5000
 2,  15.563    ,-0.15991   , 0.00000E+00,  38.790   ,   1.0873   ,
0.00000E+00,  58.090   ,  1.6000
 2,  19.803    ,-0.76792E-01, 0.00000E+00,  44.052   ,  0.71965   ,
0.00000E+00, -70.459   ,  1.7000
 2,  24.234    ,-0.58116E-02, 0.00000E+00,  44.410   ,  0.70709   ,
0.00000E+00, -79.798   ,  1.8000
 2,  28.604    , 0.65200E-01, 0.00000E+00,  42.662   ,  0.71023   ,
0.00000E+00, -34.857   ,  1.9000
 2,  32.778    , 0.13431   , 0.00000E+00,  41.257   ,  0.65275   ,
0.00000E+00,-0.32756E-02,  2.0000
 2,  36.903    , 0.19958   , 0.00000E+00,  41.257   ,  0.65267   ,
0.00000E+00,-0.35138E-03,  2.1000
 3,  4.0640    , 0.38100   , 0.00000E+00, 0.41141   ,  0.00000E+00,
0.00000E+00,  502.78   , 0.00000E+00
 3,  4.1213    , 0.37819   , 0.00000E+00, 0.73791   , -0.55989E-01,
0.00000E+00,  502.67   , 0.10000
 3,  4.2123    , 0.36988   , 0.00000E+00,  1.0862   , -0.10969   ,
0.00000E+00,  502.48   , 0.20000
 3,  4.3393    , 0.35646   , 0.00000E+00,  1.4563   , -0.15738   ,
0.00000E+00,  502.19   , 0.30000
 3,  4.5042    , 0.33862   , 0.00000E+00,  1.8458   , -0.19842   ,
0.00000E+00,  501.81   , 0.40000
 3,  4.7091    , 0.31690   , 0.00000E+00,  2.2551   , -0.23585   ,
0.00000E+00,  501.31   , 0.50000
 3,  4.9561    , 0.29144   , 0.00000E+00,  2.6897   , -0.27370   ,
0.00000E+00,  500.67   , 0.60000
 3,  5.2483    , 0.26198   , 0.00000E+00,  3.1612   , -0.31674   ,
0.00000E+00,  499.85   , 0.70000
 3,  5.5903    , 0.22770   , 0.00000E+00,  3.6919   , -0.37158   ,
0.00000E+00,  498.76   , 0.80000
```

```
 3,   5.9902    , 0.18693    , 0.00000E+00,   4.3306     , -0.44881    ,
0.00000E+00,   497.23    ,  0.90000
 3,   6.4639    , 0.13662    , 0.00000E+00,   5.2025     , -0.56597    ,
0.00000E+00,   494.74    ,   1.0000
 3,   7.0506    , 0.71741E-01,  0.00000E+00,   6.6998     , -0.74024    ,
0.00000E+00,   489.42    ,   1.1000
 3,   7.8676    , -0.97291E-02,  0.00000E+00,   10.159     , -0.84890    ,
0.00000E+00,   472.13    ,   1.2000
 3,   9.1519    , -0.97900E-01,  0.00000E+00,   14.997     ,  -1.0118    ,
0.00000E+00,   436.07    ,   1.3000
 3,   10.714    , -0.20969    , 0.00000E+00,   15.979     ,  -1.1278    ,
0.00000E+00,   427.04    ,   1.4000
 3,   12.526    , -0.23341    , 0.00000E+00,   22.940     ,  0.59048    ,
0.00000E+00,   347.20    ,   1.5000
 3,   15.600    , -0.14713    , 0.00000E+00,   38.912     ,  0.77755    ,
0.00000E+00,   55.321    ,   1.6000
 3,   19.845    , -0.93718E-01,  0.00000E+00,   44.061     ,  0.42208    ,
0.00000E+00,  -70.723    ,   1.7000
 3,   24.276    , -0.52823E-01,  0.00000E+00,   44.409     ,  0.40413    ,
0.00000E+00,  -79.812    ,   1.8000
 3,   28.645    , -0.14280E-01,  0.00000E+00,   42.641     ,  0.38149    ,
0.00000E+00,  -34.348    ,   1.9000
 3,   32.817    ,  0.23702E-01,  0.00000E+00,   41.256     ,  0.37607    ,
0.00000E+00, -0.35733E-02,   2.0000
 3,   36.942    ,  0.61306E-01,  0.00000E+00,   41.255     ,  0.37605    ,
0.00000E+00, -0.35077E-03,   2.1000
 4,   4.0640    , 0.25400    , 0.00000E+00,  0.41141     ,  0.00000E+00,
0.00000E+00,   502.75    ,  0.00000E+00
 4,   4.1221    , 0.25274    , 0.00000E+00,  0.75288     , -0.25607E-01,
0.00000E+00,   502.64    ,  0.10000
 4,   4.2150    , 0.24876    , 0.00000E+00,   1.1060     , -0.54658E-01,
0.00000E+00,   502.44    ,  0.20000
 4,   4.3439    , 0.24180    , 0.00000E+00,   1.4756     , -0.84365E-01,
0.00000E+00,   502.16    ,  0.30000
 4,   4.5107    , 0.23195    , 0.00000E+00,   1.8644     , -0.11219    ,
0.00000E+00,   501.77    ,  0.40001
 4,   4.7175    , 0.21942    , 0.00000E+00,   2.2748     , -0.13837    ,
0.00000E+00,   501.27    ,  0.50000
 4,   4.9666    , 0.20426    , 0.00000E+00,   2.7124     , -0.16525    ,
0.00000E+00,   500.62    ,  0.60000
 4,   5.2612    , 0.18623    , 0.00000E+00,   3.1885     , -0.19641    ,
0.00000E+00,   499.79    ,  0.70000
 4,   5.6063    , 0.16467    , 0.00000E+00,   3.7263     , -0.23692    ,
0.00000E+00,   498.69    ,  0.80001
 4,   6.0102    , 0.13826    , 0.00000E+00,   4.3775     , -0.29524    ,
0.00000E+00,   497.12    ,  0.90000
 4,   6.4897    , 0.10452    , 0.00000E+00,   5.2739     , -0.38682    ,
0.00000E+00,   494.55    ,   1.0000
 4,   7.0859    , 0.59057E-01,  0.00000E+00,   6.8292     , -0.53148    ,
0.00000E+00,   488.94    ,   1.1000
 4,   7.9232    , -0.93120E-03,  0.00000E+00,   10.453     , -0.63808    ,
0.00000E+00,   470.40    ,   1.2000
 4,   9.2338    , -0.67667E-01,  0.00000E+00,   15.121     , -0.75492    ,
0.00000E+00,   435.05    ,   1.3000
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4,   10.802     , -0.14927     ,  0.00000E+00,   16.049      , -0.80224     ,
0.00000E+00,   426.51     ,   1.4000
4,   12.662     , -0.16343     ,  0.00000E+00,   23.720      ,  0.37465     ,
0.00000E+00,   336.55     ,   1.5000
4,   15.832     , -0.10719     ,  0.00000E+00,   39.629      ,  0.45635     ,
0.00000E+00,   38.762     ,   1.6000
4,   20.106     , -0.78371E-01,  0.00000E+00,   44.115      ,  0.21214     ,
0.00000E+00,  -72.175     ,   1.7000
4,   24.538     , -0.58122E-01,  0.00000E+00,   44.410      ,  0.19856     ,
0.00000E+00,  -79.883     ,   1.8000
4,   28.896     , -0.40688E-01,  0.00000E+00,   42.514      ,  0.17142     ,
0.00000E+00,  -31.198     ,   1.9000
4,   33.060     , -0.22902E-01,  0.00000E+00,   41.253      ,  0.18704     ,
0.00000E+00, -0.18666E-02,   2.0000
4,   37.185     , -0.41979E-02,  0.00000E+00,   41.253      ,  0.18704     ,
0.00000E+00, -0.34654E-03,   2.1000
5,   4.0640     ,  0.12700     ,  0.00000E+00,  0.41141      ,  0.00000E+00,
0.00000E+00,   502.74     ,  0.00000E+00
5,   4.1226     ,  0.12650     ,  0.00000E+00,  0.76171      , -0.10403E-01,
0.00000E+00,   502.62     ,  0.10000
5,   4.2166     ,  0.12484     ,  0.00000E+00,   1.1197      , -0.23189E-01,
0.00000E+00,   502.42     ,  0.20000
5,   4.3470     ,  0.12182     ,  0.00000E+00,   1.4908      , -0.37268E-01,
0.00000E+00,   502.14     ,  0.30000
5,   4.5154     ,  0.11739     ,  0.00000E+00,   1.8798      , -0.51163E-01,
0.00000E+00,   501.75     ,  0.40001
5,   4.7237     ,  0.11161     ,  0.00000E+00,   2.2912      , -0.64516E-01,
0.00000E+00,   501.24     ,  0.50000
5,   4.9745     ,  0.10448     ,  0.00000E+00,   2.7311      , -0.78315E-01,
0.00000E+00,   500.59     ,  0.60000
5,   5.2712     ,  0.95868E-01,  0.00000E+00,   3.2110      , -0.94417E-01,
0.00000E+00,   499.75     ,  0.70001
5,   5.6188     ,  0.85422E-01,  0.00000E+00,   3.7549      , -0.11565     ,
0.00000E+00,   498.62     ,  0.80001
5,   6.0260     ,  0.72410E-01,  0.00000E+00,   4.4158      , -0.14683     ,
0.00000E+00,   497.03     ,  0.90000
5,   6.5102     ,  0.55432E-01,  0.00000E+00,   5.3311      , -0.19695     ,
0.00000E+00,   494.38     ,   1.0000
5,   7.1142     ,  0.31964E-01,  0.00000E+00,   6.9384      , -0.27762     ,
0.00000E+00,   488.56     ,   1.1000
5,   7.9686     ,  0.34341E-03,  0.00000E+00,   10.698      , -0.33811     ,
0.00000E+00,   468.94     ,   1.2000
5,   9.2997     , -0.35162E-01,  0.00000E+00,   15.216      , -0.39951     ,
0.00000E+00,   434.29     ,   1.3000
5,   10.873     , -0.77751E-01,  0.00000E+00,   16.117      , -0.40768     ,
0.00000E+00,   425.95     ,   1.4000
5,   12.774     , -0.83329E-01,  0.00000E+00,   24.340      ,  0.18588     ,
0.00000E+00,   327.72     ,   1.5000
5,   16.018     , -0.55558E-01,  0.00000E+00,   40.146      ,  0.20669     ,
0.00000E+00,   26.642     ,   1.6000
5,   20.312     , -0.43071E-01,  0.00000E+00,   44.154      ,  0.88569E-01,
0.00000E+00,  -73.163     ,   1.7000
5,   24.746     , -0.34685E-01,  0.00000E+00,   44.412      ,  0.81755E-01,
0.00000E+00,  -79.920     ,   1.8000
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  5,   29.095    , -0.28052E-01,  0.00000E+00,    42.416     ,  0.65367E-01,
0.00000E+00,  -28.707     ,    1.9000
  5,   33.253    , -0.20946E-01,  0.00000E+00,    41.254     ,  0.77879E-01,
0.00000E+00, -0.13445E-02,   2.0000
  5,   37.378    , -0.13158E-01,  0.00000E+00,    41.254     ,  0.77880E-01,
0.00000E+00, -0.34406E-03,   2.1000
  6,   4.0640    ,  0.00000E+00,  0.00000E+00,  0.41141     ,  0.00000E+00,
0.00000E+00,   502.74    ,  0.00000E+00
  6,   4.1228    ,  0.00000E+00,  0.00000E+00,  0.76454     ,  0.00000E+00,
0.00000E+00,   502.62    ,  0.10000
  6,   4.2171    ,  0.00000E+00,  0.00000E+00,   1.1243     ,  0.00000E+00,
0.00000E+00,   502.42    ,  0.20000
  6,   4.3480    ,  0.00000E+00,  0.00000E+00,   1.4961     ,  0.00000E+00,
0.00000E+00,   502.13    ,  0.30000
  6,   4.5169    ,  0.00000E+00,  0.00000E+00,   1.8854     ,  0.00000E+00,
0.00000E+00,   501.74    ,  0.40000
  6,   4.7258    ,  0.00000E+00,  0.00000E+00,   2.2971     ,  0.00000E+00,
0.00000E+00,   501.23    ,  0.50000
  6,   4.9773    ,  0.00000E+00,  0.00000E+00,   2.7379     ,  0.00000E+00,
0.00000E+00,   500.58    ,  0.60000
  6,   5.2748    ,  0.00000E+00,  0.00000E+00,   3.2194     ,  0.00000E+00,
0.00000E+00,   499.73    ,  0.70000
  6,   5.6233    ,  0.00000E+00,  0.00000E+00,   3.7660     ,  0.00000E+00,
0.00000E+00,   498.60    ,  0.80001
  6,   6.0319    ,  0.00000E+00,  0.00000E+00,   4.4319     ,  0.00000E+00,
0.00000E+00,   496.99    ,  0.90001
  6,   6.5181    ,  0.00000E+00,  0.00000E+00,   5.3579     ,  0.00000E+00,
0.00000E+00,   494.32    ,   1.0000
  6,   7.1259    ,  0.00000E+00,  0.00000E+00,   6.9920     ,  0.00000E+00,
0.00000E+00,   488.38    ,   1.1000
  6,   7.9884    ,  0.00000E+00,  0.00000E+00,   10.810     ,  0.00000E+00,
0.00000E+00,   468.30    ,   1.2000
  6,   9.3286    ,  0.00000E+00,  0.00000E+00,   15.258     ,  0.00000E+00,
0.00000E+00,   433.99    ,   1.3000
  6,   10.905    ,  0.00000E+00,  0.00000E+00,   16.163     ,  0.00000E+00,
0.00000E+00,   425.65    ,   1.4000
  6,   12.827    ,  0.00000E+00,  0.00000E+00,   24.634     ,  0.00000E+00,
0.00000E+00,   323.56    ,   1.5000
  6,   16.105    ,  0.00000E+00,  0.00000E+00,   40.368     ,  0.00000E+00,
0.00000E+00,   21.363    ,   1.6000
  6,   20.407    ,  0.00000E+00,  0.00000E+00,   44.171     ,  0.00000E+00,
0.00000E+00,  -73.574    ,   1.7000
  6,   24.842    ,  0.00000E+00,  0.00000E+00,   44.414     ,  0.00000E+00,
0.00000E+00,  -79.924    ,   1.8000
  6,   29.186    ,  0.00000E+00,  0.00000E+00,   42.372     ,  0.00000E+00,
0.00000E+00,  -27.562    ,   1.9000
  6,   33.342    ,  0.00000E+00,  0.00000E+00,   41.256     ,  0.00000E+00,
0.00000E+00, -0.11960E-02,   2.0000
  6,   37.468    ,  0.00000E+00,  0.00000E+00,   41.256     ,  0.00000E+00,
0.00000E+00, -0.34315E-03,   2.1000
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Modified source -- m/z 95

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  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.98    ,  0.00000E+00
  1,   4.1573    ,  0.62571    ,  0.00000E+00,  0.65325    , -0.90220E-01,
0.00000E+00,   302.80    ,  0.20000
  1,   4.3269    ,  0.60060    ,  0.00000E+00,   1.0352    , -0.15715    ,
0.00000E+00,   302.47    ,  0.40000
  1,   4.5704    ,  0.56400    ,  0.00000E+00,   1.4004    , -0.20710    ,
0.00000E+00,   302.03    ,  0.60000
  1,   4.8878    ,  0.51814    ,  0.00000E+00,   1.7776    , -0.25140    ,
0.00000E+00,   301.43    ,  0.80001
  1,   5.2832    ,  0.46310    ,  0.00000E+00,   2.1815    , -0.30100    ,
0.00000E+00,   300.62    ,   1.0000
  1,   5.7638    ,  0.39630    ,  0.00000E+00,   2.6377    , -0.37273    ,
0.00000E+00,   299.52    ,   1.2000
  1,   6.3465    ,  0.31022    ,  0.00000E+00,   3.2232    , -0.50298    ,
0.00000E+00,   297.77    ,   1.4000
  1,   7.0811    ,  0.18572    ,  0.00000E+00,   4.2616    , -0.77399    ,
