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NASA CONTRACTOR REPORT 166413

**(NASA-CR-166413) DYNAMIC MECHANICAL
ANALYSIS AND ORGANIZATION/STORAGE OF DATA
FOR POLYMERIC MATERIALS (Surface Analytic
Research, Inc.) 55 p HC A04/MF A01 CSCL 11C**

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**Dynamic Mechanical Analysis and Organization/Storage
of Data for Polymeric Materials**

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**Dynamic Mechanical Analysis and Organization/Storage
of Data for Polymeric Materials**

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I. DYNAMIC MECHANICAL ANALYSIS

Dynamic Mechanical Analysis (DMA) studies of about 90 composite samples have been completed over this period. A joint project with Dr. Ming-Ta Hsu and Mr. William Gilwee of the Chemical Research Project Office at Ames on a new series of aging measurements was started in late December. Samples involved in this aging study are: bismaleimide (H795), epoxy (5208, 934, Hitco), polystyrylpyridine (6024M), phenolic (xylok 210, benzyl), and polyimide (V378A). In addition, aging of new MY720 samples was started in late April. All samples involved have been aged in air at 177C and have been removed periodically for flexural, tensile, short beam shear, and dynamic mechanical analysis. This aging study is being continued by Dr. Hsu and Mr. Gilwee.

New versions of the operating system (RT11 V4) and a FORTRAN compiler (RT11-FORTRAN IV V2.05) were installed on the MINC computer, which controls the DMA experiments and does the DMA data analysis. The software for DMA data acquisition, data reduction and analysis have been partially converted from BASIC to FORTRAN in order to enhance system performance. A manual for the complete operation of the DMA instrument and data systems can be found under Appendix I of this report. This manual has been stored on a floppy disk labeled "DMA.TXT" under the same file name.

II. ORGANIZATION / STORAGE OF DATA FOR POLYMERIC MATERIALS

1. Hardware

The computer system, TYCHO, is a Digital Equipment Corp. (DEC) PDP 11/44 system used for real time data acquisition, data analysis and database management to support research activities in the Chemical Research Project Office at Ames. TYCHO has a large main memory to support multiple users and a floating point processor to support the FORTRAN IV+ compiler. An 11/44 configuration with an RM02 (67 megabytes) disk drive was selected as its primary mass storage device. The TS11 (45 ips, 1600 BPI, 9TR) tape drive and the TU 58 (DECTAPE II) cartridge tape drive came with the RM02 configuration. The RX02 (1 megabyte) double density disk drive is used to load diagnostics, file backups for individual users and transfer of data from laboratory instruments.

The laboratory peripheral accelerator (LPA 11) was selected as one of the communication paths to avoid the process of real time data acquisition interfering with the overall operation and the speed of 11/44. 16 RS232 lines (DZ 11E) have been installed in TYCHO. Eight of these are used by instruments and eight by terminals. An I/O processor (COMM-IOP) is also installed in TYCHO to offload as much of the I/O processing as possible from the 11/44 CPU in order to provide quicker response to interactive database and graphic users. A Trilog T100 printer/plotter is used as both a line printer and a hard copy graphics device. Tek 4025 and VT100 terminals with a Selanar graphic board installed have been used on TYCHO. In order to input data stored in graphic form from paper into the database a GTCO Digitizing Tablet is used. The LA-120 was the system console supplied in the standard configuration.

2. Software

A high level language, FORTRAN IV+, has been used to support real time application. "Software Tools" obtained from

the DECUS RSX/IAS SIG tape (1981-Spring-Miami) has been installed. BASIC +2 was selected as a powerful but easy-to-use language in simple programming. The Basic Self Paced Instruction (SPI) was also installed for the less experienced user.

When the users log on and run TYCHO, MAIN does some initialization and invokes CONTROL. CONTROL generates a menu and connects the user with the requested submodule. CONTROL maintains the current and two previous user environments within TYCHO to facilitate the command-driver and multiple-user-task features of the system.

The data system is capable of a variety of graphics output, does data reduction, data correction and manipulation of spectral data. For CRT output, there are Plot 10 compatible terminals and the Tektronic Terminal Control System (TCS), as well as Advanced Graphics II (AG II) and Interactive Graphics Language (IGL) libraries available. The International Math & Statistics Library (IMSL) is used to support the analysis module. Graphic output on the Trilog is supported with the CCSI-TRILOG plotting package.

TYCHO will provide data acquisition and instrument control capabilities. It will control the activity of and receive data from the Laboratory Peripheral Accelerator (LPA). It will also receive data from the RS-232C interfaced instruments and remote processors. It will query the user for device, run and sample information.

Datatrieve is selected as a language for database management. We have created a domain in Datatrieve for each type of analysis and a record for each test run. The records contain information on the test conditions, materials and a summary of the test results. All of these domains can be found in the PDP 11/44 computer under the data dictionary "TYCHO".

More details on the TYCHO system can be found in a paper (Appendix II) presented at the Los Angeles DECUS Meeting in December, 1981.

Another aspect of TYCHO software development is the coding of a chemical structure data manipulation system. This system can be viewed as an integral part of the overall Chemical Laboratory Management System (CLMS). A writeup on CLMS can be found in Appendix III. CLMS is the ultimate software package whereby all aspects of data acquisition, storage/retrieval, reduction, and analysis will be automated. The first phase of the chemical structure coding has been initiated and is summarized in Appendix IV under Chemical Structure Storage System (CSSS).

More recent development on chemical structure coding includes testing of the software for the generation of the so-called Morgan name based on a well-known algorithm.¹ The implementation of the Stereochemically Extended Morgan Algorithm (SEMA) is not complete. A parallel development on the data structure specification using DATATRIEVE has been completed, resulting in a procedure for the direct input of the connectivity table. These procedures are currently available under tasks SMATST (UIC 1, 322) and CSSS (UIC 1,10).

Software development has also been started on a graphics library for the Columbia microcomputer system so that it will be able to serve as the processor for the GTCO digitizing tablet. This library will provide the capability for the user to see the chemical structures as they are being inputted or to view the spectral data as they are being digitized. The library is not complete and requires further testing.

Reference

1. W.T. Wipke and T.M. Dyott, JACS 96 (1974) 4834; and references therein.

WORKING WITH MACHINES RELATED TO DMA EXPERIMENTS

I. *** Line Printer ***

1) Power Switch

The power switch for the line printer is at the back, left corner. Leave the power switch ON all time.

2) Check printer paper position at the beginning of the day after the main power is turned on.

If not aligned to top of page, do the following:

- a) Set top of page by pressing the "FORM ALIGN ↑" button until printer head is aligned with top of page. If necessary you may use the "FORM ALIGN ↓" button to back up a few lines to the top of page position.
- b) Push the "RESET" button.
- c) See if the top of page is now set by pressing the "FORM FEED" button.
- d) Repeat procedure from a) if top of page is not positioned.
- e) When top of page is aligned, press "ON LINE" button.

If it is already aligned to top of page, press ON LINE.

3) Paper Loading

"PAPER OUT" light will lit when more paper is needed. Feed paper in from back slot to front.

4) Problems

Paper Misfeeding:

Many times paper is misfed because the pile of printer paper is pressed with something on top. Remove everything from the top. Paper must always be fed in freely.

Not printing:

If the line printer is on and is not printing when a print out is expected, check the printer port at the back on the right, and the power cable on the left. Make sure they are plugged in well.

5) Setting Printer Off-line at end of the day:

At the end of each day, set the line printer off-line as follows:

- a) Press FORM FEED.
- b) Press ON-LINE. The red light should go off.

6) Paper Order

When paper supply runs low, order more from the stock supplies with:

Job Order # T4319 (subject to change)
National Stock No. 7530-00-092-2834

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I. ***** Plotter *****

1) Power Switch

Set the line switch located at right bottom front to ON (I).
Leave it ON all time.

2) Loading and Unloading Paper

Loading:

- a) Press "CHART LOAD" button
- b) Place paper in position with edges set into corners.
- c) Smooth out paper and press "CHART HOLD" button.

Unloading:

- a) Press "CHART LOAD" again.
- b) Remove paper.

3) Changing Pens

Pen Body Colors AND uses:

- i) Light grey -- standard-width. Use on transparency film only.
- ii) Black -- wide line pens. Use also on transparency film only.
- iii) Dark grey -- standard paper pen.

Change pens when you run out of ink or when you want to substitute for a pen of different color.

- a) Press appropriate pen location button (1, 2, 3, or 4) to select the pen you want to substitute.
- b) Remove pen from pen holder when plotter arm stops moving.
- c) Remove the cap of a new pen or a substitute and place it in the pen holder. The thick ring around the middle of the pen fits into the slot in the pen holder.
- d) Press "ENTER" button and pen location button. The plotter arm will put the pen in the right pen storage location.

4) Plotter Arm Controls

The plotter has 4 directional pushbutton controls for the plotter arm movement - upward, downward, left, and right. Pressing any button will move pen in the direction indicated. The direction pushbuttons can be used in X and Y combinations.

For faster movement, press "FAST" pushbutton together with a desirable direction pushbutton.

5) PEN UP and PEN DOWN

These pushbuttons are used to raise or lower the pen.

6) Pen Selection Buttons (Pen Location Buttons)

These are labeled 1, 2, 3, and 4. They are used for manual selection of pens. To select a pen, simply press appropriate pen selection button. To store the pen in the selected location, press "ENTER" pushbutton first, then press the selected location button. This operation will store and

cap the pen in place.

DO NOT LEAVE pen in the pen holder of plotter arm; the pen will dry out if not capped. ALWAYS RETURN pen to its storage location.

7) Scaling Point Pushbuttons P1 and P2

P1 and P2 direct the pen to move to the corresponding physical point on the platen. Pressing P1 gives the lower left physical point and P2 the upper right physical point of a window area you will use for plotting.

To reset scaling points, move pen to a desired physical point, press "ENTER" before pushing P1 or P2.

P1 and P2 scaling points can be used to define relative width and height of characters or symbols you want to write with the plotter.

Refer to HP Plotter Manual for more information.

8) Supplies Orders

(I) Purchase Requests needed for the following:

Seller's Address:

Hewlett/Packard
3200 Hillview Ave.
Palo Alto, CA 94303

Plotter paper:

- i) Blank paper, 11 x 17", HP #9280-0180, unit in box
- ii) 3 Cycles Loe Paper, 11 x 17", HP #9280-0168, unit in box
- iii) 2 Cycles Loe Paper, 11 x 17", HP #9280-0169, unit in box

Color pens:

- i) Standard Paper Pens, dark grey bodies,
4-Color Pack, HP #5060-6810
- ii) Pens for Transparency Films:
 - a) standard line width, light grey bodies -
 - 1) 4 Pens (black, red, blue, green), HP #5060-6818
 - 2) 4 Pens (black, orange, brown, violet), HP #5060-6834
 - b) wide line width, black bodies -
 - 1) 4 Pens (black, red, blue, green), HP #5060-6819
 - 2) 4 Pens (black, orange, brown, violet), HP #5060-6835

Solvent (used to erase on transparency films):
29.6 ml (1 fl. oz.), HP #5060-6828

Transparency Films:

8.5 x 10.5 in., 100 sheets, HP #9270-0639

(II) Order from stock supplies:

Graph Paper, grid size 10 x 15, 100 sheets -
Job Order # 03010
National Stock #7530-00-687-8331

1) POWER

Press POWER to turn the heater ON/OFF.

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2) RESET

Press RESET when power is turned ON.

Every time the heater is turned ON, you must RESET it.

But you only need to RESET it ONCE a day if the heater is to stay on all day.

3) Heater Current

The pointer deflects in a range of 0 - 4 amps in the DMA runs.

4) Light Bulbs

UNCONTROLLED : Lighted when not in use or when in use, i.e. during the experiment, indicates that heating temperature is out of control.

CONTROLLED : Indicates heating temperature is well controlled during program execution time.

5) Power Off

Turn power off at the end of your final DMA run of the day.

IV. *** MINC ***1) System Power Switch

The MINC power switch is located on the front of the MINC cart. Leave it ON all time.

