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AIPOS USER'S MANUAL



DEC-12-SQ1A-D

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PREFACE

The PDP-12 laboratory computer is prominent as a powerful assistant to scientific research. Now, as the PDP-12 LDP system, a complete, totally integrated data acquisition and manipulation facility is available for both low- and high-speed laboratory instruments. This manual details the operation of the software for the LDP system, AIPOS.

Chapter 1 includes a full explanation of the operation of the scope assisted function loader (Job Control), including optimization of available mass storage devices. All of the mathematical and display manipulation facilities for data files are described with examples of each command in Chapter 2 for the Display Oriented Research Analysis (DORA) program. Because of their similarity of operation, all the file handling functions are discussed in Chapter 3. Examples are included in all sections of the manual. The Appendices provide quick reference for loading procedures and command and error message summaries for all AIPOS users. A sequence of photographic examples of scope display can be found in Appendix C. For the experienced programmer who wishes to customize the LDP system, a series of internal descriptions are available (DEC-12-URIA-D through DEC-12-UR5A-D). Consult the glossary in the back of this manual for definitions of new terms.

Additional information on the PDP-12 computer, its operation, and programming terminology and techniques can be found in the PDP-12 System Reference Manual, DEC-12-SRZA-D, and the LAP6-DIAL Programmer's Reference Manual, DEC-12-SE2D-D.

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INTRODUCTION

AIPOS is the comprehensive operating system used on the PDP-12/40 and larger systems for real-time data acquisition and manipulation in the laboratory. It provides a convenient structure and common data base for a wide variety of functions, while retaining a simplicity and ease of use which makes it the perfect solution to the problem of effective usage of the computer in the laboratory.

The Job Control Language processor, referred to as JCL, provides a powerful link between the user and the various functions of the system. Aided by the highly interactive display, the user is guided through the specification of function requests, including input and output files, and function-qualification parameters. His function request is analyzed as he types it, thus reducing his waiting time, and permitting the dynamic detection and correction of errors.

AIPOS offers a complete set of data acquisition, data manipulation, and file handling functions. In addition, its modularity and flexibility allow AIPOS to be extended to reflect the state of the art in laboratory data acquisition, as well as the needs of highly specialized users. `

CHAPTER 1

USING THE LDP SYSTEM

1.1 SYSTEM FUNCTIONS

The many capabilities of AIPOS are grouped in units referred to as system functions. The eight system functions which provide all data manipulation and interpretation facilities are described in this manual. Briefly, they are:

- DORA Display Oriented Research Analysis display and math routines for viewing and manipulating acquired data.
- 2. File handling functions seven functions for manipulating stored data files.

Three other system functions are described in other manuals. Briefly, they are:

- 1. MIDAS Multiple Instrument Data Acquisition System data acquisition of several instruments simultaneously.
- MASH Mass Spectrometer Data Handler acquisition, interpretation, and filing for low resolution mass specs.
- RE-GC Research Gas Chromatography data acquisition and filing for up to eight GC's simultaneously and an off-line reporting program.

1.2 HARDWARE REQUIREMENTS

The minimum hardware required for AIPOS is:

PDP-12/40¹ AIP-12 Analytical Instrument Processor

Supported options include:

RK8 disk cartridge systems

1.3 JOB CONTROL

The AIPOS functions are called by issuing a function call command to <u>Job Control.</u> Essentially a program loader, Job Control verifies the Job Control can be run on a PDP-12/30. hardware configuration, activates the requested function and initializes the specified input and output files. A system function can only be requested via Job Control. Job Control is "on the air" after AIPOS is loaded initially (refer to Appendix A), after a CTRL/C is typed (refer to section 1.7), after a DX command (refer to section 1.8), and after processing is complete for a system function.

Job Control displays a series of messages to assist command input. The general format of a function call command is:

function output files = input files

As the user types in each part of the function call on the Teletype¹, it is displayed on the scope. Subsequent parts of the call are displayed on the same line. Each part of the call is interpreted by Job Control as it is typed by the user. If an error exists in the part just entered, an error message is displayed. The correct sequence may then be typed for the part in error without having to retype the whole command. The RUBOUT key can be used at any time to erase the last character typed. A backslash (\backslash) is echoed on the Teletype. The RUBOUT key can be used repeatedly to delete one additional character to the left each time it is pressed. The LINE FEED key can also be pressed to erase the entire command entered so far and to start a new function call.

1.4 MNEMONIC UNIT CODES

To specify an I/O device on a system function call to Job Control, the appropriate mnemonic code and the unit number, if needed, must be used. The codes are:

Mnemonic	Device
LTØ-7	LINCtape units Ø-7
DKØ-3	RK8 or RK12 disk units Ø-3
TTY	Console Teletype
DSP	Display scope (output device only)

Note that these codes are always followed by a colon in a system function call (refer to section 1.5).

If a nonexistent or off-line device is requested, an indicative message appears on the scope.

¹Teletype is the registered trademark of Teletype Corporation.

1.5 CALLING A SYSTEM FUNCTION

A command is entered by the following procedure. (Note that at least two mass storage devices must be on-line for a DORA function call to be accepted.)

1. Job Control always starts¹ by displaying the following initial message on the scope:

ENTER FUNCTION

DEV: FUNCTION

DEFAULT DEV= $(LT\emptyset)^2$

THEN SPACE TO SPECIFY OUTPUT, OR = TO SPECIFY INPUT.

- 2. Type the mnemonic unit code (refer to section 1.4) containing the desired system function. Terminate the three letter code with a colon. For example, LTØ indicates that LINCtape unit Ø is to be used. If the default device (refer to section 1.6) is the unit from which the function is to be loaded, then it need not be specified in the function call. Next, type the name of the function desired followed by the terminator space or the terminator equal sign if no output files are to be specified. For example, LTØ:DORA calls DORA from LINCtape unit Ø.
- 3. After a terminator is typed, Job Control checks the commands as entered so far for errors. If any are found, an error message indicating the problem is displayed. Use the RUBOUT key to delete the erroneous characters and type the correct command. (All the Job Control error messages are listed in Appendix B.1.)
- 4. If a space is typed as the terminator and no errors are found, a new message is displayed:

ENTER OUTPUT

DEV:FILENAM.EXT DEFAULT DEV = (LTØ) WHEN ALL OUTPUT HAS BEEN SPECIFIED, TYPE = TO SPECIFY INPUT

LTØ:DORA³

¹Job Control is started after loading AIPOS, typing a CTRL/C, completing a DX command or a function job. To type CTRL/C, hold down the CTRL key and type the letter C. The character C will be printed on the Teletype.

 2 The current default unit is displayed after the equal sign. Any time a terminator is typed, the unit may change. LTØ is used only as an example here.

 3 This is the start of the function call typed by the user. The command shown here is only an example. 1-3

- 5. The output devices and file codes are entered now for all output files that will be created by the requested function. The sequence DEV:FILENAM.EXT can be repeated up to eight times, once for each output file to be created, by separating each sequence with a comma. Type the mnemonic unit code (DEV), a colon, and the file name to be associated with this file. The file name is 1 to 6 characters long; the first character of the file name must be alphabetic and the file name must not already exist on the volume. An extension code of 1 to 3 alphanumeric characters may be added optionally after the file name and is always preceded by a period. In the example, some output files can be created: LTØ:DORA DK1:OUTF1,LT4:OUTF2. If the default device is the correct output device, the device and colon need not be specified; the file names are sufficient. No more than one output file can be requested for each on-line device. The extension code with a binary file, .BIN, has special meaning and can only be used for load files. After the last sequence has been entered, type as the terminator an equal sign to specify input, a semicolon to specify parameters, or a carriage return to terminate the function call.
- 6. After each comma and after the equal sign (or semicolon), Job Control checks for errors as in step 3. If the RUBOUT key is used to erase the entire output file sequence up through the space terminating the function specification, then the initial message is redisplayed and the function call may be reentered, as in step 1. When the output sequence has been accepted, another message is displayed:

ENTER INPUT

DEV:FILNAM.EXT DEFAULT DEV = (LT4) ; BEGINS PARAMETER INPUT OR RETURN BEGINS EXECUTION

LTØ:DORA DK1:OUTF1,LT4:OUTF2=

7. Specify the input files and devices in the same manner as the output files (refer to step 5). The example can be expanded to:

LTØ:DORA DK1:OUTF1,LT4:OUTF2=DK1:INF1,LT1:INF2,LT3:INF3

For an input file to be valid, it must be included in the volume's index. (Volume refers to the data on a LINCtape or disk.) Note that a maximum of 8 files (input and output, including automatically allocated working areas) can be specified in a single function call. After all files have been entered, the function call can be terminated by typing a carriage return; the command is then executed. If it is invalid, the message in step 1 is redisplayed. Alternatively, a semicolon can be typed, indicating that a parameter string will follow. As before, if RUBOUT was used to delete characters through a previous terminator (equal sign or space) the previous display appears until another terminator is typed.

8. If a semicolon is typed, the following message is displayed:

ENTER PARAMETER STRING ENDING WITH RETURN.

9. Some of the AIPOS functions may require a parameter string at the end of the function call. The format of this string is described in the appropriate chapter of this manual. In general, up to 32 characters are allowed; the legal characters are listed in Appendix A.3. Terminate the parameter string by pressing RETURN; the function call is then executed.

The following examples of complete system function calls illustrate some of the features of Job Control.

