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A MASS SPECTROMETER DATA ACQUISITION AND ANALYSIS SYSTEM

Robert B. Tucker

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

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Principal Investigator: J. Lederberg

Director, Instrumentation Research Laboratory: E. Levinthal

Instrumentation Research Laboratory, Department of Genetics

Stanford University School of Medicine

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ABSTRACT

This report describes a data acquisition and analysis system for a low resolution mass spectrometer. The system utilizes a small digital computer to acquire, interpret, and plot the mass spectra. The data can be stored on magn_tic tape for later reference. Provisions also exist for sending the data to larger computers for further analysis.

Emphasis has been placed on a high degree of user-computer interaction. A teletypewriter, display screen, and a digital plotter are used for ease of communication between the user and the computer.

CONTENTS

I. Introduction

A data gathering and analysis system has been developed for use with the low resolution Bendix Time-of-Flight mass spectrometer. Its primary functions include data gathering, data analysis, data filing, and bar graph plotting of mass spectra. The system was programmed for the LINC - a 12 bit, 2000 word computer. In addition to the basic computer, a Teletype Model 33, a Datamec 2020 digital tape unit, and a Calcomp 565 incremental plotter were employed. An interesting but not essential connection with an IBM 360/50 is also described. Mass spectra data can also be sent to a PDP-6 for further analysis.

Our principal objective was to develop a system to relieve the TOF operator of the tedious task of interpreting the traditional strip chart output of the mass spectrometer.* Also of interest was the ability to utilize the incremental plotter to make bar graphs and the storage of the spectra on tape. The availability of these data to other computers was also of conern.

Because the mass peak spacing followed a square law (discussed in the next section), the visual determination of the mass to charge ratios of the peaks of the strip chart output was very time consuming and somewhat unreliable. Placing a logarithmic amplifier between the output of the instrument and the chart recorder made the job of peak identification somewhat easier by, in effect, increasing the chart recorder's response to very small peaks. A problem then, of course, was that of

*Other participants in this project included, W. E. Reynolds, J. Bridges, and T. Coburn.

converting the significant peak amplitudes back to a linear scale. In the automated system the same logarithmic amplifier is used to increase the range of the computer's eight-bit A-D converter

The computer is used to collect the data utilizing a synchronizing pulse from the TOF to ensure that the data collection begins at the start of the scan of the mass spectrometer. The computer is later used to compensate for the unequal peak spacing that made visual interpretation difficult. A display screen on the LINC console is used to combine the talents of the user and the computer for determining the integer peak positions.

On this screen is displayed successive portions of the spectrum together with a scale (raster). The user positions the scale so that its divisions correspond to the peak position.* The computer then uses this for information to record the amplitudes of the peak positions. A detailed description of this process appears in Section IV. Finally the mass amplitudes are converted from the logarithmic scale to linear and the results are plotted as a bar graph and stored on tape.

The computer software is based on a monitor program which is used to call various subprograms. These subprograms perform the individual functions, such as data collection, data manipulation and graphic output. The structure of this software system can be seen in Figure 1. This segmentation provides for ease of modification since the subprograms are, in general, independent of one another.

*The technique is similar to that often used with the Gerber variable scale.

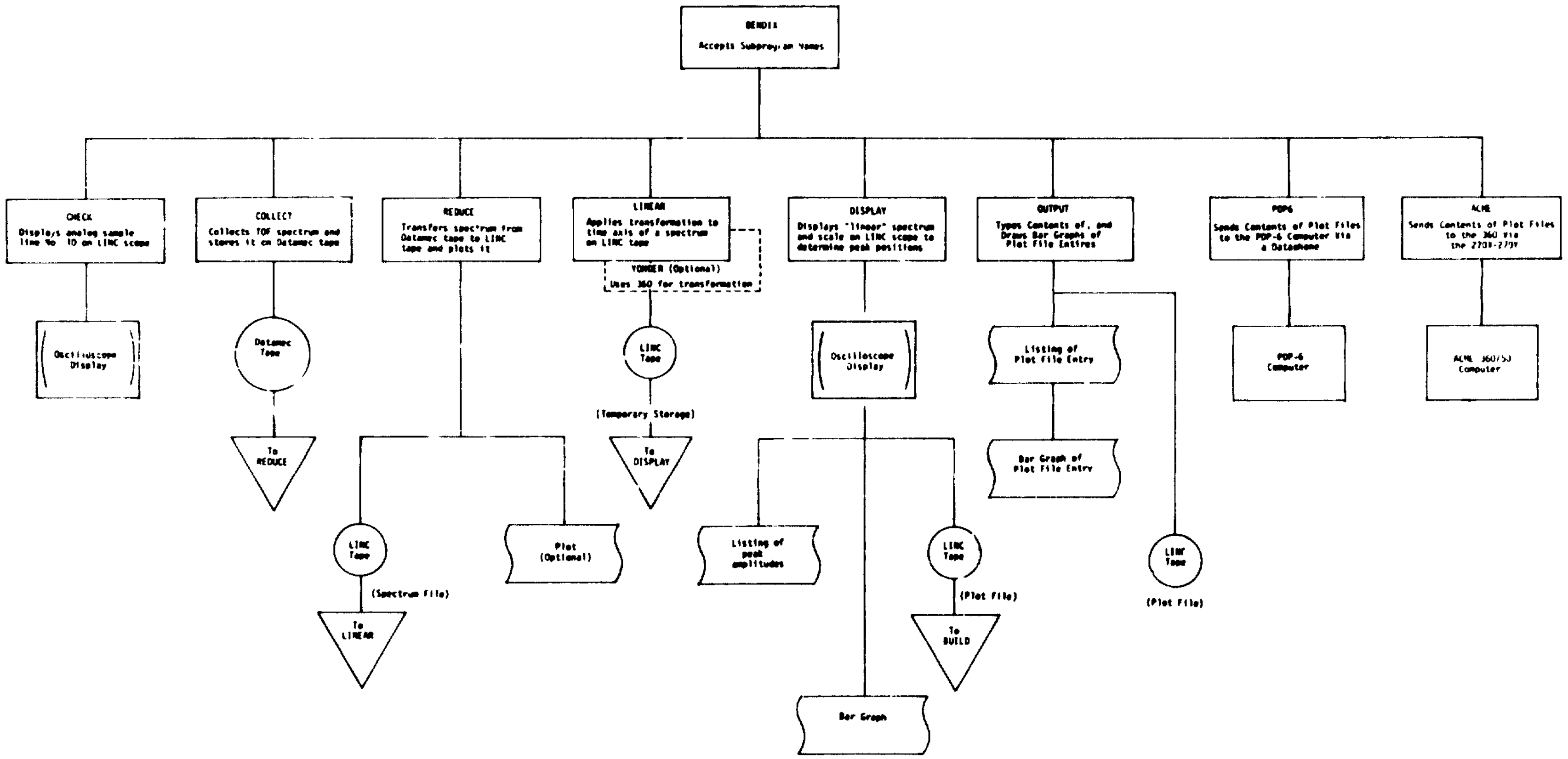

Figure 1

Software organization

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II. The Problem

The major difficulties preventing easy visual interpretation of the conventional strip chart record are: first, a square law is involved in the positioning of the mass to charge ratio responses on the time axis, and second, the absolute positions are subject to considerable drift (several a.m.u. positions at $m/e = 200$) from one run to the next, over the time span of less than an hour.

