https://ntrs.nasa.gov/search.jsp?R=19680002401 2018-07-24T04:21:18+00:00Z

A COMPUTER OPERATED MASS SPECTROMETER SYSTEM

Walter E. Reynolds
James C. Bridges
Timothy B. Coburn
Robert B. Tucker

Technical Report No. IRL-1062

November 1, 1967

Prepared under:

National Aeronautics and Space Administration
Grant NsG 81
National Institutes of Health
Grant FR 00151
Air Force Office of Scientific Research
Contract AF 49(638)-1599

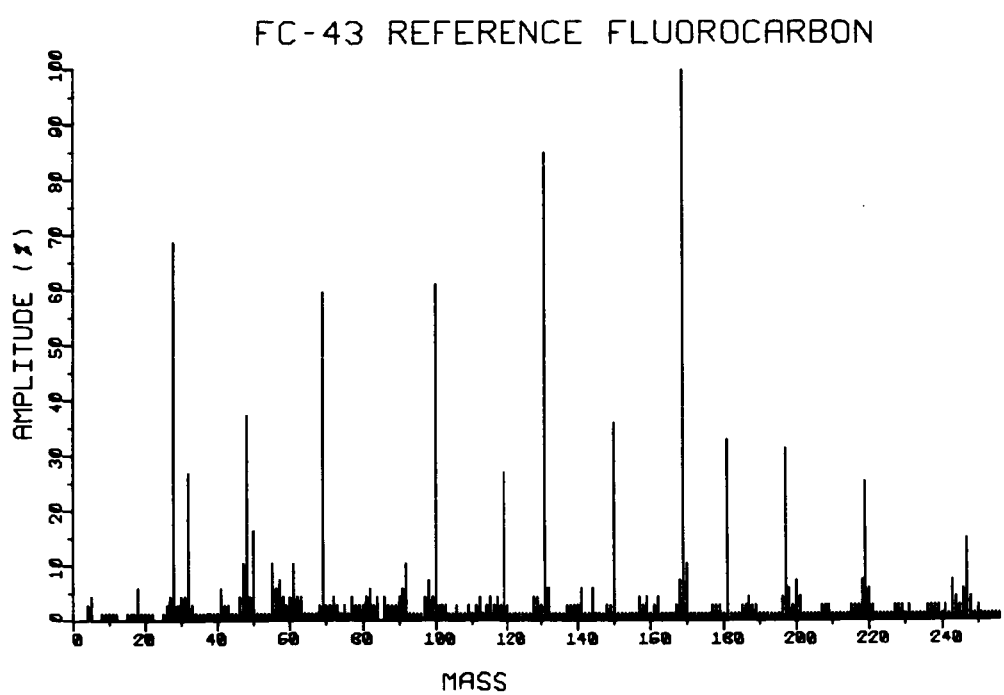
Principal Investigator: J. Lederberg

Director, Instrumentation Research Laboratory: E. Levinthal

Instrumentation Research Laboratory, Department of Genetics
Stanford University School of Medicine
Palo Alto, California

ABSTRACT

A mass spectrometer-computer system has been devised to utilize the decision-making capabilities of the modern digital computer. The system described assists the researcher user by allowing a computer to query the researcher for operating parameters. The computer translates these into detailed control functions that operate the instrument. The data acquired from the mass spectrometer is made available to the researcher in an on-line system. The system employs a small digital computer and an integer resolution quadrupole mass spectrometer. A reference gas is valved into the mass spectrometer by computer control to permit automatic calibration. Spectra processing of GLC effluent was demonstrated; the means and results are given.



CONTENTS

		Page
I.	Introduction	1
II.	Theory of Operation	5
III.	Overall Physical Description	7
IV.	The Software Structure	12
V.	Description of the Interface Electronics	15
VI.	The Software and Its Concepts	19
	A. Calibration	21
	B. Data Acquisition	23
	C. Data Manipulation	23
	D. Data Presentation	24
VII.	An Example of User-Computer Dialogue	28
VIII.	Conclusion	40
References		41
Appendix		42

ILLUSTRATIONS

Figure		Page
1	A block diagram of the computerized mass spectrometer system	8
2	The inlet system to the quadrupole mass spectrometer	9
3	Block diagram of the electronics of the IRL interface between the LINC computer and the EAI quadrupole mass spectrometer	16
4	Systems flow chart	20
5	Partitioning and flow of a routine under SPECTRUM	27
6-10	Data presentation by a Calcomp plotter	37-39
A1	The IRL interface with a local Model 33 Teletype and a 103A Data Set	43
A2	Data flow between the SEND and RECEIVE stations	44
A3	The IRL hardware modification which removes an incoming parity bit from a coded character	45
A4	Timing diagram of parity delete circuit	45

TABLES

Table		Page
1	A list of programs in SPECTRUM	13
2	Logic Outline of DISPLAY	14

I. Introduction

The use of a mass spectrometer as a research tool has been hampered by the slow development of fast and convenient methods of reducing the output to numerical data. The output (time versus intensity) is related to the mass spectrum (mass/charge versus intensity) by the characteristics of the scanning circuit and the nature of the mass analyzer (or discriminator). The theoretical relationship is marred, however, by the practical difficulties of construction and the drifts and instabilities which occur in operation. Therefore, it is difficult to establish a unique relationship between the settings of the operating controls and the output of the mass spectrometer.

A common method of mass-peak identification is to add a reference compound to the unknown sample. Then the oscillograph recording contains mass markers, corresponding to the known peaks of the reference compound. The operator counts up or down from the mass markers to identify the peaks of the unknown sample. The output of a mass spectrometer, particularly when it is used in conjunction with a gas chromatograph, provides the researcher with more information than he can process with this approach.

Several people have conceived and demonstrated systems which monitor and record digital data from a mass spectrometer at rapid (1-10 sec.) scan rates. (See references 1, 2, 3 and 4.) The usable scan rate is sometimes limited by the particular mass spectrometer used. In high resolution spectrometry, it may be limited by the sample time required to determine the mean time of arrival at the collector of

a statistically small number of ions. All of the systems described in the references deliver their data to a modern digital computer (some in real time) for processing. The system described in this report is one of many efforts to enhance the potential of the mass spectrometer through its use with a digital computer.

Our system employed the EAI QUAD 300 Quadrupole Mass Spectrometer and a LINC* computer (9). (An excellent description of the principle of the quadrupole appears in reference (5), pages 34-38.) The QUAD 300 provides integer mass resolution from mass 10 to mass 500.

There are two distinctive features of our system. One is the high level of operator involvement, making him an important system element. Through a standard Model 33 Teletype, the operator engages the computer in a conversational dialogue in which the computer requests input and/or output parameters and some branching decisions in the software algorithms. The dialogue also allows the operator to initiate output, via a Calcomp 565 digital plotter, and exercise some control over its manner of presentation. (The software is detailed later in this report.)

The human operator and the small computer perform together as a larger computer might perform alone. However, the task of programming the larger computer would be more complex. One would like to reduce the duties of the operator to merely pushing a few buttons. A push-

---

* The LINC computer in our laboratory is a small instrument computer (2K memory with built-in tape unit), designed and built as a research project at Washington University. It is very similar to the LINC 8 manufactured by the Digital Equipment Corporation (146 Main Street, Maynard, Massachusetts), and the Micro-Linc put out by Spear, Inc. (335 Bear Hill Road, Waltham, Massachusetts).

button system which would do as much as the system described in this report is beyond our present capability.

The second distinctive feature of our system is its method of mass-peak identification. Under the guidance of the operator, the computer valves in a reference compound which it uses to calibrate the scan circuit by relating the time versus intensity output to the known mass peaks of the reference. Subsequently, the control voltage which the computer interface feeds to the scan circuit is related to a mass index stored in the computer memory. This allows the output of the mass spectrometer with an unknown sample to be recorded directly as mass/charge versus intensity. In the other referenced systems, the computer receives the data of the unknown sample as time versus intensity and then converts to mass/charge versus intensity.

The spectra which are reproduced in this report show 256 as the highest recorded mass. The primary reason for this limit is the simplicity of programming effort which it afforded. Two hundred and fifty six words corresponds to one "quarter" of the LINC core memory. A quarter of LINC core may be read from or written on LINC tape with a single machine instruction.

In this system, a QUAD 300 Mass Spectrometer was used to monitor and identify the output of a Varian gas chromatograph. In a typical experiment, amino acids were coupled with an optically active reagent to give diastereoisomers resolvable by gas chromatography. The mass spectrometer was then used to identify and determine the optical purity of the stereoisomers (6,7). In a second application (8), amino acid

mixtures were derivatised to give compounds separable by gas chromatography. The QUAD 300 was then used to confirm the structure of the derivatives and to identify the volatile by-products of the reaction.

II. Theory of Operation

During spectrum data acquisition, the computer directs the mass analyzer to a program-selected mass position and reads the output intensity of the mass spectrometer. The mass analyzer is not swept in the conventional sense. It is controlled by a voltage (V) such that

$$m/e = f(V)$$

where m/e is the mass/charge ratio and f(V) is a monotonic function characterized by the mass spectrometer. V is the output of a computer directed digital-to-analog converter. For every M (M = m/e) to be passed by the mass analyzer, the computer identifies (according to the calibration program) a digital number N. Calibration programs assist the operator in determining the empirical relationship between N and M.

The procedure to measure the intensity at any M is as follows:

(1) The number N_i which corresponds to the selected mass/charge ratio (M_i) is loaded from the computer into the digital-to-analog converter. This sets the control voltage of the mass analyzer. The output of the mass spectrometer is proportional to the quantity of M_i present in the sample.

(2) An analog circuit, reset and released by the computer, integrates the output of the mass spectrometer. The output of the integrator is sent to an analog-to-digital converter in the input circuitry of the computer.

(3) Several milliseconds after the integrator is released, (the choice of integration time is supplied by the user upon program request), the computer samples the output of the converter. That digital value is stored as the intensity of M_i.

Steps (1) through (3) are repeated to acquire a complete spectrum.

The fundamental restraint upon this system is the drift of the mass spectrometer following calibration. Our experience with the QUAD 300 is that this drift causes an error in N of less than 1/8 the value from one N entry to the next in a one hour period. This is sufficiently small to allow unambiguous mass identification.

III. Overall Physical Description

The system elements referred to or mentioned in this section are explained in detail in the following sections.

Figure 1 is a block diagram of the system. The ground floor connections of the teletype and Calcomp to the LINC have been used for several years in other applications. (See Technical Report IRL-1055) They are duplicated near the site of the mass spectrometer research activity for the convenience of the principal users of the system. Except for sample injection, all input and output are through the teletype keyboard and Calcomp plotter.

The LINC computer was made available to the IRL under an NIH grant. Designed primarily for instrumentation, the LINC provides hardware inputs and outputs to several buffered registers, as well as pulse outputs and input level-sense lines. It has a 2K core memory and a built-in tape unit. "Tape Read" and "Tape Write" functions are single machine instructions.

The cable connecting the two terminal boxes contains:

(1) Twelve lines to carry the twelve bits of the LINC accumulator.

(2) A pulse line, OPR 10, to transfer the accumulator contents into a register which controls the mass position on the quadrupole.

(3) OPR 11, which clocks the contents of the accumulator into a register that controls the mass sweep, reference gas inlet, integrator reset and integrator release.