DK2:MIDAS LT3:DATA1.ASC,DK1:DATA2=LT1:SOURCE

The program MIDAS is to be called from disk unit 2 and will be used with the output files DATAL.ASC, located on LINCtape unit 3, and DATA2, located on disk unit 1, and the input file SOURCE located on LINCtape unit 1.

LTØ:TRANS DK1:PHENYL=DKØ:APHENYL

Call the TRANSFER function from LINCtape unit \emptyset and use it to transfer the input file APHENYL from disk unit \emptyset to disk unit 1 where it will be filed as PHENYL.

1.6 DEFAULT UNITS

If a device specification is omitted before a file or function name in a function call command to Job Control, the device last accessed by AIPOS when interpreting the command is the default unit. The device that is currently the default unit is displayed in all the relevant Job Control messages so the user always knows what device will be assumed. The unit from which the AIPOS Monitor is loaded is initially designated as the default unit. Thus, for a non-disk configuration, the initial default unit is LTØ; for a system loaded from disk, the

default unit is DKØ. When another unit is specified, it becomes the default unit for when a unit is not specified for a subsequent file. Thus, if at any time in the command a device is specified, that device becomes the default unit until another device is requested. For example, in the function call

DKØ:DORA FERRIC,DK1:FE26A=ETCL1,ETCL2,ETCL12

the function DORA and the output file FERRIC will be on disk unit \emptyset ; the other output file and all the input files will be on disk unit 1.

For output files, the default unit designation is more complex because no more than one output file can exist on any device. Thus, when specifying output files without requesting a particular unit, the default device is incremented after each file is accepted. Even if no output files are requested, some APOS programs require a minimum number of output (working) areas, so the system will automatically assign the appropriate number of output (working) areas. When no output device is specified, the default load unit will contain the first output area and the next sequential LINCtape will contain the second, etc. For all hardware configurations, only LINCtapes are checked for room for a second working area; no check is made for disks. (A Job Control assembly parameter must be changed for multiple disks.) The order in which devices are checked is shown graphically. The flow can be entered at any device, but note that unless a disk is explicitly requested, it is not accessed.

ORDER OF CHECKING

(after LT7, LTØ is checked next.)

For example, consider a single disk/2 LINCtape unit configuration where the LDP system device is the disk and the command request:

DORA NA1, NA2=NA3, NA4

The function DORA will be retrieved from $DK\emptyset$. The first output file, NA1, will be created on the disk also. The second output file, NA2, will be placed on the first tape unit. That tape unit will also be the device checked for the two input files, NA3 and NA4.

1.7 RETURNING TO JOB CONTROL OR DIAL

Any function in AIPOS can be interrupted at any time by typing CTRL/C which causes a return to the initial display of Job Control. The present operation is stopped immediately and another can be specified via Job Control. Note, however, that all data in the presently opened output files is lost when CTRL/C is typed.

When Job Control (or DISPLAY INDEX) is active, CTRL/D can be typed to exit from the AIPOS and load DIAL-MS¹ (the general purpose PDP-12 operating system.). If the system device is LINCtape, DIAL-MS will be loaded from tape unit \emptyset ; if the system device is disk, it is loaded from disk. Be sure DIAL-MS is on the appropriate unit; if it is not, AIPOS is restarted.

1.8 DISPLAY INDEX

In addition to the function calls, there is an auxiliary call, DISPLAY INDEX, that can be issued to Job Control. The file index of any mass storage device can be displayed by typing a command to Job Control in the format:

dev:DX

where dev is LINCtape, LTØ to LT7, or disk, DKØ to DK3. The file index contains information on the entire volume of data on the device, as well as on each file. Information displayed for the volume is its name, the starting block of the file area, and the length of the volume (number of blocks in the volume). Information displayed for an entry in the index is entry number (octal position in the volume), file name (and extension), starting block, and length of the file. An index header for the values is displayed as:

ENTRY STRT LEN

where STRT is the starting block and LEN is the length of the file in blocks. In general, the last file in the index is always WORK AREA

¹LAP6-DIAL-MS is referred to as DIAL-MS in this manual. Refer to the LAP6-DIAL Programmer's Reference Manual for information on the system.

and indicates how much space is still available (LEN) on the volume for additional files. The WORK AREA entry is not displayed if either the volume or its index is full. The first user file is entry number 3; the volume identification, the Monitor, and Job Control are entries \emptyset , 1, and 2, respectively.

The first six entries in the index are displayed as a frame when the index is initially called. A different set of six index entries can be displayed, the index can be printed, a file can be deleted or retitled, or an alias can be assigned by typing the appropriate key, as indicated in the following table.

Key

Function

F	Move display forward l frame
В	Move display backward l frame
line feed	Move display forward l line
alt mode	Move display backward l line
L	Locate display for a file
Р	Print the index on the Teletype
D	Delete a file
R	Rename a file (remove old name)
A	Create an alias for a file
return	Return to Job Control

If F is typed the next six entries in the index are displayed (or the last six entries if there are not six more); conversely, if B is typed, the previous six entries are displayed. F or B can be typed as many times as necessary to examine any section of the index.

When P is typed, the index currently displayed and header information for the volume are printed on the Teletype. In addition, the message SYSTEM or NO SYSTEM is printed after the index information so that the user will know if this is a system volume.

A specific file entry included in the index can be displayed by typing the letter L and the name of the desired file.

A file may be deleted permanently from the volume by requesting the D option.

To facilitate filing operations for special purposes, such as replacing a standard waveform, the index options Rename and Alias are provided.

When it is desired to have a new output file with the same name as an existing file on the same unit without deleting the old file, the name of the old file can be expanded to include an extension such as .BAK for backup by using the Rename option. The new file can then be created on the same volume and checked out before deleting it in the backup version. If the new file is found to be incorrect, it can then be deleted and another attempt made at creating it, or the backup version can be renamed with the correct name and used as it was initially.

The Alias feature is most commonly used for a binary program that can perform many functions. For example, the seven file handling functions described in Chapter 3 use the same basic program internally; the specific function to be performed is determined by the function name typed in by the user in the command to Job Control. This procedure relieves the user from having to issue another command to specify the exact function desired after having called the general program. Thus, using the Alias feature, one file handling program is called by any one of six names (TRANS, CREATE, etc.).

If L, D, A or R is typed, the following message appears on the scope above the index display:

ENTRY OR FILE NAME REPLY:

Type either the number or the name (and extension) of the entry to be manipulated as it appears in the display and press RETURN. If this index operation is not to be performed, press RETURN alone to redisplay the initial index display. If L and a file name are entered, the index displayed will include that file. If D and a file designation are typed, the deletion is performed immediately and the initial index display reappears. If A or R is typed, and the file designation is valid, a new message appears above the index display:

> NEW FILE NAME REPLY:

Type the alias or the new name to be assigned to the file followed by a carriage return. When the operation is completed, the initial display with the modifications appears.

A carriage return is used to exit from the DISPLAY INDEX function and return to the initial display of Job Control, incorporating all the changes requested on the volume. If CTRL/C is typed to return to Job Control during an index sequence, none of the index changes entered since requesting DISPLAY INDEX from Job Control are recorded in the volume's index.

CHAPTER 2

DISPLAY ORIENTED RESEARCH ANALYSIS

2.1 DORA'S CAPABILITIES

After acquiring data from appropriately interfaced instrumentation, the data files can be displayed and interpreted by requesting the AIPOS function DORA. Mathematical operations are executed immediately by DORA and the resultant spectrum displayed on the scope (see Appendix C). DORA consists of a large group of math commands that include, in part, capabilities to integrate or differentiate a file, calibrate the axes, straighten a sloping baseline, subtract one file from another, invert the display and many more. There are two main classes of DORA's commands - math and display. Both classes implement two cursors to define regions on the waveforms and a group of Sense Switch and A/D knob options to move the displayed files on the scope.

2.2 COMMAND FORMAT

DORA's math and display functions are requested by commands typed by the user on the Teletype. The general format for these commands is a 3 or 4 character command designation, a semicolon, and a file definition. All commands are terminated by pressing the RETURN key. RUBOUT may be used before terminating the command to delete incorrect characters. The exact syntax for each is included in the command discussion in this chapter and in the summary in Appendix A. Note, however, that DORA commands which are in a format acceptable to Job Control, but illegal to DORA (e.g., unnecessary parameters) are accepted (and ignored) by DORA and no error message is issued. It is also possible for commands that are accepted by DORA not to be accepted by Job Control. For example, illegal Job Control characters are not checked by DORA. Job Control either displays an error message or attempts to make the file name acceptable. All commands are interpreted sequentially and as much as is coherent to DORA will be executed.

2.3 WORKING AREA ASSIGNMENT

DORA is requested from Job Control by a function call in the general form:

dev:DORA outdev_i:outfile_i=indevg:infileg,indev1:infile,

where $\operatorname{outfile}_i$ is an output file and $\operatorname{infile}_{\emptyset}$ and infile_1 are input files. More than two input files can be specified in the function call, but DORA accepts only the first two requested. These files must be in floating point format; if they are not, they must be reformatted using the AIPOS TRANSFER function (refer to section 3.4.2).