The principle of operation of the time-of-flight mass spectrometer is that of accelerating a group of ions with a given electric field. Since the energy of all singly charged ions will be the same, the square of their individual velocities will depend linearly on their masses. These ions are allowed to drift down an evacuated ($\sim 10^{-5}$ Torr) flight tube. The time, t, of their arrival at the detector will be proportional to the square root of their masses,

$$t = k\sqrt{m}$$

or

$$m = Kt^2.$$

Since the flight time for the heaviest ions under consideration ($M = 450$) is about 50 μsec, a system having the effect of slowing down this time scale must be employed if anything other than an oscilloscope is going to be used to record the output. The manufacturer has incorporated such a system, referred to as an analog scanner, into the mass spectrometer. The instrument has provision for pulsing the ion accelerating field with a repetition rate of 100 microseconds, thus producing the entire spectrum at the collector repetitively. This is combined with the appropriate delays and gating operations of the analog scanner to allow a recording device to "look" at these spectra through an advancing window, similar to the operation of a sampling oscilloscope. The effect is that a single complete spectrum is recorded as the combined small portions of many spectra.

The extent to which this system faithfully reproduces a single spectrum depends on the window moving along the spectra at a uniform speed. That is, the delay between the application of the accelerating voltage and the sampling of the collector must be increasing at a uniform rate. If this is the case, the mass positions will be proportional to the square root of the masses. Unfortunately, it was found that this was not the case; the window did not move along uniformly and its performance varied slightly from one run to the next. As mentioned previously it was found that at m/e = 200, drift up to 5 a.m.u. positions would occur in a series of runs made within one hour. Though modifications to improve stability were available from manufacturers, it appeared that considerable drift would still exist.

With these drifts, it is obviously impossible to dependably identify the mass peak purely by their position. Furthermore, the effective use of reference compounds would require that they be included in the same run with the sample (thus obscuring some positions) since the device drifts in such a short time.

The use of computer techniques in identifying mass positions requires either that the peak positions be identified by their position on the time axis or by their shape and amplitude. Since their position was not dependable, attempts were made to develop various peak counting routines. Various routines were written which tried to identify peaks, attempted to predict where peaks would be, and in general used the shape of the signal to identify peak positions. The signal from the collector is processed by a log amplifier (1) in an attempt to get a meaningful signal from the small peaks and in general to increase the range of our A to D converter. However, the apparent noise level also was increased. We were unable to develop a reliable algorithm which could identify mass peaks as capably as the human operator, working by visual inspection. The algorithms which were developed were either undependable or became unstable as they were made more powerful. The use of various convolution techniques in identifying the position of peaks was found to be outside the practical limits of the small computer being used.

Since human judgment was effective in determining what was a meaningful peak and the computer had a certain capacity for estimating where peak positions should be, a software system was developed to combine these two capabilities.

III. Software Organization

The communication with the computer is done with a standard Model 33 teletype. The system is initiated by using the computer console switches to read in a simple monitor program, BENDIX (Block 400 is read into quarter 0). Starting the program (at location 20) causes the computer to type out the name BENDIX and then wait for the name of any one of nine subprograms to be entered by the user. It is these subprograms that perform the various functions necessary to collect, analyze, and present the data of the mass spectrometer (see Figure 1, Section I). Entering a question mark rather than a program name causes the typing of the names of the subprograms available. The subprograms are described in detail in the next section.

Each subprogram has a series of parameter requests designed to the needs of the function it performs. Each answer must be followed by a semicolon or carriage return. If the user makes a typing error while answering a question, striking the "rubout" key causes the question to be repeated. The entire software package is built around this question-answer concept. Some questions require just a yes-no response. In this case, any response beginning with an "N" is considered negative and all others affirmative.

The software can be thought of as existing in a series of levels with the BENDIX level being the highest, the subprogram level being next, followed by a series of parameter levels. One works down through the levels by entering names and parameters. As functions are performed control is returned to the previous applicable level. If one answers a request by striking the upward arrow key on the teletype, control reverts to the next higher level of operation until finally the BENDIX level is reached.

The subprograms are stored on the systems tape mounted on tape unit 0 (left hand unit). Each subprogram is complete by itself and can be altered without disturbing the logic of others. The only requirement is that the proper file structure be maintained. Each subprogram contains its own typewriter routines, decimal conversion routines, plotting routines, and etc. Only the double precision floating point package (2) and the Datamec control routines are shared by the subprograms. Though duplicating many of the routines is somewhat wasteful of tape storage space, the extent to which it permits easy program changing appears to make it worthwhile.

The total system involves about 7000 words of program. The convenient overlay methods permit the programming to utilize the one thousand words of programmable core quite effectively. Each subprogram is loaded into core and ready for use in less than five seconds.

Most of the coding was done in LASS, the assembler language for the LOSS system (3). The programs were assembled under LOSS and then transferred into the BENDIX system tape. The double precision floating point package and the Datamec routines exist only in absolute coding.

The system provides two forms of data storage - Spectrum Files and Plot Files.

Spectrum File entries hold digitized mass spectra in a form which corresponds to that traced on a chart recorder; simply the digitized output of the analog scanner. Each file entry is 36 blocks long (256 values per block), and is stored on tape unit 1. Sixteen such entries (numbered 0-15) can be stored on one LINC tape. These files are discussed more fully under REDUCE in the following section.

Plot Files hold only the basic information needed to generate a bar graph plot of a spectrum. A plot file entry is stored on two blocks of tape (512 words). The first 480 locations of this segment of tape hold the amplitudes of mass positions 1 to 480, the remaining locations hold an alphanumeric name of 64 characters in length. These files are held on the lower half of the tape on tape unit 0 (the systems tape). A maximum of 128 plots (numbered 0-127) can be stored on one such tape. When all locations are filed a new systems tape must be generated (see Appendix I). A further description of these files and their uses is described in the next section under OUTPUT.

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IV. The Subprograms

Since a clear understanding of the subprograms is essential to the use of the system, each one is described in some detail in this section. The following subprograms are available for use.