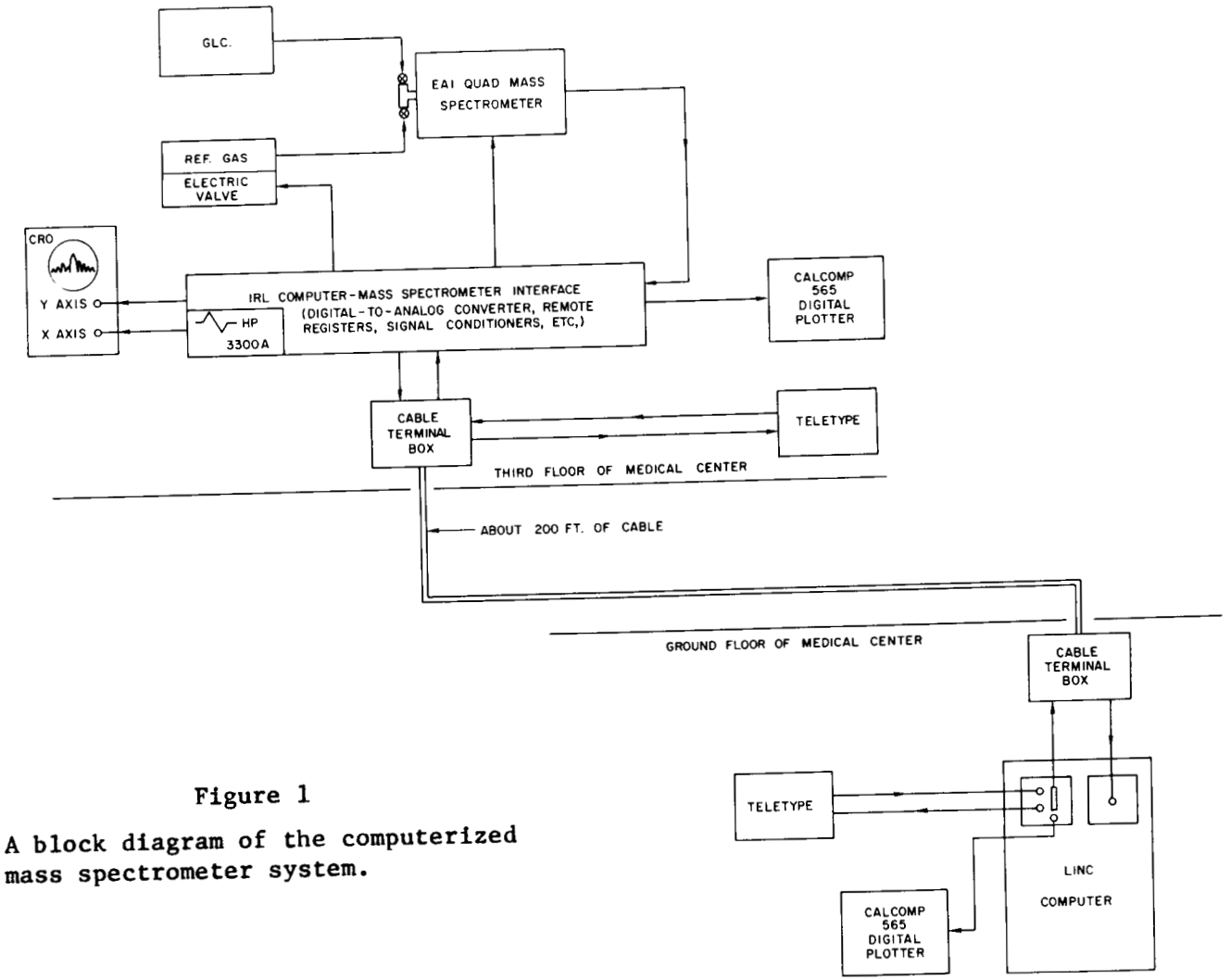


Figure 1

A block diagram of the computerized mass spectrometer system.

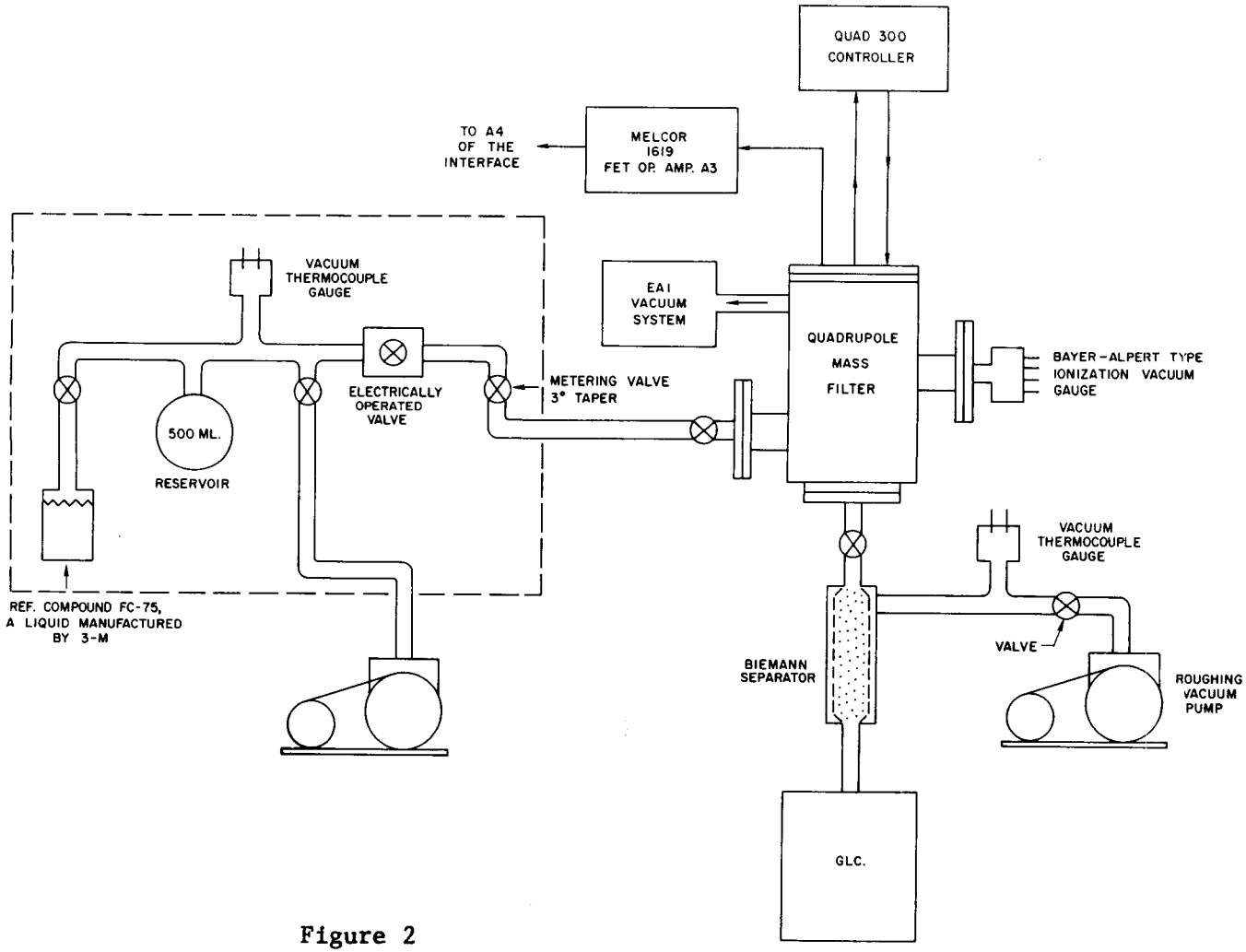


Figure 2

The inlet system to the quadrupole mass spectrometer. The portion of the diagram enclosed in dotted lines was constructed by the Instrumentation Research Laboratory.

(4) A pulse line, OPR 0, to control the Calcomp.

(5) A coaxial line to carry analog spectrum information to the LINC.

(6) Teletype communication lines.

(7) A signal line which carries the instruction to terminate data acquisition.

The inlets for the quadrupole are diagrammed in Figure 2. The gas chromatograph effluent is fed through a Biemann separator and enricher into the ionization chamber of the quadrupole. A roughing pump is used for the separator. The gas chromatograph also feeds a conventional flame detector whose output goes to a strip chart recorder. The recording is used only to monitor the run. For data processing, the equivalent output is reconstructed from the summation (total ion count) of mass spectra.

The second inlet to the ionizer is the vapor from a reference compound, stored in a 500 milliliter flask at 0.5 - 1 Torr. The pressure in the flask is maintained by manually operating the valves from the liquid reservoir or roughing pump. The flow of the reference gas into the mass spectrometer is enabled by a solenoid-actuated valve which is turned on or off by the computer.

The interface built by the Instrumentation Research Laboratory includes the digital register, digital-to-analog converter, and other electronics necessary for the computer to control all of the third floor equipment. It accepts computer commands to control mass position, inlet

of the reference gas, the teletype and the Calcomp plotter. In addition, it provides a suitable signal for displaying the mass spectrum on an oscilloscope. The interface has some manual controls for servicing.

IV. The Software Structure

The objectives of the software are to (1) operate the controls of a mass spectrometer, (2) acquire data from the mass spectrometer, and (3) to process and present that data in a manner useful to the researcher. The approach was to isolate the researcher (as much as possible) from the apparatus in order that he might spend most of his time and effort on sample analysis.

The software for this system is titled "SPECTRUM". SPECTRUM is a central pivot for a collection of several programs. Its sole function is to allow the user to call an operational program. The operational programs are listed -- along with a brief description of what each does -- in the SPECTRUM User's Guide, Table 1.

A program is called by typing its name on the teletype keyboard. The operator then gives instructions to the computer (via the teletype) to control the mass spectrometer, acquire data or present the data. Each program requests at least one decision from the user which will affect its course of action. Most of the programs also request input and/or output parameters. As an example, a flow diagram of the program called DISPLAY is given in Table 2.

Table 1

A List of Programs in SPECTRUM

(1) LOCATE: Creates a new "N table". Octal numbers are accepted as "N" entries. The user must give the corresponding mass (m/e) value as M. When two pairs have been accepted, LOCATE computes the 254 other values by straight line interpolation. This "N file" is filed under a name of the user's choice.

(2) DISPLAY: Allows visual spectra presentation. Loads an N file from tape, accepts either M or N as input, and positions the mass spectrometer gate accordingly. It also causes an auxiliary sweep about this mass position to cause a display upon an oscilloscope.

(3) MEASURE: Types amplitude values at or about a mass peak. Loads an N file from tape, accepts M or N, measures the amplitude for time T, and types out. In multiple mode the amplitudes of the 8 or so N values on either side of the specified N value are also measured.

(4) TYPE: Allows inspection of various numeric files. Requests N file, reference file, or spectrum identification and types the contents from entry 1 to 256 by increments of 1, or any arbitrary variation of these three parameters.

(5) GAS: Informs user of reference gas status, accepts on or off change if desired.

(6) TWEAK: Adjusts an N file made by LOCATE, or previous TWEAKS, by accepting a set of number pairs consisting of mass and the adjustment (error) at that mass; linear interpolation is used between the mass numbers entered.

(7) TAKE ONE: Takes a spectrum (only one), sampling for time T in milliseconds at each mass number as specified by an N file. Resulting spectrum is stored in a file from 0 to 256.