0.00000E+00,   293.78    ,   1.6000
  1,   8.1737    , -0.85326E-03,  0.00000E+00,   7.1444    ,  -1.0190    ,
0.00000E+00,   277.37    ,   1.8000
  1,   9.9105    , -0.22229    ,  0.00000E+00,   9.4784    ,  -1.2317    ,
0.00000E+00,   258.03    ,   2.0000
  1,   11.879    , -0.40414    ,  0.00000E+00,   11.479    ,  0.33172    ,
0.00000E+00,   238.17    ,   2.2000
  1,   15.261    , -0.24508    ,  0.00000E+00,   23.504    ,  0.93635    ,
0.00000E+00,   30.711    ,   2.4000
  1,   20.574    , -0.12024    ,  0.00000E+00,   27.749    ,  0.50117    ,
0.00000E+00,  -76.085    ,   2.6000
  1,   26.137    , -0.22104E-01,  0.00000E+00,   27.395    ,  0.47314    ,
0.00000E+00,  -66.448    ,   2.8000
  1,   31.358    ,  0.72401E-01,  0.00000E+00,   24.888    ,  0.45824    ,
0.00000E+00,  -1.9274    ,   3.0000
  1,   36.320    ,  0.15988    ,  0.00000E+00,   24.810    ,  0.43606    ,
0.00000E+00, -0.36814E-03,   3.2000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.88    ,  0.00000E+00
  2,   4.1559    ,  0.49597    ,  0.00000E+00,  0.61316    , -0.11230    ,
0.00000E+00,   302.73    ,  0.20000
  2,   4.3119    ,  0.46638    ,  0.00000E+00,  0.95077    , -0.17821    ,
0.00000E+00,   302.46    ,  0.40001
  2,   4.5374    ,  0.42614    ,  0.00000E+00,   1.3068    , -0.22195    ,
0.00000E+00,   302.06    ,  0.60000
  2,   4.8358    ,  0.37819    ,  0.00000E+00,   1.6813    , -0.25687    ,
0.00000E+00,   301.50    ,  0.80000
  2,   5.2118    ,  0.32337    ,  0.00000E+00,   2.0844    , -0.29212    ,
0.00000E+00,   300.74    ,   1.0000
  2,   5.6729    ,  0.26067    ,  0.00000E+00,   2.5388    , -0.33764    ,
0.00000E+00,   299.69    ,   1.2000
  2,   6.2349    ,  0.18656    ,  0.00000E+00,   3.1113    , -0.40993    ,
0.00000E+00,   298.07    ,   1.4000
  2,   6.9407    ,  0.93133E-01,  0.00000E+00,   4.0572    , -0.53423    ,
0.00000E+00,   294.68    ,   1.6000
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  2,   7.9548    , -0.25240E-01,  0.00000E+00,   6.5236    , -0.61127    ,
0.00000E+00,   281.79    ,   1.8000
  2,   9.6150    , -0.15988    ,  0.00000E+00,   9.4098    , -0.80158    ,
0.00000E+00,   259.02    ,   2.0000
  2,   11.556    , -0.30638    ,  0.00000E+00,   10.396    , -0.10185    ,
0.00000E+00,   249.78    ,   2.2000
  2,   14.599    , -0.19573    ,  0.00000E+00,   21.565    ,  0.84999    ,
0.00000E+00,   73.603    ,   2.4000
  2,   19.760    , -0.76200E-01,  0.00000E+00,   27.640    ,  0.47386    ,
0.00000E+00,  -73.297    ,   2.6000
  2,   25.324    ,  0.17255E-01,  0.00000E+00,   27.789    ,  0.47219    ,
0.00000E+00,  -77.396    ,   2.8000
  2,   30.619    ,  0.11153    ,  0.00000E+00,   25.199    ,  0.46906    ,
0.00000E+00,  -9.8174    ,   3.0000
  2,   35.586    ,  0.19498    ,  0.00000E+00,   24.801    ,  0.40690    ,
0.00000E+00, -0.40627E-03,   3.2000
  3,   4.0640    ,  0.38100    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.83    ,  0.00000E+00
  3,   4.1574    ,  0.37597    ,  0.00000E+00,  0.61992    , -0.49771E-01,
0.00000E+00,   302.69    ,  0.20000
  3,   4.3138    ,  0.36143    ,  0.00000E+00,  0.94852    , -0.94036E-01,
0.00000E+00,   302.43    ,  0.40001
  3,   4.5383    ,  0.33903    ,  0.00000E+00,   1.3007    , -0.12859    ,
0.00000E+00,   302.04    ,  0.60000
  3,   4.8355    ,  0.31038    ,  0.00000E+00,   1.6750    , -0.15754    ,
0.00000E+00,   301.49    ,  0.80000
  3,   5.2103    ,  0.27596    ,  0.00000E+00,   2.0793    , -0.18743    ,
0.00000E+00,   300.74    ,   1.0000
  3,   5.6706    ,  0.23474    ,  0.00000E+00,   2.5354    , -0.22746    ,
0.00000E+00,   299.69    ,   1.2000
  3,   6.2320    ,  0.18316    ,  0.00000E+00,   3.1084    , -0.29540    ,
0.00000E+00,   298.08    ,   1.4000
  3,   6.9369    ,  0.11227    ,  0.00000E+00,   4.0494    , -0.42838    ,
0.00000E+00,   294.72    ,   1.6000
  3,   7.9480    ,  0.91606E-02,  0.00000E+00,   6.5011    , -0.57518    ,
0.00000E+00,   281.91    ,   1.8000
  3,   9.6039    , -0.11363    ,  0.00000E+00,   9.4023    , -0.69584    ,
0.00000E+00,   259.10    ,   2.0000
  3,   11.548    , -0.24194    ,  0.00000E+00,   10.475    , -0.16372    ,
0.00000E+00,   248.92    ,   2.2000
  3,   14.589    , -0.16831    ,  0.00000E+00,   21.533    ,  0.61450    ,
0.00000E+00,   74.384    ,   2.4000
  3,   19.746    , -0.90990E-01,  0.00000E+00,   27.638    ,  0.26690    ,
0.00000E+00,  -73.244    ,   2.6000
  3,   25.311    , -0.39651E-01,  0.00000E+00,   27.797    ,  0.23537    ,
0.00000E+00,  -77.575    ,   2.8000
  3,   30.607    ,  0.73407E-02,  0.00000E+00,   25.207    ,  0.23512    ,
0.00000E+00,  -9.9636    ,   3.0000
  3,   35.575    ,  0.53149E-01,  0.00000E+00,   24.802    ,  0.22771    ,
0.00000E+00, -0.40797E-03,   3.2000
  4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.81    ,  0.00000E+00
  4,   4.1587    ,  0.25173    ,  0.00000E+00,  0.63034    , -0.23373E-01,
0.00000E+00,   302.67    ,  0.20000
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  4,   4.3173    , 0.24444    , 0.00000E+00,  0.95915    , -0.49383E-01,
0.00000E+00,   302.41    ,  0.40000
  4,   4.5438    , 0.23217    , 0.00000E+00,   1.3097    , -0.72647E-01,
0.00000E+00,   302.02    ,  0.60000
  4,   4.8428    , 0.21558    , 0.00000E+00,   1.6845    , -0.92944E-01,
0.00000E+00,   301.46    ,  0.80001
  4,   5.2197    , 0.19492    , 0.00000E+00,   2.0912    , -0.11431    ,
0.00000E+00,   300.70    ,   1.0000
  4,   5.6828    , 0.16934    , 0.00000E+00,   2.5519    , -0.14370    ,
0.00000E+00,   299.65    ,   1.2000
  4,   6.2483    , 0.13603    , 0.00000E+00,   3.1350    , -0.19490    ,
0.00000E+00,   298.01    ,   1.4000
  4,   6.9607    , 0.87834E-01, 0.00000E+00,   4.1017    , -0.29985    ,
0.00000E+00,   294.54    ,   1.6000
  4,   7.9892    , 0.13279E-01, 0.00000E+00,   6.6332    , -0.42519    ,
0.00000E+00,   281.11    ,   1.8000
  4,   9.6644    ,-0.76754E-01, 0.00000E+00,   9.4341    , -0.50025    ,
0.00000E+00,   258.89    ,   2.0000
  4,   11.621    ,-0.16602    , 0.00000E+00,   10.753    , -0.81371E-01,
0.00000E+00,   245.98    ,   2.2000
  4,   14.746    ,-0.11825    , 0.00000E+00,   22.037    ,  0.38058    ,
0.00000E+00,   63.671    ,   2.4000
  4,   19.946    ,-0.75266E-01, 0.00000E+00,   27.668    ,  0.13115    ,
0.00000E+00,  -74.067    ,   2.6000
  4,   25.511    ,-0.50845E-01, 0.00000E+00,   27.698    ,  0.95632E-01,
0.00000E+00,  -74.880    ,   2.8000
  4,   30.788    ,-0.31418E-01, 0.00000E+00,   25.118    ,  0.98475E-01,
0.00000E+00,  -7.7980    ,   3.0000
  4,   35.753    ,-0.93289E-02, 0.00000E+00,   24.801    ,  0.11224    ,
0.00000E+00, -0.39607E-03,   3.2000
  5,   4.0640    , 0.12700    , 0.00000E+00,  0.31868    ,  0.00000E+00,
0.00000E+00,   302.81    ,  0.00000E+00
  5,   4.1594    , 0.12608    , 0.00000E+00,  0.63707    , -0.96016E-02,
0.00000E+00,   302.66    ,  0.20000
  5,   4.3197    , 0.12299    , 0.00000E+00,  0.96775    , -0.21519E-01,
0.00000E+00,   302.39    ,  0.40000
  5,   4.5479    , 0.11750    , 0.00000E+00,   1.3180    , -0.33076E-01,
0.00000E+00,   302.00    ,  0.60000
  5,   4.8485    , 0.10984    , 0.00000E+00,   1.6933    , -0.43443E-01,
0.00000E+00,   301.44    ,  0.80000
  5,   5.2274    , 0.10009    , 0.00000E+00,   2.1019    , -0.54432E-01,
0.00000E+00,   300.68    ,   1.0000
  5,   5.6929    , 0.87785E-01, 0.00000E+00,   2.5666    , -0.69775E-01,
0.00000E+00,   299.61    ,   1.2000
  5,   6.2621    , 0.71399E-01, 0.00000E+00,   3.1578    , -0.97165E-01,
0.00000E+00,   297.94    ,   1.4000
  5,   6.9808    , 0.46927E-01, 0.00000E+00,   4.1466    , -0.15473    ,
0.00000E+00,   294.38    ,   1.6000
  5,   8.0245    , 0.79398E-02, 0.00000E+00,   6.7466    , -0.22367    ,
0.00000E+00,   280.41    ,   1.8000
  5,   9.7155    ,-0.39241E-01, 0.00000E+00,   9.4606    , -0.25985    ,
0.00000E+00,   258.71    ,   2.0000
  5,   11.684    ,-0.84196E-01, 0.00000E+00,   10.978    , -0.26952E-01,
0.00000E+00,   243.50    ,   2.2000
```

```
 5,   14.877     , -0.60097E-01,  0.00000E+00,    22.432      ,  0.18114     ,
0.00000E+00,    55.059     ,    2.4000
 5,   20.109     , -0.40802E-01,  0.00000E+00,    27.689      ,  0.55331E-01,
0.00000E+00,  -74.663     ,    2.6000
 5,   25.673     , -0.30761E-01,  0.00000E+00,    27.616      ,  0.34907E-01,
0.00000E+00,  -72.669     ,    2.8000
 5,   30.936     , -0.23574E-01,  0.00000E+00,    25.049      ,  0.37259E-01,
0.00000E+00,  -6.0911     ,    3.0000
 5,   35.899     , -0.14248E-01,  0.00000E+00,    24.800      ,  0.47756E-01,
0.00000E+00, -0.38762E-03,    3.2000
 6,   4.0640     ,  0.00000E+00,  0.00000E+00,   0.31868      ,  0.00000E+00,
0.00000E+00,    302.80     ,  0.00000E+00
 6,   4.1597     ,  0.00000E+00,  0.00000E+00,   0.63931      ,  0.00000E+00,
0.00000E+00,    302.65     ,  0.20000
 6,   4.3205     ,  0.00000E+00,  0.00000E+00,   0.97079      ,  0.00000E+00,
0.00000E+00,    302.39     ,  0.40000
 6,   4.5493     ,  0.00000E+00,  0.00000E+00,    1.3211      ,  0.00000E+00,
0.00000E+00,    301.99     ,  0.60000
 6,   4.8506     ,  0.00000E+00,  0.00000E+00,    1.6965      ,  0.00000E+00,
0.00000E+00,    301.44     ,  0.80000
 6,   5.2301     ,  0.00000E+00,  0.00000E+00,    2.1059      ,  0.00000E+00,
0.00000E+00,    300.67     ,    1.0000
 6,   5.6966     ,  0.00000E+00,  0.00000E+00,    2.5724      ,  0.00000E+00,
0.00000E+00,    299.60     ,    1.2000
 6,   6.2673     ,  0.00000E+00,  0.00000E+00,    3.1679      ,  0.00000E+00,
0.00000E+00,    297.92     ,    1.4000
 6,   6.9891     ,  0.00000E+00,  0.00000E+00,    4.1694      ,  0.00000E+00,
0.00000E+00,    294.31     ,    1.6000
 6,   8.0402     ,  0.00000E+00,  0.00000E+00,    6.8003      ,  0.00000E+00,
0.00000E+00,    280.10     ,    1.8000
 6,   9.7388     ,  0.00000E+00,  0.00000E+00,    9.4756      ,  0.00000E+00,
0.00000E+00,    258.64     ,    2.0000
 6,   11.714     ,  0.00000E+00,  0.00000E+00,    11.095      ,  0.00000E+00,
0.00000E+00,    242.31     ,    2.2000
 6,   14.941     ,  0.00000E+00,  0.00000E+00,    22.619      ,  0.00000E+00,
0.00000E+00,    50.922     ,    2.4000
 6,   20.188     ,  0.00000E+00,  0.00000E+00,    27.700      ,  0.00000E+00,
0.00000E+00,  -74.931     ,    2.6000
 6,   25.752     ,  0.00000E+00,  0.00000E+00,    27.578      ,  0.00000E+00,
0.00000E+00,  -71.600     ,    2.8000
 6,   31.007     ,  0.00000E+00,  0.00000E+00,    25.018      ,  0.00000E+00,
0.00000E+00,  -5.2949     ,    3.0000
 6,   35.970     ,  0.00000E+00,  0.00000E+00,    24.802      ,  0.00000E+00,
0.00000E+00, -0.38386E-03,    3.2000
```

Modified source -- m/z 143

```
  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.99    ,  0.00000E+00
  1,   4.1317    ,  0.62974    ,  0.00000E+00,  0.43736    , -0.51406E-01,
0.00000E+00,   202.87    ,  0.20000
  1,   4.2420    ,  0.61514    ,  0.00000E+00,  0.66202    , -0.92469E-01,
0.00000E+00,   202.69    ,  0.40001
  1,   4.3953    ,  0.59340    ,  0.00000E+00,  0.86950    , -0.12352    ,
0.00000E+00,   202.45    ,  0.60001
  1,   4.5897    ,  0.56617    ,  0.00000E+00,   1.0752    , -0.14797    ,
0.00000E+00,   202.15    ,  0.80000
  1,   4.8256    ,  0.53443    ,  0.00000E+00,   1.2852    , -0.16915    ,
0.00000E+00,   201.77    ,   1.0000
  1,   5.1043    ,  0.49853    ,  0.00000E+00,   1.5029    , -0.18997    ,
0.00000E+00,   201.32    ,   1.2000
  1,   5.4275    ,  0.45821    ,  0.00000E+00,   1.7320    , -0.21421    ,
0.00000E+00,   200.76    ,   1.4000
  1,   5.7984    ,  0.41221    ,  0.00000E+00,   1.9805    , -0.24813    ,
0.00000E+00,   200.07    ,   1.6000
  1,   6.2223    ,  0.35757    ,  0.00000E+00,   2.2685    , -0.30330    ,