CHECK	Checks electrical connection between LINC and TOF.
COLLECT	Collects a mass spectrum on digital tape (Datamec).
REDUCE	Reduces data onto LINC tape and plots.
LINEAR	Applies a transformation to a spectrum.
YONDER	Duplicates the function of LINEAR but performs the calculations on the ACME 360/50.
DISPLAY	Displays portions of spectrum for analysis, plots and files the results.
OUTPUT	Makes bar graphs of Plot File entries, types elements of the Plot File, builds Plot File entries.
PDP6	Sends Plot File entries to the PDP-6 for further analysis.
ACME	Sends Plot File entries to the 360/50.

The above programs are listed in the order in which they are generally used. Referring to Figure 1 (the Systems Process Chart) in Section I will assist in clarifying the relationships between the programs as will the descriptions that follow.

A. CHECK

The purpose of CHECK is to ensure that the output of the log amplifier is being properly received by the LINC through sample line ten.

The MAX and MIN levels shown in Figure 2 indicate the range of the digital to analog converter. Preliminary scans can thus be made to check for positive or negative saturation. Changing of scale on the logarithmic amplifier and/or altering a bias voltage will bring the signal into the proper range. The LINC scope is used to display the level of the signal as well as the maximum and minimum permitted by the analog to digital converter.

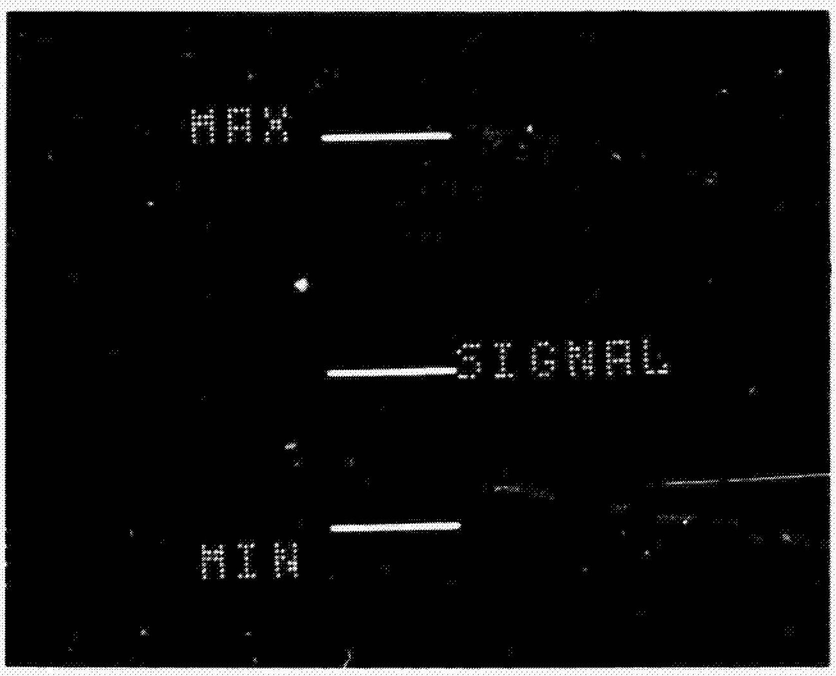

Figure 2

Oscilloscope Display Produced by CHECK

B. COLLECT

COLLECT is used to digitize the output of the TOF (via the log amplifier) and record this data continuously on the Datamec tape unit. It is the fundamental data collection step and is synchronized with the TOF as described below. It is the only program that need be run in real time with the TOF.

A write-enabled tape should be positioned at the load point, the LOW DENSITY and AUTO status lights should be illuminated, and the unit should be set to low speed. Since the operation of the Datamec is quite complex the user should consult the manual for the Model 2020 Datamec before using it (4).

The COLLECT program should now be called. If any of the above action have been improperly accomplished, pertinent error messages will be typed out followed by the word READY? Keying a semicolon will permit the program to continue after adjustments have been made. After the semicolon is typed the program will wait for a synchronizing signal on external level seven which is connected to the scan system of the TOF. When the signal is received by the starting of the TOF scan scan system, the actual data gathering will take place (via the sample line ten).

The collection is terminated by momentarily lifting sense-switch zero (one of six program interrogated console switches) on the LINC console at which time the tape will rewind to the load point and the program will return to the BENDIX level of operation. The tape thus generated can be replaced with another if the user wishes to make another collect run immediately, or it may be left in place to be read by the REDUCE subprogram. It should be noted that though this tape is a standard half inch tape, recorded at low density, it is of continuous record format and unsuitable for use with conventional computer I/O systems.

C. REDUCE

REDUCE transfers the spectrum data from the Datamec tape to the right hand LINC tape and reduces the data by averaging 16 points together. It is this operation that creates the spectrum files discussed in the previous section. The option also exists to plot the reduced data on the Calcomp plotter at this time. This plot corresponds to those conventionally plotted on a strip chart recorder and can be used to verify that the COLLECT and REDUCE operations have been performed properly (see Figure 3). As in the COLLECT operation, the Datamec tape must be set at the load point. However, the tape speed control must be set to high.

Typing the word REDUCE will initiate a request for the number of a spectrum file (from 0 to 16, inclusive) on which to store the reduced spectrum data.

Entering such a file number will cause the computer to check the status of the Datamec and note any discrepancies on the teletype. Also typed is the message PLOT? A negative answer will eliminate the plotting of the data as it is being transferred from Datamec tape to LINC tape. If only a semicolon is given or an affirmative answer followed by a semicolon the plotter must first be prepared (connected to the LINC, turned on, equipped with a pen). The program will return to the BENDIX level when completed.

D. LINEAR

The LINEAR subprogram applies a transformation to the time axis of a Spectrum File which was stored on LINC tape by REDUCE. It is intended that this transformation will alter the original spectrum such that the mass peaks will be equally spaced. As mentioned in Section II, the basic relationship between mass and time is:

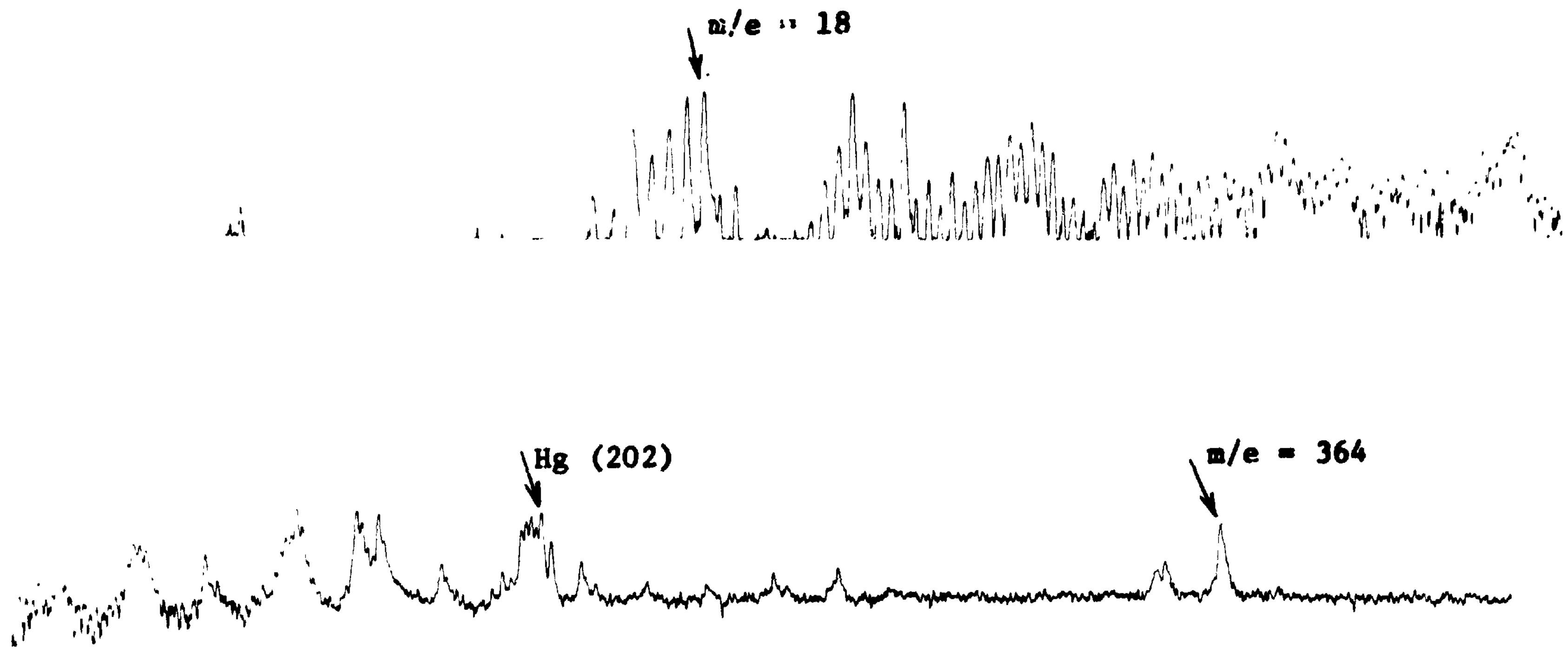

Figure 3

A digitized mass spectrum with amplitudes in logarithmic scale. The scale at the end of the spectrum (right end of lower trace) reflects the decade levels.

$$m = Kt^2.$$

Because uncertainties, considered equal for all masses, exist in the measured flight time, the relationship becomes:

$$m = K(t \pm \Delta t_o)^2$$

Where t as before, is the flight time and Δt_o is the uncertainty in the flight time. Here, t and Δt_o are in units of time corresponding to the net digitizing rate (that resulting from the REDUCE operation).

As mentioned in Section II, this attempt to develop a linear relationship between a given mass and its position on the ordinate is hindered by certain drifts in the analog scanner. For this reason, the subprogram (DISPLAY) which analyzes the output of LINEAR has been specifically designed to handle these drifts.

Calling LINEAR simply initiates a request for a Spectrum File number (output of REDUCE), applies the transformation to the spectrum, and returns control to the BENDIX level. It should be noted that the output of LINEAR is always stored on the same portion of tape, overwriting the output of a previous running.

E. YONDER

Those functions performed by LINEAR can also be performed by YONDER; the input and output is identical. The advantage with YONDER is that it is much faster, since it uses a communication link between the LINC and an IBM 360/50 operating in a time sharing mode. Though YONDER was primarily written simply to test the feasibility of this connection, it has proven quite useful. The operation consists of sending the data to the 360, performing the transformation, and returning the data to the

LINC. This is performed by YONDER and a 360 program running concurrently.

F. DISPLAY

The DISPLAY program is intended to assist the user in identifying the integer mass peaks and their amplitudes in a mass spectrum (the output from the Linear operation). This is accomplished by displaying successive portions of the spectrum on the LINC oscilloscope together with a variable scale* (see Figure 4). The program is designed to start at the lower mass positions of the digitized spectrum (on LINC tape) and proceed through the higher mass positions in response to commands by the user.

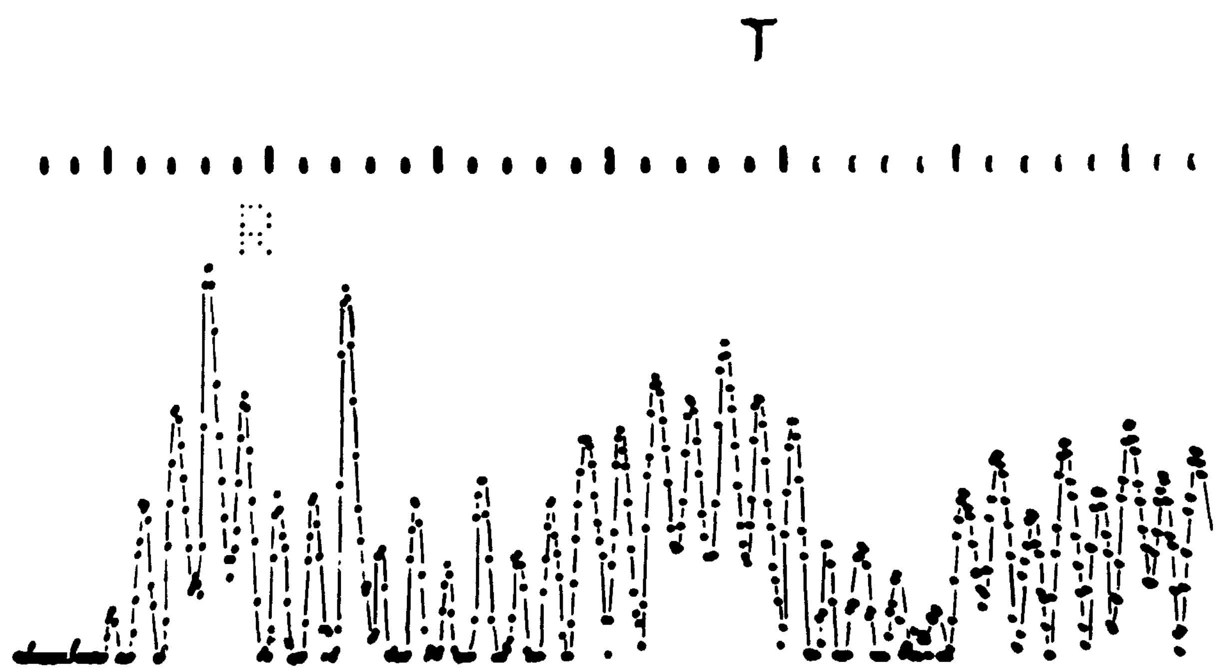

Figure 4

The above is the CRT display of a portion of the spectrum. Line segments have been added between the data points to enhance its clarity.