(8) GOGO: Takes up to 256 spectra in succession over a period of up to 20 to 40 minutes, depending on the time spent integrating at each mass; each of the spectra is stored on tape starting in file 1.

(9) SUM: Sums the individual spectra produced by GOGO, stores the result, a summation per entry, in file 0. The appearance of minus values in a spectrum indicate an End-of-File block. The resulting sums are roughly equivalent to the point values of a gas chromatograph curve as a function of time.

(10) SORT: Searches the spectra produced by GOGO, picking up a specified mass x. The resulting series of values represents the variation of mass x with time. Five separate mass numbers may be selected per SORT.

(11) PLOT: Plots any or all of the files of spectra in either a bar graph or line plot. The plots are scaled so that the maximum value in the files selected equal 100%. All other values are correspondingly smaller.

(12) ?: Indicates that the user is confused. A list of all programs available under SPECTRUM is typed out.

(13) WIPE: Indicates that the user is despondent. The computer, acting without hesitation, wipes out all software relating to the mass spectrometer. The tape will retain timing and block marks so that it may be used for other purposes.

Table 2

Logic Outline of DISPLAY

Step		Description
A.	Type < DISPLAY>	(Note: < ...> indicates a message typed out by the computer.) Turn on display sweep relay. Go to step B.
B.	Type < FILE NAME = >.	Then accept responses: a. ↑,Disable display sweep relay and return to SPECTRUM. b. 'less than four characters';, go to C. c. 'four or more characters';, then 1. if known file identifier, go to D. 2. if unknown file identifier, go to C.
C.	Type < IMPROPER ENTRY> and return to B.	
D.	Known file identifier. Read the indicated N file into core. Go to E.	
E.	Type < M OR N?>	Accept the following responses: a. ↑, go to B. b. M;, note M state is true and go to F. c. N;, note M state is false and go to G. d. anything else, go to E.
F.	Type < M=>	Accept: a. ↑, go to E. b. A decimal number within the range of 1 to 256. Look up the corresponding entry in the N table. Consider this the "N value". Go to H. c. Anything else, go to F.
G.	Type < N=>	Accept: a. ↑, go to E. b. An octal number within the range of 0 to 7777. Consider this the "N value". Go to H. c. Anything else, go to G.
H.	Type the N value as < N= 'N value'> in octal notation. Also put this N value in the external register for D-A conversion. If M state is true, then go to F, else go to G.	

V. Description of the Interface Electronics

A block diagram of the interface electronics appears in Figure 3. Most of the circuitry is housed in a short relay rack, occupying about 18 inches of vertical space. An additional 10 inches of rack space is used for the power supplies (+10 volts, ±15 volts and 3.6 volts for the integrated logic) and a precision reference voltage for the digital-to-analog converter.

The logic is a mixture of "A" series circuit cards manufactured by the Digital Equipment Corporation and low cost, epoxy, Fairchild integrated circuits. The 12 bit digital-to-analog converter was constructed of DEC cards. The Amelco 2110 BE FET was used for the electronic switches. The operational amplifiers were manufactured by Melcor; most are of the economy line.

The LINC has a "fantail cage" designed to hold custom electronics. The following input/output circuits were installed:

(1) A set of gates enabled by Relay Register 3 (in the LINC). These transmit the contents of the accumulator to the remote interface. Relay Register 3 is turned on or off by a machine instruction.

(2) A set of drivers for the operate pulses. These are OPR 10, OPR 11 and OPR 0 (LINC outputs).

(3) A resistor through which the signal current is passed and converted to a voltage suitable for the LINC's analog-to-digital converter.

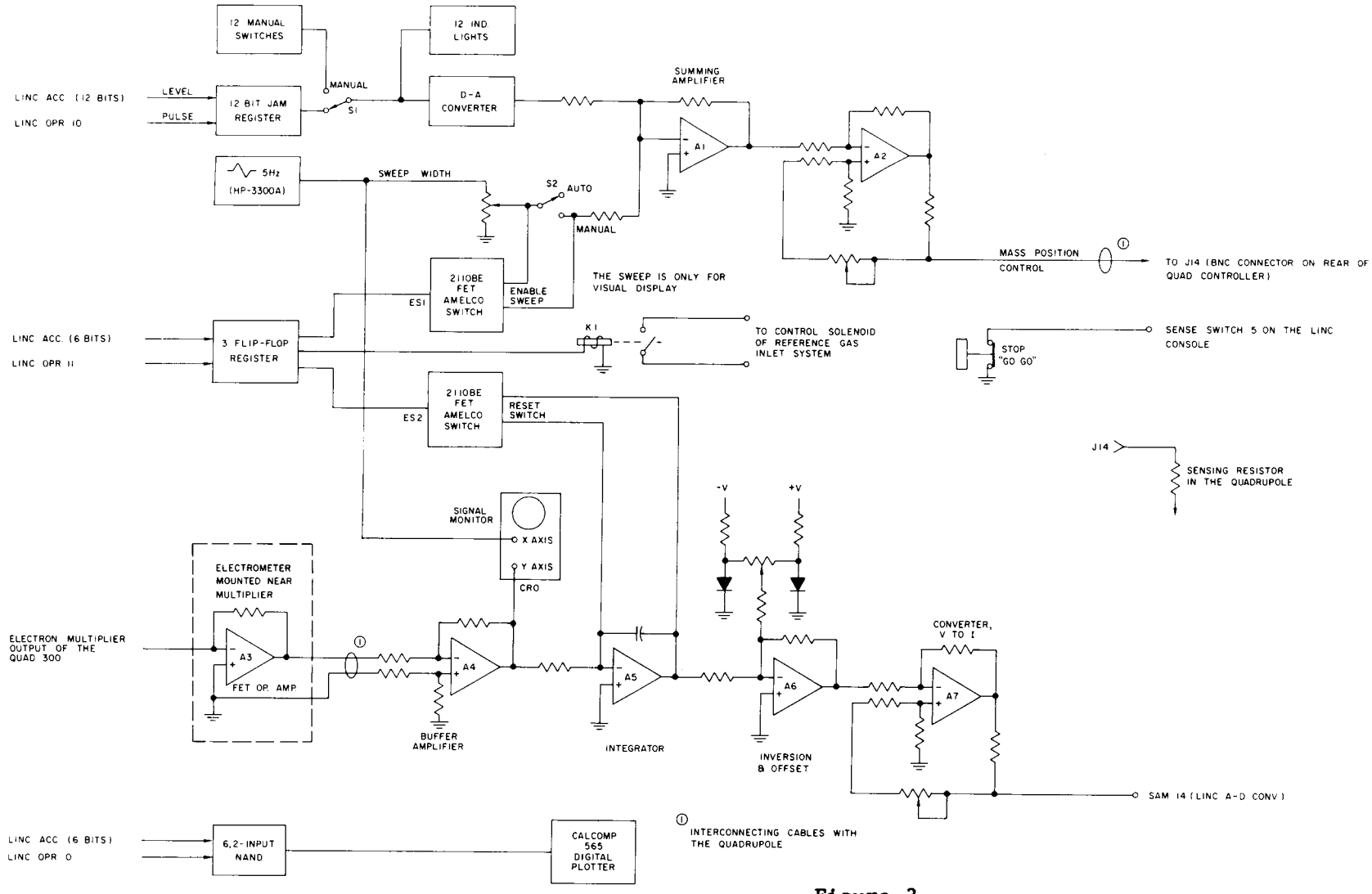


Figure 3

Block diagram of the electronics of the IRL interface between the LINC computer and the EAI quadrupole mass spectrometer.

OPR 10 clocks all 12 bits (N) of the accumulator into the jam register which feeds the digital-to-analog converter. The purpose of this jam loading is to minimize the transients caused by changing N values. If the switch S1 is in the manual position, the digital-to-analog converter is under the control of 12 manual switches mounted on the front panel of the relay rack. Above each switch is an indicator lamp. These lamps monitor the contents of the converter at all times.

OPR 11 clocks the 6 rightmost bits of the accumulator into a 3 bit jam register. The 3 bits of this register:

(1) Turn the visual display sweep of mass analyzer control voltage on or off;

(2) Permits or blocks the entrance of the reference gas into the mass spectrometer;

(3) Reset the analog integrator, A5.

OPR 0 transmits the Calcomp commands from the 6 rightmost bits of the accumulator.

The high impedance output of the digital-to-analog converter is buffered by amplifier A1. If the switch S2 is closed, either manually or by the Amelco FET, A1 sums the output of the digital-to-analog converter with the output of a triangular wave generator. This provides a visual display of the masses either side of the mass which is selected by the output of the d-to-a converter.

The ground plane in the QUAD 300 Controller was unavoidably a few millivolts different than the interface. Therefore, the output of A1 is

converted to a current (A2) before it is sent to the control circuit of the mass analyzer. Any ground loop ripple (60 Hz.) feeds the common mode of A2 and, therefore, is rejected.

The current from A2 is reconverted to a voltage by a sensing resistor installed in the quadrupole. This was the only internal modification made to the mass spectrometer.

A3 is an FET operational amplifier (Melcor 1619) which is used as an electrometer. It is mounted as close as possible to the electron multiplier output of the quadrupole. In the configuration shown, it has a bandpass exceeding 10 KHz. with 10 megohms feedback. The feedback resistor is selected to be 1, 10 or 100 megohms by a manual switch. The normal setting is at 10 megohms. A4 picks up the electrometer output at the relay rack in the differential mode, again to reject 60 Hz. ground plane ripple. A4 drives the vertical axis of a Tektronic 502 Oscilloscope and feeds an analog integrator (A5). A Hewlett-Packard 3300A Low Frequency Function Generator sweeps the horizontal axis of the 502 at about 5 Hz. The 3300A is also the source of the scan for the control voltage of the mass analyzer during visual presentation.

A5 integrates the output of A4 (across a 0.01 microfarad capacitor). Its output is converted to a current and sent over about 200 feet of cable to the LINC analog-to-digital converter.

A front panel push button, labeled "STOP GOGO", enables the operator to stop the data gathering program by that name at any time during its run.

VI. The Software and Its Concepts

The software for the computer-mass spectrometer system: (a) allows the user to acquire mass spectra of samples or a reference gas, and (b) provides information on the stability and precision of the instrument itself. The latter consideration stimulated the writing of software that might not be required for chemical application of the system but is useful in determining the reliability of the system and necessary to the development and maintenance of the instrumentation.

This mass spectrometer system utilizes the interaction, in real time, of the three major components. These components are: the computer, an instrument, and a human operator. It is apparent that the human operator is the slowest component, and in a sense the limiting factor in acquiring spectra. However, he has the greatest range of decision-making ability. This system takes advantage of this ability.

The computer-spectrometer system does not demand the contiguous location of all three components. As noted before, the computer was located three stories below the mass spectrometer. Most of the software could be operated from either location or indeed a third location. Though the mechanics of introducing the unknown chemical sample were not automated, the reference gas was valved into the instrument under computer control.