After the input files are specified to Job Control, DORA creates three working areas, each of which initially contains a copy of one of the original files, and which will, during processing, contain the current version of the data files. These areas are referred to as working areas \emptyset , 1 and T. Initially, working areas 1 and T each contain a copy of infile and working area \emptyset contains a copy of infile \emptyset . This initial allocation can be considered graphically:



The constants \emptyset and 1 are used in DORA commands to refer to the files in working areas \emptyset and 1. Using the DORA commands, files \emptyset and 1 can be modified, but the original data files are always left untouched. Thus, working areas \emptyset and 1 are temporary storage areas for the permanent files. The devices that contain the working areas are derived from the output files specification to Job Control. If two output files (and hence two devices) are specified, those devices will hold DORA's working areas. If no output file is specified, the device that will contain the working area is as defined for default devices, section 1.6. For system optimization, two output files should be specified, particularly for disk configurations that are started from LINCtape, so that Job Control is cognizant of all available devices. Devices that are not defined in the DORA call to Job Control or do not have a sufficiently large working area are not used by DORA. Working area allocation requires that sufficient space is available on the specified (or default) devices. If a disk is available, DORA tries to put both working areas there rather than one on disk and one on LINCtape for I/O optimization. For example, the call

LTØ:DORA DKØ:OF1,LT1:OF2=DKØ:IF1,IF2

creates working areas, if there is enough space on $DK\emptyset$, as:



If there is not sufficient room, the next working area allocation tried is:



It is always true that an output device with a working area that is larger than three times the size of the biggest input file plus thirty blocks is big enough to contain all of DORA's working areas. DORA requires at least one working area, i.e., output device. For I/O optimization it is recommended that LINCtape users default to one output device and specify another to Job Control. Systems with a disk need only default to the disk for output device specification.

2.4 USE OF THE DISPLAY SCOPE

The display scope is considered as having two parts, referred to as top and bottom, each of which displays a data file that is contained in the working area. The top of the scope AlWAYS contains the file in working area T; initially, the bottom contains the file in working area \emptyset . By using the MOVE command (refer to section 2.6.1) the bottom of the scope can display the contents of working area \emptyset or 1. For ease of reference, the file displayed in the top of the scope (the contents of working area T) is called file T and the one displayed in the bottom is referred to as file B. The user always knows which working area, \emptyset or 1, is currently being displayed in the bottom of the scope because the appropriate number is displayed in the lower right hand corner of the screen. Almost all of the DORA commands use the abbreviations T and B to refer to scope positions; the commands also generate changes in the appropriate working area. When necessary, an operation on file T changes the contents of working area T and an operation on file B changes the contents of working area \emptyset or 1, whichever file is currently displayed in the bottom of the scope.

The diagram in section 2.3 can be expanded to include the initially displayed files:



2.4.1 Data Display

When a new data file first appears on the display, its largest point is displayed at the top of the scope and the smallest at the bottom¹. 510 points are displayed along the X axis for floating point files; if a file has less than 510 points, enough of the file is redisplayed so that there are 510 points visible on the X-axis.

The X range of the data is determined by a moving window so that the whole file can be scanned and any contiguous section of data can be displayed at a time by locating the window over that section. The files may be displayed on a split scope with file T in the top half and file B in the bottom half or on a full scope with both files occupying the full length of the scope.

¹The scope values are single precision counterparts of the raw data and should be interpreted as relative values. Thus, a point in the middle of the scope can represent a value of 5×10^6 . The scope is considered to have limits of ± 377 .

2.4.2 Moving the Displays

Both the top and the bottom files can be moved horizontally at any time, and the top file can be moved vertically, but horizontal motion cannot be concurrent. Thus, the scope can be used to compare a modified spectrum with the original data or to compare an unknown spectrum with an identified curve.

The console Sense Switches are used to define the location and direction of the motion of the spectra, as follows:

Sense Switch	Value	Effect
ø	Ø 1	Full scope Split scope
1	Ø l	Fine horizontal motion Coarse horizontal motion
2	Ø l	Set horizontal motion for file T Set horizontal motion for file B
3	Ø 1	Inhibit vertical motion Enable vertical motion for file T

The speed at which a data file moves horizontally across the scope (the moving window) is controlled by A/D knob \emptyset . The Sense Switches must be set properly for knob \emptyset to move the desired file. Turning the knob clockwise increases the rate of motion in the forward direction; turning it counterclockwise increases the rate in the reverse direction. By centering knob \emptyset , horizontal movement of the display is halted.

Knob 4 controls vertical motion of file T like a fine tuner. The file will move only as long as the knob is rotated and then the display freezes. Knob 4 can then be rotated again to move the file another small increment. When Sense Switch 1 is set to \emptyset for fine horizontal control, knob \emptyset also becomes a fine tuner. Thus, if two spectra are to be lined up, the recommended procedure is to set Sense Switches $\emptyset=\emptyset$, 1=1, and 2=the file to be moved. Then rotate knob \emptyset until the desired segments are almost superimposed. Use knob 4 if necessary. Set Sense Switch 1= \emptyset and rotate knob \emptyset to match the spectra.

As file T is being moved in any direction by a combination of Sense Switches and A/D knobs, it will wrap around along either or both axes. Thus, the first and last points in the file appear to be contiguous and Y values that are moved past the upper limit of the axis appear at the bottom of the file's display. File B can also wrap around the X axis.



Horizontal motion of the file can produce a display, as charted above, where point a is the last point in the file and b is the first point.



Vertical motion of file T can produce this display with vertical wraparound as the spectrum moves up (or down) the scope.

2.4.3 Use of Cursors

DORA implements two cursors on the scope, referred to as cursor \emptyset and cursor 1, which appear as intensified dots and are used to mark off areas on the spectrum. Initially, both cursors are associated with file T. The X and Y coordinates of the current location on the waveform of cursor \emptyset on the scope are displayed in the upper left corner of the scope and those of cursor 1 are displayed in the lower left corner. These coordinates are relative scope values and are not the actual data values. All values are signed six digit numbers and include calibrated values. A/D knobs are used to move the cursors, as follows:

	Mot	ion
	Horizontal	Vertical
Cursor Ø	knob l	knob 5
Cursor 1	knob 2	knob 6

Rotating knob 1 or 2 clockwise moves the appropriate cursor to the right; counterclockwise moves it to the left. Similarly, for knobs 5 and 6, clockwise rotation moves the cursor upward and counterclockwise moves it downward. These cursors are said to be "fixed" initially, i.e., they can only ride along the data curve so that only the A/D knobs control-ling horizontal motion are operable. (DORA includes commands to change

the cursors' assignment. Refer to section 2.5.1.)

The following is a graphic summary of the functions of the A/D knobs and the Sense Switches.



SENSE SWITCHES

IG ATD KINOBS 10 AIND 4



A/D KNOBS

2.5 CURSOR COMMANDS

Cursors are either "fixed" or "free". A fixed cursor rides along the displayed spectrum such that only horizontal motion is permitted. A free cursor can move anywhere within its assigned section (top or bot-tom) of the scope, enabling horizontal and vertical motion. Using the cursor commands, the cursors can be assigned to different spectra, freed, or fixed so that they are properly positioned for a subsequent math command.

2.5.1 ASSIGN CURSORS

Many of DORA's math commands require one or two cursors to indicate user chosen data points in the spectrum. Using the ASSIGN CURSORS command, the two available cursors may be assigned to the same spectrum or to different spectra on the display.

The command format is:

ASCU;alpha

where alpha is T or B.

To assign both cursors to the file displayed in the top, the command is

ASCU;T

To assign both the cursors to the bottom file, the command is

ASCU;B

If the alpha parameter is omitted, cursor \emptyset is assigned to file T and cursor 1 to file B. The command is then simply

ASCU

The initial DORA display places the two cursors in the default location: both on file T. If this cursor assignment is satisfactory for the current set of data, there is no need to issue an ASSIGN CURSORS command.

2.5.2 FREE CURSORS

A FREE CURSORS command can be issued to free fixed cursors at any time and is in the format:

FRCU; numeric

where numeric is \emptyset or 1. If no numeric parameter is supplied, both cursors are freed.

When a subsequent ASSIGN CURSORS command is issued, there is no change in the "free" state of a cursor. Thus, an ASSIGN CURSORS command in the form

ASCU

associates cursor \emptyset with file T and cursor 1 with file B, and leaves both cursors in the free state.

2.5.3 FIX CURSORS

After the cursors have been freed by a FREE CURSORS command, they may be fixed by issuing a command:

FXCU; numeric

where numeric is \emptyset or l. If no numeric argument is typed, both cursors are fixed. Each cursor will be assigned to the point on the spectrum with the same X value as the cursor at the time the FIX CURSORS command is issued.

2.6 FILE MANIPULATION COMMANDS

DORA provides capabilities for moving displayed data files and for saving input files, permitting file manipulation facilities without having to return to Job Control.

2.6.1 MOVE

After calling DORA from Job Control, the first input file is assigned as file T and the second as file B and the working areas and scope are filled accordingly. At any time, these file assignments can be altered

by a MOVE command in order to compare modified data with the original file; use a different sequence of commands on the original data file; or display another file. There are six data sets that can be accessed by a MOVE command.

file T	-	currently displayed in top of scope and located in working area T
file B	-	currently displayed in bottom of scope and lo-cated in working area \emptyset or l
file Ø	-	file in working area $ otin$
file l	-	file in working area l
file X	-	original data of the input file requested first to Job Control
file Y	-	original data of the input file requested second to Job Control.