*Based on an idea of Dr. S. Liebes, Jr.

The basic idea is to display a portion of the spectrum (about 40 mass positions) and a comb, or raster, which the user can stretch and translate. Potentiometers located on the LINC console are used to enter the parameters for these adjustments. Thus the user can fit the comb to the observed mass positions (peaks) even though they are not quite equally spaced throughout the spectrum. The program uses this comb to find the amplitude of the signal at each mass position in the section of the spectrum being currently displayed. This comb also provides the user with the ability to "bridge" a group of mass positions in which little significant signal appears. Having positioned the comb properly the user can then have the series of mass positions and amplitudes typed out or recorded on tape. Figure 5 is a block diagram showing the series of functions that take place.

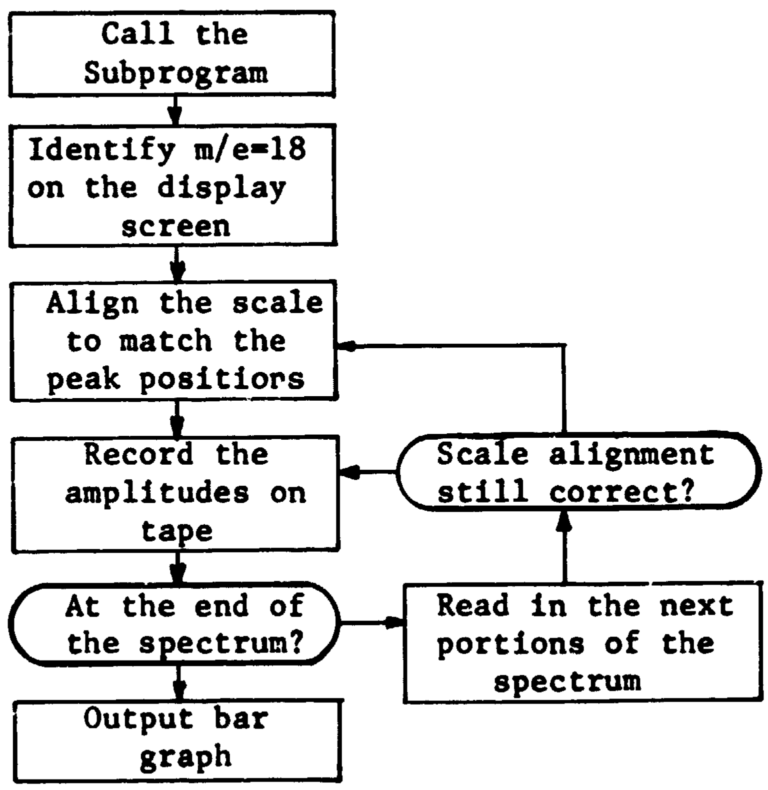

Figure 5

Upon entering DISPLAY the first four blocks of data (the spectrum) will be displayed on the scope. Also displayed are some control indicators and decimal quantities:

(1) A "T" - the tack

(2) An R - the reference mass indiator

(3) Mass number of the reference mass (left entry - top of screen)

(4) Block number of right-most data block displayed on screen (right entry - top of screen).

Using potentiometer number 2, the "T" must be moved across the screen until it coincides with mass position 18. (Determining mass position 18 is left to the cleverness of the user, though not particularly difficult.) Pot 3 can be used to raise and lower the "T" to aid in this alignment. With the T positioned at mass 18, the momentarily lifting of sense switch three will cause a raster to be developed on which every fifth mass position is enhanced. This raster can now be stretched, about the reference mass, using pot 7 until it corresponds to the mass positions of the spectrum itself. With the alignment made the mass amplitudes can be written on tape (buffered write) by momentarily lifting sense switch 4. If sense switch 0 is on during this operation the mass amplitudes are typed out rather than recorded on tape. Lifting sense switch 4 also causes the "R" to move to a mass position near the right side of the screen (this action may be considered to be a check as to whether or not the previous step was properly executed). With the "R" in the right hand portion of the screen the entire display may be moved to right by reading in the next position of the spectrum. Lifting sense switch 5 initiates this action. Note that the right-most fourth of the screen moves to the left-most fourth and new data fills the remaining portion of the screen. The raster can again be aligned with the mass positions and the process of recording on tape or typing repeated.

When the user has proceeded through as much of the spectrum as desired in the above manner, lifting sense switch 1 will initiate the request for a name and plot number. A name of up to 64 characters can be entered and terminated by a carriage return. The plot number entered must be between 0 and 128, inclusive. The CALCOMP plotter must be turned on, equipped with a pen and paper, and positioned within 1-1/2 inches of the right side of the drum. The data is normalized such that the tallest bar will be eight inches. Upon entering the plot number, the integer mass peaks will be plotted as a bar graph (Figure 6) and stored permanently on tape unit 0 in the Plot File. It is in this operation that the peak amplitudes are converted from logarithmic scale to linear. The file of plots can be referenced for replotting and typing as described in the following section.

G. OUTPUT

Three options exist under OUTPUT. (1) A Plot File entry can be plotted as a bar graph. (2) A Plot File entry can be typed out. (3) The user can manually build an entry in the Plot File by entering mass-amplitude number pairs.

The - DRAW A GRAPH - prompt enables one to plot a bar graph (Figure 6) of any plot filed under the DISPLAY subprogram or manually