There exist two levels of communication between the operator and the control system. The first (SPECTRUM level) simply accepts any one of a set of eleven subprograms which then specifies the further operation

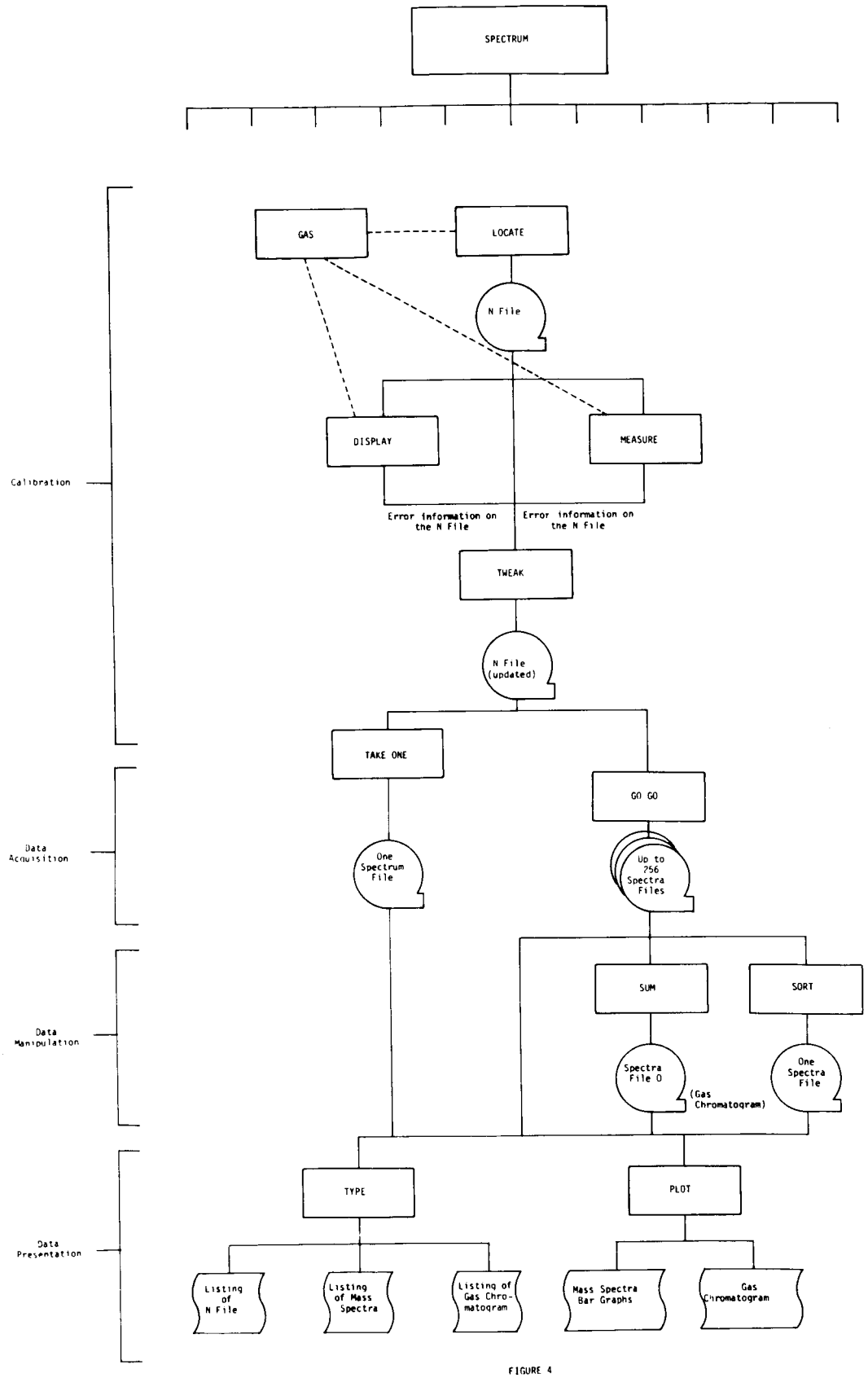


FIGURE 4

SYSTEMS FLOW CHART

of the system. Control is returned to this level upon the completion of any one of the subprograms.

Level two is that of the subprograms. It is within these subprograms that the necessary parameters are accepted for the performance of the individual tasks. These eleven subprograms can be considered in four groups according to the functions they are related to: Calibration, Data Acquisition, Data Manipulation, and Data Presentation. These four groups are indicated to the left of the systems flow chart shown in Figure 4. The figure illustrates the way the calibrate programs are used. The flow is under operator control; the lines indicate the normal paths. The result of the calibration is an accurate list of 256 numbers (an N file). These are related in a one-to-one fashion to mass numbers, so that when a number in the N file is gated into the D-A converter the resulting analog voltage allows the corresponding mass to pass through the mass analyzer. Thus a signal is available at the electrometer proportional to the abundance of that mass/charge ratio. The 256 elements in the N file correspond to mass/charge ratios 1-256.

A. Calibration

GAS allows the operator to turn on or off the reference gas. It is this reference gas that is used to develop and adjust the N file.

LOCATE creates a first approximation to an appropriate N file. It accepts two sets of coordinates each consisting of a mass number and its corresponding N value. By simple linear interpolation (and extrapolation) the remaining 254 elements in the N file are filled. The

N values corresponding to adjacent masses differ by about 15. This allows sufficient sensitivity in setting the mass analyzer to insure sensing the mass peak at its maximum rather than on the shoulders or sides.

DISPLAY provides a method for the operator to visually examine discrepancies between the N file entries created by LOCATE and the real position of the reference gas peaks. By entering a mass number, the corresponding point of the spectrum is displayed on the center of an oscilloscope. (The user can also display a point by entering any N value.) The surrounding portions of the spectrum are displayed under the control of a potentiometer. If the peak is not precisely in the center of the display, the N value calculated by LOCATE is not quite correct. The increment of error can be determined by typing in new N values until the display is correct, or by the MEASURE routine. Table 2 is a detailed flow diagram of the DISPLAY dialogue.

MEASURE samples and digitizes the electron multiplier output at a specified point or series of consecutive points. These amplitudes are typed out with their corresponding N values. The highest amplitude will indicate the center of the peak.

TWEAK accepts corrections to any N file. This may be a new file created by LOCATE or it may be one used previously that is in need of minor adjustments. These corrections can be entered for any or all of the reference gas peaks. The N file is then updated by the entered values at the designated points and by interpolation between the designated points.

Calibration of the system has been achieved using the four preceding programs in roughly fifteen minutes. An N file thus developed has been used with only minor modifications for a number of days. It appears to be as accurate as the resolving power of the mass spectrometer.

TAKE ONE provides a final check of the calibrating procedure. It uses the N file created by the operator to position the sensing gate at sequential mass positions from 1 to 256. The ion current is sampled and digitized for each position. The resulting spectrum can be plotted or typed; it should match the known reference gas spectrum.

B. Data Acquisition

GAS is used to turn off the reference gas used in the calibration procedure and provide a delay for the residual to be pumped off.

GOGO starts taking spectra at the operator's signal, continues taking spectra at intervals specified by the operator (5 second nominal), and stops on a signal from the operator or at the end of 256 spectra. Each spectrum consists of amplitude measurements at each mass value, 1-256. These spectra are stored on tape sequentially. No attempt was made to automate the starting or stopping of the data gathering, since the variability of the diffusion rate through the gas chromatograph for different substances made operator control desirable. The time scale of the operation, 10 to 25 minutes, was also appropriate for human interaction.

C. Data Manipulation

SUM adds up the amplitudes of each spectrum to produce a record

(a set of up to 256 values) of total ion current. This record is in fact a reconstructed gas chromatograph recording. It provides a quick check on the total ion peaks seen by the spectrometer and compares closely with output from the flame detector of the gas chromatograph. When the values are plotted, the scale on the horizontal axis constitutes an index to the tape locations of the individual spectra taken during the data gathering (see Fig. 6).

SORT searches through each stored spectrum picking out the amplitude at a specified mass position. The result may be plotted to show the variation of the ion current at a specific mass with time.

D. Data Presentation

PLOT is a special purpose plotting routine for displaying results as a line or bar graph. Any spectrum or the results of the SORT or SUM programs may be plotted (see Figs. 6 through 10).

TYPE is a general purpose listing routine. It lists as four digit integers any of the files or spectra produced by other programs.

This second level of communication between the operator and computer involves the entry of parameters for the specific programs. The parameters are requested individually by the program in a prompting fashion. This type of demand-response entry of parameters is very convenient from the user's point of view, although it is tedious to program. It allows a relatively inexperienced user to make use of the system without memorizing long sequences of instructions. We found that chemists with no previous computer experience could, and indeed would,

make use of the system without hesitation. Since the chemist is expected to play an integral part in the feedback system, the acceptance of his role is important. In the following section, an example of computer-operator dialogue is given.

The programming of instrument control is quite simple with the LINC computer. One instruction commands are available for the digital outputs (OPR n), and for the analog input (SAM n). Sensing the level of the digital input is a simple skip instruction (SXL n). Appropriate timing loops between these instructions are all that is required. This part of the software would require modifications for use with other systems, since it is designed specifically for the hardware involved.

Since the signal is converted to digital form by an 8 bit converter it is desirable to take full advantage of these 8 bits without saturating the converter. We achieved this by trial and error with each unknown sample. Appropriate manipulation of the integrating time by the computer could achieve the same result in a much more elegant manner.

More flexible control over the amplitude of the peaks could have been achieved by using the analog integrator in a different fashion. The amplitude of the signal seen at the computer varies with (a) the gain setting on the electrometer, (b) the amount of material injected into the spectrometer, and (c) the length of time the integration is continued. Since unknown samples can be of unknown concentration the amount of material injected is inherently variable. Altering the gain in a digital fashion would be difficult. The length of time for

integrating can be varied with great precision by examining the signal at frequent intervals.

At the instruction level of the computer, the programs consist of short mainline routines with an assortment of 50 or 60 subroutines. These subroutines vary in length from 10 instruction error checks to the 512 instruction arithmetic routines. The memory of the LINC is quite limited, 2048 twelve bit words, of which only 1024 words are programmable. The software was organized to allow extensive overlaying. The resident portion of the program requires 200 words of memory. The remaining 12,000 words of the system are read in from tape as needed. In order to improve the efficiency of the running system each of the subprograms is self-contained. This necessitated duplication of certain subroutines for each program, but allowed the majority of memory to be available when needed for high speed processes. Although this system required about 12,200 instructions on the LINC computer, it might well be duplicated in 8000 instructions on a computer where the subroutines (without duplication) could remain in core. An incentive to conserving the core memory used in this system was the desirability of extending the mass range to 500. This extension was not attempted with the quadrupole spectrometer, but the LINC memory would not have been a limiting factor.

The following diagram of Figure 5 illustrates both the partitioning and flow of a hypothetical routine under SPECTRUM. The program select table, teletype routines, and parameter table are resident in core. The number of partitions within programs vary from one to four; the program in the diagram has two partitions.