The current content of file B is indicated by the number (\emptyset or 1) displayed in the lower right corner of the scope. This number is the input file that is currently file B and is consistent with any previous MOVE commands.

The first input file specified to Job Control can be referred to by the designation X in the MOVE command and the second input file by the letter Y. The constants X and Y refer to the original input files and can not be modified by any DORA command; the designations are used only by the MOVE command to relocate the files. If a second input file was not specified in the DORA function call to Job Control, Y is an illegal parameter.

The format of the MOVE command is

MOVE; i, o

where i is the input file and is any one of the set $\{\emptyset, l, T, B, X, Y\}$ and o is the output file and is any one of the set $\{\emptyset, l, T, B\}$. Up to three pairs can be supplied at a time and the moves will be executed sequentially. When the output files are specified, the previous contents of the files are replaced. By using care in the parameter sequence of the command, however, any file of interest can be maintained. Consider the following examples.

MOVE;X,T, \emptyset ,B

File X, the original data for the first input file to Job Control, is to be moved to working area T and displayed on the top of the scope and file \emptyset , located in working area \emptyset is to be displayed in the bottom of the scope.

MOVE;Ø,T,1,B

This command will reverse the original DORA scope assignments. File \emptyset will be displayed in the top of the scope and will be placed in working area T; file 1 will be displayed in the bottom of the scope. The copy of file \emptyset that was placed in working area T initially is replaced during this MOVE command.

MOVE; T, Ø, Y, T, 1, B

A command like this one will save the file displayed in the top of the scope by moving file T to working area \emptyset , bring in a copy of the second input file and place it in working area T. File Y will be displayed in the top of the scope and file 1, the contents of working area 1, in the bottom of the scope. This is illustrated in the following chart.



2.6.2 SAVE

Any of the data files in DORA's working areas, files \emptyset , 1, T and B, can be saved on LINCtape or disk for permanent storage and subsequent retrieval. The SAVE command associates a name with the file and stores the file on the mass storage device where its working area is currently located, noting its location by a message on the Teletype. The working area units are those specified as output units to Job Control for the DORA function call (or the default devices if none were specified to Job Control). When the SAVE command is completed, it causes a return to Job Control.

To save a DORA file, issue a command in the format

where name₁ is the alphanumeric name (in the format required by Job Control) to be assigned to the file and p_1 is the parameter indicating the file to be saved in the set \emptyset ,1,T or B. For every name, a parameter must be specified. From one to three names and parameter pairs can be included in a SAVE command. No two files can be saved on the same device with the same name. If the file parameters are omitted, the sequence \emptyset ,1,T is assumed. Thus, SAVE F1,F2,F3 is equivalent to SAVE F1,F2,F3; \emptyset ,1,T. After the SAVE command is accepted, a message indicating the location (unit) of the files is printed on the Teletype in the format:

$$B, \emptyset, 1 = unit$$

T = unit

For example, after the command

SAVE SAMP1, SAMP2;1, T

a possible printout is:

$$B, \emptyset, l=DK1$$

 $T = LT2$

The SAVE command is used to save files on LINCtape or disk; for this reason there is generally no need to specify output files during a DORA function call to Job Control. Output devices need only be specified when a particular device (e.g., a second disk) is to contain the working areas and would not be called by the usual default device sequence.

2.7 TYPES OF MATH COMMANDS

DORA has two classes of mathematical routines:

- Unary only one file is manipulated; the resultant file replaces the displayed file on the scope and in the working area.
- Binary both displayed files (T and B) are manipulated; the resultant file always replaces file T on the scope and in working area T.

While most math commands are being executed, the scope is blank and is replaced with the resultant data display when the result has been calculated.

2.8 UNARY COMMANDS

The unary commands always require the file specification T or B; thus, their command format is

command; alpha

where command is the 3 or 4 character abbreviation for the operation and alpha is T or B. A cursor parameter is also used with some commands. All commands are terminated by a carriage return.

Any unary operation performed on file T changes that data in working area T; any unary operation on file B changes that data in working area \emptyset or 1, whichever file is displayed in the bottom of the scope. The data in the file is changed as specified for each command.

Some of the unary commands require specification of a value for a constant, K. The acceptable range is $-999,999 \le K \le +999,999$. Decimal points may be included providing accuracy of 1 in 10⁶. The values may also be signed (±). Thus, acceptable constants include

+3.14159 14.0067 -3.045 96487

Note that exponential notation is illegal when specifying a constant. For the commands requiring constants, a line feed can be typed before the last value is supplied to abort the command and request another.

2.8.1 OFFSET Y-AXIS

The range of a displayed spectrum along the Y-axis is initially the raw data values, but can be modified to produce a zero baseline, to view the maxima of strong absorption peaks, or to prepare the spectrum for a subsequent DORA command. The amount of offset is specified by locating one cursor at the point on the spectrum to have a Y value of zero. That value is subtracted from all the points in the data file. The point where the cursor is located will have a Y-axis value of zero in the file. The Y-axis offset operation is specified as follows:

- 1. Locate one cursor at the point on the curve to be the zero value. The other cursor can not be associated with the file to be offset. (Use an ASSIGN CURSORS command if necessary.)
- 2. Issue the command in the form

OFFY; alpha

where alpha is T or B, whichever file is to be moved. Press RETURN. The calculation is performed and the result displayed on the scope.

All scope displays are relative to a pair of normalization constants. Associated with each display is a pair of MAX-MIN values either preset (default case) or obtained from the normalization routine (NORM). This pair of MAX-MIN values is used to calculate the normalization constants. Thus, if a data file is changed and not NORMalized, it will then be displayed using the last calculated normalization constants. This factor should be remembered particularly when using the OFFY command.



Consider a file whose MAX <u>data</u> value is 1.25 and whose MIN <u>data</u> value is .25.

If the cursor is positioned at pt. a and an OFFY command is issued, the new file will have a MAX data value of (1.25-.5)=.75 and a MIN data value of (.25-.5)=-.25. However, because the data has not been normalized yet, the normalization constants have not changed and the display will be as shown in figure 1. If this data is now NORMalized, it will be displayed as in figure 2.


NOTE: A pair of coordinate axes have been included with these figures to give perspective to the data. The horizontal axis indicates the point number of the file; the vertical axis designates the corresponding file <u>data</u> values. These values are not necessarily the same as observed in the scope cursor read-out.

2.8.2 CALIBRATE X-AXIS

An X-axis value can be assigned to any data point in a displayed spectrum, thereby permitting user specification of the X-axis coordinates. From two to four values in increasing order along the X-axis can be assigned to a spectrum at a time by setting the cursor to the proper location. Only one cursor can be associated with the spectrum for this calibration; an ASSIGN CURSORS command may therefore be necessary. The assigned values are stored with the data file so that future Xaxis operations, such as baseline stripping, utilize the new parameters for the display, but the actual data values are unaltered. This calibration facility is particularly useful for spectra with wide areas that are not of interest.

To calibrate the X-axis:

1. Call the routine by typing the command

CALX;alpha

where alpha is T for the top curve or B for the bottom curve. Press the RETURN key.

2. After the message

K=

is printed on the Teleype, rotate the cursor assigned to the curve via its A/D knob to locate the cursor at the desired point on the curve. The other cursor can not be associated with the spectrum being modified. When the cursor is correctly located, type the value to be assigned to the X-axis at that point, followed by a carriage return.

- 3. The same message, K=, is printed again so that a second value may be assigned to the spectrum. Remember that the X-axis values must be specified in increasing order along the X-axis, but any value, K, can be assigned to any location in the spectrum. An error message and repeated request for the value of K will be printed if an attempt is made to assign a value in X-axis coordinates lower than or the same as the preceding coordinate.
- 4. At least two values must be assigned for K. The message K= is printed a maximum of four times; if less than four values are desired, type a carriage return after the next K= message and the calibration will be performed; if four values are desired, the calibration will be performed after the fourth value is specified.

After a CALX operation, increments along the X-axis are not necessarily equal.

2.8.3 CALIBRATE Y-AXIS

The Y-axis of a spectrum displayed as peaks may be calibrated for values in the range $1 \le K \le +1 \emptyset \emptyset$, effectively making the Y-axis a percentage scale over a user determined range. For a spectrum displayed as dips, values in the range $-1\emptyset \emptyset \le K \le 1$ can be used. By permitting negative values for inverted files, the Y minimum is always more negative than the maximum. Only one point in the data set requires specification; the rest of the Y values in the file are adjusted relative to the indicated value. The data in the file is not altered by a Y-axis calibration. Only the value of K is retained so the display is accurate.

The new value associated with any point can be determined using the proportion

$$Y_D = K \frac{Ya}{Yc}$$

where Y_D is the new value of some displayed point D; K is the value from 1 to 100 or -100 to -1 assigned to the cursor at the original scope ordinate value Y_C ; and Y_a is the scope ordinate value of the point D. Thus, if a point is one quarter of the way up the Y scale and is assigned a value of sixty, then a point that is half way up the Y scale automatically receives a value of 120, as determined by $Y_D = 60\frac{.50}{.25}$ where percentage values are used for the half and quarter way points.

To calibrate the Y axis, proceed as follows:

1. Type CALY; alpha

where alpha is T or B.