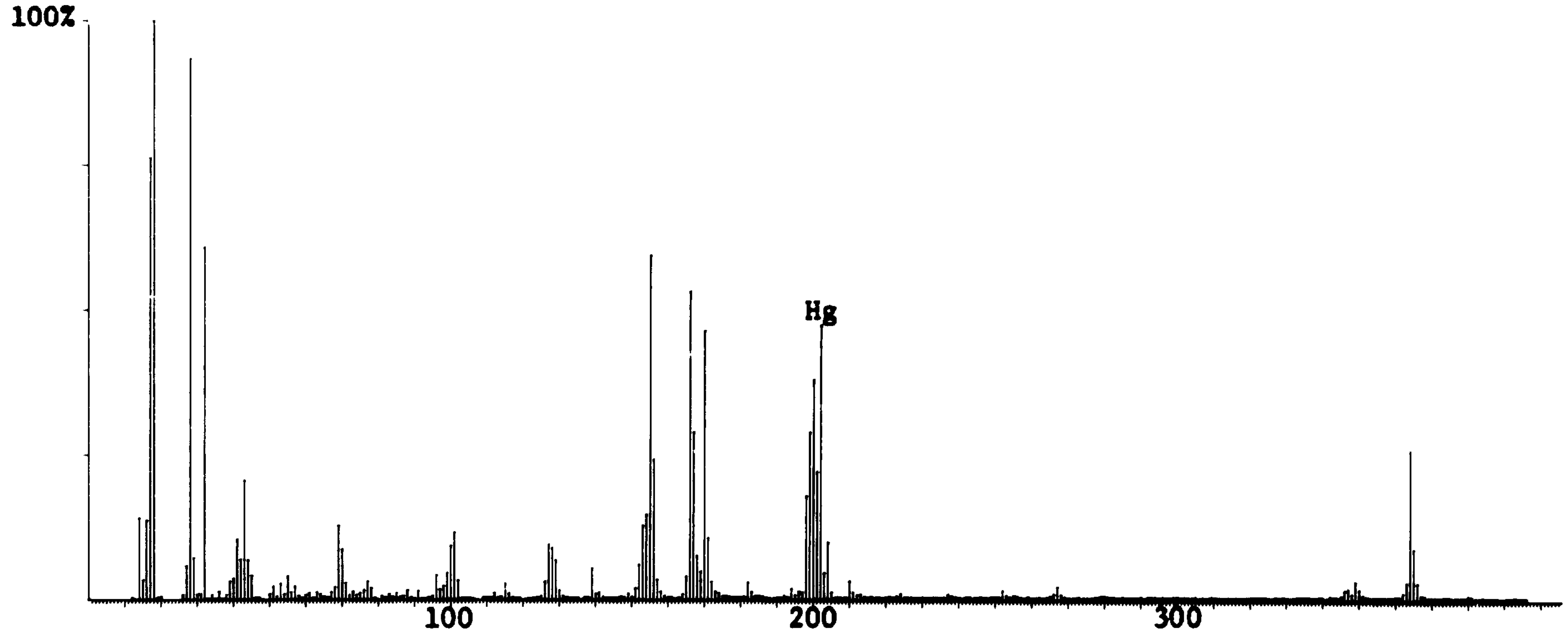

Figure 6

Typical bar graph output.

TFA-L-Prolyl (-)-Alpha-(1-Naphthyl) Ethylamine entered as described below. Since the graph is eight inches high, the plotter carriage should be placed near the right side of the plotter. At the completion of the graph, the prompt - OVERPLOT? - is typed out. An affirmative response will return the carriage to the beginning of the previous plot and request a new plot number which is plotted over the previous one. Though the second plot is slightly to the right of the first, it is recommended that a different color or ink is used to ensure readability. This capability allows two or more spectra to be easily compared. It should be noted that each spectra is normalized separately such that its highest peak is 100 percent.

The - TYPE A GRAPH - option provides for typing the contents of any Plot File entry.

By entering, yes, to the prompt - ENTER A FILE? - the user can enter a file name and number under which to file a series of mass amplitudes which are about to be entered through the teletypewriter. The entries are made in mass-amplitude number pairs. They need not be entered in increasing mass order. In fact, an entered pair can be corrected by simply retyping the mass number and the amplitude. Striking an upward arrow (↑) for an amplitude entry permits retyping the associated mass number. Striking the upward arrow for a mass number entry allows one to start the entire operation over again. The computer will request mass numbers (up to 480) and amplitudes. Entering 2000 as a mass number will terminate the entry mode and store the entered information on tape. The option just described is intended to be used when spectrum information is received from other sources (than the TOF) but the user wishes to keep the data in the Plot File for plotting, typing, or eventual transfer to another computer.

H. PDP6

This subprogram is used to send Plot File entries to the PDP-6 computer for further analysis (5) via a Model 103A Dataphone. The data involved is simply sent to the teletypewriter in the full duplex mode and is also sent to the Dataphone which is activated as described below. The PDP-6 computer receives this data in the same manner that it receives any other data transmitted via a teletypewriter; the PDP-6 is unable to determine that the data is being sent by another computer rather than by a teletypewriter.

Since in this step the user must communicate with two computers with the teletype, the user-computer dialogue becomes somewhat complex and the LINC "RESUME" lever must be lifted occasionally to complete the operation. Entering PDP6 at the teletype initiates a request for the Plot Files to be sent. Any number of Plot File entries may be sent providing their numbers are contiguous. After accepting these parameters, the LINC requests that the PDP-6 be called and then halts. The Dataphone is now used to call the PDP-6 monitor system. When the system answers, the "Data" button on the Dataphone is pressed and the connection is complete. The teletypewriter mode switch is then placed in Full Duplex and a "Control C" key is pressed (C is pressed with the CTRL key used as a shift key). This enables one to request the proper PDP-6 program and proceed with entering its parameters (6). With the parameters entered, the lifting of the LINC resume lever causes the data to be sent to the PDP-6 and stored on magnetic tape. When all data has been sent the message "HIT CONTROL Z" appears at which time the user accomplishes this to terminate the PDP-6 program. The user then terminates communication with the PDP-6. Returning the teletype mode switch to "Normal" and lifting the Resume lever brings the LINC back to the BENDIX level of operation.

I. ACME

ACME is used in conjunction with suitable 360/50 programming to send Plot File entries to the 360/50. The user is requested to indicate the Plot Files to be sent. After the entries have been made the program waits for the request from the 360/50.

The user then loads the ACME/PL1 program under the control of a 2741 communications terminal attached to the 360/50. Under the time sharing ACME system requests are sent to the LINC for successive blocks of data. After all data is sent the 360/50 system indicates that a normal termination has occurred and the LINC returns to the BENDIX level of operation.

V. User-Computer Dialogue

The following is a description of a typical dialogue between the user and the computer. It is not intended to give examples of all the computer generated messages or all of the possible responses, but only enough to illustrate the approach used. Those examples given are in the sequence in which they would normally be used. The bold face text on the left is that seen by the user at the teletype. The teletype entries which are underlined are those typed in by the user. All others are computer generated. The entries on the right are simply comments put in here for the purpose of clarity and explanation.

BENDIX	This typeout indicates the system is at the BENDIX level and waiting for the user to enter a subprogram name.
CHECK; CHECK	The user requests the CHECK subprogram. The name of the subprogram requested is repeated by the computer for confirmation.
↑ BENDIX	The user requests that the system return to the previous level (BENDIX) of operation.