2) Diskette Drives and Diskettes

MINC has two diskette drives:

0: Left hand drive. You start MINC by inserting a system diskette or a demonstration diskette or a program diskette with system in this drive labelled SY0:.

1: Right hand drive. Insert a data diskette or a program diskette in this drive labelled SY1:.

Open disk drives by pressing the black buttons underneath the doors. Close drive doors after the right diskettes are inserted.

Changing diskettes:When to change diskettes:

When the diskette in SY1: is full and you want to collect more information on a new disk, OR you want to work with a different diskette in SY1:, you change the current diskette in Drive 1.

When you want to work with a program not in the current system program disk in drive 0, you change the current diskette in BY0:

How to Change diskettes:

BY1: diskettes -

If MING is working on a program, either complete it or interrupt it with CONTROL C, before you change the diskette. Wait for READY to appear.

Then just simply remove the current diskette from drive 1 and put a new or desired diskette in.

BY0: diskettes -

You can change the system diskette in one of the two ways as follows, but preferably with procedure I if you are still new to the system.

I. When READY is displayed on screen, turn system power switch off. Remove diskette from Drive 0. Insert new system diskette. After a few seconds, turn power back on to start MING.

II. Remove diskette from Drive 0. Insert new system diskette. Leave the system power on. Press BREAK key. The terminal screen now displays a character @. Type in right after @, 1730003 This will start MING. Do not use the BREAK key other than this procedure.

Handling diskettes:

- . Label each diskette used with volume identification
- . Never write on diskettes. Always write on the label first, then put it onto diskette.
- . Do not touch diskette slot.
- . Do not bend or clean diskettes.
- . Protect them in empty envelopes.
- . Save empty envelopes in diskette envelope slot.
- . When a diskette is full, get the listing of all the files existing on the diskette by giving the command "DIR LP:" for system disk, or "DIR BY1: LP:" for diskette in drive 1. Save the diskette directories in the folder labelled DISK INDEX.

Diskette Orders:

Order more diskettes from Stock Supplies:

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Job Order #T4319
National Stock #7045-01-047-3404
Description 3740/1 Diskette from DYSAN

Quality from Dysan is better than that from Memorex.

The MING chassis contains the following 4 lab modules:

b.

- 1) Clock module (clock)
- 2) Digital-to-analog converter (d/a)
- 3) Analog-to-digital converter (a/d)
- 4) Preamplifier (Preamp)

The front panel control knobs have inner and outer knobs. Their positions are set as follows. DO NOT CHANGE ANY OF THESE SETTINGS for the DMA runs.

Clock Module

st1 Inner knob set for VAR OUT
SLOPE IN +
st2 Inner knob set for VAR OUT
SLOPE IN +

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Digital-to-Analog Converter (d/a)

0 Inner knob set at unipolar (+) selector
Outer knob set at 0-5 V
1 Inner knob at bipolar (+/-) selector
Outer knob at 5 V
2,3 same as settings of 1

Analog-to-Digital Converter (a/d)

0,1,2,3 All outer knobs set at TEST position

Preamplifier

A,B,C,D All inner knobs set at V mode
All outer knobs set at full clockwise position
P, programmable gain condition

4) Terminal Keyboard

Special keys:

DELETE Used to correct typing mistakes. If you make a typing mistake, press the DELETE key as many times as necessary to back up to the error and erase it. Then resume typing.

RETURN Used to end a message to MING. When you type a command or input a value to the computer, you end it by pressing the RETURN key.

CTRL. The CTRL key is used, in combination with another key, to identify a special function for that key. The CTRL/C function is used to interrupt MING. When you want MING to stop its current activity, you hold down the CTRL key and press the C key twice.

NO SCROLL

The NO SCROLL key is used to temporarily stop MIRC from displaying lines on the terminal screen. You use this key when MIRC is displaying many lines of information faster than you can read them. Press the NO SCROLL key to stop the display. When you are ready to continue, press the NO SCROLL key again and MIRC resumes its display.

ENTER

Can be used as a RETURN key.

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Numeric Keypad:

The numeric keypad enables numbers to be entered in calculator fashion.

BREAK

DO NOT use the BREAK key except for changing system diskette in drive Q.

5) Brightness of Terminal Screen Display

Brightness can be adjusted by pressing SFT UP key followed by pressing the ↑ key to increase or the ↓ key to decrease to the desired brightness of the display. Then press the SFT UP key again.

6) Basic Commands

When MIRC displays the READY message, it waits for you to type a command. The following Basic commands are used all time doing the DMA runs.

The DIRECTORY Command

You can see the names of all the program files, data files and other files that you save on a volume with the DIRECTORY command, DIR. The directory includes the current date, the volume identifier, the owner, the list of files, and a description of the available and used space. The Volume ID and the Owner were named by you or someone else when the volume was initialized. Refer to INITIALIZATION. You can use the DIR command as shown below:

READY	MIRC now waits for you to type in a command.
<u>DIR</u>	MIRC displays the directory of the diskette at SY0:
<u>DIR SY1:</u>	MIRC displays the directory of the diskette at SY1:

The INITIALIZATION Command

Before using a new volume, i.e., a new diskette, you must initialize it. When you initialize a volume, MIRC formats it - setting up a directory area and an area available for files. It also erases any previous information stored on the volume, if you try to initialize a used volume. Always check with the DIR command before initializing a used volume to avoid erasing the files you want to keep.

With a system volume in SY0:, place a new volume to be initialized in SY1:. A complete example of initializing a new volume follows:

READY
INI SY1:

Install volume to be initialized in SY1:, and press RETURN

Current volume id:eeeeeeeeeeeeee

Current owner: eeeeeeeeeeeeeee

Proceed with initialization (Y or N)? Y

Type new Volume id: (Type the identification name you wish to give)

Type new owner name: (Type your initials)

After two minutes, MINC prints the message:

Initialization is complete; found 000 Bad blocks

Now you can use this new volume to store programs, a system or data.

If MINC shows that there are some number of bad blocks, put aside the volume with bad blocks. Initialize another new volume.

The RUN Command

If you want to run a program stored on the volume, type:

RUN filename

filename = the name of the program you want to run

for example:

RUN DMA

or

RUN PLOT

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Error messages occur when you have input a wrong filename or when the data disk is full.

?MINC-F-Specified or default volume does not have file named

indicates that you may have input a wrong filename not stored in the volume or the desired program file is not on the volume.

Check the volume directory with DIR command and type the correct filename again.

?MINC-F-No suitable free space on volume for file on line xxxxx

warns you that your data disk is full. Initialize a new volume and collect data on the new initialized volume.

The DUPLICATE Command

You can use the DUP command to copy an entire volume or diskette including the MINC system files for back-ups. The DUP command prompts you to put the volume to be duplicated in SY0: and the backup volume in SY1:. The DUP command then copies the entire contents of the volume in SY0: to the volume in SY1:, destroying all of the previous contents of the volume in SY1:. MAKE SURE THAT YOU ARE NOT USING A VALID VOLUME WHICH YOU WANT TO KEEP, IN SY1: AS A BACKUP DISK. It is safe to use a new diskette in this duplicating process.

The following example shows the entire procedure for duplicating a volume.

install volume to be initialized in SY1: and press RETURN

Current volume id:
 Current owner:
 Proceed with initialization (Y or N)? Y - for new diskette
 N - for unora diskette inserted

Type new Volume id:
 Type new owner name:
 Initialization is complete: found 000 Bad blocks

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READY
 VERIFY SY1: (type this command in)
 There were no bad blocks found

READY
 DUP (type the command in)
 Install volume to be duplicated in SY0:
 Install initialized, empty volume in SY1:, are you ready (Y or N)?

SY1 volume id is:
 SY1 owner is: (these two information are what you save during INT)

Do you want to duplicate another volume (Y or N)? N

Re-install system volume in SY0, and then press RETURN.

MING BASIC V1.1

MING displays an identifying message on the terminal screen the same way you start up the system. It prompts you for the date and time.

IMPORTANT NOTE:

Never type CTRL /C while using the DUPLICATE command. A CTRL /C typed during duplication can destroy data on the source volume in SY0:. Either wait for DUPLICATE to finish or turn off the MING.

The COPY Command

You can use the COPY command to transfer a file from one volume to another, or to list a file on a line printer.

The form of the COPY command is:

COPY from-filespec to-filespec

where:

from-filespec is the file specification of the file to be copied. The default device is SY0:. The default file type is .BAS. The name of the file to be copied must be present.

to-filespec is the file specification of the new file that holds the copy. The default file name is the from-file name. The default file type is the from-file type. The default device is SY0:. LP: prints the file on the line printer.

The following are some of the COPY command examples you can use:

If you want to copy the DMA file from your SY0: diskette to diskette in SY1:, use one of the following commands. Since it is a basic file you

and use the file type code in your command.

COPY SYO:DMA.BAS SY1:DMA.BAS
OR
COPY DMA SY1:DMA

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If you want to get a hard copy of the DMA file on the line printer, type:

COPY DMA LP:

Your DMA file is in SYO:.

If you want to copy a text file other than a basic file, type the file with its file type: (file type is specified with the last three characters followed by a period after the file-name)

COPY SY1:DMA.TXT LP:

The DISPLAY..CLEAR Command

To erase a graph displayed on the terminal screen, type in the following command:

READY
DISPLAY..CLEAR

3) MINC Service Center

For any service requested, provide our serial # WF05314.
DEC Field Service (408)727-0200 Ext. 2339 Ask for Sheri
MINC Product Services Center 1-800-554-4013
Ask for Lorrie Freedman

V. *** Dynamic Mechanical Analyzer ***

1) Power Switch

Power switch is the left toggle at the back of the DMA. Set toggle at UP position to turn power ON, and leave it ON all time.

2) Controls and Indicators

Name	Position
OSC.FREQUENCY (check switch)	NORMAL.
OSC.FREQUENCY (range switch)	LOW
OSC.AMPLITUDE	0.0 mm during driven arm centering 0.2 mm during passive arm alignment
A/Z GAIN	0% during driven arm centering 50% during passive arm alignment
MODE switch	MAN. ALIGN. during level arm alignment and

3) Operating Procedures

Remove the thermal cover by loosening the thumbscrews and pushing back the flange clamps.

- i) Centering the Driven Arm
- ii) Mounting a Sample
- iii) Manual alignment of Passive Arm

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All these routine three procedures are described in the DMA program section in detail. Refer to DMA operation manual for other operating procedures.

* CALCULATIONS USED FOR DMA ANALYSIS *

There are two sets of equations which can be used for the DMA analysis. We have been using the old set of equations in the DMA experiments. Results obtained from calculations using the new set of equations still need to be verified for compatibility with DuPont's results. Although in the DMA room temperature runs we keep records of both results obtained from old and new equations, we only use the old equations in our current DMA programmed runs.

a) Old DMA Equations: (for rectangular equations)

$$C = (D_0 * F_0^2) / (2.19 * V_0 * D_1)$$

$$\tan d = V_1 * C / F^2$$

$$E = ((4 * \pi^2 * I^2 * J - K) / (2 * W * ((L/2) + D)^2)) * (L/T)^3$$

where

- D₀ = offset of spring steel stan. (MV)
- F₀ = frequency of standard (Hz)
- V₀ = damping of standard (MV)
- D₁ = value obtained from table (refer to DMA manual, appendix section, p.2), for oscillation amplitude of .2mm, D₁ is 174 MV
- V₁ = damping
- J = single arm moment of inertia (kg.m²)
- C = tan d constant
- F = sample frequency (Hz)
- W = sample width (mm)
- L = sample length (mm)
- T = sample thickness (mm)
- D = clamping distance (mm)
- E = flexural modulus

b) New DMA Equations: (for rectangular samples)

$$B' = (2 * I * (\omega^2 - \omega_0^2) * L) / (A * R^2 * (1 + L^2 / (24 * K^2 * (1 + \delta)))) * (1 - (\omega^2 - \omega_0^2) / (\omega_a^2 - \omega_0^2))^{-1}$$

$$B'' = (R * \eta^2 * I * C * (V - V_0) * L) / (A * R^2) * (1 + L^2 / (24 * K^2 * (1 + \delta))) *$$

$$E' = 2 * (1 + \nu) * G'$$

$$E'' = 2 * (1 + \nu) * G''$$

$$\tan d = 4 * \pi^2 * C * (V - V_0) / (\omega^2 - \omega_0^2)$$

where

- J = single arm moment of inertia (kg.m²)
- $\omega = 2 * \pi * F$ where F = sample frequency (Hz)
- $\omega_0 = 2 * \pi * F_0$ where F₀ = sample-free frequency (Hz)
- $\omega_a = 2 * \pi * F_a$ where F_a = rigid running frequency (Hz)
- A = cross-section area = Width * Thickness = W * T
- B = distance between arm center = Length + 2 * Clamping Distance
= L + 2 * D
- K = sample cross-section radius of gyration
= (Thickness²/12)^{0.5} = (T²/12)^{0.5}
- ν = poisson ratio
- C = tan d constant (same C calculated in old DMA equations)
- G' = shear storage modulus
- G'' = shear loss modulus
- E' = Young's storage modulus
- E'' = Young's loss modulus

The most recent DMA program files are stored in the following volumes:

- 1) DMA OLD#14A (used for plotting with old set of DMA equations)
- 2) MINC DMA#14 (used for plotting with new set of DMA equations)

Please note:

Use the volume labelled DMA OLD#14 until results with new DMA equations are verified.