2. After the message K= is printed, use the A/D knob associated with the cursor to locate it at the desired point on the spectrum. The cursor can not be located at the bottommost (-377) Y location when typing positive K values. (The other cursor can not be associated with this curve.) Then type in the relative value (K in the equation above) from 1 to 100 to be associated with this point. When the command is executed, the only visible change in the display is the cursor readout for the Y value.

2.8.4 SCALE

If the entire Y range of a set of data is too large or too small for a useful scope display, each Y value in the file can be multiplied by a constant, K, to bring the data into a suitable range using the SCALE command. The constant is specified in the same manner as the constant for the calibrate commands; after issuing the command as

SCA; alpha

where alpha is T or B for the top or bottom spectrum, the message K= is printed. Type the scale factor and press RETURN. The scaled spectrum is displayed in its portion of the scope and the file is altered in its working area. The other spectrum is unmodified.

2.8.5 STRIP BASELINE

A sloping baseline can be subtracted from any section of a data set by placing the two scope cursors so they define the slope of the baseline to be stripped. The line that is subtracted is the straight line between the cursors. The value subtracted from any Y value is the ΔY between the cursor line and a baseline created through the lower cursor. Note that the cursors may or may not be fixed to the curve; only the slope of the line between them is important. A baseline can not be "added"; the STRIP BASELINE command only subtracts values from the curve starting from the smaller Y value. Remember that any previous changes to the data by other DORA routines are considered in this calculation.

The procedure for subtracting a baseline is as follows:

- 1. The cursors must be properly positioned before the command is issued. If a baseline is to be stripped from all the data points, set the two cursors so they demark a line with the desired slope. If a baseline is to be stripped from only a portion of the data points, locate the two cursors so that, in addition to creating a line with the desired slope, one is on or above the first point in the baseline to be altered and the other is similarly located for the last point.
- 2. Call the routine by typing:

BLS;alpha,C

where alpha is T or B, and C is optional; if the baseline indicated by the two cursors is to be subtracted only from those points between the cursors, then the argument C is required in the command. If that baseline is to be subtracted from all the data points, the argument C is omitted.

2.8.6 STRIP PEAK

A peak or any section of a spectrum can be stripped from the data and replaced by a linear data set using the PEAK STRIP command. The cursors are located on the curve to indicate the region to be replaced and may include any displayed region of the spectrum. The peaks are stripped between the cursors from the lower X value to the higher X value.

An unlimited number of peaks can be removed; each will result in the straight line formed between the cursors replacing the data. Because both cursors must be on the same curve before issuing the command, an ASSIGN CURSORS statement may be necessary. If a CALX operation has already been performed on that part of the data to be peak stripped, then two connecting lines with different slopes may replace the peak. The procedure to strip out a section of data is:

1. Locate the cursors on the curve so they mark the beginning and end of the data to be replaced by a straight line with the slope indicated by the cursors.

2. Type the command as:

PKS; alpha

where alpha is T or B for the curve to be peak stripped.

2.8.7 NORMALIZE

When DORA displays a set of data after some mathematical operations, the points that are larger than the scope limits of ± 377 appear at the top of the scope with no definition of the large peaks. Also, the smaller peaks may not be sufficiently resolved. The NORMALIZE command performs two functions:

- 1. Brings the entire file within scope limits.
- Enlarges the file so that user's specified maximum and minimum points are the scope Y-axis limits. (This function requires that both cursors be assigned to the spectrum.)

NORMALIZE does not change the data in the working area. Instead, the necessary constants are stored with the data so that the file displayed after other commands includes the effect of the NORMALIZE command, leaving the actual data unaltered.

To normalize the entire file to scope limits, issue the command as

NORM; alpha

where alpha is T or B for the file to be normalized.

The second function enlarges small peaks by normalizing them to the scope limits. Position the cursors so that one defines the Y-axis minima and the other the Y-axis maxima and type the command as

NORM; alpha, C

The entire file is enlarged and Y values that are larger than +377 appear as points at the top of the scope and those smaller than -377 appear as points at the bottom.

2.8.8 INTEGRATE

An integration can be performed for a displayed spectrum that uses the algorithm:

$$A = \sum_{i=0}^{n} \frac{(Y_i + Y_{i+1})}{2} \Delta X$$

where $\Delta X = X_{i+1} - X_i$.

The X_i values used are the calibrated values resulting from a preceding CALX command, if issued. The first data value of the file is assigned a value of \emptyset .

The command format is:

INT; alpha, C

where alpha is T or B and C is optional. If the entire spectrum is to be integrated, the argument C is omitted from the command. If only a portion of the curve is to be integrated, locate the cursors at the initial and final points to be calculated and then issue the INT command with the argument C after alpha. The integrated data replaces the old data in the working area.

For best results with the INT command, it may be helpful before issuing the command to:

- 1. use the OFFY function to set the baseline to \emptyset
- 2. use the CALX function to assign the proper X range

2.8.9 DIFFERENTIATE

The derivative of a whole or part of a spectrum is calculated by the five point differentiation algorithm where the first two and last two points in the file can not be differentiated:

For
$$F = \{ (X_i, F(X_i)) \}$$

 $D'F = \frac{\Delta Y}{\Delta X} = \frac{Y_{n+4} - Y_n}{X_{n+4} - X_n}$ for Y_n = some data value
for X_n = some calibrated point count

Multi-depth derivatives can be determined. The derivative curve is displayed immediately after it is calculated. The command format is

DIFF; alpha, C

where alpha is T or B, and C is included only if the part of the spectrum between cursors is to be differentiated. If only part of the curve is to be differentiated, locate the cursors so they mark off that portion of the spectrum before issuing the command. If the whole spectrum is to be differentiated, cursor location does not matter.

2.8.10 SMOOTH

Noise can be smoothed from an entire spectrum or from the portion that lies between the two cursors by a least (7 point) squares curve fit routine. At least seven data points must be included between the cursors. The algorithm used is:

$$Y'_{i} = C_{1}(Y_{i+3} + Y_{i-3}) + C_{2}(Y_{i+2} + Y_{i-2}) + C_{3}(Y_{i+1} + Y_{i-1}) + C_{4}(Y_{i})$$

where Y_i = point to be smoothed Y'_i = smoothed point

The format of the SMOOTH command is

SMO;alpha,C

where alpha is T or B and C is included only if the portion between cursors is to be smoothed. Locate the cursors so they denote the portion of the waveform to be smoothed before issuing the SMOOTH command.

2.9 BINARY COMMANDS

The binary commands use both files T and B and place the resultant data in file T. The length of the resultant file is always equal to the length of the shorter input file. Because no parameters are needed, each of the four binary commands is issued simply by typing the appropriate code followed by a carriage return. Each of the binary commands is described below.

2.9.1 ADD

File B is added to file T and the sum file displayed in the top of the scope (as file T) by the command ADD.

2.9.2 SUBTRACT

File B is subtracted from file T and the difference is placed in file T by using the command SUB.

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2.9.3 INVERSE SUBTRACTION

The SUBTRACT operation can be reversed via the ISB command; file T is subtracted from file B and the difference is placed in file T by the inverse subtraction routine.

2.9.4 OFFSET X-AXIS

When two spectra are displayed at the same time, an OFFSET X-AXIS command can be issued to line up any two points on each spectra, so that the spectra have common X-axis values. The cursors are used, one on each spectrum, to determine the corresponding points. When the command is executed, the file with more points to the left of the cursor location has sufficient points deleted from its start so that the two X-axis values coincide.

To offset the X-axis, locate the cursors at the X locations that are to correspond with each other, one on each curve, and type the command OFFX. Note that the resultant file must be at least one block long or the files can not be offset.

2.10 DISPLAY COMMANDS

In addition to the math routines, DORA implements several commands to maximize scope interaction which can be issued to invert the spectrum, remove a spectrum from the scope or generate a hard copy on an inter-faced X-Y plotter. These commands are called in the standard DORA format.

2.10.1 VIEW

At any time while using DORA, a single file can be viewed on the scope. If only one file is currently displayed, the VIEW command re-enables the inactive display. The format of the VIEW command is:

VIEW; alpha

where alpha is T or B for the file to be displayed. Only one alpha value can be specified. If no parameters are entered after VIEW, then any file not currently displayed because of a previous VIEW command is redisplayed.

2.10.2 INVERT DISPLAY

A spectrum displayed on the scope can be inverted (peaks to dips and vice versa) and its complement displayed. Math commands can then be performed on the inverted file. One or two spectra can be polarized on the inverted file. One or two spectra can be polarized by a statement in the form

INVR; alpha

where alpha is T or B. To invert both displayed files, the command is

INVR;T,B

An INVERT command issued without any parameters returns all displayed files to their original state (peaks or dips). (If both parameters are the same, e.g., INVR;T,T, no effective operation is performed.)

The INVR command leaves the baseline invariant for both full and split scope, i.e., points that are displayed at the bottom or middle of the scope are never inverted:





*NOT INVERTED

Users who would like a real INVR can always scale by -1 with the realization that the original data was modified. Note that if the scope is inverted prior to a MOVE command, it remains inverted after the command. In general, the INVR command is invariant with the MOVE command.

2.10.3 PLOT

The PLOT command can be used to print up to six line plots of any displayed spectrum on an interfaced X-Y plotter permitting multiple plots of a file. When a PLOT command is issued, the scope is cleared. At this time, turn the plotter to start; plotting is then initialized by typing any key on the Teletype (not including CTRL/C or RUBOUT) and a moving dot traces across the scope. When the plot is completed, the scope is again cleared. Turn off the plotter, then type a key. When the display reappears, another DORA operation can be requested.