COLLECT;	COLLECT is requested by the user.
COLLECT	
	The system checks the status of the Datamec tape unit and notes any changes to be made by the user.
PRESS "AUTO" SET SPEED SELECT TO LOW	
	The user indicates the changes have been made.
READY?YES;	At this time, the computer waits for the synchronizing signal from the TOF and then begins collecting the data.
BENDIX	By momentarily lifting console switch one, the user terminates the collection and returns to the BENDIX level.
REDUCE;	REDUCE is called.
REDUCE	
	The request is made for the number of a Spectrum
FILE NUMBER = 15;	File on which to store the data.
PLOT ?YES;	The option exists at this time to plot the Spectrum File.
BENDIX	
LINEAR;	The user calls LINEAR and indicates that the output of the previous step is to be used.
LINEAR FILE NUMBER = 15;	
BENDIX	

DISPLAY;	DISPLAY is called by the user.
DISPLAY	
	Successive portions of the spectrum (output of LINEAR) are displayed on the LINC oscilloscope for mass peak identification.

```
NAME: TFA-L-PROLYL (-)-ALPHA-(1-NAPHTHYL)ETHYLAMINE
PLOT NUMBER=45;
```

When the identification portion of the operation is completed, a name and Plot File number are requested under which to file the spectrum information. The bar graph of the spectrum is then plotted and the data stored on tape.

BENDIX	The BENDIX level is returned to.
	If the user wishes to replot the data, OUTPUT
OUTPUT;	can be called.
OUTPUT DO YOU WANT TO: DRAW A GRAPH?YES; PLOT NUMBER=45;	The user indicates that he wants a graph to be drawn and indicates the file number of it.

```
TFA-L-PROLYL (-)-ALPHA-(1-NAPHTHYL)ETHYLAMINE
```

The name of the sample (as entered under DISPLAY above) is typed out and the graph is then drawn.

OVERPLOT? NO;

The "overplot" option appears and is rejected.

The series of questions is repeated. This time the user requests that the contents of the Plot File entry be typed out.

DO YOU WANT TO:
DRAW A GRAPH?NO;
TYPE A GRAPH?YES;
PLOT NUMBER=45;
TFA-L-PROLYL (-)-ALPHA-(1-NAPHTHYL)ETHYLAMINE

Again the name is typed out.

12	3
13	1
14	113
15	28
16	110
17	610
18	800
19	3
20	5
26	7
27	47
28	747
29	58
30	8
31	8
32	487
33	2

The contents is typed out in mass-amplitude number pairs (only a portion of which is shown). Control returns to the initial series of questions.

DO YOU WANT TO:
DRAW A GRAPH?NO;
TYPE A GRAPH?NO;
ENTER A GRAPH?YES;

The OUTPUT subprogram can also be used to construct manually a Plot File entry.

NAME: REFERENCE COMPOUND
PLOT NUMBER=46;

A name is given, and a plot number on which to file the entered data.

```
M=28;
A=60;
M=32;
A=29;
M=41;
A=10;
M=47;
A=19;
M=50;
A=22;
M=69;
A=65;
M=100;
A=71;
M=119;
A=33;
M=131;
A=85;
M=150;
A=39;
M=169;
A=100;
M=181;
A=32;
M=219;
A=27;
M=247;
A=17;
M=2000;
```

The data is then entered as mass-amplitude number pairs.

A mass entry of 2000 indicates that all values have been entered.

```
DO YOU WANT TO:
DRAW A GRAPH?YES;
PLOT NUMBER=46;
REFERENCE COMPOUND

OVERPLOT? ↑
BENDIX
```

This data could then, of course, be plotted.

```
BENDIX
PDP6;
PDP6
SEND PLOT NUMBER 45;
TO PLOT NUMBER 45;
CALL THE PDP-6 PROGRAM
```

The following dialogue is used to send Plot Files to the PDP-6.

The plot numbers to be sent are entered here.

The LINC program halts. The user calls the PDP-6 on the Dataphone.

The PDP-6 program is loaded.

```
↑C

.A DTA3
DTA3 ASSIGNED
JOB4
STANFORD 2.8/09A

.R PIP2

*DTA3:F←TTY:


(SETQ S:TFA.L.PROLYL (.).ALPHA.(1.NAPHTHYL)ETHYLAMINE   (QUOTE (
(    12 .      3)
(    13 .      1)
(    14 .    113)
(    15 .     28)
(    16 .    110)
(    17 .    610)
(    18 .    800)
(    19 .      3)
(    20 .      5)
(    26 .      7)
(    27 .     47)
(    28 .    747)
(    29 .     58)
(    30 .      8)
(    31 .      8)
(    32 .    487)
(    33 .      2)
HIT CONTROL Z
```

Lifting the resume lever on the LINC control panel initiates the sending of the plot name followed by the mass-amplitude number pairs.

A "control Z" is struck by the user to terminate the PDP-6 program.

Lifting the resume lever returns the LINC to the BENDIX level.

```
BENDIX
```

VI. Hardware Description

The following is a brief description of the hardware used in the system (see Figure 7). Since most of the equipment is commercially available and adequately described in the manufacturer's literature the discussion here will deal only with the general layout.

A. The Mass Spectrometer

The instrument used is a Model 12 Bendix Time-of-Flight Mass Spectrometer utilizing a 180 cm drift tube (7). It is equipped with an analog scanner (see Section II) the output of which is digitized by LINC sample line ten after it is converted to a logarithmic scale as described in the next section.

B. Logarithmic Amplifier

The logarithmic amplifier used is a locally developed unit (Model 1010) specifically intended for use with mass spectrometers (1). Its use greatly increases the usefulness of the 6 bit analog to digital converter used. By incorporating the amplifier the need to make several recordings of various levels of attenuation was eliminated. One data collection step digitizing only one channel suffices. Of course the need exists to convert the signal back to linear at some step prior to final data presentation. Digital resolution does, of course, suffer for large signal amplitudes. Using the device, the output signal of the TOF over a five decade range can easily be digitized.