Both volumes have the same program file names as follows:

Related Programs for DMA Programmed Runs:

DMA .BAS
DMA2
TFC

DMA Parameter File Printout Related Programs:

EXCHGE.BAS
PARFIL.BAS

Related Programs for Terminal Display of DMA Data:

CRT .BAS
CRT1

Related Programs for DMA Data Plots:

PLOT .BAS
PLOT1
PLOT2
PLOT3
PLOT4
PLOT5
PLOT6
PLOT7

STATUS.BAS

Program for View Graphs of DMA Data:

VGFL0T.BAS

Program for Writing View Graph Characters:

VGCHAR.BAS

Related Programs for DMA Room Temperature Runs:

DMART .BAS
DMART1

Calculational Programs:

WTLOSS.BAS - % Wt. Loss
AVERAG.BAS - Average Modulus

DMA Room Temperature Data File Entry Program:

RTD .BAS

DMA Room Temperature Data Files Output Programs:

RTDFIL.BAS Rosenberg's asins samples data
 starting 1/28/81
RTDLST.BAS Rosenberg, Gilwee and Hsu's asins samples
 data starting 12/28/81 AND 4/30/82

Program for DMA Room Temperature Data Plots:

DATAPL.BAS

* PROCEDURES FOR DMA ROOM TEMPERATURE RUNS *

Note: Power switch in each machine is always left ON except in the heater. The main power switch controls power for all instruments.

1) Initial Preparation:

- Remove asins samples from oven and cool.
- Weigh each pan with samples in it.
- Measure the width and thickness of each sample.

2) MINC Start-Up

- . Turn main power switch on.
- . MINC will display an identifying message on the terminal screen

and ask you to enter the date.

Type the date in the following format:

dd-mmm-yy <press RETURN>

for example:

12-MAY-82 <RETURN>

- Next, MINC asks you for the correct time of the day. Type the time in 24-hour format as follows:

hh:mm:ss <RETURN>

You can omit the seconds if you wish.

for example:

16:35

- After about 15 seconds, MINC displays the message READY on the screen, indicating that it is ready to run programs, perform calculations or collect data.

3) Start DMA Run

- Set the CAPS LOCK key so that all letters typed are in big letters.
- You can now type:

RUN DMART

DMART is a program written for DMA room temperature runs.

- Remove the thermal cover by loosening the thumbscrews and pushing back the flange clamps.

5) Procedures for running the DMART program

Input information as asked and follow through the following steps:

(Remember to terminate your information input with the RETURN key.

Typing errors must be corrected before pressing the RETURN key. Use the DELETE key for this purpose.)

Terminal Display	Operator's response
SAMPLE?	Type in sample name. <RETURN> e.g. BENZYL
RUN #?	Type in sample run #. <RETURN> Maximum of 6 characters long. e.g. R10A or R7E
OPERATOR?	Type your initials. <RETURN>
TYPE OF SAMPLE: (1) RECTANGULAR, (2) SPRING, (3) OTHER?	Type 1. <RETURN> Samples are usually rectangular.
WIDTH?	Type width measured in mm. <RETURN>
THICKNESS?	Type thickness measured in mm. <RETURN>

A series of numbers is now being scrolled up continuously on the terminal screen.

Make sure that the MODE control is set at MAN. ALIGN position.

If the sample is the very FIRST ONE, center the driven arm as follows (Refer to figure 3-2). NO SAMPLE is mounted at this point. You only need to do this once a day. Skip driven arm centering for the rest of the samples.

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Centering Driven Arm:

15:

- . Without any sample being mounted; set osc. amplitude at 0.00mm. Turn the knob all the way to your left.
- . Set A/Z Gain to 0%. Turn the knob all the way to left
- . Switch the LEFT toggle at the back of DMA DOWN.
- . Loosen the driven arm hold-down screw and slowly turn the zero adjust cam until the figures displayed on screen is within + or - 3mm of 0.
- . Tighten the hold-down screw.
- . Flip the LEFT toggle at back UP.

Mount the sample: (See figure 3-6)

- . Loosen sample clamp screws.
- . Insert the sample in the sample clamps with the sample being centered within the clamps and perpendicular to the arms.
- . Tighten the sample clamp screws.
- . Locate the sample thermocouple as close to the sample as possible without interfering with the vibrating arms.

For every sample including the first one in the day, perform manual alignment of the passive arm as follows: (See figure 3-10)

Passive Arm Alignment:

- . Switch LEFT toggle at back DOWN.
- . Set osc. amplitude to .20mm. Turn knob clockwise till a 2 appeared in top slot aligned with 0 at bottom scale.
- . Set A/Z Gain at 50%, half way clockwise.
- . Loosen the passive arm hold-down screw.
- . Rotate the pivot block cam until figures displayed on screen are within + or - 3mm of 0.
- . Tighten the hold-down screw.
- . Switch LEFT toggle at back UP.

Hit '8' on terminal keyboard to stop the number scrollline.

LENGTH?

Measure length between sample clamps in mm. Add 6.35mm to your reading. This gives you the correct length. Type length in mm. <RETURN>

SAMPLE TYPE (1) RESIN, (2) RUBBER?

Type 1. <RETURN>

Usually the sample is resin.

A/Z GAIN?

Type 50. <RETURN>

980 Operation

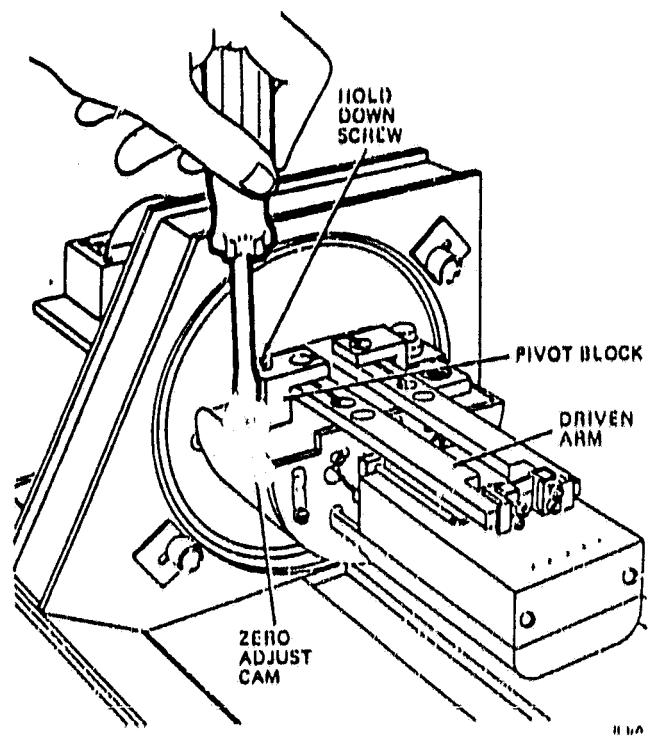


Figure 3-2. Centering the Driven Arm.

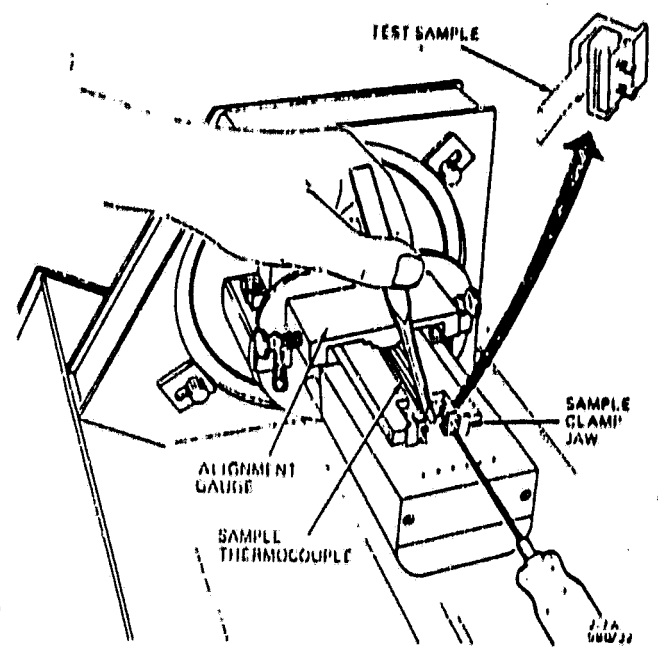


Figure 3-6. Solid Sample Loading.

3-5

Du Pont Instruments

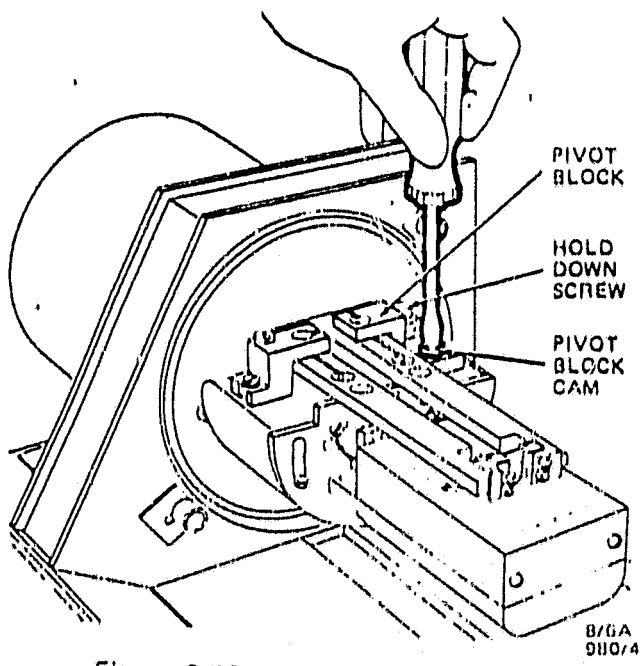


Figure 3-10. Manual Alignment of Passive Arm.

REP APPLIED?

DO YOU WISH TO CHANGE ANY
PARAMETER?

After a few seconds, values
of different moduli, frequency,
damping, time, temperature
are displayed on terminal
screen.

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SAMPLE?

TYPE '20' RETURN

Type 'Y' if you have made a mistake.
Type 'N' or Just a RETURN if no change
is to be made.
<RETURN>

Now set MODE to RUN position.

Watch time change. When it reaches
.8 min, hit "S" and then the NO
SCROLL key to terminate run and
stop screen scrolling.
Now, record Flexural Modulus,
Shear Storage and Loss Moduli,
Flexural Storage and Loss Moduli,
Frequency and Damping.

Hit the NO SCROLL key again and
set MODE to MAN. ALIGN position.
Unscrew the sample clamp screws and
remove sample.

Mount a new sample and continue the
room temperature runs as above.
To terminate the experiment, press
the CTRL. and C keys together.
READY appears when program is
terminated.

You can run some other programs if
you like; Just say RUN program-name.
In place of program-name type name
of the program you want to run.
e.g. RUN AVERAG for calculating
average modulus.
RUN WTLOSS for calculating % wt.
loss.