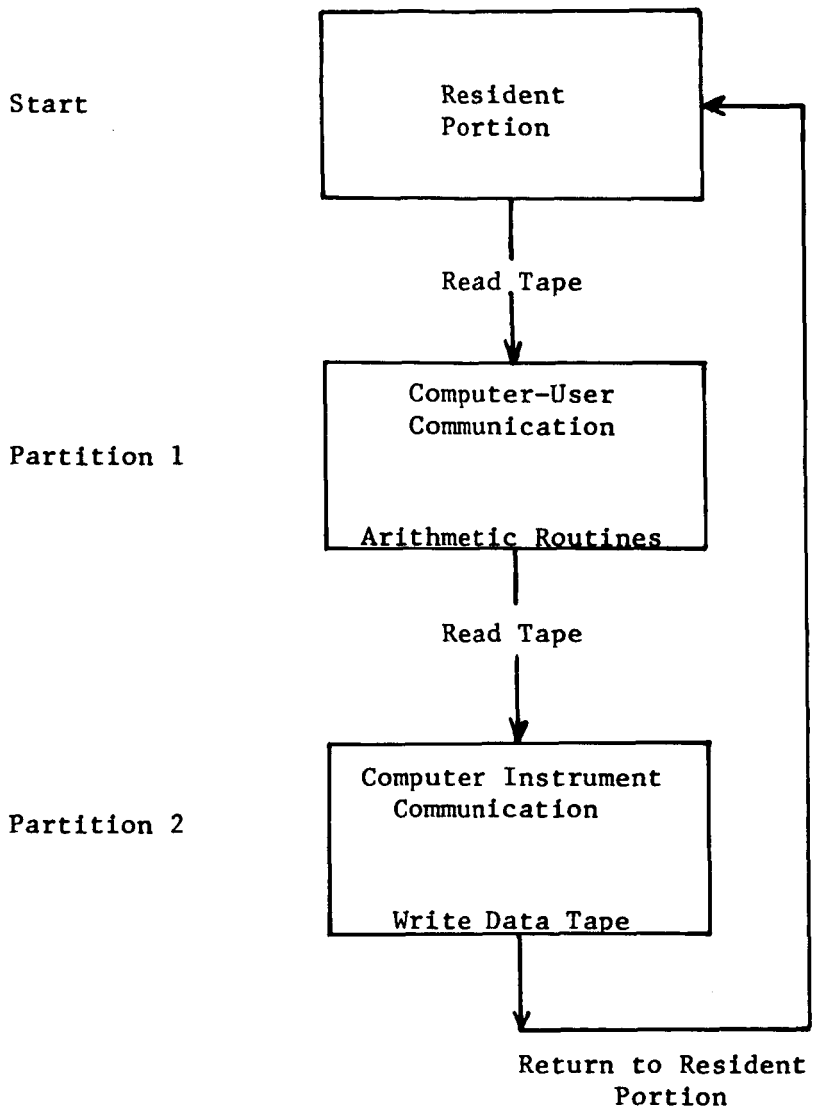


Figure 5

Partitioning and Flow of a Routine under SPECTRUM

VII. AN EXAMPLE OF USER-COMPUTER DIALOGUE

In this section a typical dialogue between the user and the computer system is reproduced. The example will probably give the reader a quicker feel for the flow of the communication. It is presumed that this is a "cold start"; there was no prior calibration. The example goes through the complete calibration phase and a data acquisition from a gas chromatograph run.

The teletype listing is reproduced on the left. Normally most lines have some output, but here lines are skipped to keep the comments in step with the teletype listing. The comments are on the right.

All computer output is left as it appeared. The user's typing is underscored for identification. One other user key used was the < rubout>. This leaves no character on the paper; the program simply ignores what was on that line and advances the paper and repeats. Where rubout was used, the legend "< rubout>" has been inserted.

Teletype Listing:	Comments:
SPECTRUM	"SPECTRUM" was typed by the computer. This indicates it is ready to execute any program stored in SPECTRUM.
GAS;	The program selected by the user is "GAS".
REFERENCE GAS IS OFF! DO YOU WANT IT ON ?YES; WAIT 15 SECS.	In this case the user indicates he wants the reference gas valved in. The computer gates it into the mass ionizer and instructs the user to wait for the gas pressure to stabilize in the analyzer source.
SPECTRUM LOCATE;	The next program the user calls is "LOCATE". LOCATE illustrates the method of initially establishing an "N Table". The computer must be given the known N value and m/e identification for two known masses. LOCATE also enables the display of the spectrum on the oscilloscope, centered about the last N which was entered.
LOCATE	
N= 1600;	The first guess is 1600. (This can also be done manually by switches.) This causes the spectrum to be displaved centered about 1600.
M=↑	Next the computer asks for "M", the m/e value. Apparently the operator is not ready to identify the peak, or the peak is not centered. Thus the operator answers with an upward arrow (↑).
N= 1610; M= ↑	This causes the program to ask the previous question, "N=".

	The operator guesses 1610 and then is satisfied with 1606.
N= 1606+	The entry 1606+ is rejected by the program as meaningless.
N= 1606;	It again asks for N.
M= 69;	Finally at N=1606 the operator is satisfied that this is the best value for m/e = 69; thus he answers 69 to the query M=.
N= 4000;	The guess and try method identifies 4572 as the position for mass 169.
M= ↑	
N= 5000;	
M= 4400; IMPROPER ENTRY	Mass 4400 is beyond the range of the mass spectrometer.
M= ↑	
N= 4400;	
M= ↑	
N= 4500;	
M= 4600; IMPROPER ENTRY	
M= ↑	
N= 4600;	
M= ↑	
N= 4560;	
M= ↑	
N= 4570;	
M= ↑	
N= 4573;	
M= 457↑	
N= 4572;	
M= 169;	After the second identified M, the program types the parameters for verification and asks for acceptance. If the user had indicated non-acceptance, the program would have backed up to the beginning and allowed the work to be redone.
N= 1606 M= 0069	
N= 4572 M= 0169	
ACCEPT? YES;	
	The program computes the other 254 N values from the relationship, N = k·m/e + b. k and b are computed from the two known points. This file of 256 values must be stored in a manner so that it may be called for use whenever desired. The program asks for a FILE NAME.
FILE NAME = REPORTS;	The user responds with "REPORTS".
	This N Table is now available under the identifier, "REPORTS".
SPECTRUM	The program returns the user to "SPECTRUM", level one.
DISPLAY;	The user now will call DISPLAY to verify, or determine the errors in N Table. DISPLAY only displays the spectrum on the oscilloscope. The display center is the N value output from the computer. The manual width control is typically set so that integer peaks have a separation of one centimeter. This is the user call.
DISPLAY	The computer responds. DISPLAY program is now active.
FILE NAME = REPORTS;	What file? User types "REPORTS", and the program loads that table.
M OR N?M;	Query. Does the user wish to direct by N entry or by M entry? (The computer looks up the N entry.) User answers that he wishes to direct by mass entry.
M= 69; N= 1606	He asks for mass 69. The program looks up the table, finds 1606 and outputs it to the mass spectrometer interface. It then types the N value for operator information.
M= 169; N= 4572	Same with 169. Note that these are the two points given in LOCATE.
M= 100; N= 2537	Now mass 100 is tried. Apparently the user is not too happy with this; the peak does not seem to be exactly centered.

M= ↑	So now upward arrow causes the program to back up a question.
M OR N?N;	The user indicates by "N" that he wishes to enter N numbers directly.
N= 2542; N= 2542 N= 2544; N= 2544 N= ↑ M OR N? NOTE 2544 GOOD AT MASS 100	In two more tries he finds that mass 100 is at N entry 2544. Backs up again, and this time writes himself a note about mass 100.
M OR N?M;	This is meaningless to the computer, so the program retypes "M OR N"?. This time the user answers M.
	Now let us recap what happened. The N entry at mass 100 is 5 off. (All N numbers are in octal.) The error is +5, since it is necessary to add it to the entry in the REPORTS N Table.
SS <rubout> SS↑	In typing this note, the user overran the buffer. The SS is meaningless. Doing a <rubout> does no good.
M OR N?↑ FILE NAME = ↑	The user can recover. The program responds to ↑ by going one level nearer to SPECTRUM.
SPECTRUM	Three upward arrows get the user clear back to SPECTRUM.
DISPLAY;	Now DISPLAY is called again. The program is reread from the tape. The user goes through the list of reference peaks, checking each one.
DISPLAY FILE NAME = REPORTS; M OR N?M;	
M= 100; N= 2537 M= 28; N= 0426 M= 47; N= 1067 M= 50; N= 1145 M= 69; N= 1606 M= 100; N= 2537 M= 119; N= 3200 M= 131; N= 3467 M= 150; N= 4130 M= 169; N= 4572	
M= 81 <rubout> M= 181; N= 5060 M= 197; N= 5444 M= 219; N= 6164 M= 231; N= 6452	Between 169 and 181 he makes a typing error, but notices it before typing a semicolon. A <rubout>, one of the teletype keys, cancels the line.
M= 247; N= 7036	Presumably the user has noted the position errors, if any, for each listed mass. These errors will be needed soon. The actual process, similar to that shown for mass 100, takes about an hour for a new setup. For day to day checking, it takes only about 10 to 20 minutes.
M= ↑ M OR N?↑ FILE NAME = ↑	Upward arrows bring the user back to SPECTRUM.
SPECTRUM	

```
MEASURE;
MEASURE
FILE NAME = REPORTS;
SINGLE? NOPE;
M= 181;
T= 25;
```

"MEASURE" may also be used to check the N Table.
Here it is called and the N Table "REPORTS" is requested.

Multiple readings are desired.
At mass 181.
Each reading is to be integrated for 25 milliseconds.

```
   N    AMP.

5031    0002
5050    0074
5051    0161
5052    0207
5053    0223
5054    0236
5055    0241
5056    0235
5057    0217
5060    0173
5061    0134
5062    0114
5063    0057
5064    0036
5065    0023
5066    0033
5067    0011
5070    0014
5107    0007
```

These are the results. For a span equal to about that between two integer mass positions, each N number is tried. Also two points, 1.5 mass divisions up and down, are included to give a good base reference. The results are typed as shown. Inspection here shows that mass 181 is actually centered about N=5055. This is in contrast with the N=5060 in the REPORTS table. Hence the error is -3.

```
M=↑
M OR N?↑
SINGLE? ↑
FILE NAME =↑
```

Again, upward arrows bring the user back to SPECTRUM.

```
SPECTRUM
TWEAK;
TWEAK
M= 28;
E= 112;
M= 47;
E= 32;
M= 50;
E= 15;
M= 100;
E= 5;
M= 119;
E= 10;
M= 131;
E= 7;
M= 150;
E= 3;
M= 169;
E= 0;
M= 181;
E= -3;
M= 197;
E= -7;
M= 219;
E= -15;
M= 231;
E= -17;
M= 247;
E= -24;
M= 2000;
```

The program TWEAK is now called to correct the N file.
The user types in pairs of numbers, masses and errors that he has determined at those masses.

Mass 100.
Error in the table of REPORTS for mass 100 is +5.

When the user has completed his list he signals that fact by typing 2000.

```
ERROR ENTRIES  COMPLETED
```

The program notes this and recypes the entries for verification.

```
   28 0112
   47 0032
   50 0015
  100 0005
  119 0010
  131 0007
  150 0003
  169 7777
  181 7772
  197 7770
  219 7762
  231 7760
  247 7753
ACCEPT? YES;
```

The program then gives the user a chance to accept or reject. Upon acceptance, the program prepares to use these points to make corrections to an N Table.

```
FILE NAME=REPORTS;
```

It asks what N table to correct. REPORTS is the answer.

```
CALIBRATION COMPLETE
```

Then the N table and the errors are merged to form a new corrected table. Mass positions between calibrated points are corrected by straight line interpolation of the error function.