To generate line plots:

- 1. Request all math and display operations so that the file on the screen is exactly the plot desired.
- 2. Up to six plots can be requested for either displayed file or any combination of them. The plots will be drawn in the order in which they are specified in the command. The format is:

PLOT; alpha, alpha, alpha, alpha, alpha, alpha

where any one alpha is T or B. Specify the PLOT command with 1 to 6 alpha parameters and press RETURN. (If no parameters are specified, file T then file B are plotted.)

- 3. When the screen becomes blank, turn the plotter on, then type a key on the Teletype.
- 4. During plotting a moving dot traces across the scope. Turn the plotter off; then type a key on the Teletype. The display will reappear.
- 5. If more than one file is being plotted, an additional Teletype key must be typed between the plots (i.e., a total of 2 keys); one to terminate the current plot and one to initiate the next plot.

CHAPTER 3

FILE HANDLING FUNCTIONS

3.1 FILE MANIPULATIONS

AIPOS includes extensive file handling facilities that are implemented using a one word code in the function call to Job Control, as follows:

Code	Operation
MOVE	Move data files specified either by AIPOS file name or by starting block and number of blocks or points between tape and disk.
TRANS	Change the data format of the file during a file transfer.
PRINT	Print a data file and its header on the Teletype.
DISHDR	Display the header information of a data file on the scope.
FIXHDR	Create and store the primary header block.
INTERP	Interpolate input file to a specified output file size.
CREATE	Create data files on tape or disk.

Any of the seven file handling functions¹ is requested by typing the code for that function and the files it is to use in the same manner as any other call to Job Control, at any time when the system is under Job Control.

3.2 DATA FORMATS

Some of the file handling functions (TRANS, INTERP, CREATE) require specification of the file's data format. There are four acceptable data formats:

single precision signed integers double precision signed integers double precision signed fractions floating point

After requesting those functions, a message is displayed to permit specification of the output file format:

Do not use the Alias or Rename feature of the DISPLAY INDEX function to rename any of the file handling commands.

```
OUTPUT FORMAT

1 = S.P. INT.

2 = D.P. INT.

3 = D.P. FRAC.

4 = FLT. PT.

REPLY
```

The format is specified by typing the appropriate number (1-4) and pressing RETURN. A reply other than 1 to 4 causes the message to be redisplayed. An input file that is not an AIPOS file also requires format specification. For that purpose, the above message is displayed with the header INPUT FORMAT and is answered in the same manner as the output format messages.

It is possible to change the format of a file by using the TRANS function. It should be noted however that each format has its own characteristics; therefore numbers which may be represented in one format may be nonexistent in another. For example, the floating point number 3.5 is a 3 in double precision integer format. In general, any file may be converted to floating point format without losing any precision. When changing the format of a file, values in the input file that are out of the range of the output file are set to the closest limit of the format of the output file. The format ranges used:

-2Ø48	Single	precision	integers	2Ø47	
99999 <u>9</u>	Double	precision	fractions	+.999999	
838861×10^{7}	Double	precision	integers	+.838861 x	: 1Ø7

3.3 FUNCTION CALL FORMAT

Each of the six file handling functions is called through Job Control by a statement in the form:

dev:function outdev:outfile=indev:infile

The normal sequence of Job Control messages are displayed and answered as described in section 1.5. Default devices are determined in the same manner as explained in section 1.5. All of the file handling functions return to Job Control after completing the requested operation.

It is possible to specify an input and/or output file by starting block and number of blocks or points rather than by file name by simply not including the name in the function call. Thus, legal calls include:

```
dev:function outdev:outfile=indev:infile
dev:function outdev:outfile
dev:function=indev:infile
dev:function
```

When an input specification is omitted in a function call, the following message is displayed (after the file format message):

INPUT

ENTER DEV: STARTING BLOCK, POINTS AS PXXXXX OR BLOCKS AS BXXX RETURN

Note: When input definition is required during a MOVE command, the message is as follows:

INPUT

ENTER DEV: STARTING BLOCK, BLOCKS, RETURN REPLY:

Three parameters must be specified. First, a mnemonic unit code is typed followed by a colon to locate the file. The starting block number (octal) is entered next and followed by a comma. Legal block numbers are \emptyset to 1577 for LINCtape and \emptyset to 6257 for disk. The file length is specified as number of points or number of blocks. To indicate the number of points, type P followed by a decimal number in the range 1 to 999,999. To indicate the number of blocks, type B¹ followed by the octal number of blocks in the range 1 to 16 \emptyset for tape and 1 to 626 \emptyset for disk.

If the output file name was omitted, the display is

OUTPUT

ENTER DEV: STARTING BLOCK, RETURN REPLY:

Respond to this display with the same parameter restrictions as the INPUT display. (There is no need to enter the number of blocks or number of points.)

Both replies are terminated by pressing the return key. An illegal response causes the message to be redisplayed.

¹The B is not required during a MOVE command.

For example, to specify an input file that starts at block $2\emptyset$ on LINC-tape unit 4 and is 47 blocks long, a correct reply to the input file message is

LT4,2Ø,B47

If this same file contains $3\emptyset\emptyset\emptyset$ points, a correct reply is

 $LT4, 2\emptyset, P3\emptyset\emptyset\emptyset$

Note that input data files requested in this manner are treated as if no header block were present. Similarly, output files are created without a header block.

3.4 THE FUNCTIONS

3.4.1 MOVE

The MOVE command is used to copy files onto another tape or disk or to duplicate the file on the same device. To move the file LEUCO from disk unit 2 to tape unit 2, and assign it the name ALEUCO, the call to Job Control, assuming LTØ is the system device, is

LTØ:MOVE LT2:ALEUCO=DK2:LEUCO

This command can also be used to copy an entire volume of data by requesting only the function from Job Control and then replying to the input and output file displays. For example, to copy the tape on unit 4 to unit 6, the call to Job Control and the file specifications are:

```
LTØ:MOVE
LT4,Ø,16ØØ
LT6,Ø
```

Note that no data format changes are possible during a MOVE command.

3.4.2 TRANSFER

In addition to moving a file between I/O devices, the TRANSFER command changes the format of the data. The OUTPUT FORMAT message is displayed so that the format can be specified. Thus, after a call to Job Control such as

DK1:TRANS LT1:BUTAMD=LT1:BUTAMS

the OUTPUT FORMAT display appears. In this case, the file will be on the same device in two different formats (or the same format if it is chosen). TRANS must be used when an LDP file is to be created from a non-LDP data file.

3.4.3 PRINT

A data file and its header (if present) can be printed on the Teletype by a PRINT request to Job Control. The data in the primary header block is printed in the following format:

> NAME n HEADER BLOCKS n DATA BLOCKS DESCRIPTION OF FORMAT n POINTS THE MAXIMUM VALUE IS ±.aE±b THE MINIMUM VALUE IS ±.aE±b

The contents of the file is printed as follows:

POINT	VALUE
ø	± .aE≠b
•	•
•	•
•	•
•	•
n	≠ .aE±b

For the values in both the header and data blocks, a is six digits and b is 3 digits.

CTRL/C may be typed at any time to abort the printing.

Only the input file need be specified in the call to Job Control. For example, to print the file C6HCL5 located on disk unit 2, the correct call is

DKØ:PRINT=DK2:C6HCL5

for a disk system.

3.4.4 DISPLAY HEADER

The information in the primary header block is displayed on the scope in the same format as in the PRINT command. The call to Job Control requires specification of the input file only, so that the call

DKØ:DISHDR=DK2:C6HCL5

will display the header block of the file C6HCL5 on disk unit 2. Type CTRL/C to return to Job Control.

3.4.5 FIX HEADER

The primary header block can be created and stored for an LDP data file that is already present on the volume. The first block of the file must be a free block. Only the data file requires specification, as the input file, in the call to Job Control:

dev:FIXHDR=indev:infile

The data format message is then displayed for the input file. When that has been specified, the total number of header blocks and data points is requested by the display:

> ENTER NUMBER OF HEADER BLOCKS NUMBER OF DATA POINTS REPLY:

Type the total number of header blocks, in the range 1-7, that the data file contains, followed by a comma.

Then type the total number of data points in the file and press RETURN. Note that FIX HEADER computes only the primary header block. Secondary header blocks, if present, are the user's responsibility.

3.4.6 INTERPOLATE

An output file can be created that is an interpolated subset or superset of an input file. INTERPOLATE can provide increased file resolution with no loss of accuracy by requesting a larger number of points in the output file. In addition, two spectra of the same compound that contain a different number of points can be compared by expanding or decreasing the number of points in one file.

The call to Job Control is in the standard format:

dev:INTERP outdev:outfile=indev:infile

The data format message is displayed next so that the output file can be in a different format than the input file.

The number of points in the output file is requested after the call to Job Control by the message on the scope

OUTPUT SIZE REPLY:

Type the decimal number of points desired and press RETURN.

Thus the sequence of responses

LTØ:INTERP LT3:RNA=LT1:RNA 4 2ØØ

interpolates file RNA on LINCtape unit 1 to a file of $2\emptyset\emptyset$ floating point format points on LINCtape unit 3 called RNA.