* PROCEDURES FOR DMA PROGRAMMED RUNS *

1) MINC Start-Up

Skip this procedure if the system is already on.
Refer to MINC Start-Up section under PROCEDURES FOR DMA ROOM
TEMPERATURE RUNS if you need to turn on the system.

2) Start DMA Run

- . Set the CAPS LOCK key for typing in his letters.
- . Program written for this experiment is named DMA.BAS.
Type: RUN DMA

3) Turn heater power ON and RESET it.
Remove thermal cover.

4) Procedures for running the DMA program

Terminal Display

Operator's Response

SAMPLE?

Enter sample name written on baggie. Write what kind of sample it is, and/or with its ID #.
e.g. BISMALIMIDE 2SLI-24
or BENZYI

RUN #?

Enter next number in sequence available in the log book. When the same piece of material is run more than once, keep the same run # for it but add a suffix A, B, or C, etc. to the number.
e.g. You run bismaleimide 3 times.
Your 1st run has a run # 120.
2nd run has 120A.
3rd run has 120B.
Record full name and id of the sample tested with the current run #.

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OPERATOR?

For all questions asked from OPERATOR till DO YOU WISH TO CHANGE ANY PARAMETER, follow through the description of this section in the PROCEDURES FOR DMA ROOM TEMPERATURE RUNS.

*Refer to
p. 14 - 17*

DO YOU WISH TO CHANGE ANY PARAMETER?

TEMPERATURE PROGRAM - LEG NUMBER.
(1) ISOTHERMAL, (2) LINEAR,
(3) END OF PROGRAM?

Select 1 if you do an isothermal run.
2 when you do a linear run.
3 to terminate the run.

ISOTHERMAL TEMPERATURE?

You have selected 1 from above. Enter the isothermal temperature at which you like to maintain your run. The temperature range allowable is -100C to 499C.

TIME AT ISOTIME (IN MIN)?

You have selected 1 from above. Enter how long (in minutes) you like to do the isothermal run.

PROGRAM RATE?

You have selected 2 from above. Enter 5
The recommended heating rate is 5 degrees per minute.

FINAL TEMPERATURE?

For a linear run, select the final temperature you want to reach. The temperature range allowable is -100C to 499C.
Normally for your first run for the sample, select final temp at 300C. Enter 300.
If your first run of the sample does not show a glass-transition temperature, you need to do a 2nd run on the same sample.
For a second run of the sample, select final temperature at 480C.

HEAT STARTING TEMPERATURE?

Enter current temperature of sample.
Type 99 for room temperature.
If your first run has reached the end
and you are starting a second run
up to 480°C, you don't need to cool
the sample down to room temperature.
You may start at 300 or so.

Push the ON LINE button in the line
printer. If paper is not aligned
to top of page, refer to the Line
Printer section in this manual and
reset the paper position.

DO YOU WISH TO CHANGE THE
TEMPERATURE PROGRAM?

Enter Y or N.

Put the thermal cover back on. Secure
the O-rings in its groove. Tighten
the thumbscrews.
Set MODE at RUN position.

Turn on liquid nitrogen.
Check the nitrogen flow rate; maintain
rate at 6 l/min. Do not turn the
black valve at the back of the DMA;
this way you can maintain a constant
flow continuously.

Close the box.

The line printer outputs the DMA
parameter file for the current
sample tested.

Data collected from the DMA
on the Frequency and Dampins
are displayed in a graph on
the terminal screen.

Take note of the controlled temp. and
sample temp. displayed at bottom of
graph.

MAX. HEAT

Sample is being overheated. Sample
temperature is much higher than that
of the controlled or set temp.

COOLING

Set temperature or controlled temp is
too high for the sample; the sample
cannot catch up with the set temp.

Either way, watch the temperature
difference between the controlled
and sample temperatures. If the
difference is above 10°C and the
CONTROLLED green light never sets
turned on for a few minutes, you
can do the following:

Lift the lid up on MINC.
Slightly Jiggle the lab module
MNCAS by the handle.
If this doesn't help, terminate
the program by hitting 'S'.

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Watch the frequency curve on graph. If it drops close to the base line, around 5.0 Hz, and the damping has also dropped, terminate the program by hitting "Q" to prevent sample melting or decomposing.

RUN COMPLETED

It indicates that the run is terminated normally or is discontinued.

Cool down to a desired temperature before you do a run again on the same sample.

You may run the STATUS program to see how agreeable the controlled and sample temperatures are. Then start another run when cooled down.

Enter information from the previous DMA parameter file for your repeated runs.

* STATUS PROGRAM *

The STATUS program displays the temperature status of the sample. To run the program, type:

RUN STATUS

To terminate this program, hit "Q".

* DMA PLOTS *

You may want to know the glass-transition temperature if there is any in your run. Run the CRT program which allows you to select a point of interest on the graphic plot of DMA data. Do not select a "Y" axis in your plot if you are to see the coordinates of a point.

Type RUN CRT

RUN CRT

Enter run #

SELECT VARIABLES TO PLOT

- 1. SAMPLE TEMPERATURE (TEMP C)
- 2. TAN DELTA

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3. MODULUS (GPa)
4. DAMPING (V)
5. FREQUENCY (Hz)
6. SAMPLE TEMPERATURE (V)
7. ELAPSE TIME (MIN)
8. LOG (TIME (MIN))
9. NO PLOT
10. LOG10 (TAN DELTA)

X-AXIS? Enter 1

Y-AXIS? Enter 2

Y'-AXIS? Enter 2 if you want to read a pt.

UPPER LIMIT FOR X-AXIS? Enter 500

LOWER LIMIT FOR X-AXIS? Enter -100

UPPER LIMIT FOR Y-AXIS? Enter .4

LOWER LIMIT FOR Y-AXIS? Enter 0

UPPER LIMIT FOR Y'-AXIS? If chosen for 3, Modulus, enter 50

LOWER LIMIT FOR Y'-AXIS? Enter 0

SELECT START TEMPERATURE (DEG C)? Enter 0 for first point of data.
Otherwise, enter a desired temp.

INVALID TEMPERATURE It indicates you have selected a
starting temp the program does not
recognize.
Re-select a reasonable starting temp.

DO YOU WISH TO CHANGE ANY
PARAMETER? Y or N

MINC displays the graph on screen.

DO YOU WANT TO MEASURE A VALUE
FROM THE GRAPH? Answer Y or N. If you want to read
a point, answer with Y.

MOVE BRND TO POINT OF INTEREST
AND HIT RETURN Use arrow indicator buttons to move
marker to the peak center.

DO YOU WANT ANOTHER POINT? Answer Y or N.

DO YOU WANT TO PLOT MORE DATA
FROM THIS RUN? Answer Y or N.

DO YOU WANT A HARD COPY ON THE
9872A? Answer Y.
Refer to the PLOTTER PAPER LOADING
AND UNLOADING section.
Load paper to plotter.

THE TYPE OF PLOT IS -

- (1) STANDARD PROG. RUN,
- (2) ISOTHERMAL RUN,
- (3) PARA. FROM FILE,
- (4) NONSTANDARD PLOT

Select 1 if a standard plot is desired
Standard plot has the following:

X-axis	Sample Temp	-100 to 5000
Y-axis	Tan Delta	0 to .4
Y'-axis	Modulus (GPa)	0 to 50

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Select for blank or log paper.
Select axes and their limits.
Ask for grid if plotted on blank
paper. Log paper and Graph paper
don't need grids.

STARTING TEMPERATURE (DEG C)?

Enter 0 for the first data point.

The plotter now starts plotting
automatically as programmed.
Other than loading paper at the
beginning, you don't have to
worry about touching any other
buttons on plotter.

DO YOU WANT TO PLOT MORE DATA
FROM THIS RUN?

Type Y or N.

* DMA PLOTS WITHOUT INITIAL PLOTTING ON CRT *

The PLOT.BAS program plots out data on the plotter without first going
through the CRT.BAS program. Insert the data diskette which has the data
for the sample you want. Check with DIR SY1: command to see if the desired
data are stored in the diskette. If your data exists in SY1: diskette,
type RUN PLOT, and provide appropriate information when asked.

The PLOT program prompts you for the following information:

RUN #?

THE TYPE OF PLOT IS - (1) STANDARD PROG. RUN, (2) ISOTHERMAL RUN,
(3) PARA. FROM FILE, (4) NONSTANDARD PLOT?

Usually selections are made on 1 or 4, sometimes 2.

Standard Plots have the following axes and limits:

x-axis	Sample Temperature (Deg C)	from -100 to 500
y-axis	Tan Delta	from 0 to .4
y'-axis	Modulus (GPa)	from 0 to 50

If selection of above is 1, then:
STARTING TEMPERATURE?

If selection is 2, then:
WHAT IS THE ISOTHERMAL TEMPERATURE (DEG C)?
SHALL I PLOT A GRID (Y OR N)?

If selection is 4, then:
TYPE OF CHART PAPER: DUPONT (1), BLANK PAPER (2), GRAPH PAPER (3),
LOG GRAPH PAPER (4)?

Normally use blank paper for the DMA plots.
Log paper is used when you like to reveal a small peak.

SELECT THE VARIABLES TO PLOT

1. SAMPLE TEMPERATURE (DEG C)

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- 1. TAN DELTA
- 2. MODULUS (GPa)
- 3. DAMPING (V)
- 4. FREQUENCY (Hz)
- 5. NO PLOT
- 6. ELAPSED TIME (MIN)
- 7. TIME (MIN) (LOG PLOT)
- 8. TAN DELTA (LOG PLOT, 2 CYCLES)
- 9. TAN DELTA (LOG PLOT, 3 CYCLES)

X-AXIS?
 Y-AXIS?
 Y'-AXIS?

UPPER LIMIT FOR X-AXIS?
 LOWER LIMIT FOR X-AXIS?
 UPPER LIMIT FOR Y-AXIS?
 LOWER LIMIT FOR Y-AXIS?
 UPPER LIMIT FOR Y'-AXIS? If you have selected for this axis.
 LOWER LIMIT FOR Y'-AXIS?

STARTING TEMPERATURE (DEG C)?
 INVALID TEMPERATURE. If you have input a temp not recognizable.

DO YOU WANT A GRID?

DO YOU WISH TO CHANGE ANY PARAMETERS?

TURN ON PLOTTER AND LOAD PAPER THAN PUSH RETURN.

DO YOU WANT TO PLOT MORE DATA FROM THIS RUN?

 * DMA ROOM TEMPERATURE CALCULATIONS *

Average Modulus Calculations:

READY
RUN AVERAGE

OF SAMPLES Enter # of samples you want to calculate the modulus for. i.e. the # of samples you have for a run #, 3 or 5.

THE MODULUS OF THE SAMPLE Enter modulus for each sample.

AVERAGE VALUE OF THE MODULUS Displays the average modulus. Record the average in lab book.

OF SAMPLES Repeat for next sample, or type CONTROL C to terminate calculations.

Percent Weight Loss Calculations:

READY

QDN UTILITIES

HOW MANY SAMPLES?

Enter # of % wt. losses you want to calculate for a sample.

PAN WEIGHT?

Type sample pan weight.

INITIAL WEIGHT?

Type sample initial weight with pan before asins.

NEW WEIGHT?

Type a new weight for the same sample.

A percent wt. loss is displayed.

NEW WEIGHT?

Type another new weight for the same sample.

.
. .
. .
. .

HOW MANY SAMPLES?

Continue calculations for another sample or terminate with a CONTROL C.