The new corrected file must be put somewhere. This time the query "FILE NAME=" is for this purpose. The user responds with "SUPER". Apparently this file name has already been used.

```
FILE NAME=SUPER; OVERWRITE?GO AHEAD;
```

Reuse of this name causes whatever is in SUPER to be erased. The program will not do this unless expressly directed to. That is why it asks "OVERWRITE?". The answer is affirmative, so old SUPER is erased. Now the new file is in SUPER.

```
SPECTRUM
```

The program gives control back to SPECTRUM.

```
DISPLAY;
```

The user has recalled DISPLAY.

```
DISPLAY
FILE NAME = SUPER;
```

And the file SUPER.

```
M OR N?M;
M= 28;    N= 0540
M= 32;    N= 0622
```

He is investigating the behavior around masses 28 to 50.

```
M= 40;    N= 0770
M= 50;    N= 1162
M= 231;    N= 6433
M= 69;    N= 1617
M= ↑
M OR N?N;
N= 614;    N= 0614
N= 616;    N= 0616
N= 770;    N= 0770
N= 762;    N= 0762
N= 6
N= 764;    N= 0764
N= 765;    N= 0765
N= ↑
M OR N?↑
FILE NAME = ↑
```

He goes back to SPECTRUM. He apparently has noted more errors.

```
SPECTRUM
```

```
TWEAK;                          Calls TWEAK again.
TWEAK
M= 1;                           Note that he says no error at 1 and 28.  This will insure
E= 0;                           that no changes are made at those inclusive masses.
M= 28;
E= 0;
M= 32;                          He did note errors at 32 and 40.
E= -4;
M= 40;
E= -3;
M= 50;                          But 50 through 255 is pegged by specifying these errors
E= 0;                           to be zero.
M= 255;
E= 0;
M= 2000;
ERROR ENTRIES   COMPLETED

    1 7777
   28 7777
   32 7773                      And this is typed out for verification.  (The notation is
   40 7774                      octal, one's complement.)
   50 7777
  255 7777

ACCEPT? YES;
FILE NAME=SUPER;                The correction is made to SUPER.
CALIBRATION COMPLETE

FILE NAME=SUPER;OVERWRITE?YES;
                                The new table is filed under SUPER.  (The old one has
                                been erased.)

SPECTRUM
DISPLAY;                        Now DISPLAY is called for a final verification.

DISPLAY
FILE NAME = SUPER;
M OR N?M;
M= 28;    N= 0540
M= 32;    N= 0616
M= 50;    N= 1162               All seems well.
M= 40;    N= 0765
M= 131;    N= 3476
M= 219;    N= 6147
M= ↑
M OR N?↑                        Return to SPECTRUM.
FILE NAME = ↑

SPECTRUM

TAKE ONE;                       TAKE ONE will read each mass point from 1 to 256.  The time
                                for integration at each peak is remembered from the last
TAKE ONE                        time TAKE ONE was used.  To change this parameter, upward
FILE NAME = ↑                   arrow must be used here.  The time is set to 17 milliseconds
T= 17;                          per peak.
FILE NAME = SUPER;              The N Table to be used is SUPER.  Now the spectrum is
                                taken.
                                In about 3 seconds it is complete.
                                The user may elect to take another.

SPECTRUM FILED AT 1.            Since the reference gas has been left on all this time, the
REPEAT?  NO;                    plotted results of this would be similar to first illustra-
                                tion in this report.
```

SPECTRUM

GAS;	Now GAS is called.
REFERENCE GAS IS ON DO YOU WANT IT OFF YES PLEASE; WAIT 15 SECS.	It reports its condition. And the user requests that it be turned off.
SPECTRUM	After the due wait for the system to pump out, the program returns the user to SPECTRUM. The system is now fully calibrated.
GOGO; GOGO	GOGO is the program that will take a sequence of mass spectra during a gas chromatograph run.
FILE NAME=SUPER; MOUNT TAPE;	The N file must be specified. At this point the user may mount a new tape if he wishes to retain the data on magnetic tape.
MSEC PER PEAK=17;	And last the milliseconds per peak integration is specified. Actual data acquisition starts with the semi-colon after the "17". This continues for about 18 minutes. The program would have come to a normal halt at the end of about 21 minutes. However, the operator was watching a strip chart recording of the signal from the flame detector of the GLC. He noted that the last peak of interest has passed and pressed the terminal button.
SPECTRUM	Control is passed back to SPECTRUM.

SUM;
SUMMING TAKES TIME WAIT 5 OR 10

FILE# 0. #OF POINTS=0217	SUM is the program that adds up each individual spectrum. There were 217 spectra. The sum of each was put in file 0.

SPECTRUM

PLOT;	PLOT causes Calcomp plots of the results.
NAME: GLC OF NCS-AMINO ACID METHYL ESTER MIXTURE;	
FILE #S: 0;	This call of PLOT plots the result of SUM.
J TO K BY I.	
J= 1;	
K= 22;	This and the next entry are in error.
I= 240;	
X DIMEN.= ↑	Typist correcting his error.
I= ↑	
K= 240;	
I= 1;	The error is corrected.
X DIMEN.= 16;	The plot is to be 16 inches wide.
Y DIMEN.= 7;	And 7 inches high.
BAR GRAPH? NO;	Since this is a total ion plot, it is the equivalent of a GLC chart. The numbers on the x axis refer to the spectra. Since a spectrum was taken every 5 seconds, this axis is also a measure of time. Also, the plot is a good index to the spectrum of interest. The plot is shown in Figure 6.

```
SPECTRUM
PLOT;

NAME: NCS-ALANINE METHYL ESTER;
FILE #S: 16;
J TO K BY I.
J= 20;
K= 250;
I= 1;
X DIMEN.= 15;
Y DIMEN.= 6;
BAR GRAPH? YES;
```

This is the first plot of a mass spectrum of this group. As can be seen in Figure 6, file 16 indexes the first GLC peak. The operator, from his knowledge of the GLC plot, identifies and titles it. This is shown in Figure 7.

```
SPECTRUM
PLOT;

NAME: NCS-METHIONINE METHYL ESTER;
FILE #S: 156;
J TO K BY I.
J= 20;
K= 250;
I= 1;
X DIMEN.= 15;
Y DIMEN.= 6;
BAR GRAPH? YUSP;
```

This is another of the 217 spectra available. The program asks the user for certain items. First is the Name. This becomes the title of the plot. Then the range of interest (J to K). The size of the plot and if it is to be a bar or connected line plot. This "YUSP" was interpreted correctly as "YES". See Figure 8.

```
SPECTRUM
SORT;
```

SORT will go through the spectra and get the time history of the amplitude on any 5 mass peaks.

```
SORT SPECTRA FOR MASS #S:
MASS(1)= 159;
MASS(2)= 143;
MASS(3)= 145;
MASS(4)= 203;
MASS(5)= 205;
WAIT...
STORE IN FILES 0507, 0508, 0509, 0510, 0511.
```

In this case mass 159, 143, 145, 203 and 205 are requested.

```
SPECTRUM
PLOT;

NAME: MASS 145 (NCS-ALANINE METHYL ESTER);
FILE #S: 509;
J TO K BY I.
J= 1;
K= 240;
I= 1;
X DIMEN.= 16;
Y DIMEN.= 6;
BAR GRAPH? NOPE;
```

File 509 contains the time history of mass 145 (see above). This, as can be seen in Figure 7, appears to be the molecular peak of NCS-Alanine Methyl Ester. The connected line graph is shown in Figure 9.

```
SPECTRUM
PLOT;

NAME: MASS 203 (NCS-ASPARI <rubout>
```

The user corrected himself.

```
NAME: MASS 203 (NCS-ASPARTIC ACID DIMETHYL ESTER);
FILE #S: 510;
```

This is a similar plot of mass 203 shown in Figure 10.

```
J TO K BY I.
J= 1;
K= 240;
I= 1;
X DIMEN.= 16;
Y DIMEN.= 6;
BAR GRAPH? NOT NOW;
```

SPECTRUM

About 30 to 45 minutes have elapsed since the end of the GLC run. SUM took the longest time, about 12 minutes. The plots took about 4 to 5 minutes each.

All of this control, listing, and plotting took place in the laboratory right next to the mass spectrometer.

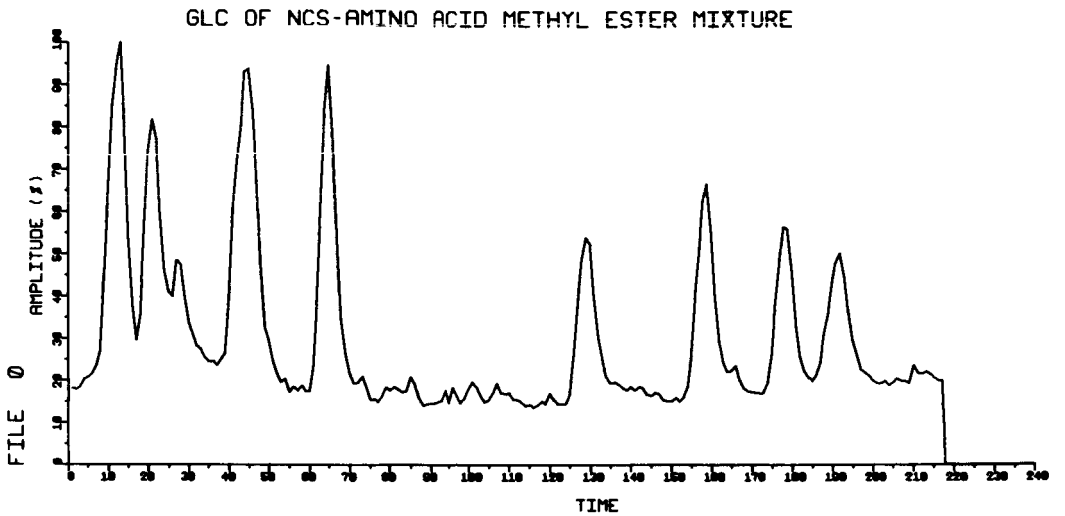


Figure 6

Each unit on the abscissa represents five seconds. There was one spectra taken during each such unit. The ordinate is the sum of all mass peaks or total ion current. Hence, this is an index to the mass spectra recorded and a GLC representation.

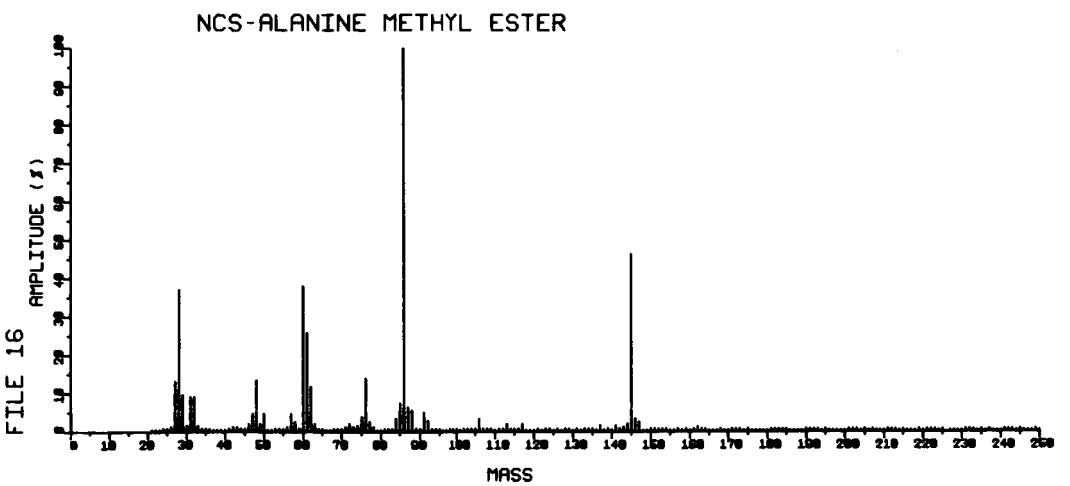


Figure 7

The spectra of the 16th time slot of Figure 6, the first GLC peak.