0.00000E+00,   199.14    ,   1.8000
  1,   6.7119    ,  0.28788    ,  0.00000E+00,   2.6519    , -0.40437    ,
0.00000E+00,   197.69    ,   2.0000
  1,   7.3013    ,  0.19027    ,  0.00000E+00,   3.3201    , -0.58593    ,
0.00000E+00,   194.60    ,   2.2000
  1,   8.0917    ,  0.54749E-01,  0.00000E+00,   4.7469    , -0.73558    ,
0.00000E+00,   185.92    ,   2.4000
  1,   9.2099    , -0.94203E-01,  0.00000E+00,   6.2132    , -0.77612    ,
0.00000E+00,   173.95    ,   2.6000
  1,   10.493    , -0.25714    ,  0.00000E+00,   6.5272    , -0.83129    ,
0.00000E+00,   170.93    ,   2.8000
  1,   11.848    , -0.36957    ,  0.00000E+00,   7.6919    ,  0.64564E-01,
0.00000E+00,   159.15    ,   3.0000
  1,   13.828    , -0.30354    ,  0.00000E+00,   12.799    ,  0.73803    ,
0.00000E+00,   81.255    ,   3.2000
  1,   17.055    , -0.18628    ,  0.00000E+00,   18.496    ,  0.38830    ,
0.00000E+00,  -50.601    ,   3.4000
  1,   20.886    , -0.12265    ,  0.00000E+00,   19.456    ,  0.28875    ,
0.00000E+00,  -77.558    ,   3.6000
  1,   24.788    , -0.65679E-01,  0.00000E+00,   19.539    ,  0.28287    ,
0.00000E+00,  -79.950    ,   3.8000
  1,   28.548    , -0.14099E-01,  0.00000E+00,   17.941    ,  0.25602    ,
0.00000E+00,  -35.562    ,   4.0000
  1,   31.975    ,  0.36669E-01,  0.00000E+00,   16.558    ,  0.24310    ,
0.00000E+00, -0.17352    ,   4.2000
  1,   35.286    ,  0.85062E-01,  0.00000E+00,   16.551    ,  0.24187    ,
0.00000E+00, -0.43170E-03,   4.4000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.90    ,  0.00000E+00
  2,   4.1315    ,  0.50107    ,  0.00000E+00,  0.42147    , -0.65907E-01,
0.00000E+00,   202.81    ,  0.20001
  2,   4.2341    ,  0.48320    ,  0.00000E+00,  0.60665    , -0.10941    ,
0.00000E+00,   202.66    ,  0.40000
```

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 2,   4.3749     ,  0.45822     ,  0.00000E+00,  0.80187      , -0.13858     ,
0.00000E+00,   202.45     ,  0.60001
 2,   4.5553     ,  0.42826     ,  0.00000E+00,   1.0031      , -0.16003     ,
0.00000E+00,   202.18     ,  0.80001
 2,   4.7766     ,  0.39449     ,  0.00000E+00,   1.2110      , -0.17722     ,
0.00000E+00,   201.83     ,   1.0000
 2,   5.0403     ,  0.35748     ,  0.00000E+00,   1.4276      , -0.19288     ,
0.00000E+00,   201.40     ,   1.2000
 2,   5.3484     ,  0.31727     ,  0.00000E+00,   1.6562      , -0.20967     ,
0.00000E+00,   200.88     ,   1.4000
 2,   5.7040     ,  0.27331     ,  0.00000E+00,   1.9040      , -0.23107     ,
0.00000E+00,   200.22     ,   1.6000
 2,   6.1124     ,  0.22418     ,  0.00000E+00,   2.1887      , -0.26260     ,
0.00000E+00,   199.34     ,   1.8000
 2,   6.5848     ,  0.16695     ,  0.00000E+00,   2.5559      , -0.31405     ,
0.00000E+00,   198.03     ,   2.0000
 2,   7.1492     ,  0.96509E-01,  0.00000E+00,   3.1483      , -0.39506     ,
0.00000E+00,   195.49     ,   2.2000
 2,   7.8855     ,  0.97666E-02,  0.00000E+00,   4.3669      , -0.45802     ,
0.00000E+00,   188.66     ,   2.4000
 2,   8.9370     , -0.83591E-01,  0.00000E+00,   6.0381      , -0.50062     ,
0.00000E+00,   175.73     ,   2.6000
 2,   10.206     , -0.19392     ,  0.00000E+00,   6.5104      , -0.58340     ,
0.00000E+00,   171.28     ,   2.8000
 2,   11.536     , -0.29299     ,  0.00000E+00,   7.0304      , -0.14878     ,
0.00000E+00,   166.33     ,   3.0000
 2,   13.324     , -0.25304     ,  0.00000E+00,   11.235      ,  0.51808     ,
0.00000E+00,   109.27     ,   3.2000
 2,   16.290     , -0.13975     ,  0.00000E+00,   17.824      ,  0.43892     ,
0.00000E+00,  -32.611     ,   3.4000
 2,   20.068     , -0.67035E-01,  0.00000E+00,   19.392      ,  0.33214     ,
0.00000E+00,  -75.794     ,   3.6000
 2,   23.965     , -0.12375E-02,  0.00000E+00,   19.532      ,  0.32810     ,
0.00000E+00,  -79.838     ,   3.8000
 2,   27.784     ,  0.65519E-01,  0.00000E+00,   18.297      ,  0.33548     ,
0.00000E+00,  -45.202     ,   4.0000
 2,   31.275     ,  0.13221     ,  0.00000E+00,   16.649      ,  0.31474     ,
0.00000E+00,  -2.4904     ,   4.2000
 2,   34.586     ,  0.18649     ,  0.00000E+00,   16.548      ,  0.26690     ,
0.00000E+00, -0.52259E-03,   4.4000
 2,   37.896     ,  0.23987     ,  0.00000E+00,   16.548      ,  0.26690     ,
0.00000E+00, -0.34076E-03,   4.6000
 3,   4.0640     ,  0.38100     ,  0.00000E+00,  0.25974      ,  0.00000E+00,
0.00000E+00,   202.86     ,  0.00000E+00
 3,   4.1325     ,  0.37819     ,  0.00000E+00,  0.42720      , -0.27863E-01,
0.00000E+00,   202.77     ,  0.20000
 3,   4.2357     ,  0.36998     ,  0.00000E+00,  0.60658      , -0.53808E-01,
0.00000E+00,   202.63     ,  0.40000
 3,   4.3759     ,  0.35698     ,  0.00000E+00,  0.79700      , -0.75375E-01,
0.00000E+00,   202.43     ,  0.60000
 3,   4.5551     ,  0.34012     ,  0.00000E+00,  0.99614      , -0.92510E-01,
0.00000E+00,   202.17     ,  0.80000
 3,   4.7749     ,  0.32017     ,  0.00000E+00,   1.2034      , -0.10672     ,
0.00000E+00,   201.83     ,   1.0000
```

```
  3,   5.0371    ,  0.29751    ,  0.00000E+00,   1.4201    , -0.11987    ,
0.00000E+00,   201.40   ,   1.2000
  3,   5.3437    ,  0.27215    ,  0.00000E+00,   1.6492    , -0.13417    ,
0.00000E+00,   200.88   ,   1.4000
  3,   5.6980    ,  0.24355    ,  0.00000E+00,   1.8978    , -0.15287    ,
0.00000E+00,   200.22   ,   1.6000
  3,   6.1052    ,  0.21034    ,  0.00000E+00,   2.1825    , -0.18157    ,
0.00000E+00,   199.35   ,   1.8000
  3,   6.5762    ,  0.16954    ,  0.00000E+00,   2.5481    , -0.23122    ,
0.00000E+00,   198.06   ,   2.0000
  3,   7.1385    ,  0.11531    ,  0.00000E+00,   3.1331    , -0.31848    ,
0.00000E+00,   195.56   ,   2.2000
  3,   7.8702    ,  0.41203E-01,  0.00000E+00,   4.3362    , -0.41193    ,
0.00000E+00,   188.86   ,   2.4000
  3,   8.9156    , -0.42881E-01,  0.00000E+00,   6.0163    , -0.43439    ,
0.00000E+00,   175.93   ,   2.6000
  3,   10.183    , -0.13600    ,  0.00000E+00,   6.5098    , -0.48722    ,
0.00000E+00,   171.31   ,   2.8000
  3,   11.515    , -0.22100    ,  0.00000E+00,   7.0605    , -0.18194    ,
0.00000E+00,   165.95   ,   3.0000
  3,   13.295    , -0.20267    ,  0.00000E+00,   11.174    ,  0.33257    ,
0.00000E+00,   110.28   ,   3.2000
  3,   16.245    , -0.12583    ,  0.00000E+00,   17.774    ,  0.27707    ,
0.00000E+00,  -31.281   ,   3.4000
  3,   20.019    , -0.85003E-01,  0.00000E+00,   19.387    ,  0.17090    ,
0.00000E+00,  -75.659   ,   3.6000
  3,   23.916    , -0.51784E-01,  0.00000E+00,   19.531    ,  0.16416    ,
0.00000E+00,  -79.826   ,   3.8000
  3,   27.738    , -0.21633E-01,  0.00000E+00,   18.318    ,  0.14528    ,
0.00000E+00,  -45.790   ,   4.0000
  3,   31.233    ,  0.74359E-02,  0.00000E+00,   16.668    ,  0.14469    ,
0.00000E+00,  -2.9894   ,   4.2000
  3,   34.544    ,  0.35711E-01,  0.00000E+00,   16.546    ,  0.14092    ,
0.00000E+00, -0.53392E-03,   4.4000
  3,   37.853    ,  0.63895E-01,  0.00000E+00,   16.546    ,  0.14092    ,
0.00000E+00, -0.34098E-03,   4.6000
  4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.84   ,  0.00000E+00
  4,   4.1332    ,  0.25276    ,  0.00000E+00,  0.43361    , -0.12656E-01,
0.00000E+00,   202.75   ,  0.20000
  4,   4.2379    ,  0.24883    ,  0.00000E+00,  0.61408    , -0.26814E-01,
0.00000E+00,   202.61   ,  0.40000
  4,   4.3795    ,  0.24208    ,  0.00000E+00,  0.80310    , -0.40382E-01,
0.00000E+00,   202.41   ,  0.60000
  4,   4.5597    ,  0.23281    ,  0.00000E+00,   1.0010    , -0.52053E-01,
0.00000E+00,   202.15   ,  0.80000
  4,   4.7805    ,  0.22138    ,  0.00000E+00,   1.2080    , -0.61995E-01,
0.00000E+00,   201.81   ,   1.0000
  4,   5.0436    ,  0.20805    ,  0.00000E+00,   1.4252    , -0.71302E-01,
0.00000E+00,   201.38   ,   1.2000
  4,   5.3514    ,  0.19280    ,  0.00000E+00,   1.6555    , -0.81594E-01,
0.00000E+00,   200.86   ,   1.4000
  4,   5.7071    ,  0.17519    ,  0.00000E+00,   1.9061    , -0.95324E-01,
0.00000E+00,   200.19   ,   1.6000
```

```
  4,  6.1163    , 0.15416    , 0.00000E+00,  2.1945    , -0.11678    ,
0.00000E+00,  199.31    ,  1.8000
  4,  6.5904    , 0.12741    , 0.00000E+00,  2.5674    , -0.15458    ,
0.00000E+00,  197.99    ,  2.0000
  4,  7.1578    , 0.90237E-01, 0.00000E+00,  3.1669    , -0.22333    ,
0.00000E+00,  195.43    ,  2.2000
  4,  7.8990    , 0.37108E-01, 0.00000E+00,  4.3991    , -0.29989    ,
0.00000E+00,  188.49    ,  2.4000
  4,  8.9568    ,-0.23983E-01, 0.00000E+00,  6.0578    , -0.31180    ,
0.00000E+00,  175.60    ,  2.6000
  4,  10.229    ,-0.89924E-01, 0.00000E+00,  6.5233    , -0.34223    ,
0.00000E+00,  171.26    ,  2.8000
  4,  11.569    ,-0.14845    , 0.00000E+00,  7.1977    , -0.11431    ,
0.00000E+00,  164.53    ,  3.0000
  4,  13.386    ,-0.13778    , 0.00000E+00,  11.472    ,  0.22973    ,
0.00000E+00,  105.37    ,  3.2000
  4,  16.390    ,-0.90425E-01, 0.00000E+00,  17.927    ,  0.15512    ,
0.00000E+00, -35.337    ,  3.4000
  4,  20.176    ,-0.69417E-01, 0.00000E+00,  19.401    ,  0.81858E-01,
0.00000E+00, -76.083    ,  3.6000
  4,  24.074    ,-0.53781E-01, 0.00000E+00,  19.532    ,  0.76564E-01,
0.00000E+00, -79.862    ,  3.8000
  4,  27.886    ,-0.41814E-01, 0.00000E+00,  18.248    ,  0.54411E-01,
0.00000E+00, -43.914    ,  4.0000
  4,  31.367    ,-0.30763E-01, 0.00000E+00,  16.622    ,  0.61906E-01,
0.00000E+00, -1.8865    ,  4.2000
  4,  34.678    ,-0.16874E-01, 0.00000E+00,  16.545    ,  0.70136E-01,
0.00000E+00,-0.50947E-03,  4.4000
  5,  4.0640    , 0.12700    , 0.00000E+00, 0.25974    ,  0.00000E+00,
0.00000E+00,  202.84    , 0.00000E+00
  5,  4.1337    , 0.12651    , 0.00000E+00, 0.43753    , -0.50998E-02,
0.00000E+00,  202.74    , 0.20000
  5,  4.2393    , 0.12488    , 0.00000E+00, 0.61968    , -0.11328E-01,
0.00000E+00,  202.60    , 0.40000
  5,  4.3820    , 0.12196    , 0.00000E+00, 0.80865    , -0.17782E-01,
0.00000E+00,  202.40    , 0.60000
  5,  4.5633    , 0.11781    , 0.00000E+00,  1.0061    , -0.23625E-01,
0.00000E+00,  202.14    , 0.80001
  5,  4.7851    , 0.11257    , 0.00000E+00,  1.2130    , -0.28699E-01,
0.00000E+00,  201.80    ,  1.0000
  5,  5.0492    , 0.10635    , 0.00000E+00,  1.4305    , -0.33471E-01,
0.00000E+00,  201.37    ,  1.2000
  5,  5.3582    , 0.99145E-01, 0.00000E+00,  1.6619    , -0.38781E-01,
0.00000E+00,  200.84    ,  1.4000
  5,  5.7154    , 0.90718E-01, 0.00000E+00,  1.9143    , -0.45947E-01,
0.00000E+00,  200.17    ,  1.6000
  5,  6.1265    , 0.80489E-01, 0.00000E+00,  2.2059    , -0.57333E-01,
0.00000E+00,  199.28    ,  1.8000
  5,  6.6033    , 0.67193E-01, 0.00000E+00,  2.5846    , -0.77740E-01,
0.00000E+00,  197.93    ,  2.0000
  5,  7.1752    , 0.48232E-01, 0.00000E+00,  3.1972    , -0.11529    ,
0.00000E+00,  195.30    ,  2.2000
  5,  7.9250    , 0.20572E-01, 0.00000E+00,  4.4557    , -0.15678    ,
0.00000E+00,  188.15    ,  2.4000
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  5,   8.9935    , -0.11264E-01,  0.00000E+00,   6.0920    , -0.16166    ,
0.00000E+00,   175.34    ,   2.6000
  5,   10.269    , -0.45242E-01,  0.00000E+00,   6.5343    , -0.17553    ,
0.00000E+00,   171.20    ,   2.8000
  5,   11.616    , -0.74570E-01,  0.00000E+00,   7.3029    , -0.51983E-01,
0.00000E+00,   163.35    ,   3.0000
  5,   13.464    , -0.69185E-01,  0.00000E+00,   11.714    ,  0.11744    ,
0.00000E+00,   101.19    ,   3.2000
  5,   16.511    , -0.46862E-01,  0.00000E+00,   18.046    ,  0.67937E-01,
0.00000E+00,  -38.467    ,   3.4000
  5,   20.306    , -0.38220E-01,  0.00000E+00,   19.413    ,  0.31729E-01,
0.00000E+00,  -76.402    ,   3.6000
  5,   24.205    , -0.32252E-01,  0.00000E+00,   19.533    ,  0.28969E-01,
0.00000E+00,  -79.886    ,   3.8000