* DMA ROOM TEMPERATURE DATA ENTRY *

We have collected the following room temperature DMA data on the two diskettes:

Diskette Id:

DMA Data

DMA #77

Rosenberg's asins samples starting 1/23/81 -

DMA #111

Rosenberg, Gilwee, and Hsu's asins samples starting 12/28/81 & 4/30/82

Rosenberg's asins samples starting 1/23/81 -

Code #	Run #	File Names	Sample Names
1	1.23	PAN26	Phosphorylated bis-maleimide
2	2.21	PAN7	MXG 6070
3	3.24	NASAB	Hitco-epoxy
4	4.25	PSPM	PSP 6024M
5	5.27	NASAC	Bismaleimide B
6	6.30	PAN8	NASA #1006B Benzyl
7	7.29	PAN1B	polyphenylsulfone
8	8.26	PAN1C	polyethersulfone
9	9	KS38	PSP KS38
10	10.22	7W630	10% ATBN

11	11	ZM44	10% ATBN
12	12,28	PSP	PSP
13	13,20	FX3046	Fiberite HMF 330 B/34
14	14	PAN4	934 Fiberite Epoxy
15	15	FPCN	Fron 828
16	16	MY720S	MY720
17	101	ATBN	MY720 + 2% ATBN
18	103	MY720	MY720 DDS
19	104	PSFP	PSP
20	106	M751	M751
21	108	H795	H795
22	111	DGRFF	DGRFF-TMB

Rosenberg, Gilwee and Hsu's aging samples starting 12/28/82 & 4/30/82

Sample Id:/Run #	File Names	Sample Names
R-1	EPOXYB	Pan #1 Epoxy Hitco #7-9 NASA # 1021B
R-2	BENZYL	Pan #8 Benzyl
R-3	PSP	PSP 6024M/W133
R-4	IMIDES	Pan #7 Polyimide Celion 6000/ V378A Hitco #8-9
R-5	EPOXYD	Pan #1 Epoxy Hitco #7-9 NASA # 1021D
R-6	IMIDES	Pan #7 Polyimide Celion 6000/ V378A Hitco #6-1
R-7	XYLOK	Pan #5 Xylok 210
R-8	H795	Pan #8 Celion 6000/H795 BMI
R-9	934	Epoxy Celion 6000/934
R-10	5208	5208/133 S Harness Satin
R-11	AR98	AR-98 BT
R-12	CTRN10	AR-101 10% CTRN
R-13	CTRN2	AR-111 2% CTRN

Insert the appropriate data diskette in drive 1 and enter the collected room temperature data from the lab book to the diskette.

READY
RUN RTD

SAMPLE NAME? Refer the listings above, type the File Name of the sample for which you wish to update the data collected.
e.g. BENZYL

SAMPLE AGING TEMPERATURE? Type 177 or 200

NEW FILE? Type Y if you are creating a new data file.
N if you are updating the data.

TYPE IN '*' TO TERMINATE YOUR INPUT. This is an instruction for terminating your data input.

RECORD # Tells you MIND is ready to accept new data in the file with the given file-name under this given record #.

TIME (DAYS)? If the Record # shown above is 1, enter the number of days of aging for the sample for your data set.

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If the Record # is some number other than 1, 26, you may type #. This will enable you to see a list of all your data entered previously. Now you know where to start updating your data.

MODULUS (GPa)?

Enter modulus corresponding to the aging time.

WEIGHT (GRAMS)?

Enter percent weight loss calculated for the sample corresponding to the aging time.

TIME (DAYS)?

Enter data for next available aging period.

.
. .
. .
. .
. .

TIME (DAYS)?

Type * to terminate input.

XX RECORDS IN FILE.

Tells you how many records you already have in this sample data file.

Displayed is all the data collected in file.

DO YOU WANT TO CHANGE ANY RECORD?

Type Y or N after checking all the data displayed on screen.

ENTER THE NUMBER OF RECORD YOU WANT TO CHANGE.

If you have answered Y in the above question, type the record # in which you wish to make a change.

Displayed is the data collected under record you asked to be changed.

IS THIS THE ENTRY YOU WANT TO CHANGE?

Check the data displayed answer appropriately.

NEW TIME (DAYS)?
NEW MODULUS (GPa)?
NEW WEIGHT (GRAMS)?

Enter correct data for each of these.

DO YOU WANT TO CHANGE ANY RECORD?

You can continue making changes if necessary.

.
. .

DO YOU WANT TO ENTER DATA FOR NEXT SAMPLE?

Type Y or N.

SAMPLE NAME?

Enter new sample name.

* DMA ROOM TEMPERATURE DATA FILE PRINTOUT *

You may want to pull out the DMA Room Temperature Data Files for your record. Insert either Diskette labelled DMA #77 (Rosenberg's aging samples data) or Diskette DMA #111.(Rosenberg, Gilwee and Hsu's aging samples data) in drive 1, SY1:

READY
RUN RTDFIL (for Rosenberg's data)

or

RUN RTDLST (for Rosenberg, Gilwee and Hsu's data)

With RUN RTDFIL, answer the following questions:

HOW MANY DATA FILES DO YOU WANT PRINTED OUT? Enter a number.

REFER TO RTD INDEX AND ENTER NECESSARY INFO. FOR EACH SAMPLE. Refer to listings in the section of DMA ROOM TEMPERATURE DATA ENTRY.

CODE #? Enter code #, not run #.
e.s. 4

SAMPLE NAME? Enter File Name not Sample Name.
File Name is the condensed Sample Name to a maximum of 6 characters.
e.s. PSPM

SAMPLE AGING TEMPERATURE? Type 177 or 200.

CODE #? Enter information for the following samples.

.
. .
. .
. .
. .

Wait for line printer outputs of requested data files.

With RUN RTDLST answer the following questions:

HOW MANY DATA FILES DO YOU WANT PRINTED OUT? Enter a number.

ID #? Enter sample Id/run #.
e.s. R-7

SAMPLE NAME? Enter a file name.
e.s. XYLOK

Type 177 or 200.

ID #?

Repeat input for other samples.

Wait for hard-copies of requested data files.

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* DMA ROOM TEMPERATURE DATA PLOTS *

Insert appropriate room temperature data disk in 8Y1:
This program allows you to plot out data points of a few samples on the same graph, either Modulus vs Time or % Wt. Loss vs Time.

READY
RUN DATAPL

SAMPLE NAME?

Enter appropriate File Name from the listing in the section, DMA ROOM TEMPERATURE DATA ENTRY.

SAMPLE AGING TEMPERATURE?

Type 177 or 200.

DO YOU WANT TO PLOT MODULUS VS TIME?

Type Y or N.

UPPER LIMIT FOR X-AXIS?

Time is the x-axis.

INCREMENT FOR X-AXIS?

UPPER LIMIT FOR Y-AXIS?

Y-axis is either Modulus or % Wt. Loss.

INCREMENT FOR Y-AXIS?

LOAD PAPER AND THEN TYPE RETURN.

DO YOU WANT TO SKIP TO DATA PLOT?

Type Y if you don't want a grid for plot.

The HP plotter draws and labels the x- and y- axes if you have chosen a grid for plot.

WHAT SYMBOL DO YOU WANT PLOTTED?

Type a unique symbol for each sample.

LINE TYPE (0-6)?

Type RETURN for solid line or
0- specifies dots only at plotted pts.
1-
2- - - - -
3- _____
4- _____
5- _____

Push one of the pen selector buttons
to select desired color for the plot.

t if you wish.

STARTING POINT?

Plotting!

DO YOU WANT TO PLOT MORE DATA?

Type Y or N.
You may continue plotting for other
samples as the plot allows.
If you want to change paper and start
another plot, quit at this point
re-run the program later.
Modulus vs Time and % Wt. Loss vs Time
two separate plots.

* DRAWING VIEW GRAPHS *

Loading Transparency Films:

It is important to keep the transparency films clean. Handle with
care. Press CHART LOAD button. Set the transparency film into corners
of the HP plotter. Place a sheet of blank paper on top. Press CHART
HOLD button and smoothen it out. Remove the top blank paper.

DMA Room Temperature Data Plots:

Insert the right data diskette in SY1:
Run the DATAPL program.

Data Plots for DMA Programmed Runs:

Insert the right data diskette in SY1:
Run VEPLDT program.

READY
RUN VEPLDT

RUN # Enter a run# stored in SY1: disk.

- SELECT VARIABLES TO PLOT:
1. SAMPLE TEMPERATURE (DEG C)
 2. TAN DELTA
 3. MODULUS (GPa)
 4. DAMPING (V)
 5. FREQUENCY (Hz)
 6. SAMPLE TEMPERATURE (V)
 7. ELAPSED TIME (MIN)
 8. NO PLOT

X-AXIS?

Y'-AXIS?

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UPPER LIMIT FOR X-AXIS?
LOWER LIMIT FOR X-AXIS?
UPPER LIMIT FOR Y-AXIS?
LOWER LIMIT FOR Y-AXIS?
UPPER LIMIT FOR X'-AXIS?
LOWER LIMIT FOR X'-AXIS?

DO YOU WISH TO CHANGE ANY
PARAMETERS?

TURN ON PLOTTER AND LOAD PAPER
THEN PUSH RETURN.

SHALL I PLOT A GRID?

Plotting a grid if chosen.

START POINT?

LINE TYPE (0-6)?

Refer to description in DMA ROOM
TEMPERATURE PLOTS.

SELECT PEN (0-4)?

Push a pen selector button for color
variation.

DO YOU WANT TO PLOT MORE DATA
FROM THIS RUN?

DO YOU WANT TO PLOT DATA FROM
ANOTHER RUN?

If you want to plot data from another
run on a separate diskette, you need
to exit from this program with a
CTRL/C first. When READY is
displayed on screen, insert the
right data diskette in SY1: and
continue plotting with the command,
RUN. This will get you back on
where you were.

* WRITING CHARACTERS ON VJFW GRAPHS *

Refer to description in Plotter section, for Pen Selection Buttons
and Scaling Point Pushbuttons P1 and P2.

READY
RUN VQCHAR

Define relative width and height of characters or symbols you want to
write with the scaling point pushbuttons P1 and P2.

Select a pen.

Move pen to where you want to start writing.

Enter the character string you want to write.

Press RETURN when ready to write.
You may draw straight with any of the four direction pushbutton controls while the pen is in PEN DOWN condition.

* DMA PARAMETER FILE PRINTOUT *

Keep all DMA parameter files in the DMA Log. Sometimes the line printer is not on-line when a parameter file output has already been sent to the printer during the DMA run, you may not get a complete printout on the parameter file for the current run. To obtain a complete copy of the output, do the following:

READY
RUN EXCHGE

RUN # Enter the run # for which you want a parameter file output.

READY
RUN PARFIL

RUN # Enter the same run # provided for EXCHGE.

The line printer prints out the complete file.

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* SUMMARY *

SYSTEM START-UP/SHUT-OFF:

Turn the main power switch ON at the beginning of the day, and OFF at the end of the day. Except for the heater, power on all other instruments should be left ON.

Turn off liquid nitrogen if used, at the end of the day.

DMA ROOM TEMPERATURE RUNS:

1. Remove aging samples from oven.
2. Weigh samples in pans.
3. Measure sample width, thickness.
4. RUN DMART
5. Mount sample, measure length.
6. Run for .3 minute.
7. RUN AVERAGE to calculate average modulus for each sample.

8. RUN WTLOSS to calculate % weight loss of samples. 32.
9. RUN RTD to enter current room temperature data or data not entered prior to this run for updating data.
10. Optional: RUN RTDFIL (Rosenberg's data) or RUN RTDLST (Rosenberg, Gilwee, and Hsu's data) to get hard-copies on all data files.
11. Optional: RUN DATAPL to plot out results on paper or on transparency film.
12. Optional: RUN VGCHAR to write characters or symbols on plots.

DMA PROGRAMMED RUNS:

1. RUN DMA
2. RUN CRT to plot out data on the terminal screen.
You can obtain a hard-copy of the results through the CRT program at the end.
3. Optional: RUN PLOT to get a hard-copy of data plot if the CRT program is skipped.
4. Optional: RUN VBPLT for view-graph plotting.
5. Optional: RUN VGCHAR to write characters or symbols on view-graphs.
6. RUN STATUS for current sample temperature status.
7. Cool down the sample after each run before starting another run.