3.4.7 CREATE

A data file can be built by typing in the values on the Teletype in the order desired and pressing RETURN after each. Only the output file and device need to be specified in the CREATE call to Job Control. To create a file on LINCtape unit 3 and call it PYRINE, the call for a LINCtape system is:

LTØ:CREATE LT3:PYRINE

Scientific (exponential) or decimal notation may be used for entering the values. Exponential numbers are specified as $aE\pm b$ where a is a six digit decimal number and b is a three digit decimal number in the range \emptyset to ± 599 . Both formats can include a decimal point and can be signed. Up to six digits of accuracy can be obtained.

Examples of acceptable values are:

1Ø	.1	-1Ø.5875
lø.	1E-1	1Ø5875E+2
1ØE+1	1.ØE-1	-1Ø5875E-4

If an unacceptable value is entered, a question mark (?) and carriage

return/line feed are echoed on the Teletype and the incorrect value is ignored. When all values have been entered, type CTRL/S to store the data in the specified file and return to Job Control.

CHAPTER 4

FOCAL.12

4.1 USING FOCAL.12

The AIPOS system allows its users to acquire, reformat, transfer, manipulate, and display data files. However, most users require that more specific tasks be performed on their data. For this reason the AIPOS system contains a version of FOCAL-12 (called FOCAL.12 in AIPOS) that is capable of manipulating AIPOS files.

4.2 LOADING FOCAL.12

To use FOCAL.12 issue the following command to Job Control:

DEV:LOAD=DEV:FOCAL.12

When FOCAL.12 has been successfully loaded, it will respond with *. At this time, the user may enter any of the FOCAL-12 commands as described in the PDP-12 manual FOCAL-12 (DEC-12-AJAA-D).

4.3 FOCAL.12 vs FOCAL-12

FOCAL-12 differs from DIAL FOCAL-12 in the following ways:

All file names specified in L M, L O, L L, and L S commands must be in the AIPOS file name format (i.e., six characters followed by a character extension).

ALIASed AIPOS files must not be replaced via L M or L S commands.

An LDP RETURN (abbreviation L R) allows the user to close all files and return to the AIPOS Job Control.

All AIPOS files contain a primary header block and a data area. If a user creates a data file using FOCAL.12 and wishes to manipulate it using DORA or any other AIPOS function he must first create the primary header block. This may be accomplished with the FIXHDR command (refer to section 3.4.5).

APPENDIX A

SUMMARIES

A.1 STARTING PROCEDURES

A.1.1 LINCtape

To start AIPOS from LINCtape:

- 1. Press the STOP console switch. Set the scope channel indicator to 1 & 2.
- 2. Mount the LDP system tape containing the Monitor and Job Control on tape unit \emptyset . (If required, mount another LDP system tape (or disk) on a unit 1-7 (or 1-3).
- 3. Set the tape units to REMOTE and WRITE ENABLE. (Turn the disk on if it is being used.)
- 4. Clear all the console switches. (A switch is cleared when the front part of the rocker is raised.)
- 5. Set the Left Switches to $\emptyset 7 \emptyset \emptyset$ by pushing down the front part of the switches indicated by + and the back part of the switches indicated by + in the following diagram:

 $\uparrow \uparrow \uparrow \downarrow \downarrow \downarrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow \uparrow$

Left Switches

- 6. Press the I/O PRESET switch.
- 7. Press the DO switch.
- 8. Press the START 20 switch.

A.1.2 Disk

To start AIPOS from RK8 for RK12 disk:

- 1. Press the STOP console switch. Set the scope channel indicator to 1 & 2.
- 2. Mount the LDP system disk containing the Monitor and Job Control in disk unit \emptyset . If required, mount another LDP system tape or disk on a tape unit 1-7 or a disk unit 1-3.
- 3. Set the disk START switch. If the SAFE light does not go out in a few seconds, the disk must be re-mounted. Return to step 2.

- 4. When the drive Ø light goes on, clear all the console switches. (A switch is cleared when the front part of the rocker is raised.)
- 5. Set the mode switch to 8 mode.
- 6. Set the Left Switches to $\emptyset \emptyset 2\emptyset$ and the Right Switches to 6733 by pushing down the front part of the switches indicated by \downarrow and the back part of the switches indicated by \uparrow in the following diagram.

ተተተ ተተተ ተ¥ተ ተተተ	** * * ** * **
Left Switches	Right Switches

- 7. Press the FILL switch, then press the FILL STEP switch.
- 8. Set the Right Switches to $5\emptyset 21$. The switches are set as follows (refer to step 6):

↓↑↓ ↑↓↑ ↑↓↑

Right Switches

9. Press the FILL STEP, I/O PRESET and START 20 switches, in that order.

If AIPOS was successfully loaded, it signals that it is ready for a function call command by displaying the first Job Control message on the scope. A command to Job Control can now be issued.

If the AIPOS tape or disk on unit \emptyset does not contain the AIPOS Monitor and Job Control, NO is displayed on the scope. Mount the correct tape or disk and start again.

A.2 DORA COMMANDS.

Cursors

	ASCU;alpha FRCU;numeric FXCU;numeric	Assign cursors Free cursors Fix cursors
File	MOVELLO	Mowo
	SAVE; name; ; pi	Save
Math	~~7	
Unai	OFFY:alpha	Offset V-avis
	CALX; alpha	Calibrate X-axis
	CALY; alpha	Calibrate Y-axis
	SCA; alpha	Scale
	BLS;alpha(,C)	Strip baseline
	PKS;alpha	Strip peak
	NORM; alpha(,C)	Normalize
	INT; alpha(,C)	Integrate
	SMO:alpha(,C)	Smooth
		0

```
Binary
                                                               Add
        ADD
        SUB
                                                               Subtract
                                                               Inverse subtract
        ISB
        OFFX
                                                               Offset X-axis
Display
        VIEW;alpha
INVR;alpha(,alpha)
                                                              View
                                                              Invert display
                                                              Plot (up to six alphas)
        PLOT; alpha
        alpha = T or B

numeric = \emptyset or 1

i = one of \emptyset, 1, T, B, X, Y

o = one of \emptyset, 1, T, B

name<sub>i</sub> = filename (paired with a parameter p_i)
        p. = one of {Ø, 1, T, B}
(<sup>1</sup>) = optional parameter
C = means use cursor
A.3 LEGAL CHARACTERS
А
                                                               $
в
                                                               &
С
                                                                (
D
                                                               )
*
Е
                                                               +
\mathbf{F}
G
Н
                                                               _
Ι
                                                                .
                                                               /ø
123
J
к
\mathbf{L}
М
Ν
                                                               4
5
0
Ρ
                                                                6
Q
                                                                7
ñ
S
                                                                8
т
                                                               9
U
                                                                :
V
                                                                ;
Ŵ
                                                                <
Х
                                                               =
Y
                                                               >
\mathbf{Z}
                                                               ?
[ (SHIFT/K)
∖ (SHIFT/L)
                                                                9
                                                               LINE FEED
] (SHIFT/M)
                                                               RETURN
                                                               ALTMODE
ϯ
                                                               RUBOUT
\rightarrow
SPACE
                                                               CONTROL/I (TAB)
```

1

A.4 USING INIT

The initialization program, INIT, creates LINCtapes and disks that can be used by the LDP system by placing the necessary index information and the AIPOS system (Monitor and Job Control) on the tape. To prepare an LDP tape/disk:

- 1. Start the LDP system by the appropriate procedure in Appendix A.
- 2. When the initial Job Control display appears, type INIT and press the return key.
- 3. The first display of the INIT program appears:

LDP UNIT TO INITIALIZE:

LTØ-7 LINCTAPE DKØ-3 DISK

REPLY:

- 4. Type the mnemonic unit code for the device containing the volume to be initialized for the LDP system. This volume must be a marked LINCtape or formatted disk. Then press the return key. RETURN may be pressed alone as the reply to this display to return to Job Control.
- 5. When an acceptable response is typed, the next display appears:

ENTER UP TO TEN CHARACTERS FOR VOLUME IDENTIFICATION

REPLY:

Up to ten printing DIAL characters may be typed in for volume identification purposes. The information entered this time appears as the first entry in an index display (DX). It may be helpful to use the date created as the volume identifier.

6. After the volume identifier is entered and accepted, the next display is:

HOW MANY INDEX BLOCKS SHOULD BE ALLOCATED? (1 TO $1 \emptyset$ OCTAL) DEFAULT IS 4

REPLY:

The number of index blocks to be allocated to this volume is specified now. This value should be large enough to accommodate all future files because additional index blocks can only be allotted by reinitializing the volume, thereby losing all files currently on the volume. Use the following parameters as a guide in determining the number of blocks to allocate. 321 d index entries/index block

lst index block requires 3 entries for system use.

Each file, alias, and deletion requires an index entry. It is suggested that a tape have at least four index blocks and a disk have ten blocks.

- 7. Type the number of blocks to be used for the index and press the RETURN key.
- 8. If it is a LINCtape that is being initialized, the next display is:

REPLY:

If the tape was marked (via MARK12) for $1\emptyset\emptyset\emptyset$ blocks, type $1\emptyset\emptyset\emptyset$; if it was marked for $16\emptyset\emptyset$ blocks, type $16\emptyset\emptyset$. Then press the return key. If the volume being initialized is an RK8 disk, a length of $626\emptyset_8$ blocks is assumed.

9. The next display is:

WHERE ARE THE SYSTEM BINARIES?