  5,   28.008    , -0.28623E-01,  0.00000E+00,   18.191    ,  0.15280E-01,
0.00000E+00,  -42.371    ,   4.0000
  5,   31.479    , -0.25392E-01,  0.00000E+00,   16.597    ,  0.23355E-01,
0.00000E+00,  -1.2539    ,   4.2000
  5,   34.789    , -0.19806E-01,  0.00000E+00,   16.546    ,  0.28324E-01,
0.00000E+00, -0.49156E-03,   4.4000
  6,   4.0640    ,  0.00000E+00,  0.00000E+00,  0.25974    ,  0.00000E+00,
0.00000E+00,   202.83    ,  0.00000E+00
  6,   4.1338    ,  0.00000E+00,  0.00000E+00,  0.43879    ,  0.00000E+00,
0.00000E+00,   202.74    ,  0.20000
  6,   4.2398    ,  0.00000E+00,  0.00000E+00,  0.62161    ,  0.00000E+00,
0.00000E+00,   202.60    ,  0.40000
  6,   4.3829    ,  0.00000E+00,  0.00000E+00,  0.81067    ,  0.00000E+00,
0.00000E+00,   202.40    ,  0.60000
  6,   4.5646    ,  0.00000E+00,  0.00000E+00,   1.0080    ,  0.00000E+00,
0.00000E+00,   202.13    ,  0.80000
  6,   4.7867    ,  0.00000E+00,  0.00000E+00,   1.2148    ,  0.00000E+00,
0.00000E+00,   201.79    ,   1.0000
  6,   5.0512    ,  0.00000E+00,  0.00000E+00,   1.4325    ,  0.00000E+00,
0.00000E+00,   201.36    ,   1.2000
  6,   5.3606    ,  0.00000E+00,  0.00000E+00,   1.6643    ,  0.00000E+00,
0.00000E+00,   200.83    ,   1.4000
  6,   5.7184    ,  0.00000E+00,  0.00000E+00,   1.9175    ,  0.00000E+00,
0.00000E+00,   200.16    ,   1.6000
  6,   6.1303    ,  0.00000E+00,  0.00000E+00,   2.2107    ,  0.00000E+00,
0.00000E+00,   199.26    ,   1.8000
  6,   6.6084    ,  0.00000E+00,  0.00000E+00,   2.5929    ,  0.00000E+00,
0.00000E+00,   197.91    ,   2.0000
  6,   7.1827    ,  0.00000E+00,  0.00000E+00,   3.2132    ,  0.00000E+00,
0.00000E+00,   195.25    ,   2.2000
  6,   7.9369    ,  0.00000E+00,  0.00000E+00,   4.4836    ,  0.00000E+00,
0.00000E+00,   188.00    ,   2.4000
  6,   9.0104    ,  0.00000E+00,  0.00000E+00,   6.1080    ,  0.00000E+00,
0.00000E+00,   175.22    ,   2.6000
  6,   10.288    ,  0.00000E+00,  0.00000E+00,   6.5411    ,  0.00000E+00,
0.00000E+00,   171.18    ,   2.8000
  6,   11.640    ,  0.00000E+00,  0.00000E+00,   7.3610    ,  0.00000E+00,
0.00000E+00,   162.78    ,   3.0000
  6,   13.502    ,  0.00000E+00,  0.00000E+00,   11.837    ,  0.00000E+00,
0.00000E+00,   99.075    ,   3.2000
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  6,   16.570    , 0.00000E+00, 0.00000E+00,   18.101    , 0.00000E+00,
0.00000E+00,  -39.942    ,   3.4000
  6,   20.370    , 0.00000E+00, 0.00000E+00,   19.418    , 0.00000E+00,
0.00000E+00,  -76.549    ,   3.6000
  6,   24.269    , 0.00000E+00, 0.00000E+00,   19.534    , 0.00000E+00,
0.00000E+00,  -79.897    ,   3.8000
  6,   28.068    , 0.00000E+00, 0.00000E+00,   18.164    , 0.00000E+00,
0.00000E+00,  -41.613    ,   4.0000
  6,   31.534    , 0.00000E+00, 0.00000E+00,   16.589    , 0.00000E+00,
0.00000E+00,  -1.0278    ,   4.2000
  6,   34.844    , 0.00000E+00, 0.00000E+00,   16.546    , 0.00000E+00,
0.00000E+00, -0.48358E-03,   4.4000
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Modified source -- m/z 286

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  1,   4.0640    ,  0.63500    ,  0.00000E+00,  0.18367     ,  0.00000E+00,
0.00000E+00,   102.99    ,  0.00000E+00
  1,   4.1652    ,  0.62675    ,  0.00000E+00,  0.33992     , -0.39560E-01,
0.00000E+00,   102.85    ,  0.40000
  1,   4.3366    ,  0.60514    ,  0.00000E+00,  0.51382     , -0.66639E-01,
0.00000E+00,   102.63    ,  0.80000
  1,   4.5753    ,  0.57469    ,  0.00000E+00,  0.67968     , -0.84374E-01,
0.00000E+00,   102.33    ,   1.2000
  1,   4.8806    ,  0.53838    ,  0.00000E+00,  0.84758     , -0.96468E-01,
0.00000E+00,   101.95    ,   1.6000
  1,   5.2539    ,  0.49788    ,  0.00000E+00,   1.0197     , -0.10588     ,
0.00000E+00,   101.47    ,   2.0000
  1,   5.6971    ,  0.45347    ,  0.00000E+00,   1.1977     , -0.11698     ,
0.00000E+00,   100.88    ,   2.4000
  1,   6.2138    ,  0.40293    ,  0.00000E+00,   1.3894     , -0.13863     ,
0.00000E+00,   100.14    ,   2.8000
  1,   6.8144    ,  0.33842    ,  0.00000E+00,   1.6266     , -0.19248     ,
0.00000E+00,   99.049    ,   3.2000
  1,   7.5385    ,  0.23881    ,  0.00000E+00,   2.0506     , -0.31806     ,
0.00000E+00,   96.645    ,   3.6000
  1,   8.5184    ,  0.92389E-01,  0.00000E+00,   2.8938     , -0.37470     ,
0.00000E+00,   90.398    ,   4.0000
  1,   9.7856    , -0.51099E-01,  0.00000E+00,   3.3216     , -0.35657     ,
0.00000E+00,   86.481    ,   4.4000
  1,   11.137    , -0.19230    ,  0.00000E+00,   3.4596     , -0.31890     ,
0.00000E+00,   85.134    ,   4.8000
  1,   12.777    , -0.24612    ,  0.00000E+00,   5.1077     , -0.95771E-02,
0.00000E+00,   64.348    ,   5.2000
  1,   15.664    , -0.16397    ,  0.00000E+00,   9.5548     ,  0.19411     ,
0.00000E+00,  -32.351    ,   5.6000
  1,   19.887    , -0.11804    ,  0.00000E+00,   11.012     ,  0.77543E-01,
0.00000E+00,  -76.706    ,   6.0000
  1,   24.320    , -0.88974E-01,  0.00000E+00,   11.110     ,  0.70686E-01,
0.00000E+00,  -79.932    ,   6.4000
  1,   28.527    , -0.68152E-01,  0.00000E+00,   9.6793     ,  0.48983E-01,
0.00000E+00,  -35.832    ,   6.8000
  1,   32.079    , -0.46293E-01,  0.00000E+00,   8.3420     ,  0.74150E-01,
0.00000E+00, -0.11226    ,   7.2000
  1,   35.415    , -0.16305E-01,  0.00000E+00,   8.3374     ,  0.75029E-01,
0.00000E+00, -0.42052E-03,   7.6000
  2,   4.0640    ,  0.50800    ,  0.00000E+00,  0.18367     ,  0.00000E+00,
0.00000E+00,   102.92    ,  0.00000E+00
  2,   4.1633    ,  0.49731    ,  0.00000E+00,  0.31842     , -0.49483E-01,
0.00000E+00,   102.81    ,  0.40000
  2,   4.3210    ,  0.47152    ,  0.00000E+00,  0.47210     , -0.76938E-01,
0.00000E+00,   102.62    ,  0.80000
  2,   4.5418    ,  0.43723    ,  0.00000E+00,  0.63260     , -0.93250E-01,
0.00000E+00,   102.36    ,   1.2000
  2,   4.8277    ,  0.39771    ,  0.00000E+00,  0.79803     , -0.10359     ,
0.00000E+00,   102.00    ,   1.6000
  2,   5.1809    ,  0.35474    ,  0.00000E+00,  0.96890     , -0.11102     ,
0.00000E+00,   101.55    ,   2.0000
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  2,   5.6038    ,  0.30888    ,  0.00000E+00,   1.1468     , -0.11864    ,
0.00000E+00,   100.99    ,    2.4000
  2,   6.1001    ,  0.25918    ,  0.00000E+00,   1.3385     , -0.13131    ,
0.00000E+00,   100.28    ,    2.8000
  2,   6.6798    ,  0.20188    ,  0.00000E+00,   1.5709     , -0.15896    ,
0.00000E+00,   99.268    ,    3.2000
  2,   7.3753    ,  0.12772    ,  0.00000E+00,   1.9498     , -0.21740    ,
0.00000E+00,   97.259    ,    3.6000
  2,   8.2954    ,  0.29876E-01,  0.00000E+00,   2.7232     , -0.25740    ,
0.00000E+00,   91.874    ,    4.0000
  2,   9.5245    , -0.74010E-01,  0.00000E+00,   3.2896     , -0.26939    ,
0.00000E+00,   86.812    ,    4.4000
  2,   10.866    , -0.18386    ,  0.00000E+00,   3.4099     , -0.26503    ,
0.00000E+00,   85.625    ,    4.8000
  2,   12.392    , -0.22717    ,  0.00000E+00,   4.6457     ,  0.38073E-01,
0.00000E+00,   70.971    ,    5.2000
  2,   14.939    , -0.13986    ,  0.00000E+00,   8.7239     ,  0.29563    ,
0.00000E+00,  -9.9804    ,    5.6000
  2,   19.016    , -0.49081E-01,  0.00000E+00,   10.930     ,  0.19211    ,
0.00000E+00,  -74.170    ,    6.0000
  2,   23.437    ,  0.26731E-01,  0.00000E+00,   11.102     ,  0.18915    ,
0.00000E+00,  -79.777    ,    6.4000
  2,   27.742    ,  0.10788    ,  0.00000E+00,   10.013     ,  0.21004    ,
0.00000E+00,  -45.731    ,    6.8000
  2,   31.411    ,  0.19015    ,  0.00000E+00,   8.3845     ,  0.16122    ,
0.00000E+00,  -1.2962    ,    7.2000
  2,   34.746    ,  0.23753    ,  0.00000E+00,   8.3335     ,  0.11475    ,
0.00000E+00, -0.49384E-03,    7.6000
  3,   4.0640    ,  0.38100    ,  0.00000E+00,   0.18367    ,  0.00000E+00,
0.00000E+00,   102.89    ,  0.00000E+00
  3,   4.1643    ,  0.37658    ,  0.00000E+00,   0.31997    , -0.21771E-01,
0.00000E+00,   102.78    ,  0.40001
  3,   4.3216    ,  0.36401    ,  0.00000E+00,   0.46845    , -0.40200E-01,
0.00000E+00,   102.61    ,  0.80000
  3,   4.5402    ,  0.34518    ,  0.00000E+00,   0.62614    , -0.53058E-01,
0.00000E+00,   102.35    ,    1.2000
  3,   4.8234    ,  0.32213    ,  0.00000E+00,   0.79055    , -0.61627E-01,
0.00000E+00,   102.00    ,    1.6000
  3,   5.1735    ,  0.29618    ,  0.00000E+00,   0.96117    , -0.67926E-01,
0.00000E+00,   101.56    ,    2.0000
  3,   5.5933    ,  0.26777    ,  0.00000E+00,   1.1392     , -0.74449E-01,
0.00000E+00,   101.00    ,    2.4000
  3,   6.0866    ,  0.23603    ,  0.00000E+00,   1.3311     , -0.85586E-01,
0.00000E+00,   100.30    ,    2.8000
  3,   6.6631    ,  0.19744    ,  0.00000E+00,   1.5623     , -0.11111    ,
0.00000E+00,   99.300    ,    3.2000
  3,   7.3541    ,  0.14252    ,  0.00000E+00,   1.9338     , -0.17045    ,
0.00000E+00,   97.351    ,    3.6000
  3,   8.2652    ,  0.61131E-01,  0.00000E+00,   2.6975     , -0.22138    ,
0.00000E+00,   92.079    ,    4.0000
  3,   9.4883    , -0.24349E-01,  0.00000E+00,   3.2853     , -0.21175    ,
0.00000E+00,   86.876    ,    4.4000
  3,   10.830    , -0.11002    ,  0.00000E+00,   3.4112     , -0.20936    ,
0.00000E+00,   85.632    ,    4.8000
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 3,   12.349    , -0.15553    ,  0.00000E+00,   4.5975     , -0.15530E-01,
0.00000E+00,   71.620    ,   5.2000
 3,   14.864    , -0.11156    ,  0.00000E+00,   8.6224     ,  0.16972     ,
0.00000E+00,  -7.3314    ,   5.6000
 3,   18.922    , -0.67542E-01,  0.00000E+00,   10.919     ,  0.74839E-01,
0.00000E+00,  -73.802    ,   6.0000
 3,   23.340    , -0.39636E-01,  0.00000E+00,   11.101     ,  0.67986E-01,
0.00000E+00,  -79.752    ,   6.4000
 3,   27.655    , -0.15292E-01,  0.00000E+00,   10.051     ,  0.56454E-01,
0.00000E+00,  -46.836    ,   6.8000
 3,   31.339    ,  0.72924E-02,  0.00000E+00,   8.4184     ,  0.55423E-01,
0.00000E+00,  -2.1121    ,   7.2000
 3,   34.675    ,  0.28486E-01,  0.00000E+00,   8.3325     ,  0.52707E-01,
0.00000E+00, -0.50992E-03,   7.6000
 4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.18367     ,  0.00000E+00,
0.00000E+00,   102.87    ,  0.00000E+00
 4,   4.1653    ,  0.25203    ,  0.00000E+00,  0.32384     , -0.10077E-01,
0.00000E+00,   102.77    ,  0.40001
 4,   4.3241    ,  0.24582    ,  0.00000E+00,  0.47152     , -0.20782E-01,
0.00000E+00,   102.59    ,  0.80000
 4,   4.5436    ,  0.23570    ,  0.00000E+00,  0.62760     , -0.29367E-01,
0.00000E+00,   102.34    ,   1.2000
 4,   4.8272    ,  0.22268    ,  0.00000E+00,  0.79118     , -0.35360E-01,
0.00000E+00,   101.99    ,   1.6000
 4,   5.1775    ,  0.20762    ,  0.00000E+00,  0.96170     , -0.39831E-01,
0.00000E+00,   101.55    ,   2.0000
 4,   5.5976    ,  0.19079    ,  0.00000E+00,   1.1402     , -0.44577E-01,
0.00000E+00,   100.99    ,   2.4000
 4,   6.0916    ,  0.17150    ,  0.00000E+00,   1.3334     , -0.52848E-01,
0.00000E+00,   100.28    ,   2.8000
 4,   6.6695    ,  0.14709    ,  0.00000E+00,   1.5676     , -0.72069E-01,
0.00000E+00,   99.275    ,   3.2000
 4,   7.3638    ,  0.11026    ,  0.00000E+00,   1.9457     , -0.11767     ,
0.00000E+00,   97.298    ,   3.6000
 4,   8.2810    ,  0.52874E-01,  0.00000E+00,   2.7143     , -0.15718     ,
0.00000E+00,   91.971    ,   4.0000
 4,   9.5087    , -0.66206E-02,  0.00000E+00,   3.2915     , -0.14444     ,
0.00000E+00,   86.844    ,   4.4000
 4,   10.852    , -0.64705E-01,  0.00000E+00,   3.4182     , -0.14176     ,
0.00000E+00,   85.588    ,   4.8000
 4,   12.382    , -0.97876E-01,  0.00000E+00,   4.6386     , -0.24020E-01,
0.00000E+00,   71.044    ,   5.2000
 4,   14.929    , -0.74895E-01,  0.00000E+00,   8.7111     ,  0.91610E-01,