When a data diskette is full:

1. Get disk index of the diskette; type DIR SY1: LP:
Save in DISK INDEX folder.
2. When READY, remove data diskette from drive 1, SY1:
3. Label a new diskette.
4. Insert the labelled new diskette in drive 1, SY1:
5. Type INI SY1:

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TYCHO - A CHEMICAL LABORATORY
SYSTEM USING A PDP 11/44

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ABSTRACT

The design and development of the hardware configuration and application software for "TYCHO" are presented. TYCHO is a Digital Equipment Corp. (DEC) PDP 11/44 system used for real time data acquisition, data analysis, and database management. The system supports the operation of a chemical research laboratory and collects data from a variety of instruments, both analog and digital. Interactive and real time communications requirements are met with a laboratory peripheral accelerator (LPA) and other DEC communications hardware. DATATRIEVE is used to provide the user with interactive database management support.

INTRODUCTION

In this paper we present a detailed description of a dedicated computer system that supports various research efforts in the Chemical Research Projects Office at the NASA/Ames Research Center. This laboratory conducts both basic and applied research in polymer, computational, physical and organic chemistry. One of the projects being pursued by this office is the development of improved binder resins for use in advanced aerospace composites. The researchers of the Chemical Research Projects Office are involved in all phases of new resin development: selection, synthesis, curing, characterization, and testing of new polymer structures. This project has been under way for several years and the mass of data collected necessitated the development of a computer system to support the office's activities.

SYSTEM REQUIREMENTS

The computer system, "TYCHO" must be able to capture data directly from the laboratory instruments during routine testing, do the required data analysis, and store the results in the database. Data that have been previously collected or data supplied by other sources must also be able to be easily entered into the database. The data in the database must be accessible either by type of material, test results, or for use in correlations and models. This information must be able to be displayed on various devices either graphically or in tabular form. The users will be research chemists and the "TYCHO" system must be easy to learn (tutorial), simple to use, and highly interactive.

HARDWAREOverview

In developing the hardware configuration we took into account the following requirements:

- o Multi User
- o Real Time Data Acquisition
- o Data Base Management

- o Analog and Digital I/O
- o Video Graphics
- o Hard Copy Graphics
- o Ability to Manipulate Large Virtual Arrays (Spectra)
- o Reasonable Response Time
- o All Data Maintained Online

The systems hardware configuration is shown in Figure 1, and is described in three parts: processor, storage, and communication.

Processor

The PDP 11/44 was selected as the processor for "TYCHO" because it could support all of the above requirements and was the smallest PDP 11 that could provide 1 megabyte of main memory. We felt that a large main memory was necessary to support multiple users manipulating large virtual arrays, such as spectral data. The floating point processor was a necessity both because of the type of application and to support the Fortran IV+ compiler.

Mass Storage

We selected an 11/44 configuration that had an RM02 (67 megabytes) disk drive as its primary mass storage device. An additional RM02 could be added as the system growth demanded more capacity to store the full database online. Data will only be removed when a material is no longer considered a viable candidate. In this case, all the data associated with that material will be moved offline to tape. The newly announced RAS0 (121 megabyte) Winchester disk drive would be a logical substitute for the second RM02. The RAS0 offers a larger capacity than the RM02 and has its own disk controller allowing simultaneous disk transfers for faster system operation. The modest increase in cost would be well worth the extra performance. The TS11 (45 ips, 1600 BPI, 9TR) tape drive and the TU58 (DECTAPE II) cartridge tape drive were standard peripherals that came with the RM02 configuration. We initially had a great deal of hardware trouble with the TS11. However, once fixed, the TS11 has been adequate. The TS11 is a

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slow tape drive, a faster tape drive such as the TU77 (125 ips, 800/1600 BPI, 9TR) may be well worth the extra cost. We have found no occasion to use the TU58 cartridge tape drive since the system was installed. On the other hand the RX02 (1 megabyte) double density disk drive has been invaluable; we use it to load diagnostics, file backups for individual users, and transfer of data from laboratory instruments.

Communication

There are three communication paths aside from the 11/44's UNIBUS: the laboratory peripheral accelerator (LPA 11), the asynchronous RS232 lines (DZ 11), and the IEEE bus (120 11). The LPA 11 was selected so that the process of real time data acquisition would not interfere with the overall operation and speed of the 11/44. The LPA 11 has its own UNIBUS as shown in Figure 1 and controls the operation of the analog-to-digital converter (AD 11), the digital-to-analog converter (AA 11), the digital I/O modules (DR 11), and the real time clock (KW 11). The LPA 11 has two microprocessors: one controls the operation of the LPA's I/O modules and the other handles the Direct Memory Access (DMA) transfer of the data from local buffers to main memory. The LPA will support up to eight simultaneous users. Table 1 shows the instruments that will be directly connected to TYCHO and the type of interface employed. For each instrument we first tried to implement an RS232 interface rather than use LPA 11 interfaces. Analog data acquisition has the problems of signal conditioning, calibration, and it is more susceptible to Electro-Magnetic Interference (EMI).

We currently have 16 RS 232 lines (DZ 11E) installed in TYCHO. Eight of these lines are used by instruments and eight by terminals. These instruments could easily burden the 11/44 CPU with a glut of I/O processing. We are currently installing an I/O processor (COMM-IOP) in TYCHO. This is a microprocessor (KMC 11) that handles the I/O processing for the DZ 11's. Our plan has been to offload as much of the I/O processing as possible from the 11/44 CPU so that it will be able to respond quickly to interactive database and graphics users.

We had initially planned to have a four color plotter (HP 9872A) interfaced on the IEEE bus. The development of the IEEE bus software has been very time consuming and was postponed for later development. We have heard that DEC may be refining the software to run the IEEE bus so that this development may be easier to implement in the future.

We selected a Trilog T100 printer/plotter to serve as both a line printer and a hard copy graphics device. It has 100 dots per inch resolution and being a dot matrix impact printer is inexpensive to operate, and has been trouble-free so far. Figure 2 shows a plot made on the Trilog directly from the screen of a Tektronix 4025 raster terminal. The resolution on this plot is limited by the terminal not the Trilog. This figure is a graphical representation of a portion of a platinum tetra cyanate structure, one of a class of one-dimensional conductors studied at the Chemical Research Projects Office Laboratories.

Several years ago we selected the Tek 4025 CRT terminals for TYCHO because we needed a relatively

low cost, high quality graphics terminal. Since then there has been an explosion of graphics terminals on the market. This past year on TYCHO we have used VT100 with a Selanar graphics board installed. This combination has proved to be very powerful. We can use the VT100 features of the system like the keyboard editors (KED, ED2) and the "Set Guide" mode in Datatrieve (DTR), and can also display graphics using standard Tektronix Plot-10 commands. The Tek 4025 is a very nice terminal and has several features not found in the Selanar modified VT100's. However, for our application the price and performance of the modified VT100's have made them the terminal of future choice.

In order to input data stored in graphic form from paper into the database we are using a GTCO Digitizing Tablet. It has its own microprocessor and can scale the digitized data to user units. It digitizes data in several modes such as x-axis increment or a vector distance from last point. This is a rapid way to convert graphic data into arrays that can be used by the database.

The LA-120 was the system console supplied in the standard configuration and has proven to be trouble free.

SOFTWARE

Overview

The software module design is shown in Figure 3. We produced a document that defines each module in a high level design language. We desired a structured language that would support real time applications like Praxis which was under development at the time (1,2) at the Lawrence Livermore National Laboratory (LLNL). With the difficulty experience in getting Praxis to run properly on a PDP 11, we decided to use Fortran IV+ (F4P). Recently we have installed "Software Tools" (3) that were obtained from the DECUS RSX/TAS SIG tape (1981-Spring-Miami). We are now considering using the RAIFOR (4) preprocessor included for future software development.

After the initial design phase we described the practical features of the design to all of the users in a seminar and distributed a brief written description and user suggestion form. We received several comments and incorporated them where possible. One recurring request was that the users wanted a simple programming language to use. We selected Basic +2 as a powerful but easy-to-use language. We also installed the Basic Self Paced Instruction (SPI) so that inexperienced users could easily get started.

Main & Control

When the users log on and run TYCHO, MAIN does some initialization and invokes CONTROL. CONTROL generates a menu and connects the user with the requested submodule. CONTROL maintains the current and two previous user environments within "TYCHO". This facilitates the command-driver and multiple-user-task features of the system. Thus, as an example, the user could start up data acquisition task, leave the acquisition running and perform interactive graphics on other data, all without

leaving the program. Even if the user logs off, the environments are saved and the program will check the status of 'outstanding' acquisition tasks upon starting the next session.

Analysis

The analysis module does data reduction, data correlation, and manipulation of spectral data such as spectral addition or subtraction. This module is capable of a variety of graphics output. We are working on a device-independent graphics package where a standard plot file is constructed and can be processed by a device-specific module which will produce the output. For CRT output all of our terminals are Plot 10 compatible and we have used Tektronix Terminal Control System (TCS), Advanced Graphics II (AG II) and Interactive Graphics Language (IGL) libraries. We found TCS usable but primitive, AG II was easy to use but restrictive, and IGL wouldn't work properly with the Fortran IV+ (F4P) compiler. We plan to use the IGL library, which has the best set of features, for this application as soon as we get the primary command set to work with F4P.

We are using the International Math & Statistics Library (IMSL) to support the analysis module. It takes up a fair amount of disk space but is very complete and well supported.

To support graphic output on the Trilog we are using the CCSI-TRILOG plotting package. This package provides high level commands plus a rasterizing program for output to the Trilog T100.

Acquisition

This system will provide data acquisition and instrument control capabilities. It will control the activity of and receive data from the Laboratory Peripheral Accelerator (LPA). It will also receive data from the RS-232C interfaced instruments and remote processors. It will query the user for device, run and sample information.

An acquisition module for each lab instrument is required. The instruments connected to the LPA will use the Fortran routines supplied by DEC to program the LPA devices data acquisition. Acquisition on devices connected through the LPA will be facilitated via tasks separate from TYCHO. These tasks will be communicated with via executive calls, event flags, AST's and constructed inter-process communication buffers in memory or on disk. It is important to note that these tasks are created 'autonomous' and are not spawned. This is done so that the issuing task (TYCHO) may go on to do other things or even terminate without affecting data acquisition, unless effects are explicitly directed.

RS-232C compatible devices will acquire data and store it locally when possible, and send it to TYCHO at the end of the analysis. When the data are not stored locally these acquisition tasks will also run as autonomous tasks.

Data Base Management

We looked at all the database management software available, some of it very elaborate and expensive. We selected Datatrieve as a relatively inexpensive

language that would fulfill our requirements. We have created a domain in Datatrieve for each type of analysis and a record for each test run. The records contain information on the test conditions, materials, and a summary of the test results. Large arrays of spectral data are kept in separate data files which are pointed to by a data field in the record.

CONCLUSION

A clear indication of how the 11/44's performance measures up to the tasks assigned is not possible at this time since many of the applications are still undergoing development. Our evaluation at this time of the TYCHO system is that it will be able to perform it's initial function well, however, as new applications are moved onto TYCHO they will have to be evaluated individually to assess the impact on the systems operation.

The user's response to the system thus far has been encouraging. Users are moving more applications from both large mainframes and small desktop systems over to the 11/44 as their awareness of the computer system increases and they see the advantages of a dedicated minicomputer. They are beginning to write their own applications programs and we are seeing an interest in programming among previously 'non-computing' professionals.