LTØ-7	LDP TAPE
dkø-3	LDP DISK
DIAL	DIAL-MS FILES
NO	OMIT SYSTEM

REPLY:

If a system from another LDP volume is to be copied onto this volume, type the mnemonic unit designation for the device containing that volume. If carriage return alone is typed, the system will be copied from the current system residence device. If a new system is to be created from DIAL-MS binary files, type DIAL, which will cause the following display to appear:

ENTER NAME, COMMA, AND DIAL UNIT OF LDP MONITOR BINARY

REPLY:

Type the DIAL name and unit of the device where the LDP Monitor resides. For the Monitor on LINCtape DEC-12-SQAA-UO, the DIAL name is MØ1 (for version 1). The unit number is as in DIAL-MS: Ø-7 for tape and 1Ø-15, 2Ø-25, 3Ø-35 and 4Ø-45 for RK8 disk. If no system is desired on the volume being initialized (e.g., it is to be used for data only), type NO. All replies are followed by RETURN.

10. After the Monitor is copied from the specified unit onto this volume, the following display appears:

ENTER NAME, COMMA, AND DIAL UNIT OF LDP JOB CONTROL BINARY

REPLY:

Type the DIAL name and unit number of the device where Job Control resides. For the Job Control binary on LINCtape DEC-12-SQAA-UO, the DIAL name is JOBCTL. After it is copied, the message in step 3 reappears. Another volume may then be initialized or Job Control can be reentered.

Note that it is very poor practice to initialize the system unit because the system may be copied to different tape blocks than it had before initialization.

APPENDIX B

ERROR MESSAGES

All the AIPOS programs alert the user to unacceptable command input by an error message. These messages are listed here by system program.

B.1 JOB CONTROL

As a command is entered to Job Control, it is checked for errors after every delimiter. If an error is found, a message is displayed on the scope indicating the type of error. Generally, the errors require specification of a different name to eliminate duplication or of another device to provide sufficient room. For this purpose, RUBOUT can be used to remove the faulty characters in the command and the correct characters can then be typed in. Line feed can be typed to delete the entire line. All the messages are listed below.

REQUESTED FILE DOES NOT EXIST.

INVALID CHARACTER OR IMPROPER SYNTAX. PLEASE CORRECT.

NOT AN LDP VOLUME.

OUTPUT FILE ALREADY EXISTS.

INSUFFICIENT SPACE TO CREATE FILE.

INDEX IS FULL.

ONLY ONE OUTPUT FILE ALLOWED ON ANY DEVICE.

NO MORE FILES ALLOWED.

TOO MANY CHARACTERS IN PARAMETER STRING.

UNABLE TO SAVE name

name IS INVALID OR DUPLICATE FILE NAME. SAVE AS ? REPLY:

Job Control also has a pause message which appears if a nonexistent or off-line device is requested: WAITING FOR device PLEASE READY IT, OR TYPE CONTROL/C TO RESTART

The next error message indicates insufficient room on the requested (or default) device for the file. A new volume is required with enough free space.

UNABLE TO ALLOCATE WORKING AREAS. CONTROL/C TO RESTART.

B.2 DISPLAY INDEX

After a DX error message is displayed, press RETURN to redisplay the last index shown. Its messages are:

SPECIFIED FILE DOES NOT EXIST.

A nonexistent file was requested.

SORRY, NEW NAME ALREADY EXISTS.

New name (after R or A) is already associated with a file.

INDEX IS FULL.

This alias request can not be filled because there is no more room in the index of this volume.

B.3 MONITOR

Under certain conditions, the Monitor may detect programming or unrecoverable hardware errors. In this event, an error message is printed on the console Teletype and it halts near location 712. The LDP system should then be reloaded. The errors are:

Message	Meaning
?Ø	Attempt to execute an unimplemented Monitor command. May also be caused by jumping to page zero illegally.
?1	Too many interrupt pushes: probably routine which called INTPSH did not call INTPOP.
?2	Too many interrupt pops: opposite of ?1.

B**-2**

Message	Meaning
?3	Too many SETINTs. Program is setting up too many interrupt handlers, and not deleting unused ones.
?4	Invalid I/O unit. I/O request for a nonexistent unit.
?5	I/O request on a busy control block. Program failed to wait for completion of the preceding operation.
?6	Unrecoverable disk error.

÷.

B.4 DORA

DORA has its own set of error messages to indicate an illegal operation or request that can not be completed. The message is printed on the Teletype as a question mark and a two digit number. The meaning of each code follows. If the display has been cleared to execute the command, the display is reactivated after the error message is printed.

Code	Meaning
?4Ø	Undefined command - illegal characters or command can not be performed on requested file.
?41	Improper syntax - too many characters, illegal file names or any syntax error in command.
?42	Illegal parameter string - illegal characters, string too long or too short, or undefined file requested.
?43	Invalid command file requested is not currently visible on scope.
?44	Cursor error - cursors positioned improperly.
?45	OFFX error - too few or too many points to move.
?46	FPP arithmetic error - number out of acceptable range.
?47	Division by zero requested - this is an illegal opera- tion.
?48	Illegal value - numeric input outside of acceptable range, or CALY cursor error.
?49	Invalid files - no input files requested or an input file is in an illegal format (e.g., binary). Returns to Job Control.
?5Ø	Working area too small - input file does not fit in assigned working area. Returns to Job Control.
?51	INVR error - an operation between cursors can not be performed on an inverted file.
?52	Vertical OFFX error - OFFX is not needed because cur- sors are positioned on identical file points.

в-3

B.5 FILE HANDLING FUNCTIONS

The following error messages can be printed during a file handling operation.

Code	Meaning
?61	Illegal device.
?62	Insufficient output area.
?64	Illegal load file
?65	Not an LDP data file.

B.6 BUIID/INIT

To resume operation after any of the following error messages, press RETURN.

```
BINARY IS TOO BIG
FOR THIS VOLUME.
INVALID FILENAME.
INVALID UNIT.
NO SUCH BINARY.
NOT A DIAL UNIT.
ERROR: BINARY LOADS
OVER MONITOR.
NOT AN LDP SYSTEM VOLUME.
```

APPENDIX C

Examples of Display Frames

The following pages include photographic examples of some of the display oriented AIPOS programs with explanations of the highlights of each photo. These examples maybe useful as supplementary descriptions of Job Control and DORA.

1. Job Control Initial Display



When the AIPOS system is loaded initially and after CTRL/C or a DX command, the above message is displayed. Any command to Job Control can be entered at this time.

2. Job Control Final Display



For a command that includes a parameter string, the format of the display before terminating the statement is as above.

This example requests DORA, which is on disk unit \emptyset , to use the input files GCl, which is on tape unit 1, and GC2, which is on tape unit 2 and to create the output files BENZEN and METHAC on tape unit 2. A comment on the sequence, EXPERIMENTAL RUN 128, is also included in the command.

All of the following photos have been cropped to illustrate only the areas of interest. For example, some photos do not include cursor readouts.

3. Initial DORA Display



This photo is of a typical initial DORA display of two input files in split scope.



This photo is of the same spectra displayed full screen.

C-2

The following photos illustrate DORA operations on one spectrum.

4. Initial Display



The input file.

5. Differentiation and Normalization



The derivative curve after normalization to the max,min of the entire spectrum for the file displayed in example 4.

6. Integration



The integral of the file and the original spectrum are displayed together in full scope.

7. Peak Strip



The third peak displayed in the original file (example 4) has been removed via the PKS command.

8. Initial Display



Notice that this data requires smoothing and scaling in order to define the peaks on the display.

9. Scaled Curve



The file in example 8 was scaled via the SCA command to generate this display.

10. Smoothed Data

NAMANY

The same file after smoothing.

11. Free Cursors



Both cursors were freed by a FRCU command with no argument to generate this display.
12. Adding Files

before



after

The file on the bottom has been added to the file on the top.

GLOSSARY

.

Constant	A user specified six digit number which can include a decimal point.		
Cursor	A bright dot displayed on the scope that is moved via A/D knobs and used to mark a parti- cular location on a spectrum.		
Default unit	The device accessed by Job Control when a de- vice specification is omitted in a function call.		
Device	A hardware storage unit - LINCtape or RK8 disk drive.		
Disk unit	An RK8 or tape drive set to a particular unit number. A volume of data is mounted on the unit.		
File	A named set of data stored on LINCtape or disk which can be displayed and modified.		
Function call	A loading command issued to Job Control to call the desired program, initialize the chosen in- put files and create output files from the specified device.		
Job Control	The part of AIPOS that calls system functions and data files and creates storage files from a function call. Used as the system loader.		
LINCtape unit	A LINCtape drive set to a particular unit num- ber. A volume of data is mounted on the unit.		
Mnemonic code	An alphanumeric abbreviation used to specify a device and unit number to Job Control.		
Monitor	The main controller for AIPOS. Contains all I/O and interrupt facilities, decodes user in- put, and coordinates all AIPOS activities.		
Moving window	A data file is displayed by showing sections of the spectrum continuously across the scope. Thus, the portion displayed at any moment is that part of the file where the moving window is currently located.		
System functions	Programs such as DORA, TRANSFER and CREATE.		
Volume	All of the stored data (index and files) on a tape or disk. A volume of data can be mounted on any tape or disk unit.		
Working Area	Space allocated on a volume for function out- put.		

INDEX

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