0.00000E+00,  -9.5570    ,   5.6000
 4,   19.004    , -0.54909E-01,  0.00000E+00,   10.929     ,  0.24874E-01,
0.00000E+00,  -74.122    ,   6.0000
 4,   23.424    , -0.46615E-01,  0.00000E+00,   11.102     ,  0.19140E-01,
0.00000E+00,  -79.774    ,   6.4000
 4,   27.731    , -0.43376E-01,  0.00000E+00,   10.020     ,  0.19438E-02,
0.00000E+00,  -45.870    ,   6.8000
 4,   31.403    , -0.42142E-01,  0.00000E+00,   8.4004     ,  0.12881E-01,
0.00000E+00,  -1.6597    ,   7.2000
 4,   34.738    , -0.33191E-01,  0.00000E+00,   8.3335     ,  0.23231E-01,
0.00000E+00, -0.49932E-03,   7.6000
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   5,   4.0640    , 0.12700    , 0.00000E+00,  0.18367    ,  0.00000E+00,
0.00000E+00,   102.87    ,  0.00000E+00
   5,   4.1659    , 0.12622    , 0.00000E+00,  0.32642    , -0.40858E-02,
0.00000E+00,   102.76    ,  0.40000
   5,   4.3258    , 0.12361    , 0.00000E+00,  0.47441    , -0.89407E-02,
0.00000E+00,   102.59    ,  0.80000
   5,   4.5464    , 0.11915    , 0.00000E+00,  0.62978    , -0.13175E-01,
0.00000E+00,   102.33    ,   1.2000
   5,   4.8307    , 0.11323    , 0.00000E+00,  0.79287    , -0.16232E-01,
0.00000E+00,   101.99    ,   1.6000
   5,   5.1817    , 0.10627    , 0.00000E+00,  0.96335    , -0.18527E-01,
0.00000E+00,   101.54    ,   2.0000
   5,   5.6025    , 0.98394E-01, 0.00000E+00,   1.1423    , -0.20985E-01,
0.00000E+00,   100.98    ,   2.4000
   5,   6.0975    , 0.89238E-01, 0.00000E+00,   1.3367    , -0.25338E-01,
0.00000E+00,   100.27    ,   2.8000
   5,   6.6773    , 0.77359E-01, 0.00000E+00,   1.5737    , -0.35617E-01,
0.00000E+00,   99.247    ,   3.2000
   5,   7.3750    , 0.58804E-01, 0.00000E+00,   1.9575    , -0.60124E-01,
0.00000E+00,   97.234    ,   3.6000
   5,   8.2983    , 0.29301E-01, 0.00000E+00,   2.7307    , -0.80760E-01,
0.00000E+00,   91.854    ,   4.0000
   5,   9.5301    ,-0.94338E-03, 0.00000E+00,   3.2959    , -0.72755E-01,
0.00000E+00,   86.811    ,   4.4000
   5,   10.875    ,-0.30113E-01, 0.00000E+00,   3.4231    , -0.71099E-01,
0.00000E+00,   85.550    ,   4.8000
   5,   12.414    ,-0.47302E-01, 0.00000E+00,   4.6786    , -0.15459E-01,
0.00000E+00,   70.486    ,   5.2000
   5,   14.991    ,-0.37432E-01, 0.00000E+00,   8.7924    ,  0.39354E-01,
0.00000E+00,  -11.661    ,   5.6000
   5,   19.081    ,-0.30172E-01, 0.00000E+00,   10.938    ,  0.53804E-02,
0.00000E+00,  -74.408    ,   6.0000
   5,   23.503    ,-0.28905E-01, 0.00000E+00,   11.103    ,  0.22842E-02,
0.00000E+00,  -79.793    ,   6.4000
   5,   27.802    ,-0.30954E-01, 0.00000E+00,   9.9894    , -0.89187E-02,
0.00000E+00,  -44.975    ,   6.8000
   5,   31.462    ,-0.34106E-01, 0.00000E+00,   8.3875    ,  0.11700E-02,
0.00000E+00,  -1.3329    ,   7.2000
   5,   34.797    ,-0.31044E-01, 0.00000E+00,   8.3334    ,  0.82173E-02,
0.00000E+00, -0.49019E-03,   7.6000
   6,   4.0640    , 0.00000E+00, 0.00000E+00,  0.18367    ,  0.00000E+00,
0.00000E+00,   102.87    ,  0.00000E+00
   6,   4.1661    , 0.00000E+00, 0.00000E+00,  0.32728    ,  0.00000E+00,
0.00000E+00,   102.76    ,  0.40001
   6,   4.3264    , 0.00000E+00, 0.00000E+00,  0.47547    ,  0.00000E+00,
0.00000E+00,   102.58    ,  0.80000
   6,   4.5474    , 0.00000E+00, 0.00000E+00,  0.63064    ,  0.00000E+00,
0.00000E+00,   102.33    ,   1.2000
   6,   4.8320    , 0.00000E+00, 0.00000E+00,  0.79355    ,  0.00000E+00,
0.00000E+00,   101.98    ,   1.6000
   6,   5.1833    , 0.00000E+00, 0.00000E+00,  0.96402    ,  0.00000E+00,
0.00000E+00,   101.54    ,   2.0000
   6,   5.6044    , 0.00000E+00, 0.00000E+00,   1.1432    ,  0.00000E+00,
0.00000E+00,   100.98    ,   2.4000
```

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   6,   6.0998    , 0.00000E+00, 0.00000E+00,   1.3381     ,  0.00000E+00,
0.00000E+00,   100.26    ,   2.8000
   6,   6.6804    , 0.00000E+00, 0.00000E+00,   1.5767     ,  0.00000E+00,
0.00000E+00,   99.235    ,   3.2000
   6,   7.3800    , 0.00000E+00, 0.00000E+00,   1.9641     ,  0.00000E+00,
0.00000E+00,   97.206    ,   3.6000
   6,   8.3064    , 0.00000E+00, 0.00000E+00,   2.7383     ,  0.00000E+00,
0.00000E+00,   91.800    ,   4.0000
   6,   9.5399    , 0.00000E+00, 0.00000E+00,   3.2975     ,  0.00000E+00,
0.00000E+00,   86.796    ,   4.4000
   6,   10.885    , 0.00000E+00, 0.00000E+00,   3.4255     ,  0.00000E+00,
0.00000E+00,   85.530    ,   4.8000
   6,   12.429    , 0.00000E+00, 0.00000E+00,   4.6969     ,  0.00000E+00,
0.00000E+00,   70.228    ,   5.2000
   6,   15.020    , 0.00000E+00, 0.00000E+00,   8.8289     ,  0.00000E+00,
0.00000E+00,  -12.627    ,   5.6000
   6,   19.117    , 0.00000E+00, 0.00000E+00,   10.942     ,  0.00000E+00,
0.00000E+00,  -74.535    ,   6.0000
   6,   23.539    , 0.00000E+00, 0.00000E+00,   11.103     ,  0.00000E+00,
0.00000E+00,  -79.802    ,   6.4000
   6,   27.834    , 0.00000E+00, 0.00000E+00,   9.9755     ,  0.00000E+00,
0.00000E+00,  -44.566    ,   6.8000
   6,   31.489    , 0.00000E+00, 0.00000E+00,   8.3834     ,  0.00000E+00,
0.00000E+00,  -1.2130    ,   7.2000
   6,   34.824    , 0.00000E+00, 0.00000E+00,   8.3333     ,  0.00000E+00,
0.00000E+00, -0.48637E-03,   7.6000
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Modified source -- m/z 382

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  1,   4.0640     ,  0.63500     ,  0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.990     ,  0.00000E+00
  1,   4.1750     ,  0.62590     ,  0.00000E+00,  0.30012     , -0.34708E-01,
0.00000E+00,   77.843     ,  0.50000
  1,   4.3641     ,  0.60242     ,  0.00000E+00,  0.45383     , -0.57427E-01,
0.00000E+00,   77.611     ,   1.0000
  1,   4.6279     ,  0.56991     ,  0.00000E+00,  0.60161     , -0.71507E-01,
0.00000E+00,   77.299     ,   1.5000
  1,   4.9660     ,  0.53180     ,  0.00000E+00,  0.75135     , -0.80233E-01,
0.00000E+00,   76.895     ,   2.0000
  1,   5.3798     ,  0.49012     ,  0.00000E+00,  0.90405     , -0.86372E-01,
0.00000E+00,   76.393     ,   2.5000
  1,   5.8707     ,  0.44512     ,  0.00000E+00,   1.0609     , -0.94538E-01,
0.00000E+00,   75.780     ,   3.0000
  1,   6.4426     ,  0.39362     ,  0.00000E+00,   1.2305     , -0.11493     ,
0.00000E+00,   75.002     ,   3.5000
  1,   7.1098     ,  0.32389     ,  0.00000E+00,   1.4558     , -0.17426     ,
0.00000E+00,   73.772     ,   4.0000
  1,   7.9369     ,  0.20906     ,  0.00000E+00,   1.9160     , -0.28242     ,
0.00000E+00,   70.603     ,   4.5000
  1,   9.0579     ,  0.69063E-01,  0.00000E+00,   2.5034     , -0.25853     ,
0.00000E+00,   65.484     ,   5.0000
  1,   10.356     , -0.57406E-01,  0.00000E+00,   2.6465     , -0.25236     ,
0.00000E+00,   64.033     ,   5.5000
  1,   11.723     , -0.17030     ,  0.00000E+00,   2.9896     , -0.14377     ,
0.00000E+00,   60.303     ,   6.0000
  1,   13.618     , -0.19282     ,  0.00000E+00,   5.0512     ,  0.15769     ,
0.00000E+00,   27.474     ,   6.5000
  1,   17.127     , -0.12963     ,  0.00000E+00,   8.4241     ,  0.54670E-01,
0.00000E+00,  -62.451     ,   7.0000
  1,   21.510     , -0.11571     ,  0.00000E+00,   8.9069     ,  0.16894E-01,
0.00000E+00,  -79.004     ,   7.5000
  1,   25.959     , -0.10989     ,  0.00000E+00,   8.6132     , -0.44599E-02,
0.00000E+00,  -68.816     ,   8.0000
  1,   29.860     , -0.11097     ,  0.00000E+00,   7.0073     , -0.10848E-02,
0.00000E+00,  -19.156     ,   8.5000
  1,   33.089     , -0.97070E-01,  0.00000E+00,   6.2788     ,  0.52794E-01,
0.00000E+00, -0.16928E-02,   9.0000
  1,   36.228     , -0.70668E-01,  0.00000E+00,   6.2788     ,  0.52807E-01,
0.00000E+00, -0.37198E-03,   9.5000
  2,   4.0640     ,  0.50800     ,  0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.921     ,  0.00000E+00
  2,   4.1724     ,  0.49625     ,  0.00000E+00,  0.27982     , -0.43172E-01,
0.00000E+00,   77.809     ,  0.50000
  2,   4.3463     ,  0.46838     ,  0.00000E+00,  0.41755     , -0.66033E-01,
0.00000E+00,   77.613     ,   1.0000
  2,   4.5908     ,  0.43183     ,  0.00000E+00,  0.56104     , -0.78986E-01,
0.00000E+00,   77.331     ,   1.5000
  2,   4.9081     ,  0.39029     ,  0.00000E+00,  0.70868     , -0.86536E-01,
0.00000E+00,   76.957     ,   2.0000
  2,   5.3002     ,  0.34573     ,  0.00000E+00,  0.86047     , -0.91457E-01,
0.00000E+00,   76.484     ,   2.5000
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  2,   5.7694    , 0.29876    , 0.00000E+00,   1.0175    , -0.96863E-01,
0.00000E+00,   75.898    ,   3.0000
  2,   6.3197    , 0.24793    , 0.00000E+00,   1.1874    , -0.10815    ,
0.00000E+00,   75.152    ,   3.5000
  2,   6.9641    , 0.18773    , 0.00000E+00,   1.4045    , -0.13707    ,
0.00000E+00,   74.024    ,   4.0000
  2,   7.7538    , 0.10607    , 0.00000E+00,   1.8050    , -0.19040    ,
0.00000E+00,   71.447    ,   4.5000
  2,   8.8164    , 0.70284E-02, 0.00000E+00,   2.4273    , -0.19584    ,
0.00000E+00,   66.226    ,   5.0000
  2,   10.097    ,-0.92602E-01, 0.00000E+00,   2.6322    , -0.20391    ,
0.00000E+00,   64.169    ,   5.5000
  2,   11.438    ,-0.18782    , 0.00000E+00,   2.8029    , -0.13076    ,
0.00000E+00,   62.386    ,   6.0000
  2,   13.155    ,-0.19874    , 0.00000E+00,   4.3028    ,  0.11744    ,
0.00000E+00,   41.299    ,   6.5000
  2,   16.303    ,-0.91631E-01, 0.00000E+00,   8.0591    ,  0.17599    ,
0.00000E+00,  -50.676    ,   7.0000
  2,   20.620    ,-0.16035E-01, 0.00000E+00,   8.8799    ,  0.14312    ,
0.00000E+00,  -78.179    ,   7.5000
  2,   25.078    , 0.55577E-01, 0.00000E+00,   8.9263    ,  0.14885    ,
0.00000E+00,  -79.827    ,   8.0000
  2,   29.140    , 0.13715    , 0.00000E+00,   7.3195    ,  0.16228    ,
0.00000E+00,  -28.143    ,   8.5000
  2,   32.455    , 0.20282    , 0.00000E+00,   6.2761    ,  0.70095E-01,
0.00000E+00, -0.10867E-01,   9.0000
  2,   35.593    , 0.23749    , 0.00000E+00,   6.2757    ,  0.69306E-01,
0.00000E+00, -0.40535E-03,   9.5000
  3,   4.0640    , 0.38100    , 0.00000E+00,  0.15892    ,  0.00000E+00,
0.00000E+00,   77.892    , 0.00000E+00
  3,   4.1734    , 0.37611    , 0.00000E+00,  0.28064    , -0.19217E-01,
0.00000E+00,   77.785    , 0.50001
  3,   4.3465    , 0.36235    , 0.00000E+00,  0.41371    , -0.34927E-01,
0.00000E+00,   77.600    ,   1.0000
  3,   4.5884    , 0.34210    , 0.00000E+00,  0.55489    , -0.45239E-01,
0.00000E+00,   77.327    ,   1.5000
  3,   4.9024    , 0.31777    , 0.00000E+00,  0.70167    , -0.51551E-01,
0.00000E+00,   76.961    ,   2.0000
  3,   5.2909    , 0.29090    , 0.00000E+00,  0.85325    , -0.55762E-01,
0.00000E+00,   76.493    ,   2.5000
  3,   5.7565    , 0.26195    , 0.00000E+00,   1.0104    , -0.60416E-01,
0.00000E+00,   75.913    ,   3.0000
  3,   6.3033    , 0.22963    , 0.00000E+00,   1.1802    , -0.70405E-01,
0.00000E+00,   75.174    ,   3.5000
  3,   6.9438    , 0.18877    , 0.00000E+00,   1.3953    , -0.97541E-01,
0.00000E+00,   74.068    ,   4.0000
  3,   7.7269    , 0.12651    , 0.00000E+00,   1.7868    , -0.15428    ,
0.00000E+00,   71.573    ,   4.5000
  3,   8.7800    , 0.44261E-01, 0.00000E+00,   2.4138    , -0.15849    ,
0.00000E+00,   66.354    ,   5.0000
  3,   10.057    ,-0.32497E-01, 0.00000E+00,   2.6308    , -0.15317    ,
0.00000E+00,   64.194    ,   5.5000
  3,   11.398    ,-0.10597    , 0.00000E+00,   2.7973    , -0.11752    ,
0.00000E+00,   62.429    ,   6.0000
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  3,   13.098    , -0.13183    ,  0.00000E+00,   4.2518     ,  0.29128E-01,
0.00000E+00,   42.182    ,   6.5000
  3,   16.199    , -0.80253E-01,  0.00000E+00,   7.9990     ,  0.75257E-01,
0.00000E+00,  -48.765    ,   7.0000