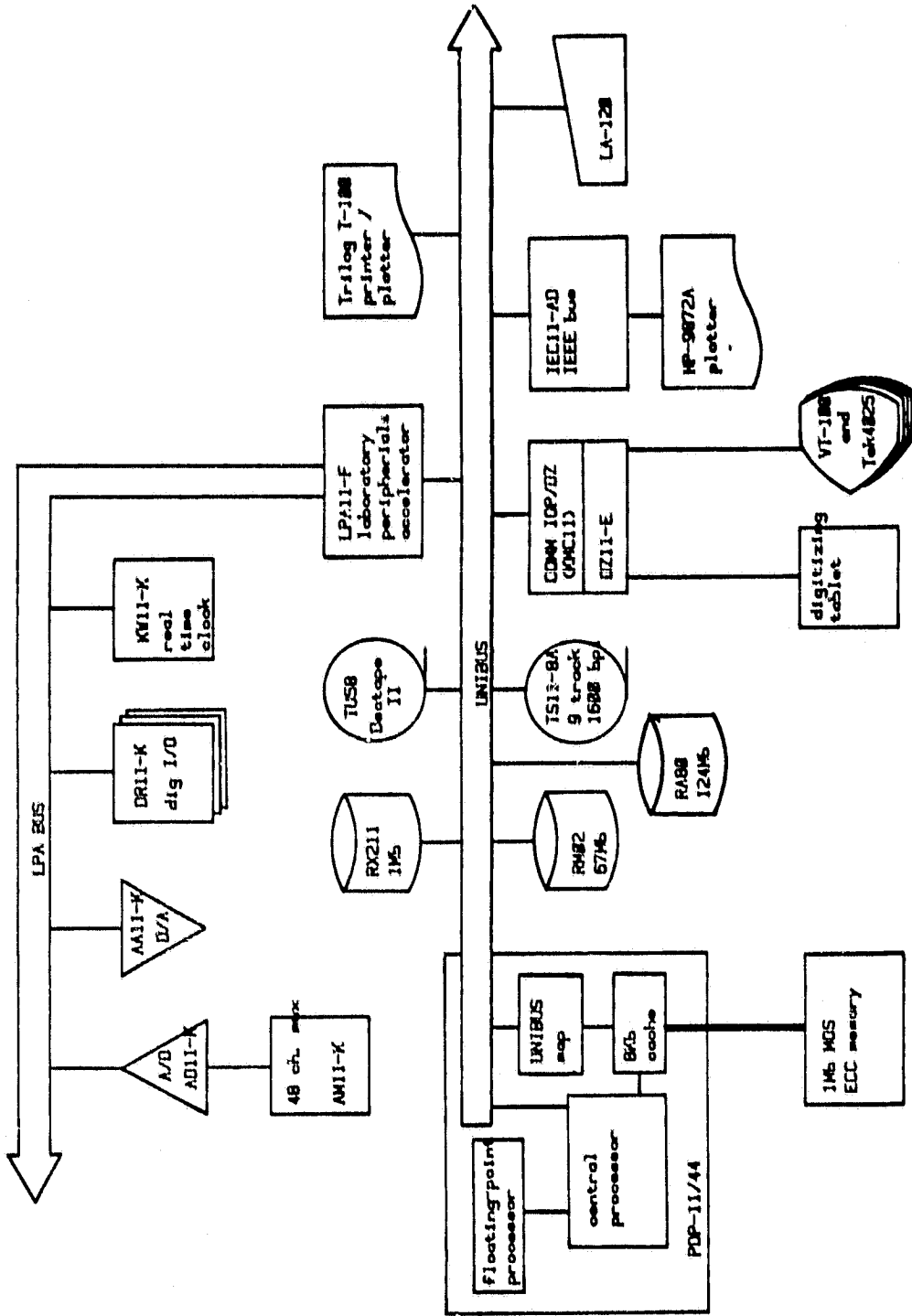
If we were to start over on the development of this system, but were equipped with the lessons learned thus far, we would consider some of the following:

- 1) We would try to avoid the problems associated with signal conditioning and running long analog data acquisition lines. This could be done by using recently developed 'smart' data acquisition modules or by implementing a local network using MINC 11/23's running LAB-RSX to control acquisition.
- 2) We would consider a 32-bit minicomputer, probably the VAX 11/750 for the processor. At the time we developed TYCHO's configuration there were no competitively priced 32-bit machines available. The VAX would ease development of software that requires large data areas and provide an easier path for growth. The additional speed would improve response time for all the interactive applications, some of which were not originally anticipated.

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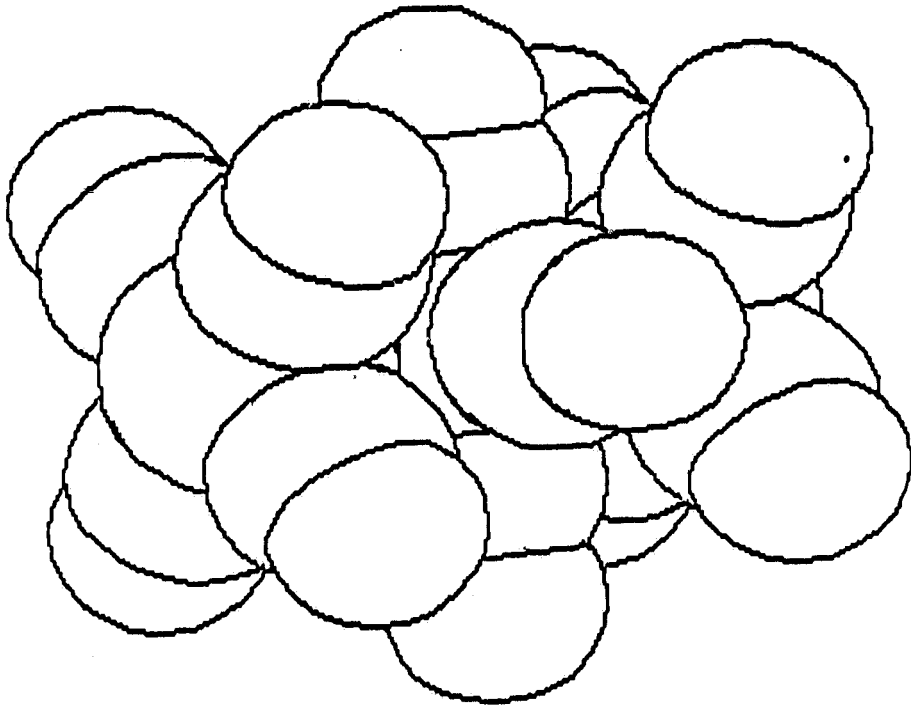
Figure 1. 'TYCHO' Hardware Configuration



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FIGURE 2

EXAMPLE OF GRAPHICS OUTPUT



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FIGURE 3
TYCHO SOFTWARE DESIGN

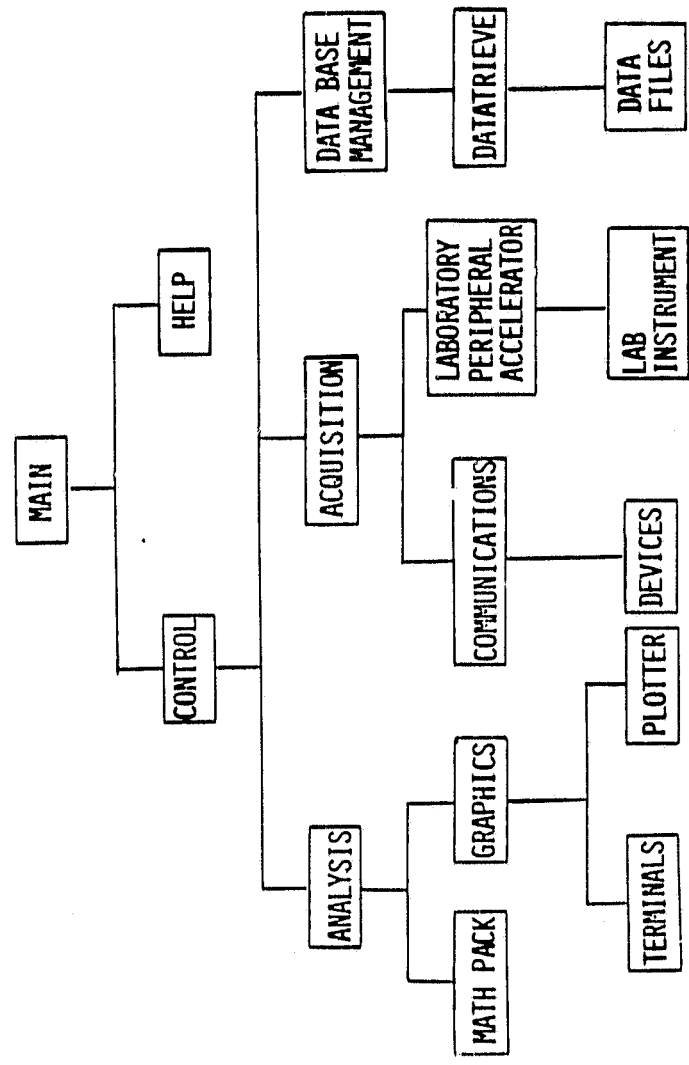


TABLE 1

TYPE	MODEL	ASSOCIATED PROCESSOR	INTERFACE
Digitizing Tablet and Graphics Terminal	GTCO	Z-88A	RS-232C
Fourier Transform Infrared Spec.	NICOLE MX1		RS-232C
Gas Chromatograph/ Mass Spec.	HP-5933A	HP 2100	RS-232C
Mechanical Testor	INSTRON	PDP 11/03	RS-232C
Thermal Analysis	DUPONT 990 (3 each)		A/D
Thermal Analysis	DUPONT 1090		RS-232C
Liquid Chromatography	WATERS	Spectra Physics SP 4000	RS-232C
NBS Smoke Chamber		HP 9835	RS-232C
PMR	VARIAN EM390		A/D, D/A
Toxicology			A/D
Gas Chromatography	HP-5830A		RS-232C
EPR	BRUCKER-ER200tt		A/D, D/A
DMA	DUPONT 901	MINC-11	RS-232C

ACKNOWLEDGEMENT

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CHEMICAL LABORATORY MANAGEMENT SYSTEM

Abstract :

The Chemical Laboratory Management System (CLMS) is a collection of integrated chemical application systems installed on a FDP-11/44 at NASA/Ames Chemical Research Projects Office. CLMS is a system for the acquisition, analysis, storage, management, and representation of chemical data and information related to composites, polymers, and other materials. CLMS is comprised of the following systems :

CDMS Chemical Database Management System
CSSS Chemical Structure Storage System
SPMS Structure-Properties Modelling System
DAAS Data Acquisition and Analysis System
DIGS Device Independent Graphics System.

These systems are designed to be :

- 1) highly interactive
- 2) simple to use
- 3) easy to learn.

These systems are command driven. Many of the commands and options are presented to the user in a menu format. This improves the simplicity of use.

Hardware features in the terminals will be exploited whenever possible. If a terminal has programmable function keys, a system will program the keys on a menu-by-menu basis to simplify interaction and reduce user typing.

Introduction :

The following list describes the systems which comprise the CLMS at CRPO :

CDMS Chemical Database Management System

This is the 'kernel' or the core of the systems developed for CRPO. It provides access to all the databases installed on TYCHO for the users directly and for the other application systems.

Interfaces to the databases will be made through DATATRIEVE-11 and RMS-11. The RMS-11 interface is provided to support database access from within programming languages.

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CSSS Chemical Structure Storage System

This system will maintain access and provide data entry utilities for a database of chemical structure and topology information. It will be capable of structure and substructure searches of the database.

This system will be interfaced to the Structure-Properties Modelling System which will rely on CSSS for its DBM support.

SPMS Structure-Properties Modelling System

This system will perform semi-empirical modelling of resin systems based on software models installed on the computer, information in the structure and topology database, and information in the properties database.

Since it will perform pattern matching for approximate substructure similarities. A relatively sophisticated AI (artificial intelligence) capability will necessary.