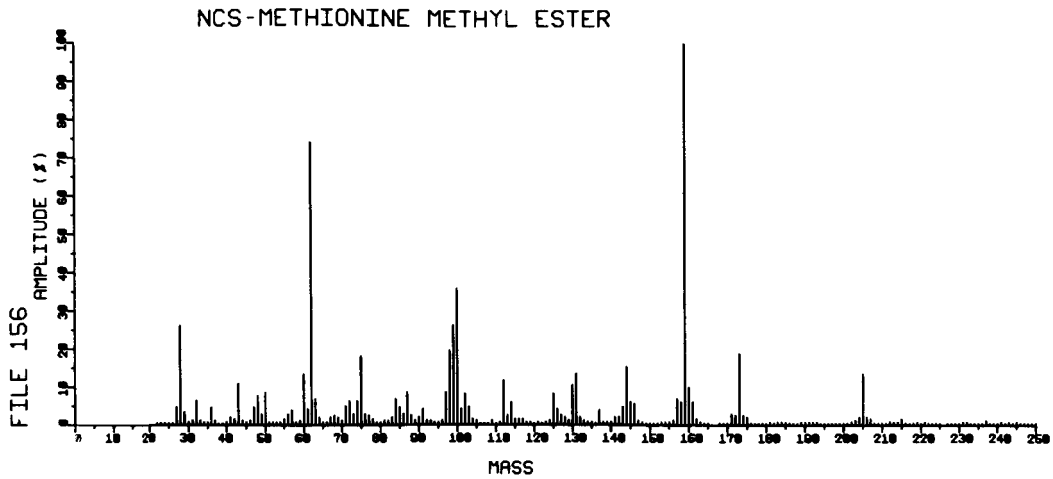


Figure 8

A spectrum from the third peak from the end. As can be expected from the longer retention times, this fraction has a higher molecular weight.

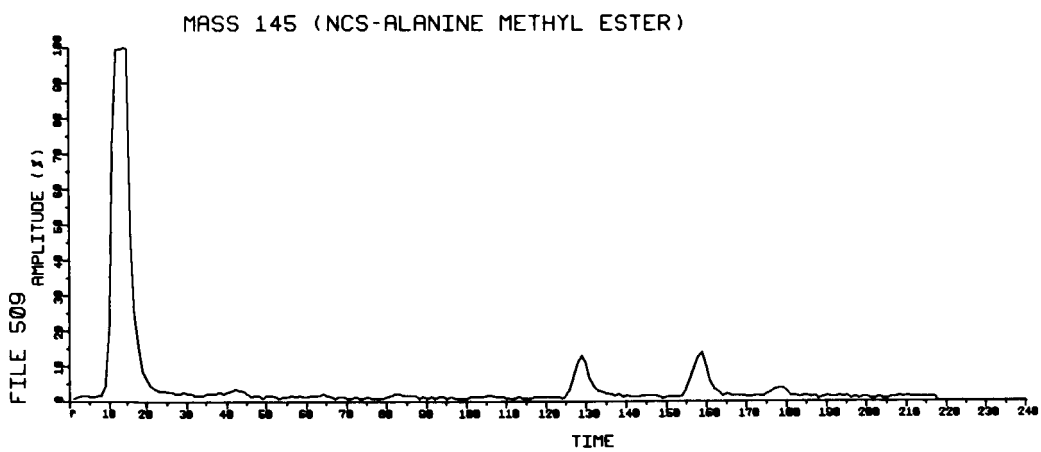


Figure 9

The occurrence of mass 145 versus time. The time scale is the same as Figure 6.

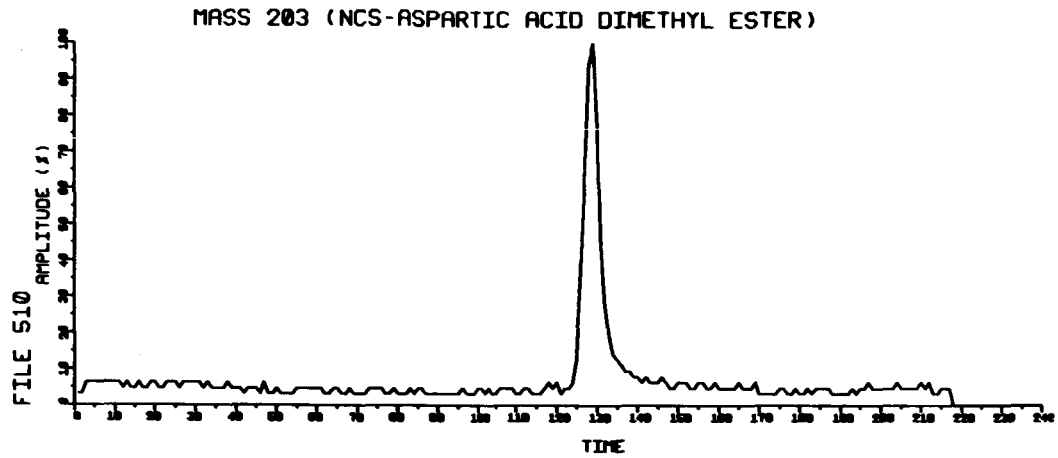


Figure 10

A time plot of mass 203.

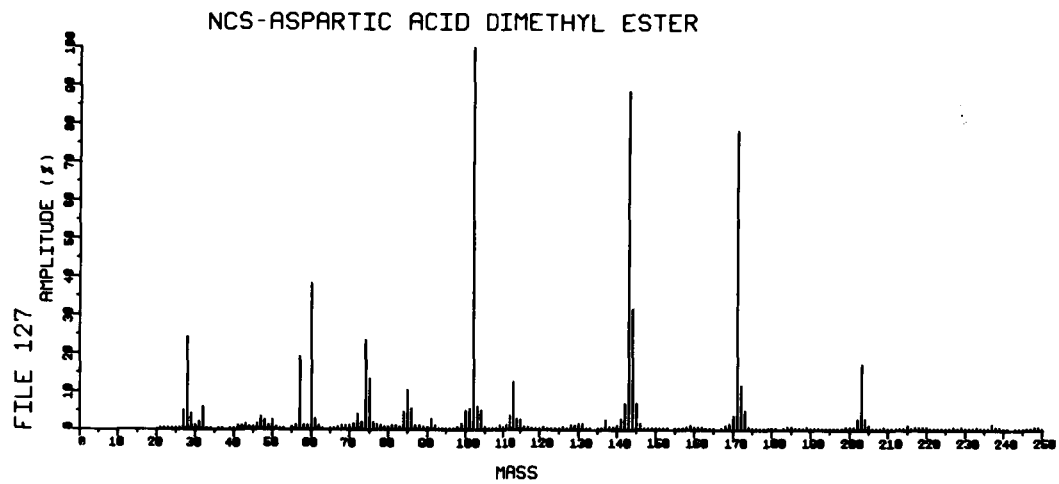


Figure 11

Another spectra indexed by Figure 6.

VIII. Conclusion

This system demonstrates the use of a computer in the operation of a mass spectrometer. By thoughtful programming techniques, a complex arrangement of hardware is made easily accessible to a user. The operator-computer dialogue is particularly useful in the processing and presentation of data. The software of the system significantly reduces the time required for sample analysis, releasing the researcher to explore the potential of the mass spectrometer..

The calibration of a mass spectrometer provides a reference for measuring the precision and stability of the instrument. Computer monitoring of the operating parameters of a mass spectrometer will provide data needed to improve these characteristics. We are working on ways to make the calibration more automatic, limited only by the time constants of the mass spectrometer. This would involve using a given N file to take a spectrum of the reference gas. The computer would then compare the spectrum data to a manually entered spectrum of the reference gas which would be filed on tape. After comparing the two, adjustments would be made to the N file. This would permit a calibration before every GLC run.

It is feasible to build a limited purpose computer and a quadrupole mass spectrometer as one unit, forming a compact instrument with features similar to the system presented in this report. Some of the software could be embodied in hardware circuits. Alternatively, the system could be interfaced with a larger time-shared computer. We expect to investigate this possibility.

References

(1) R. A. Hites and K. Biemann, "Computer Recording and Processing of Low Resolution Mass Spectra", International Mass Spectrometry Conference, Berlin, September 1967.

(2) R. A. Hites and K. Biemann, "A Computer-Compatible Digital Data Acquisition System for Fast-Scanning, Single-Focusing Mass Spectrometers", Anal. Chem., 39, 965, 1967.

(3) H. C. Bowen, D. J. Shields, and H. M. Stanier, "Experience with Fast Processing of High-Resolution Mass Spectra using Direct Transfer of Data to an On-Line Digital Computer Without Intermediate Recording", International Mass Spectrometry Conference, Berlin, September 1967.

(4) C. Merritt, Jr., P. Issenberg, and M. L. Bazinet, "Design and Performance of A Direct-Coupled, Real-Time, Spectrum Digitizer and a Rapid-Scanning, High-Resolution Mass Spectrometer", International Mass Spectrometry Conference, Berlin, September 1967.

(5) C. A. McDowell, Ed., Mass Spectrometry, McGraw-Hill, New York, 1963.

(6) B. Halpern, J. W. Westley, E. C. Levinthal, and J. Lederberg, "The Pasteur Probe: An Assay for Molecular Asymmetry", Life Sciences and Space Research IV, M. Florkin and A. Dollfus, Eds., p. 239-249, North-Holland, Amsterdam, 1967.

(7) B. Halpern, J. W. Westley, I. von Wredenhagen, and J. Lederberg, "Optical Resolution of DL Amino Acids by Gas Chromatography and Mass Spectrometry", Biochem. Biophys. Res. Comm., 20, 710, 1965.

(8) "Cytochemical Studies of Planetary Microorganisms - Explorations in Exobiology", Status Report Covering Period April 1, 1967 to October 1, 1967, IRL-1061, Instrumentation Research Laboratory, Genetics Department, Stanford University.

(9) "LINC - Programming and Use, 1", Vol. 16, Washington University, Computer Systems Laboratory, 724 South Euclid Avenue, St. Louis, Missouri.

(10) H. L. Friedman, H. W. Goldstein and G. A. Griffith, "Mass Spectrometric Thermal Analysis of Polymer Decomposition Products", Conference Proceedings of Fifteenth Annual Conference on Mass Spectrometry and Allied Topics, ASTM Committee E-14, Denver, Colorado, May 1967.