  3,   20.505    , -0.55654E-01,  0.00000E+00,   8.8755     ,  0.38267E-01,
0.00000E+00,  -78.035    ,   7.5000
  3,   24.962    , -0.37166E-01,  0.00000E+00,   8.9290     ,  0.35406E-01,
0.00000E+00,  -79.927    ,   8.0000
  3,   29.044    , -0.25380E-01,  0.00000E+00,   7.3607     ,  0.23433E-01,
0.00000E+00,  -29.341    ,   8.5000
  3,   32.374    , -0.12292E-01,  0.00000E+00,   6.2748     ,  0.31809E-01,
0.00000E+00, -0.31380E-01,   9.0000
  3,   35.511    ,  0.36463E-02,  0.00000E+00,   6.2735     ,  0.31881E-01,
0.00000E+00, -0.41284E-03,   9.5000
  4,   4.0640    ,  0.25400    ,  0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.880    ,  0.00000E+00
  4,   4.1744    ,  0.25182    ,  0.00000E+00,  0.28382     , -0.89428E-02,
0.00000E+00,   77.771    ,  0.50001
  4,   4.3490    ,  0.24497    ,  0.00000E+00,  0.41587     , -0.18202E-01,
0.00000E+00,   77.587    ,   1.0000
  4,   4.5916    ,  0.23402    ,  0.00000E+00,  0.55555     , -0.25155E-01,
0.00000E+00,   77.318    ,   1.5000
  4,   4.9056    ,  0.22024    ,  0.00000E+00,  0.70162     , -0.29587E-01,
0.00000E+00,   76.954    ,   2.0000
  4,   5.2941    ,  0.20467    ,  0.00000E+00,  0.85309     , -0.32599E-01,
0.00000E+00,   76.487    ,   2.5000
  4,   5.7597    ,  0.18759    ,  0.00000E+00,   1.0106     , -0.36025E-01,
0.00000E+00,   75.905    ,   3.0000
  4,   6.3069    ,  0.16800    ,  0.00000E+00,   1.1817     , -0.43489E-01,
0.00000E+00,   75.162    ,   3.5000
  4,   6.9488    ,  0.14199    ,  0.00000E+00,   1.3998     , -0.63973E-01,
0.00000E+00,   74.044    ,   4.0000
  4,   7.7353    ,  0.99658E-01,  0.00000E+00,   1.7957     , -0.10769    ,
0.00000E+00,   71.528    ,   4.5000
  4,   8.7929    ,  0.42042E-01,  0.00000E+00,   2.4208     , -0.10929    ,
0.00000E+00,   66.307    ,   5.0000
  4,   10.072    , -0.97370E-02,  0.00000E+00,   2.6335     , -0.10203    ,
0.00000E+00,   64.186    ,   5.5000
  4,   11.415    , -0.58977E-01,  0.00000E+00,   2.8093     , -0.81831E-01,
0.00000E+00,   62.299    ,   6.0000
  4,   13.126    , -0.81215E-01,  0.00000E+00,   4.2946     ,  0.75081E-02,
0.00000E+00,   41.431    ,   6.5000
  4,   16.254    , -0.56878E-01,  0.00000E+00,   8.0317     ,  0.27927E-01,
0.00000E+00,  -49.767    ,   7.0000
  4,   20.566    , -0.52413E-01,  0.00000E+00,   8.8785     ,  0.41287E-03,
0.00000E+00,  -78.114    ,   7.5000
  4,   25.024    , -0.52857E-01,  0.00000E+00,   8.9288     , -0.43283E-02,
0.00000E+00,  -79.891    ,   8.0000
  4,   29.095    , -0.62937E-01,  0.00000E+00,   7.3394     , -0.19950E-01,
0.00000E+00,  -28.697    ,   8.5000
  4,   32.418    , -0.67386E-01,  0.00000E+00,   6.2754     ,  0.13699E-01,
0.00000E+00, -0.24098E-01,   9.0000
  4,   35.555    , -0.60368E-01,  0.00000E+00,   6.2744     ,  0.14059E-01,
0.00000E+00, -0.40939E-03,   9.5000
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  5,   4.0640      , 0.12700     , 0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.875     , 0.00000E+00
  5,   4.1751      , 0.12613     , 0.00000E+00,  0.28599     , -0.36325E-02,
0.00000E+00,   77.764     , 0.50001
  5,   4.3508      , 0.12325     , 0.00000E+00,  0.41810     , -0.78628E-02,
0.00000E+00,   77.579     ,  1.0000
  5,   4.5943      , 0.11841     , 0.00000E+00,  0.55706     , -0.11316E-01,
0.00000E+00,   77.311     ,  1.5000
  5,   4.9090      , 0.11214     , 0.00000E+00,  0.70267     , -0.13583E-01,
0.00000E+00,   76.948     ,  2.0000
  5,   5.2980      , 0.10495     , 0.00000E+00,  0.85409     , -0.15134E-01,
0.00000E+00,   76.481     ,  2.5000
  5,   5.7642      , 0.96971E-01, 0.00000E+00,   1.0120     , -0.16918E-01,
0.00000E+00,   75.897     ,  3.0000
  5,   6.3123      , 0.87681E-01, 0.00000E+00,   1.1842     , -0.20867E-01,
0.00000E+00,   75.148     ,  3.5000
  5,   6.9560      , 0.74969E-01, 0.00000E+00,   1.4052     , -0.31835E-01,
0.00000E+00,   74.014     ,  4.0000
  5,   7.7464      , 0.53525E-01, 0.00000E+00,   1.8056     , -0.55089E-01,
0.00000E+00,   71.466     ,  4.5000
  5,   8.8087      , 0.24142E-01, 0.00000E+00,   2.4274     , -0.55136E-01,
0.00000E+00,   66.252     ,  5.0000
  5,   10.090      ,-0.17110E-02, 0.00000E+00,   2.6351     , -0.50630E-01,
0.00000E+00,   64.175     ,  5.5000
  5,   11.434      ,-0.26219E-01, 0.00000E+00,   2.8206     , -0.41432E-01,
0.00000E+00,   62.192     ,  6.0000
  5,   13.157      ,-0.38449E-01, 0.00000E+00,   4.3391     ,  0.13468E-02,
0.00000E+00,   40.674     ,  6.5000
  5,   16.312      ,-0.29141E-01, 0.00000E+00,   8.0635     ,  0.74739E-02,
0.00000E+00,  -50.795     ,  7.0000
  5,   20.629      ,-0.30265E-01, 0.00000E+00,   8.8804     , -0.67177E-02,
0.00000E+00,  -78.191     ,  7.5000
  5,   25.088      ,-0.34015E-01, 0.00000E+00,   8.9244     , -0.11608E-01,
0.00000E+00,  -79.770     ,  8.0000
  5,   29.148      ,-0.44006E-01, 0.00000E+00,   7.3166     , -0.19687E-01,
0.00000E+00,  -28.042     ,  8.5000
  5,   32.463      ,-0.49692E-01, 0.00000E+00,   6.2752     ,  0.47152E-02,
0.00000E+00, -0.19229E-01,  9.0000
  5,   35.600      ,-0.47231E-01, 0.00000E+00,   6.2744     ,  0.49344E-02,
0.00000E+00, -0.40621E-03,  9.5000
  6,   4.0640      , 0.00000E+00, 0.00000E+00,  0.15892     ,  0.00000E+00,
0.00000E+00,   77.874     , 0.00000E+00
  6,   4.1753      , 0.00000E+00, 0.00000E+00,  0.28672     ,  0.00000E+00,
0.00000E+00,   77.761     , 0.50000
  6,   4.3515      , 0.00000E+00, 0.00000E+00,  0.41893     ,  0.00000E+00,
0.00000E+00,   77.577     ,  1.0000
  6,   4.5953      , 0.00000E+00, 0.00000E+00,  0.55767     ,  0.00000E+00,
0.00000E+00,   77.308     ,  1.5000
  6,   4.9103      , 0.00000E+00, 0.00000E+00,  0.70312     ,  0.00000E+00,
0.00000E+00,   76.945     ,  2.0000
  6,   5.2994      , 0.00000E+00, 0.00000E+00,  0.85451     ,  0.00000E+00,
0.00000E+00,   76.478     ,  2.5000
  6,   5.7659      , 0.00000E+00, 0.00000E+00,   1.0126     ,  0.00000E+00,
0.00000E+00,   75.894     ,  3.0000
```

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  6,   6.3144    , 0.00000E+00,  0.00000E+00,    1.1854     ,  0.00000E+00,
0.00000E+00,   75.143    ,   3.5000
  6,   6.9591    , 0.00000E+00,  0.00000E+00,    1.4080     ,  0.00000E+00,
0.00000E+00,   74.002    ,   4.0000
  6,   7.7515    , 0.00000E+00,  0.00000E+00,    1.8110     ,  0.00000E+00,
0.00000E+00,   71.437    ,   4.5000
  6,   8.8160    , 0.00000E+00,  0.00000E+00,    2.4297     ,  0.00000E+00,
0.00000E+00,   66.228    ,   5.0000
  6,   10.098    , 0.00000E+00,  0.00000E+00,    2.6355     ,  0.00000E+00,
0.00000E+00,   64.171    ,   5.5000
  6,   11.443    , 0.00000E+00,  0.00000E+00,    2.8258     ,  0.00000E+00,
0.00000E+00,   62.135    ,   6.0000
  6,   13.171    , 0.00000E+00,  0.00000E+00,    4.3607     ,  0.00000E+00,
0.00000E+00,   40.321    ,   6.5000
  6,   16.337    , 0.00000E+00,  0.00000E+00,    8.0765     ,  0.00000E+00,
0.00000E+00,  -51.230    ,   7.0000
  6,   20.657    , 0.00000E+00,  0.00000E+00,    8.8809     ,  0.00000E+00,
0.00000E+00,  -78.223    ,   7.5000
  6,   25.115    , 0.00000E+00,  0.00000E+00,    8.9181     ,  0.00000E+00,
0.00000E+00,  -79.607    ,   8.0000
  6,   29.170    , 0.00000E+00,  0.00000E+00,    7.3063     ,  0.00000E+00,
0.00000E+00,  -27.766    ,   8.5000
  6,   32.482    , 0.00000E+00,  0.00000E+00,    6.2743     ,  0.00000E+00,
0.00000E+00, -0.18133E-01,   9.0000
  6,   35.618    , 0.00000E+00,  0.00000E+00,    6.2735     ,  0.00000E+00,
0.00000E+00, -0.40496E-03,   9.5000
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Modified source -- m/z 572

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  1,  4.0640   ,  0.63500    ,  0.00000E+00,  0.12987     ,  0.00000E+00,
0.00000E+00,   52.991    ,  0.00000E+00
  1,  4.1700   ,  0.62684    ,  0.00000E+00,  0.23517     , -0.25932E-01,
0.00000E+00,   52.860    ,  0.60000
  1,  4.3465   ,  0.60579    ,  0.00000E+00,  0.35090     , -0.42930E-01,
0.00000E+00,   52.657    ,   1.2000
  1,  4.5902   ,  0.57668    ,  0.00000E+00,  0.46138     , -0.53179E-01,
0.00000E+00,   52.388    ,   1.8000
  1,  4.9003   ,  0.54288    ,  0.00000E+00,  0.57249     , -0.58816E-01,
0.00000E+00,   52.046    ,   2.4000
  1,  5.2774   ,  0.50673    ,  0.00000E+00,  0.68452     , -0.61330E-01,
0.00000E+00,   51.627    ,   3.0000
  1,  5.7217   ,  0.46950    ,  0.00000E+00,  0.79671     , -0.62845E-01,
0.00000E+00,   51.134    ,   3.6000
  1,  6.2336   ,  0.43071    ,  0.00000E+00,  0.90997     , -0.67521E-01,
0.00000E+00,   50.559    ,   4.2000
  1,  6.8155   ,  0.38605    ,  0.00000E+00,   1.0333     , -0.84803E-01,
0.00000E+00,   49.841    ,   4.8000
  1,  7.4833   ,  0.32219    ,  0.00000E+00,   1.2094     , -0.13514    ,
0.00000E+00,   48.639    ,   5.4000
  1,  8.2990   ,  0.22374    ,  0.00000E+00,   1.5344     , -0.17833    ,
0.00000E+00,   45.952    ,   6.0000
  1,  9.3068   ,  0.12956    ,  0.00000E+00,   1.7774     , -0.13707    ,
0.00000E+00,   43.606    ,   6.6000
  1,   10.394  ,  0.50712E-01,  0.00000E+00,   1.8344     , -0.12947    ,
0.00000E+00,   43.002    ,   7.2000
  1,   11.519  , -0.27353E-01,  0.00000E+00,   1.9758     , -0.12726    ,
0.00000E+00,   41.419    ,   7.8000
  1,   12.917  , -0.95042E-01,  0.00000E+00,   2.8016     , -0.85581E-01,
0.00000E+00,   29.753    ,   8.4000
  1,   15.341  , -0.10308    ,  0.00000E+00,   5.4548     , -0.14814E-01,
0.00000E+00,  -35.188    ,   9.0000
  1,   19.063  , -0.13548    ,  0.00000E+00,   6.5859     , -0.80090E-01,
0.00000E+00,  -75.568    ,   9.6000
  1,   23.059  , -0.18765    ,  0.00000E+00,   6.6918     , -0.90216E-01,
0.00000E+00,  -79.742    ,   10.200
  2,  4.0640   ,  0.50800    ,  0.00000E+00,  0.12987     ,  0.00000E+00,
0.00000E+00,   52.926    ,  0.00000E+00
  2,  4.1678   ,  0.49744    ,  0.00000E+00,  0.21999     , -0.32441E-01,
0.00000E+00,   52.826    ,  0.60000
  2,  4.3302   ,  0.47224    ,  0.00000E+00,  0.32258     , -0.49816E-01,
0.00000E+00,   52.656    ,   1.2000
  2,  4.5557   ,  0.43918    ,  0.00000E+00,  0.42930     , -0.59471E-01,
0.00000E+00,   52.415    ,   1.8000
  2,  4.8459   ,  0.40177    ,  0.00000E+00,  0.53847     , -0.64616E-01,
0.00000E+00,   52.100    ,   2.4000
  2,  5.2022   ,  0.36219    ,  0.00000E+00,  0.64950     , -0.67013E-01,
0.00000E+00,   51.708    ,   3.0000
  2,  5.6255   ,  0.32158    ,  0.00000E+00,  0.76165     , -0.68306E-01,
0.00000E+00,   51.238    ,   3.6000
  2,  6.1165   ,  0.27996    ,  0.00000E+00,  0.87569     , -0.70962E-01,
0.00000E+00,   50.684    ,   4.2000
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 2,    6.6781     ,  0.23526     ,  0.00000E+00,  0.99918     , -0.79629E-01,
0.00000E+00,   49.994     ,   4.8000
 2,    7.3234     ,  0.18139     ,  0.00000E+00,   1.1641     , -0.10317     ,
0.00000E+00,   48.923     ,   5.4000
 2,    8.1004     ,  0.11002     ,  0.00000E+00,   1.4519     , -0.13052     ,
0.00000E+00,   46.671     ,   6.0000
 2,    9.0691     ,  0.34376E-01,  0.00000E+00,   1.7413     , -0.11928     ,
0.00000E+00,   43.938     ,   6.6000
 2,    10.144     , -0.36408E-01,  0.00000E+00,   1.8220     , -0.11810     ,
0.00000E+00,   43.089     ,   7.2000
 2,    11.252     , -0.10553     ,  0.00000E+00,   1.8950     , -0.10289     ,
0.00000E+00,   42.299     ,   7.8000
 2,    12.545     , -0.14204     ,  0.00000E+00,   2.5389     , -0.29051E-01,
0.00000E+00,   33.858     ,   8.4000
 2,    14.616     , -0.97367E-01,  0.00000E+00,   4.8150     ,  0.12768     ,
0.00000E+00,  -15.828     ,   9.0000
 2,    18.138     , -0.37626E-01,  0.00000E+00,   6.4890     ,  0.81189E-01,
0.00000E+00,  -71.894     ,   9.6000
 2,    22.112     ,  0.96904E-02,  0.00000E+00,   6.6821     ,  0.78347E-01,