DAAS Data Acquisition and Analysis System

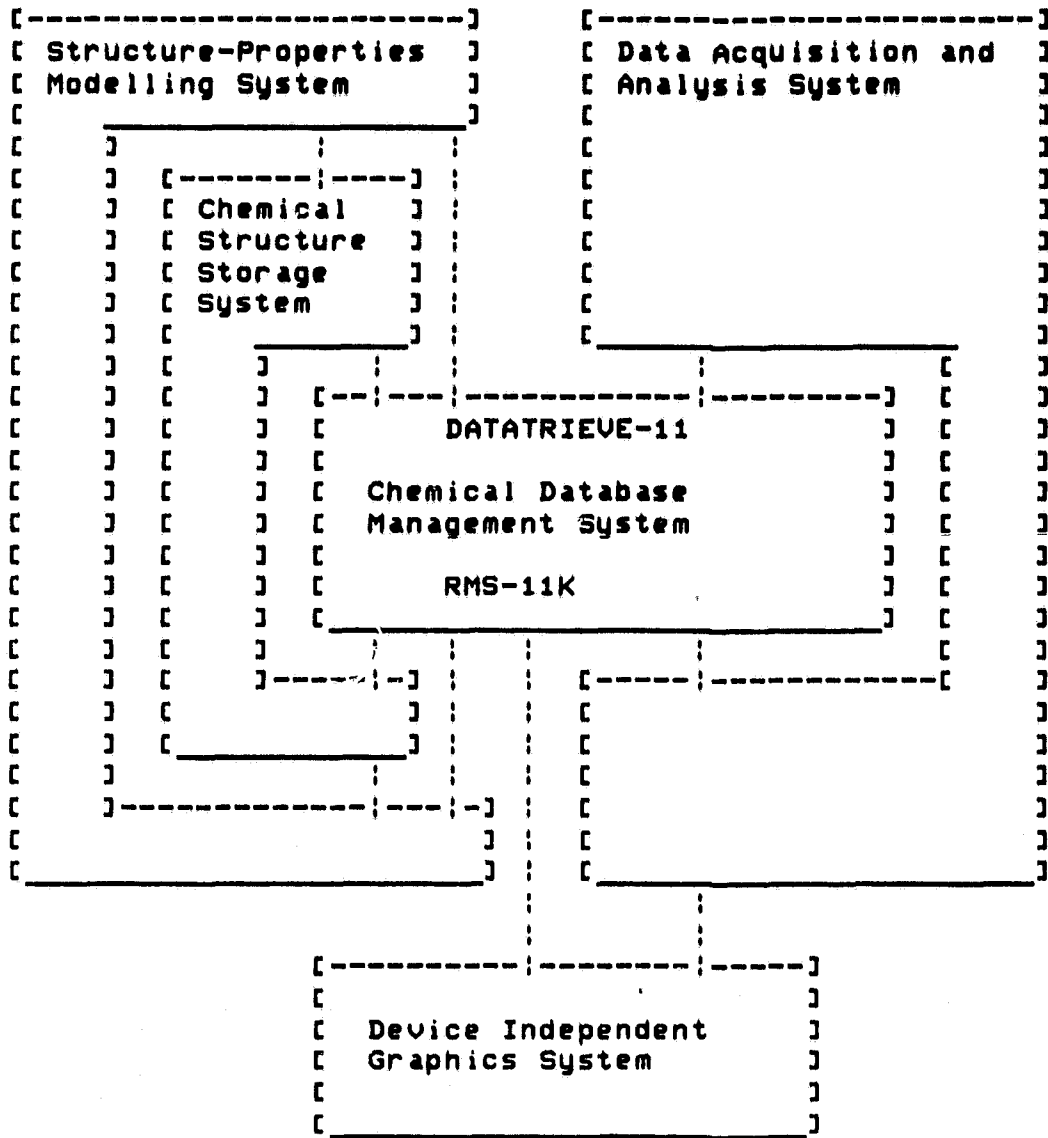
This system will control and monitor data acquisition from instruments throughout the building. It will perform varying degrees of analysis on that data. It will provide some data entry support to the properties database.

DIGS Device Independent Graphics System

This system is actually a utility that will be used in several of the other systems, as well as user applications.

DIGS will provide device and language independent graphics support for the system. It will also provide an interactive graphics utility with device independence.

Chemical Laboratory Management System
Hierarchy



APPENDIX IV.

CHEMICAL STRUCTURE STORAGE SYSTEM -- (CSSS)

Overview

This system will maintain a database of structure and topology information on materials of interest to CRPO. It will maintain the ability to encode the structure from a variety of sources and obtain topology from the user or from codes which will calculate approximate topologies (via bond optimization). It will have the ability to search the database for matching structures and common substructures.

The output from the system will be in the form of candidate materials, with or without accompanying physical properties data. The output can be represented tabularly, graphically as structure diagrams, or graphically as space-filling models.

Following is a brief description of some of the chemical structure coding algorithms that can be used, and a tentative description of the implementation of the system.

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Selection of a Chemical Structure Coding/Decoding Algorithm

We are designing a system which will store chemical structure information and, in addition, search this collection of information for similar structures and substructures.

One of the first steps in the design of this system is the selection of an algorithm for coding the structure data into the computer. For expediency, an existing algorithm should be used. Three of these algorithms will be considered here.

The selection criteria for a structure coding algorithm include the following points :

- 1) ease of use for coding/decoding
- 2) compactness of representation
- 3) compactness of resulting database
- 4) ease and speed of search
- 5) must include stereochemical information
- 6) readability

* Connectivity Tables

A chemical structure diagram can be thought of as a graph, consisting of a collection of nodes and edges. Connectivity tables (or connection tables -- CT) are simply a tabular representation of that graph. This is, in principle, a more straightforward and readable notation than WLN. The CT consist of a set of lists. Each atom is assigned a number. An atom type is associated with each number (the atomic number or character symbol for that element). The next list contains the numbers of all atoms connected to the current atom. The next list enumerates the types of connections made in the previous list (single bond, double bond, etc.). More lists can be added as necessary to include isotopic information or some other special information. CT's are not as compact as WLN, but substructure searches are much easier and quicker to perform, and CT's can easily be used to generate the chemical structure diagram.

A CT coding example : 2-chloro-cyclohexanol

1	C	2,7	S,S
2	C	1,3	S,S
3	C	2,4	S,S
4	C	3,5	S,S
5	C	4,6,7	S,S,S
6	O	5	S
7	C	5,8,1	S,S,S
8	Cl	7	S

Because of the ease in translation between CT and structure diagrams, no matter which algorithm is chosen for structure storage, the CT will either be present or generated for each diagram.

*** Stereochemically Extended Morgan Algorithm**

The SEMA notation is based on keeping track of extended connectivity. Extended connectivity includes the connectivity of neighbor atoms with the connectivity of the central atom. The order of extended connectivity is the limit of how removed the neighbors are that are being included in the extended connectivity (ie. second order implies connectivity out to neighbors twice removed). SEMA provides an index of how centrally involved an atom is in a structure. SEMA is a set of rules for constructing a unique searchable index. Structures can be searched very rapidly using SEMA. Substructures can also be searched, but not as easily. It is a relatively compact notation. There is commercial and public domain software for coding and decoding SEMA. Since it is built from a type of connectivity table, translation between CT and SEMA is quite straightforward.

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Tenative Implementation of Chemical Structure Storage System

We currently plan to store the structure information as follows :

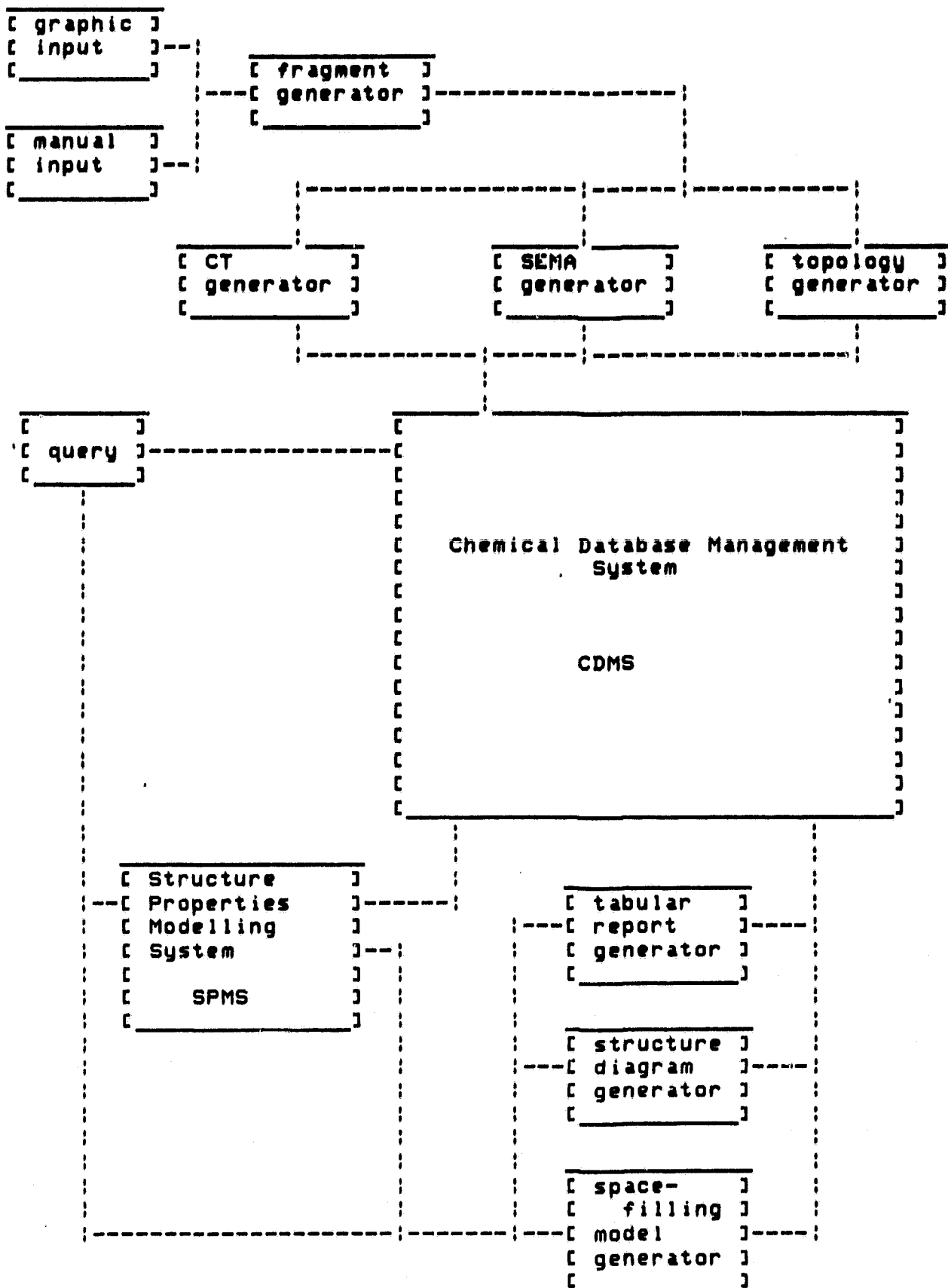
- 1) From INPUT, generate exhaustive list of component fragments and connectivity table
- 2) Code structure and fragments by their SEMA codes and percent composition (before cataloging, a search of the SEMA codes on the database will be done to eliminate redundant entries)
- 3) The database will be entered into DATATRIEVE-11 domains. This implementation will greatly reduce the time needed to develop the database and will simplify the interface between the structure database and the properties database, which is already implemented using DATATRIEVE-11.
 - a) Two sets of cross-referenced records will be installed :
 - i) for the structures, a list of all associated fragments and percent composition
 - ii) for the fragments, a list of all associated structures and percent composition
- 4) The connectivity tables will be cross-referenced by SEMA code and will have optionally extended fields that contain additional topology information (eg. atomic coordinates in Angstroms)

Using DATATRIEVE-11 to store the fragments will probably be slower to search than ordering the fragment list, as is done by Friedrich and Ugi (see references). But this loss in speed is compensated by a reduction in the time to develop the database and in the simplified interface between the structures database and the properties database. The loss in speed is also made less important by the fact that the database will not contain a large number of different materials (other structure databases are designed to handle tens of thousands to millions of different materials).

Initially, structure information obtained from physical properties and properties obtained from structure information will be limited to correlations between the two databases.

Chemical Structure Storage System Hierachy

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CT/topology file :

There will be a record for each fragment(material) for which there is a SEMA code on record in the system.

- A) SEMA number
- B) CT with optional extension (repeat for each atom)
 - 1) atom number
 - 2) atom type
 - 3) connections
 - 4) connection types
 - 5) X,Y,Z coordinates

Material Structure File :

There will be a record for each material on record in the system.

- A) SEMA number
- B) fragment list (repeat for each fragment present)
 - 1) SEMA
 - 2) percent composition

Fragment Structure File :

There will be a record for each fragment on record in the system

- A) SEMA number
- B) material list (repeat for each material in which fragment is found)
 - 1) SEMA
 - 2) percent composition