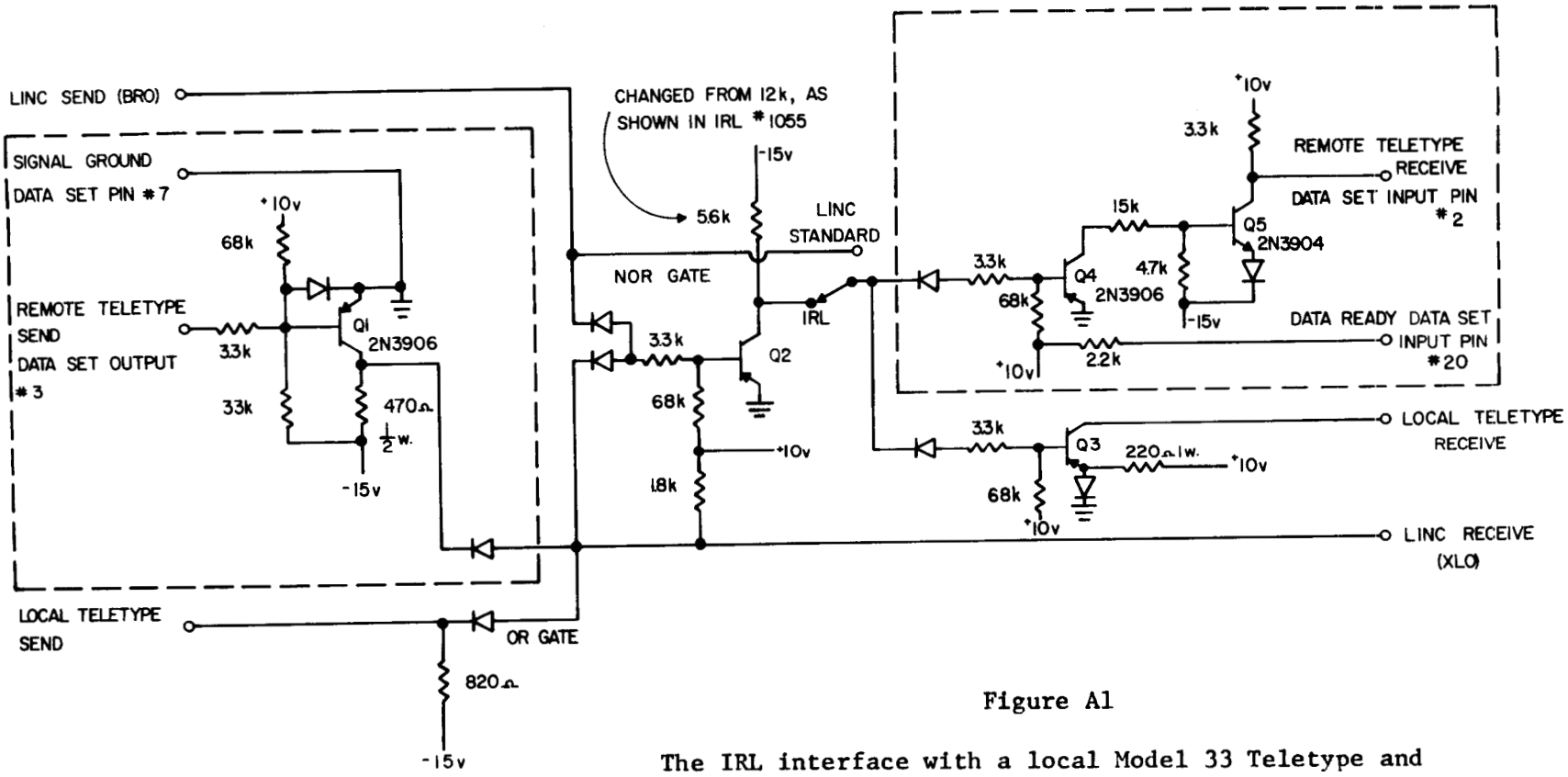
APPENDIX

IRL Interface with the Telephone Company Lines

The Instrumentation Research Laboratory's connection of a Model 33 Teletype to its LINC computer has been previously described in Appendix A of Technical Report No. IRL-1055. To further demonstrate the possibility of remote access to LINC - QUAD 300 system, the connection was modified to permit interfacing with a 103 A Data Set. This Data Set, rented from the phone company, transmits to and receives from similar units any serial, digital code. Such units are available throughout the Bell Telephone service area.

The Data Phone has a TALK and a DATA mode of operation. In the TALK mode the Data Phone may be used for voice communication; in the DATA mode the flow of information is digital and through the Data Set connector. By connecting the LINC to a Data Set it is possible to call and control the program from any Data Phone-Data Set combination in the Bell system. In particular, we wished to call the LINC from locations having a Teletype connection to the local Data Set, since the Teletype is our local input-output device. The phone company does, in fact, present this type of connection in one package. A Model 33 KSR Teletype can be obtained with a Data Set and Data Phone built into its mounting rack. This type of unit appears, for example, in the offices of those who subscribe to news services such as the Associated Press.

The basic IRL hookup is shown in Figure A1. The data flow is indicated by the table of Figure A2.



ALL RESISTORS ARE $\frac{1}{4}$ WATT UNLESS NOTED OTHERWISE.

ALL DIODES ARE SILICON.

Figure A1

The IRL interface with a local Model 33 Teletype and a 103A Data Set. The circuitry enclosed in dotted lines has been added to the previous IRL circuit described in Figure 1 of Appendix A in IRL Report No. 1055.

SEND

		LINC	Remote Teletype on Data Phone	Local Teletype Permanently Connected to the LINC
	LINC		Q1, OR	OR
RECEIVE	Remote Teletype on Data Phone	NOR, Q4 Q5	Q1, NOR, Q4, Q5	OR, NOR, Q4, Q5
	Local Teletype Connected to LINC	NOR, Q3	Q1, NOR, Q3	OR, NOR, Q3

FIGURE A2

Data Flow between the SEND and RECEIVE stations.

A problem came up in the use of IRL software with the remote Teletype. Those Teletypes with built-in Data Sets put out a parity bit as the last unit of its character code. Those characters which included this parity bit were not recognized by our LINC Teletype routine. However, the remote Teletype did not demand parity, as evidenced by the fact that it accepted our output, without parity, from the LINC. It was

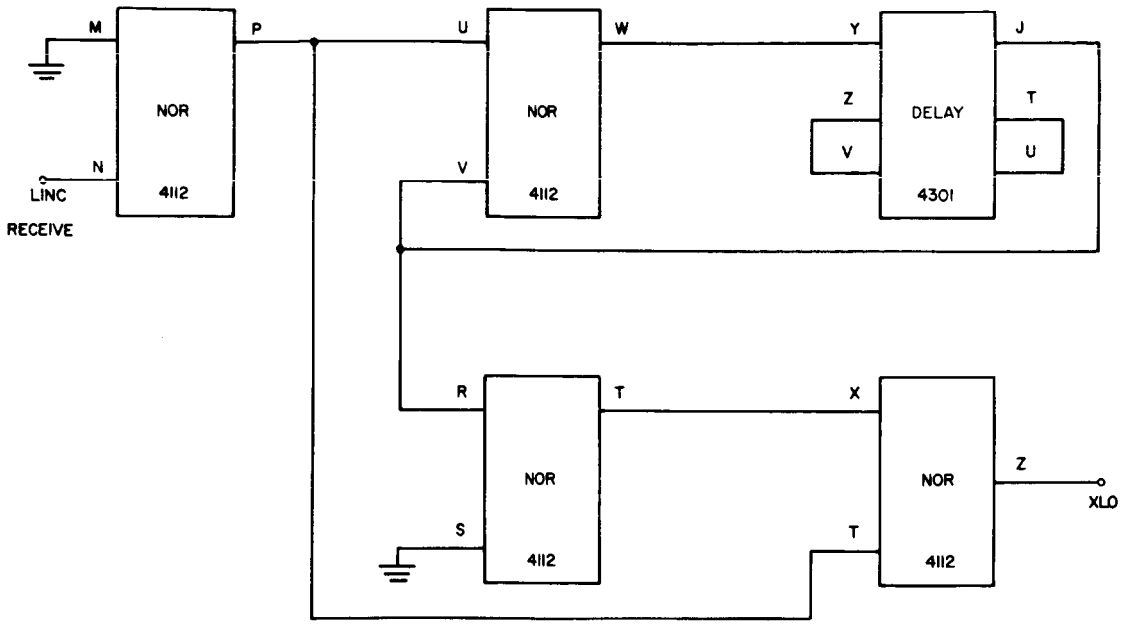


Figure A3

The IRL hardware modification which removes an incoming parity bit from a coded character.

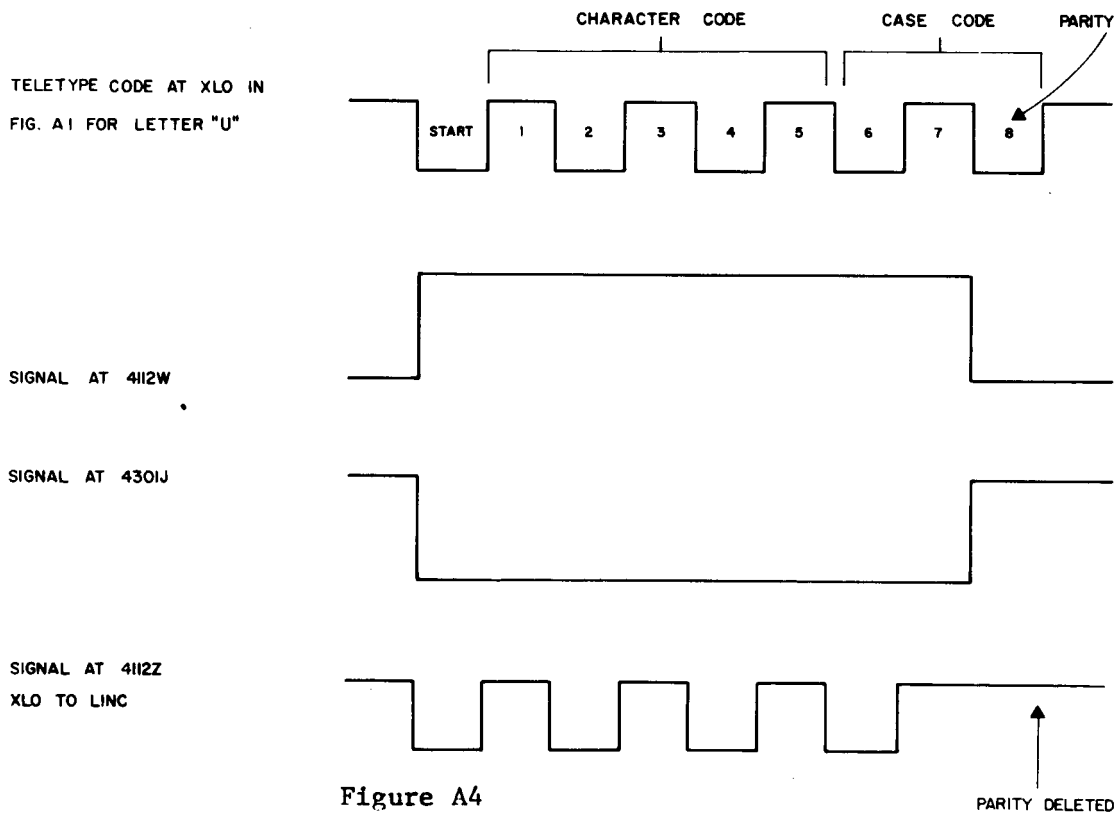


Figure A4

Timing diagram of parity delete circuit.

decided that the easiest way to solve this problem was to remove this parity bit at the input to the LINC with a hardware modification. This modification, shown in figure A3, makes it possible to use all of our past and present software from either our local Teletype or the remote Data Phone Teletype, via the telephone lines. The circuit was implemented with two DEC logic cards of the 4000 series. The NOR blocks which are shown in figure A3 are all on one 4112 card. The letters are the pin connections. The circuit, in use, intercepts the output line marked LINC Receive in figure A1.

The timing diagram, figure A4, illustrates the manner of deleting the parity bit.