0.00000E+00,  -79.428     ,   10.200
 2,    26.102     ,  0.59071E-01,  0.00000E+00,   6.3579     ,  0.93744E-01,
0.00000E+00,  -66.907     ,   10.800
 2,    29.527     ,  0.11463     ,  0.00000E+00,   5.0708     ,  0.91942E-01,
0.00000E+00,  -23.299     ,   11.400
 2,    32.240     ,  0.15573     ,  0.00000E+00,   4.2285     ,  0.21151E-01,
0.00000E+00, -0.46362E-01,   12.000
 2,    34.776     ,  0.16758     ,  0.00000E+00,   4.2267     ,  0.19613E-01,
0.00000E+00, -0.49151E-03,   12.600
 2,    37.312     ,  0.17934     ,  0.00000E+00,   4.2267     ,  0.19612E-01,
0.00000E+00, -0.34474E-03,   13.200
 3,    4.0640     ,  0.38100     ,  0.00000E+00,  0.12987     ,  0.00000E+00,
0.00000E+00,   52.900     ,  0.00000E+00
 3,    4.1687     ,  0.37665     ,  0.00000E+00,  0.22059     , -0.14264E-01,
0.00000E+00,   52.804     ,  0.60000
 3,    4.3303     ,  0.36437     ,  0.00000E+00,  0.31945     , -0.25986E-01,
0.00000E+00,   52.644     ,   1.2000
 3,    4.5532     ,  0.34629     ,  0.00000E+00,  0.42408     , -0.33619E-01,
0.00000E+00,   52.412     ,   1.8000
 3,    4.8399     ,  0.32469     ,  0.00000E+00,  0.53235     , -0.37920E-01,
0.00000E+00,   52.104     ,   2.4000
 3,    5.1925     ,  0.30123     ,  0.00000E+00,  0.64302     , -0.40013E-01,
0.00000E+00,   51.718     ,   3.0000
 3,    5.6118     ,  0.27687     ,  0.00000E+00,  0.75514     , -0.41166E-01,
0.00000E+00,   51.253     ,   3.6000
 3,    6.0990     ,  0.25162     ,  0.00000E+00,  0.86932     , -0.43455E-01,
0.00000E+00,   50.703     ,   4.2000
 3,    6.6567     ,  0.22367     ,  0.00000E+00,  0.99254     , -0.51198E-01,
0.00000E+00,   50.021     ,   4.8000
 3,    7.2974     ,  0.18722     ,  0.00000E+00,   1.1549     , -0.73721E-01,
0.00000E+00,   48.979     ,   5.4000
 3,    8.0672     ,  0.13288     ,  0.00000E+00,   1.4375     , -0.10413     ,
0.00000E+00,   46.790     ,   6.0000
 3,    9.0290     ,  0.73624E-01,  0.00000E+00,   1.7346     , -0.87961E-01,
0.00000E+00,   44.000     ,   6.6000
```

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  3,   10.102     ,  0.23860E-01,  0.00000E+00,    1.8199     , -0.80869E-01,
0.00000E+00,   43.105    ,   7.2000
  3,   11.208     , -0.24483E-01,  0.00000E+00,    1.8888     , -0.78687E-01,
0.00000E+00,   42.356    ,   7.8000
  3,   12.487     , -0.63917E-01,  0.00000E+00,    2.5041     , -0.53427E-01,
0.00000E+00,   34.354    ,   8.4000
  3,   14.511     , -0.65465E-01,  0.00000E+00,    4.7075     ,  0.28860E-01,
0.00000E+00,  -12.743    ,   9.0000
  3,   17.996     , -0.61768E-01,  0.00000E+00,    6.4694     , -0.13629E-01,
0.00000E+00,  -71.119    ,   9.6000
  3,   21.966     , -0.73544E-01,  0.00000E+00,    6.6808     , -0.22419E-01,
0.00000E+00,  -79.364    ,   10.200
  3,   25.963     , -0.89870E-01,  0.00000E+00,    6.4077     , -0.42781E-01,
0.00000E+00,  -68.762    ,   10.800
  3,   29.416     , -0.11452     ,  0.00000E+00,    5.1175     , -0.40282E-01,
0.00000E+00,  -24.680    ,   11.400
  3,   32.149     , -0.12764     ,  0.00000E+00,    4.2299     ,  0.20733E-01,
0.00000E+00, -0.74841E-01,   12.000
  3,   34.685     , -0.11423     ,  0.00000E+00,    4.2268     ,  0.22516E-01,
0.00000E+00, -0.50720E-03,   12.600
  3,   37.221     , -0.10072     ,  0.00000E+00,    4.2268     ,  0.22517E-01,
0.00000E+00, -0.34600E-03,   13.200
  4,   4.0640     ,  0.25400     ,  0.00000E+00,  0.12987     ,  0.00000E+00,
0.00000E+00,   52.889    ,  0.00000E+00
  4,   4.1696     ,  0.25207     ,  0.00000E+00,  0.22292     , -0.65704E-02,
0.00000E+00,   52.791    ,  0.60001
  4,   4.3325     ,  0.24604     ,  0.00000E+00,  0.32098     , -0.13370E-01,
0.00000E+00,   52.633    ,   1.2000
  4,   4.5559     ,  0.23638     ,  0.00000E+00,  0.42431     , -0.18463E-01,
0.00000E+00,   52.404    ,   1.8000
  4,   4.8425     ,  0.22431     ,  0.00000E+00,  0.53180     , -0.21479E-01,
0.00000E+00,   52.099    ,   2.4000
  4,   5.1946     ,  0.21091     ,  0.00000E+00,  0.64213     , -0.22977E-01,
0.00000E+00,   51.714    ,   3.0000
  4,   5.6134     ,  0.19686     ,  0.00000E+00,  0.75424     , -0.23844E-01,
0.00000E+00,   51.250    ,   3.6000
  4,   6.1001     ,  0.18213     ,  0.00000E+00,  0.86877     , -0.25583E-01,
0.00000E+00,   50.699    ,   4.2000
  4,   6.6577     ,  0.16538     ,  0.00000E+00,  0.99294     , -0.31405E-01,
0.00000E+00,   50.013    ,   4.8000
  4,   7.2992     ,  0.14221     ,  0.00000E+00,    1.1572     , -0.48412E-01,
0.00000E+00,   48.963    ,   5.4000
  4,   8.0707     ,  0.10542     ,  0.00000E+00,    1.4401     , -0.71751E-01,
0.00000E+00,   46.776    ,   6.0000
  4,   9.0336     ,  0.65111E-01,  0.00000E+00,    1.7359     , -0.58047E-01,
0.00000E+00,   43.994    ,   6.6000
  4,   10.107     ,  0.33074E-01,  0.00000E+00,    1.8206     , -0.51301E-01,
0.00000E+00,   43.103    ,   7.2000
  4,   11.213     ,  0.20958E-02,  0.00000E+00,    1.8901     , -0.52520E-01,
0.00000E+00,   42.341    ,   7.8000
  4,   12.495     , -0.27947E-01,  0.00000E+00,    2.5089     , -0.46064E-01,
0.00000E+00,   34.277    ,   8.4000
  4,   14.526     , -0.40298E-01,  0.00000E+00,    4.7231     , -0.48983E-02,
0.00000E+00,  -13.193    ,   9.0000
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  4,   18.017     , -0.52700E-01,  0.00000E+00,    6.4720      , -0.35612E-01,
0.00000E+00,  -71.236     ,    9.6000
  4,   21.987     , -0.77273E-01,  0.00000E+00,    6.6807      , -0.43604E-01,
0.00000E+00,  -79.374     ,    10.200
  4,   25.983     , -0.10626     ,  0.00000E+00,    6.3999      , -0.62782E-01,
0.00000E+00,  -68.494     ,    10.800
  4,   29.432     , -0.14273     ,  0.00000E+00,    5.1102      , -0.59811E-01,
0.00000E+00,  -24.486     ,    11.400
  4,   32.160     , -0.16423     ,  0.00000E+00,    4.2284      ,  0.18576E-01,
0.00000E+00, -0.63725E-01,    12.000
  4,   34.696     , -0.15191     ,  0.00000E+00,    4.2259      ,  0.20741E-01,
0.00000E+00, -0.50452E-03,    12.600
  4,   37.231     , -0.13946     ,  0.00000E+00,    4.2259      ,  0.20742E-01,
0.00000E+00, -0.34583E-03,    13.200
  5,   4.0640     ,  0.12700     ,  0.00000E+00,  0.12987      ,  0.00000E+00,
0.00000E+00,   52.884     ,  0.00000E+00
  5,   4.1702     ,  0.12624     ,  0.00000E+00,  0.22451      , -0.26508E-02,
0.00000E+00,   52.785     ,  0.60000
  5,   4.3341     ,  0.12372     ,  0.00000E+00,  0.32260      , -0.57267E-02,
0.00000E+00,   52.626     ,    1.2000
  5,   4.5583     ,  0.11948     ,  0.00000E+00,  0.42531      , -0.82354E-02,
0.00000E+00,   52.398     ,    1.8000
  5,   4.8453     ,  0.11403     ,  0.00000E+00,  0.53230      , -0.97765E-02,
0.00000E+00,   52.094     ,    2.4000
  5,   5.1976     ,  0.10791     ,  0.00000E+00,  0.64239      , -0.10548E-01,
0.00000E+00,   51.710     ,    3.0000
  5,   5.6166     ,  0.10144     ,  0.00000E+00,  0.75452      , -0.11001E-01,
0.00000E+00,   51.246     ,    3.6000
  5,   6.1036     ,  0.94619E-01,  0.00000E+00,  0.86939      , -0.11920E-01,
0.00000E+00,   50.693     ,    4.2000
  5,   6.6618     ,  0.86718E-01,  0.00000E+00,  0.99454      , -0.15019E-01,
0.00000E+00,   50.002     ,    4.8000
  5,   7.3048     ,  0.75401E-01,  0.00000E+00,    1.1608      , -0.24083E-01,
0.00000E+00,   48.939     ,    5.4000
  5,   8.0789     ,  0.56878E-01,  0.00000E+00,    1.4447      , -0.36265E-01,
0.00000E+00,   46.744     ,    6.0000
  5,   9.0438     ,  0.36702E-01,  0.00000E+00,    1.7377      , -0.28561E-01,
0.00000E+00,   43.980     ,    6.6000
  5,   10.118     ,  0.21146E-01,  0.00000E+00,    1.8214      , -0.24714E-01,
0.00000E+00,   43.099     ,    7.2000
  5,   11.225     ,  0.61171E-02,  0.00000E+00,    1.8926      , -0.26126E-01,
0.00000E+00,   42.320     ,    7.8000
  5,   12.511     , -0.98607E-02,  0.00000E+00,    2.5188      , -0.25781E-01,
0.00000E+00,   34.131     ,    8.4000
  5,   14.556     , -0.19108E-01,  0.00000E+00,    4.7538      , -0.92542E-02,
0.00000E+00,  -14.064     ,    9.0000
  5,   18.057     , -0.29492E-01,  0.00000E+00,    6.4776      , -0.25166E-01,
0.00000E+00,  -71.458     ,    9.6000
  5,   22.028     , -0.46377E-01,  0.00000E+00,    6.6809      , -0.29648E-01,
0.00000E+00,  -79.392     ,    10.200
  5,   26.022     , -0.67194E-01,  0.00000E+00,    6.3859      , -0.50577E-01,
0.00000E+00,  -67.969     ,    10.800
  5,   29.463     , -0.96786E-01,  0.00000E+00,    5.0970      , -0.48686E-01,
0.00000E+00,  -24.094     ,    11.400
```

```
  5,   32.187    , -0.11573    ,  0.00000E+00,   4.2278     ,  0.57043E-02,
0.00000E+00, -0.64808E-01,   12.000
  5,   34.722    , -0.11154    ,  0.00000E+00,   4.2251     ,  0.71131E-02,
0.00000E+00, -0.50111E-03,   12.600
  5,   37.257    , -0.10727    ,  0.00000E+00,   4.2251     ,  0.71136E-02,
0.00000E+00, -0.34550E-03,   13.200
  6,   4.0640    ,  0.00000E+00,  0.00000E+00,  0.12987     ,  0.00000E+00,
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0.00000E+00,   52.783    ,  0.60000
  6,   4.3347    ,  0.00000E+00,  0.00000E+00,  0.32321     ,  0.00000E+00,
0.00000E+00,   52.623    ,   1.2000
  6,   4.5591    ,  0.00000E+00,  0.00000E+00,  0.42573     ,  0.00000E+00,
0.00000E+00,   52.396    ,   1.8000
  6,   4.8464    ,  0.00000E+00,  0.00000E+00,  0.53254     ,  0.00000E+00,
0.00000E+00,   52.092    ,   2.4000
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  6,   6.1049    ,  0.00000E+00,  0.00000E+00,  0.86972     ,  0.00000E+00,
0.00000E+00,   50.691    ,   4.2000
  6,   6.6635    ,  0.00000E+00,  0.00000E+00,  0.99536     ,  0.00000E+00,
0.00000E+00,   49.997    ,   4.8000
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0.00000E+00,   43.976    ,   6.6000
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0.00000E+00,   43.097    ,   7.2000
  6,   11.230    ,  0.00000E+00,  0.00000E+00,   1.8939     ,  0.00000E+00,
0.00000E+00,   42.310    ,   7.8000
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0.00000E+00,  -23.919    ,   11.400
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0.00000E+00, -0.69439E-01,   12.000
  6,   34.735    ,  0.00000E+00,  0.00000E+00,   4.2254     ,  0.00000E+00,
0.00000E+00, -0.50004E-03,   12.600
  6,   37.270    ,  0.00000E+00,  0.00000E+00,   4.2254     ,  0.00000E+00,
0.00000E+00, -0.34535E-03,   13.200
```

APPENDIX B

MS SPECTRA--DEVELOPMENTAL PHASES

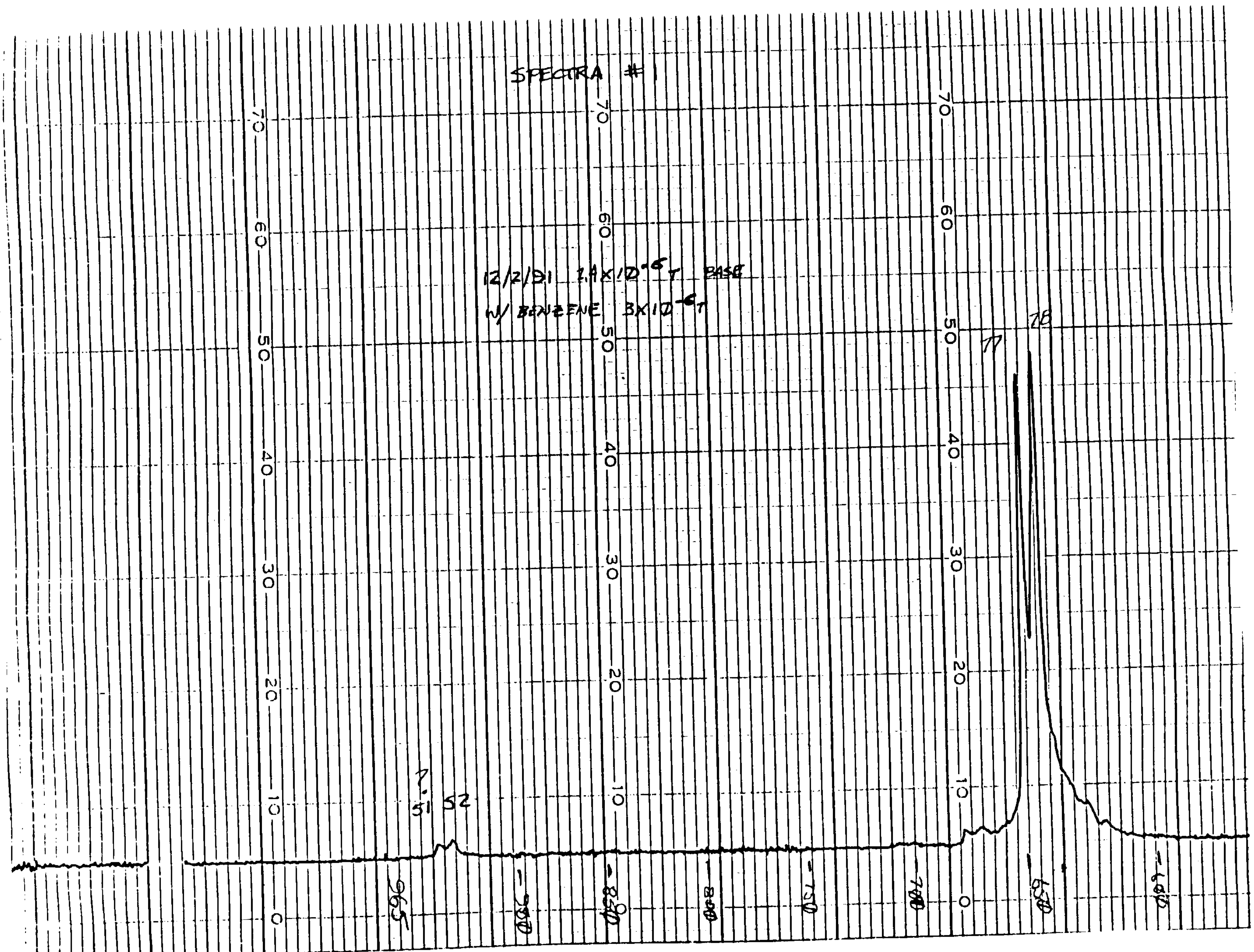
The process of developing the system involved many configurations and in the course of this work the spectra taken with the instrument passed through many stages. Some of the steps along the development path can be illustrated with the output traces that were collected and analyzed. The following pages show selected MS outputs as examples and are provide for information purposes only.

Spectra 1 shows a typical sweep of benzene. Peaks at 51,52 and 77,78 can be seen. The bottom scale is acceleration voltage of the source. The spectra included in this section were taken with different magnetic sector strengths, so some of the peaks may not match others, i.e., the m.v. constant varies over the included spectra.

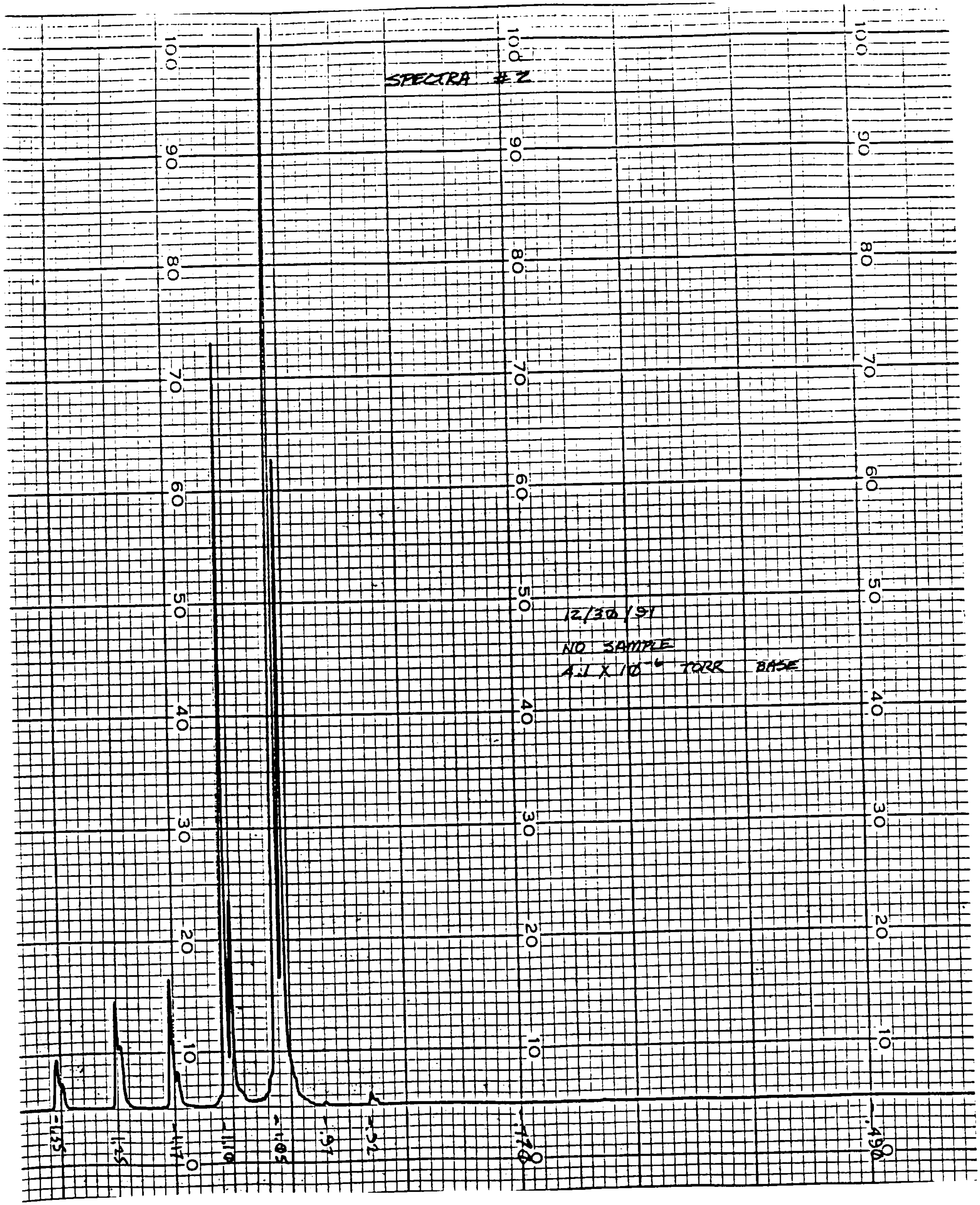
Spectra 2 shows a background scan and Spectra 3 shows the addition of TCE (trichloroelthylene). Note that the peak heights do not match the standard data. This is due to a high mass peak intensity reduction; one of our main goals was to increase high mass so that this effect would be less of a problem for quantitative measurements. These spectra are but a sampling of scan data taken, but are representative of the data in general.

The following pages are a brief guide to system setup and operation of the MS/MS prototype unit.