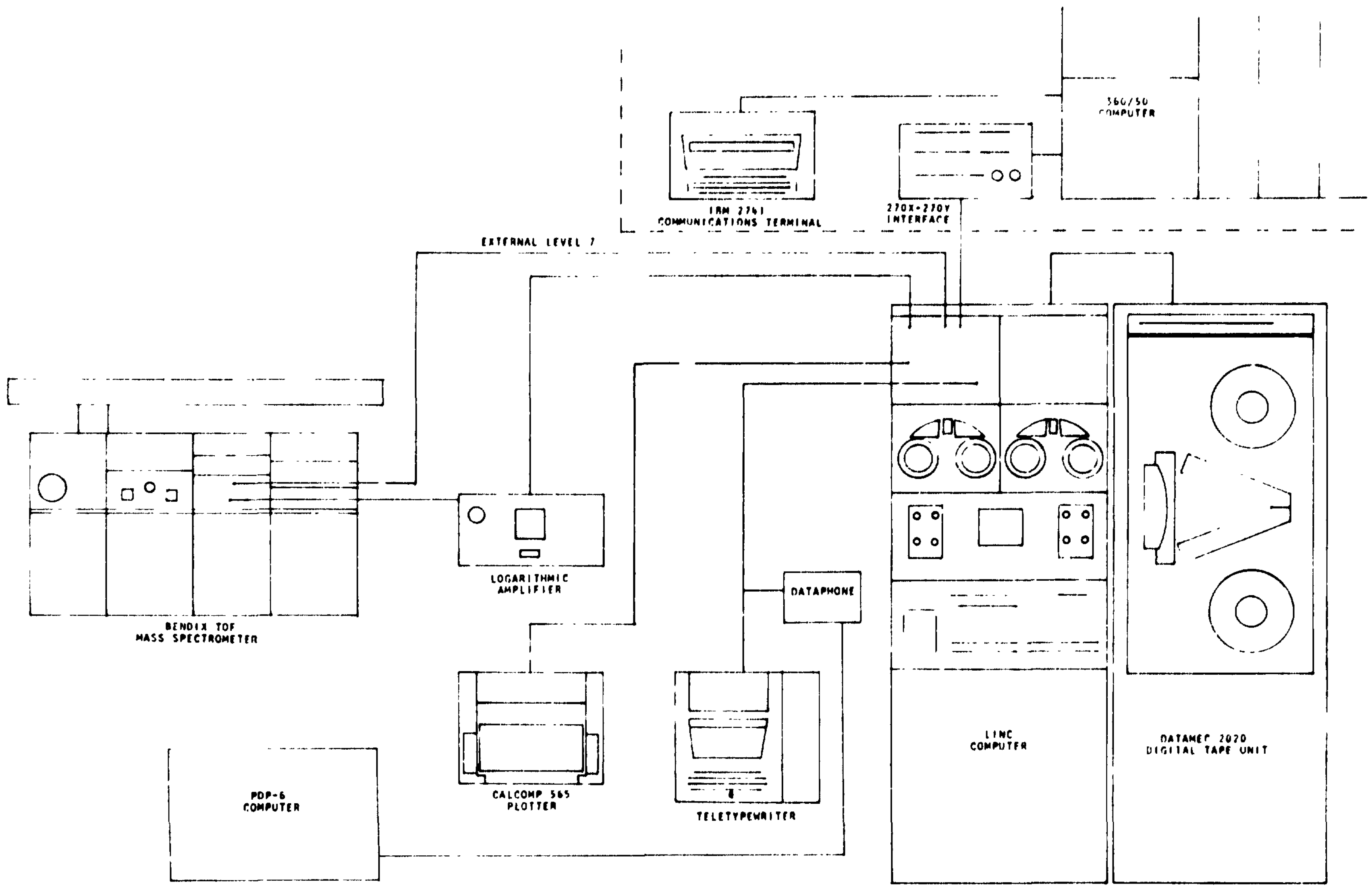

Figure 7

Block diagram of the hardware used.

C. The LINC Computer

The computer, a LINC, is a twelve bit, 2000 word digital computer (8). It was developed at the Massachusetts Institute of Technology under an NIH program for the development of medical computer capability. Incorporated in it is a 16 channel 8 bit analog to digital conversion system, digital output busses, and level sensing terminals. It has an eight microsecond cycle time with most instructions requiring two or three cycles.

Also included is a locally interfaced Datamec 2020, seven channel, digital tape unit. The interfacing provides only the minimum control necessary to read and write tape. All timing, parity checking, and blocking is done under program control. A Model 33 KSR Teletype is connected to the LINC, utilizing external level zero for input and relay register zero for output. Reference should be made to entry 2 in the list of references for a complete description of this interface.

A digital incremental plotter manufactured by California Computer Products (Model 565) is used to plot the Spectrum Files (see Section II) and produce the bar graphs of the spectra. It operates under the control of the OPR 0 instruction and a code in the right half of the accumulator. Entry 2 in the list of references describes this interface in detail.

D. IBM 360/50 Interface

Communication between the LINC and the 360/50 is via an IBM 270X-270Y general purpose digital interface (9). It was designed for our laboratory to be used in interfacing a variety of digital equipment to the 360/50. Thus the LINC is attached to the multiplexer channel of the

360/50. It then becomes simply another I/O device, like a tape unit, for the 360/50.

Programs can be written and executed from a 2741 communications terminal which reference the LINC for input and output. These operations take place under the locally written ACME time sharing system.

E. PDP-6 (Digital Equipment Corporation)

The PDP-6 has 128 thousand, 36 bit, words of memory. It is equipped with eight DEC tape units, a Datamec 2020 tape unit, a line printer, and presently provisions for connecting up to sixteen teletypewriters. It is normally used in a time sharing mode described in reference (6).

REFERENCES

1. W. E. Reynolds, The Use of a Logarithmic Amplifier in Data Processing of Analog Signals, NASA Technical Report No. IRL-1017, Instrumentation Research Laboratory, Genetics Department, Stanford University, 1965.

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3. R. [illegible] Moore, An Operating System for the LINC Computer, NASA Technical Report No. IRL-1038, Instrumentation Research Laboratory, Genetics Department, Stanford University, 1965.

4. Datamec Model 2020 Instruction, Maintenance, and Spare Parts Manual, Datamec Division of Hewlett-Packard, Mountain View, Calif.

5. G. Sutherland, DENDRAL-A Computer Program for Generating and Filtering Chemical Structures, Stanford Artificial Intelligence Laboratory Memo No. 49, Stanford University, 1967.

6. A. Grayson, et al, How to Begin Using the PDP6 Time Sharing System, Stanford Artificial Intelligence Laboratory Operating Note No. 3, Stanford University, 1967.

7. Instruction Manual for Models 1003 and 1005 (Basic Model 12) Bendix Time-of-Flight Mass Spectrometer, IM-63-CDE-07(B636250-11), The Bendix Corp., Cincinnati Div., Cincinnati, Ohio, 1963.

8. LINC-Programming and Use-1, Vol. 16, Washington University, Computer Systems Laboratory, St. Louis, Missouri, 1965.

9. R. N. Hontzeborn and C. H. Sederholm, IBM Research Report to be published.

APPENDIX

The Systems Tape

The BENDIX systems tape must be regenerated after all Plot File positions (128) have been utilized. Transferring blocks 400_8 to 434_8, inclusive, to another tape will provide the user with a new systems tape. Listed below are the locations of the various subprograms on this tape.

Block (octal)	Subprogram
400	BENDIX (calling program)
401	unused
402	CHECK
403	COLLECT
404-406	Datamec Routines
407-411	REDUCE
412-413	LINEAR
414-415	Floating Point Routines
416-423	DISPLAY
424-427	OUTPUT
430	DISPLAY
431-432	YONDER
433-434	PDP6

Blocks 470 to 476 are used as a temporary storage area by the DISPLAY subprogram. Blocks 500 to 560 hold the output of LINEAR which then is also the input data for DISPLAY. All blocks on the upper half of the tape, other than those mentioned above, are unused.