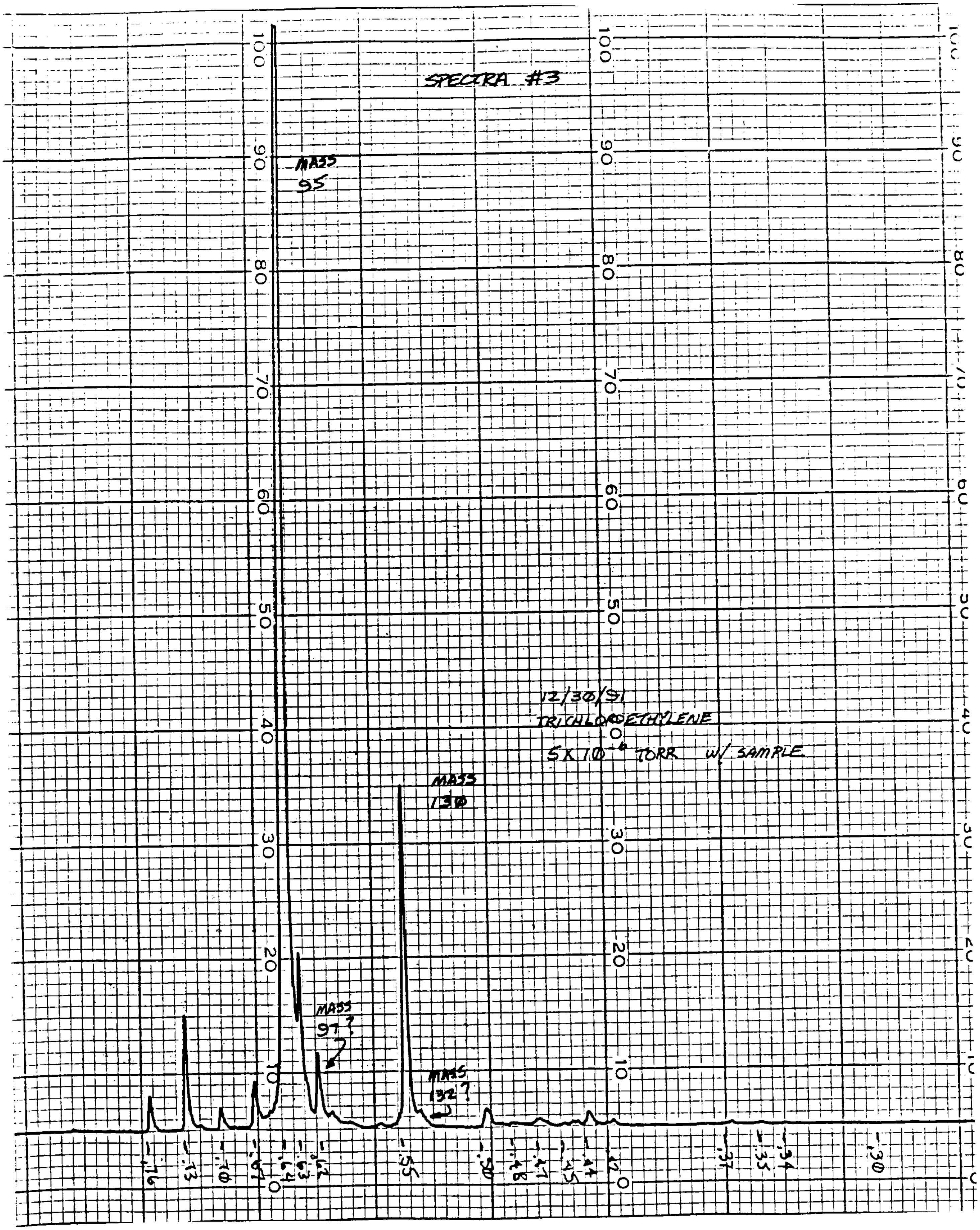
Tuning the MS/MS can be quite difficult; patience is required. Keep in mind that if hard copies of data (spectra) are needed, a strip chart recorder connected to the electrometer output makes a good data acquisition system. As the power supply scans (H.V. capacitor discharges), the power advances and captures peaks (if any) over time. In fact, that is how the majority of these spectra were taken. Although a computer did compile some data, this system was very experimental.


SPECTRA #1
12/2/91 1.4X10-6T BASE
W/ BENZENE 3X10-6T
77
78
51 52
965
900
850
800
750
700
650
600

Spectra 1



Spectra 2


SPECTRA #3
MASS 95
12/30/91
TRICHLOROETHYLENE
5 X 10^{-6} TORR w/ SAMPLE
MASS 130
MASS 97?
MASS 132?
-.76
-.73
-.70
-.67
-.64
-.63
-.62
-.55
-.50
-.48
-.47
-.45
-.44
-.42
-.37
-.35
-.34
-.30

Spectra 3

Test Stand Initial Setup

1. Uncrate cabinet, do not tilt, handle with care!

2. Upon arrival, the unit should be under at least 10^{-5} Torr vacuum. If not, check the system over for resulting damage.

   NOTE: No damage should occur, but the system will take approximately 1 week to evacuate to a usable state.

3. Connect a forepump, such as a Sargent-Welch 1405 or similar pump, to the foreline hose noted on inside of cabinet. <u>Use an oil filter to prevent back-streaming of pump oil</u>. If you do not, damage to unit will occur!

4. Obtain a multi-plug outlet strip for plugging in the various systems. The outlet strip should be rated for at least 10 amps and 120 VAC.

5. The vent valve should only be used when shipping the unit or back filling with argon during maintenance of the chamber (source).

6. An ion gauge controller, such as an HP 59822B, should be used to monitor high vacuum.

7. A thermocouple gauge on the forepump line should also be connected, although it is not absolutely necessary if the forepump is known to be in good condition and you are familiar with high vacuum procedures.

8. Continue to Test Stand Operation.

Test Stand Operation
(Refer to Figure B-1 for Operation)

1. While holding main flange and top firmly against their respective o-rings, turn on forepump and open roughing valve.

   NOTE: It will be necessary to have more than one person to accomplish Step #1. In addition, the main and top flanges may need very firm pressure to allow a rough vacuum to take place.

2. When rough vacuum is $<10^{-2}$ Torr, start turbopump, close rough valve.

3. Plug in turbo cooling fan.

4. Wait till vacuum is $<10^{-6}$ to operate system (approximately 2 days).

5. When vacuum is approximately 5×10^{-6} Torr, plug in source power supply, plug in detector power supply.

6. Turn on source power supply.

7. Rotate filament current variac slowly until current reads approximately 1.8 amps and filament emission reads approximately 1 mA (100 mA x 10). Do not operate filament (or H.V.) if vacuum is above 5×10^{-5} Torr!

8. Rotate scan voltage variac slowly until accelerating voltage reads approximately 1 kV (check voltage with an H.V. probe and meter to get a true reading).

9. Hook up an electrometer (such as a Keithley 616) to Detector #1 and monitor detector. Scale should be approximately 10^{-8} amps.

   If no ions are present at or near 1 kV (O_2), then the system needs adjustment, go to the next section, Adjustments/Finding Ion Beams.

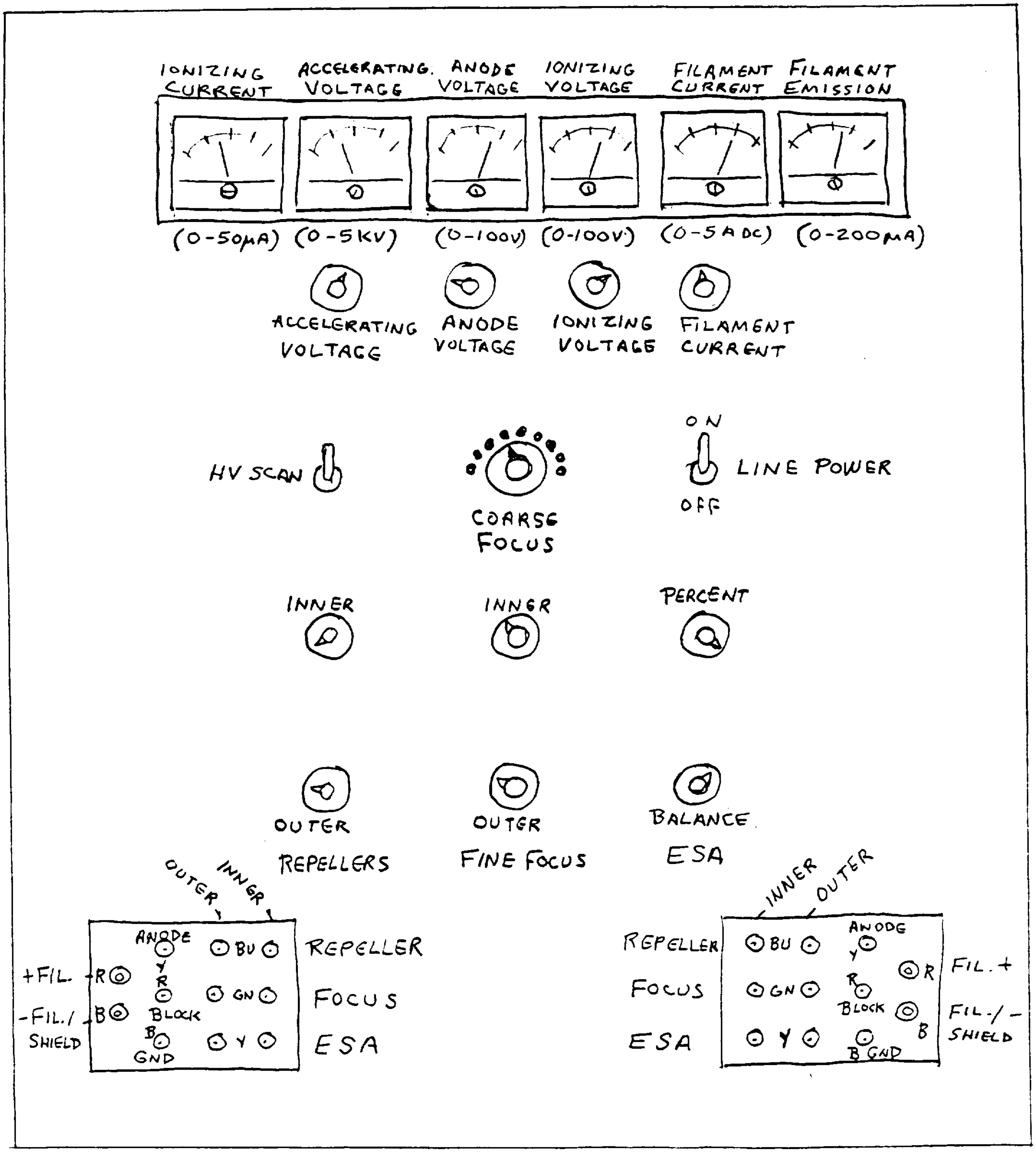
10. Vary the focus, repeller, scan, ESA balance, ESA percentage, filament bias, anode voltage, and saddle lens to get the highest detector current possible for mass 32 (O_2).

    NOTE: It may also be necessary to adjust magnet position. Do it carefully; it is a touchy adjustment.

    Figure B-2 shows a typical voltage setup (reference only).

11. Adjust the scan voltage to approximately 780 volts and observe the detector. Slow scans from 820 to 770 volts should produce an argon and/or a CO_2 peak, as in Figure B-3.

    NOTE: Argon may not always be seen if large amounts of H_2O and CO_2 are being sampled into the system.



MASS SPECTROMETER BENCH TESTING
POWER SUPPLY

1-90

Figure B-1

MEASUREMENTS OF E.B. MASS SPEC P.S.

THE NUMBER OF DATA SHEETS TO FOLLOW IS 2

NAME ARON BACS

DATE 12/30/91

*MEASURED AT 2.ØØ4 KILOVOLTS

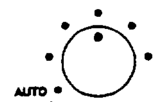
READ FROM METERS ON FRONT PANEL

REF	NAME	ACTUAL	NOMINAL
10	IONIZING CURRENT	2 uA	
11	ACCELERATING VOLTAGE	2.15 KV	
12	ANODE VOLTAGE	8ØV	
13	IONIZING VOLTAGE	64V	
14	FILAMENT CURRENT	1.8 A	
15	FILAMENT EMISSION	65Ø uA	

MEASURED FROM METER WITH H.V. PROBE

REF	NAME	ACTUAL	NOMINAL
1	ESA INNER (−)	−.145 kV	
2	ESA OUTER (+)	+.148 KV	
3	FOCUS OUTER	1.14Ø KV	
4	FOCUS INNER	1.118 KV	
5	BLOCK	2.11 KV	
6	REPELLER	2.11 KV	
	SADDLE	1.8Ø KV	
	COLLIMATOR	−.Ø7 KV	
* +	FILAMENT (+)	2.Ø4 KV	
−	FILAMENT (−) / SHIELD	2.Ø4 KV	

ELECTROMETER SCALE



$1Ø^{-8}$ AMPS

RECORDER DATA

CHART SPEED
4Ø SEC/DIV

CHART SCALE
2.Ø VOLTS/DIV

VACUUM DATA
6.Ø X10^{-6} TORR

COMMENTS

* FILAMENT USED AS REF.

Figure B-2

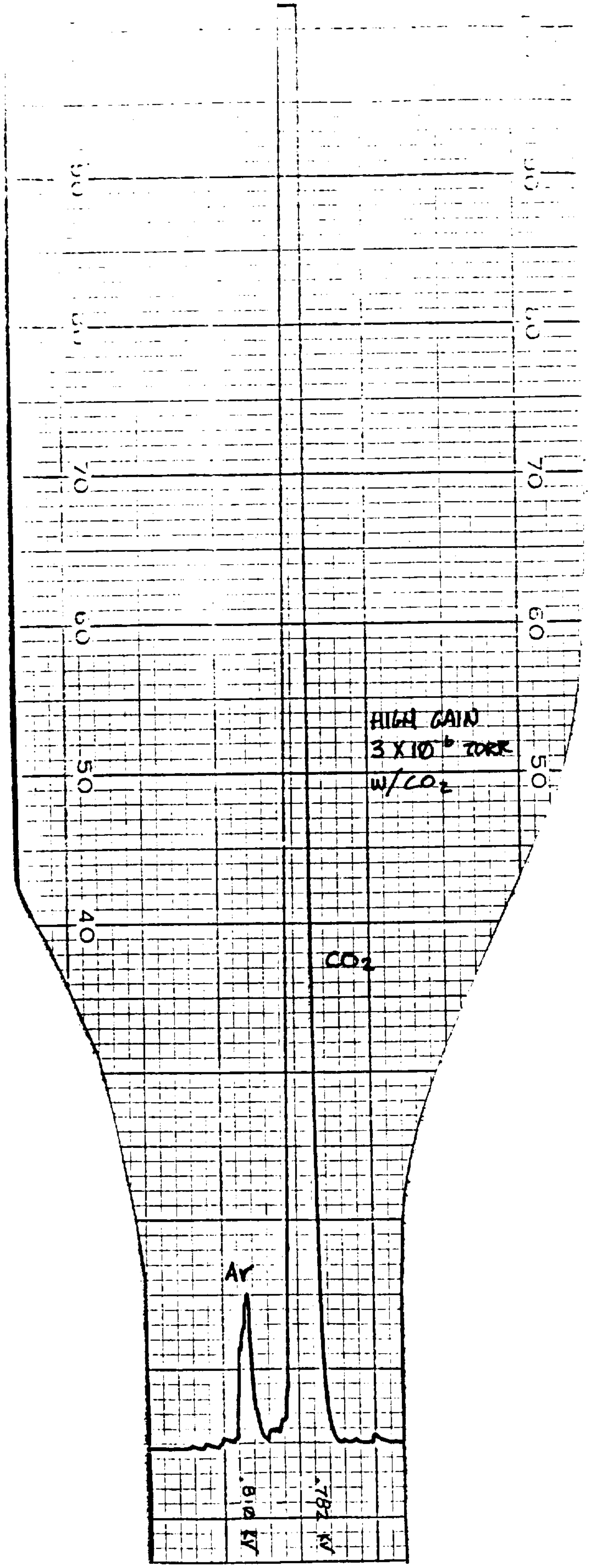


Figure B-3

12. Keep adjusting the scan supply to maximize Detector #1's signal.

13. Connect a power supply to E-sector #2 and make sure polarities are correct for the E-sector +V outer, -V inner. The power supply should be well regulated and adjustable betwen 150 to 800 VDC and have dual polarity about ground potential. For example, as V+ varies from 150V to 800V, V- varies from -150 to -800V.

    NOTE: Detector #2 must first be installed when proceeding past Step 13.

    Also, connect a power supply to the focus lens of E-sector #2. It must be able to adjust from approximately 0V to -1kV.

14. Observe Detector #2 with an electrometer. As you adjust the surface plate into the ion beam (in front of Detector #1), you should see an increase of background noise on Detector #2. E-sector #2 voltages should be approximately 250V, -250V and E-sector focus lens should be approximately -500V.

15. As the E-sector #2 voltages are varied from 150 to 800V, the secondary (or daughter) spectrum should appear at Detector #2. As of 3/15/92, only a level shift at approximately 650 volts on E-sector #2 was seen. More work on lensing should probably help the resolution of E-sector #2.

16. Turn off all voltages, adjust filament current slowly to 0, and turn off scan supply until further operation is needed.

Adjustments/Finding Ion Beams

1. If no signal is seen at Detector #1, make sure surface plate is not blocking Detector #1.

2. Monitor the beta (or intermediate) slit for ion current with an electrometer.

   As you adjust the various lenses for maximum signal, you should observe, by adjusting the ESA percent, a double or triple peaking of the signal on the beta slit. Figure 4 shows a typical triple peak and where you should adjust the ESA percent.

3. If you still cannot get a signal on either Detector #1 or the beta slit, you must check all connections to the source or disassemble the vacuum system and check for shorted or open connections from the ion source, E-sectors, detectors, etc.

4. Return to Step #10 and continue.

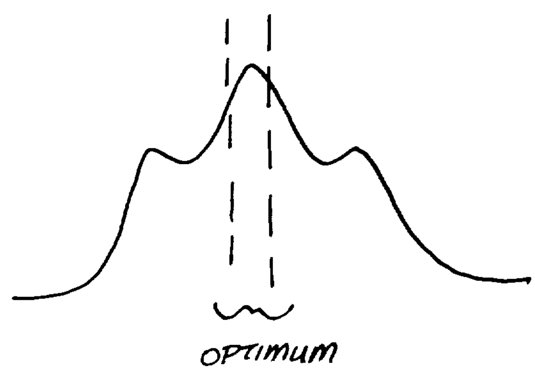


Figure B-4