

DEC-12-UW5A-D  
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## NMRSIM(E)

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## 1.0 ABSTRACT

NMRSIM(E)<sup>1</sup> is designed to calculate theoretical spectra of compounds containing nuclei of spin one-half, including hydrogen, fluorine, and carbon-13. Chemical shifts for each nucleus and coupling constants between nuclei are input from the Teletype. Calculated line spectra are displayed on the VR12 scope. Twenty-five calibration points are displayed across the X axis. Output is to LINCtape and high- or low-speed paper tape punch, as well as to the Teletype. NMRSIM has options that allow varying all the parameters as well as offsets for enhancement of resolution. Chemical shifts and coupling constants may be adjusted continuously until the displayed theoretical spectrum is acceptable. Spectra may be read back and displayed from LINCtape or paper tape; several spectra may be merged in this mode of operation, thereby allowing the simulation of large spin systems or mixtures of compounds.

## 2.0 EQUIPMENT

A PDP-12A equipped with KW12A real time clock and MC12 4K Memory Extension is required.

## 3.0 OPERATING PROCEDURES

NMRSIM(E) is loaded from a LAP6-DIAL<sup>2</sup> tape containing the program by the command

```
→ LO NMRSIM(E),Ø )
```

Refer to the LAP6-DIAL Programmer's Manual, DEC-12-SE2B-D for further details.

The restarting procedure is as follows:

- 1) Press the STOP key on the PDP-12A.
- 2) Press I/O PRESET.
- 3) Press START.

NMRSIM then returns to the display mode.

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NMRSIME utilizes the EAE option for the PDP-12.

<sup>2</sup>LAP6-DIAL is hereafter referred to as DIAL.

#### 4.0 SPECTRUM GENERATION

After the program is loaded, it prints a series of messages on the Teletype to specialize the parameters for the experiment. The user types a reply to each message and terminates the response by pressing the RETURN key. If an illegal response is typed, a ? is printed on the Teletype and the message is repeated. The RUBOUT key can be used to erase incorrectly typed characters before a terminator is typed. The messages are listed below with their acceptable responses. Refer to section 8.0 for a sample dialogue.

#### 4.1 COMMENTS:

Any amount of commentary can be typed at this time using any of the Teletype keys. After entering appropriate titles, type CTRL/A to advance to the next message.

#### 4.2 WANT PAPER TAPE I/O?

Only a response of Y or N is acceptable. A reply of N stores the position and intensity of all calculated transitions on LINtape only. A reply of Y outputs the position and intensity of all calculated transitions on paper tape in addition to LINtape. After a reply of Y, a second question is printed:

WANT HIGH SPEED READER-PUNCH?

Type Y to use the high-speed punch, type N to output to the Teletype punch.

#### 4.3 NO. OF SPINS =

Enter the number of spins; values from 1 through 6 are acceptable.

#### 4.4 OFFSET & WIDTH

These two parameters define the range of the X axis on the scope. OFFSET is the value in Hz of the first point displayed along the horizontal axis. WIDTH is the total range in Hz of the horizontal axis. It is important to keep in mind that the axis will be displayed from right to left corresponding to the standard display mode for NMR data.

#### 4.5 CHEMICAL SHIFTS:

Enter the value in Hz of the CHEMICAL SHIFTS in order. Type a comma to separate values:

1, 2, . . . , n

#### 4.6 COUPLING CONSTANTS

Enter the value in Hz of the coupling constants in order:

$J_{1\ 2}, J_{1\ 3}, J_{1\ 4}, \dots, J_{1n}, J_{2\ 3}, J_{2\ 4}, \dots, J_{2n}, \dots, J_{(n-1)n}$

Specify every coupling constant required, even if the value is zero. Type a comma after each value.

#### 4.7 BLOCK, U:

Type the starting block in octal notation, a comma, and the number of the LINCtape transport unit to be used to store the peak parameters of the calculated transitions. The number of blocks required is dependent upon the size of the spin system desired.

The computer now calculates the theoretical spectra and automatically stores the data on the LINCtape.

#### 5.0 COMMANDS

When displaying a line spectrum the Teletype is active and can be used to issue commands defining the next task for the computer. Six options are available to the user at this time. Each of these commands is issued by typing the appropriate letter followed by a colon. The command may be changed by using the RUBOUT key before the colon has been typed. The display can be scaled with Right Switches 9, 10 and 11.

#### 5.1 R (RESTART)

Restart prints the message COMMENTS (section 4.1) and restarts the program. It is used to calculate a complete set of new data. Note that paper tape status can not be changed after the initial responses to the messages.

## 5.2 C (COUPLING CONSTANTS)

Returns to section 4.6 and requests new parameters. Used for open loop iteration to find the best coupling constants.

## 5.3 O (OFFSET & WIDTH)

This command allows a new section of the X axis to be displayed on the scope so that any section of the calculated spectrum can be displayed on the scope. The OFFSET option is useful for resolution enhancement. To exercise this option, there must be NMR data on LINCtape or paper tape (prepared by the P: command). If paper tape was requested during initialization (section 4.2), the question

TAPE INPUT?

is asked. Type Y to read data from the high speed or Teletype reader and write it on LINCtape before display. Type N to read data from LINCtape.

## 5.4 D (DIAL)

Program returns control to the DIAL Operating System.

## 5.5 L (LIST)

The L command lists intensity and energy data on the Teletype in tabular format. After typing L, the message

MIN. INTENSITY:

is printed. Type an integer number between 0 and 1000. If the intensity of the transition is greater than the entered value, the transition will be in the output list. This question thus serves as a threshold on the intensities that are listed. A second question

DISPLAY LIST

is then printed. Type Y to output only the lines which are displayed on the scope. Type N to output all lines in the table. There are usually many more lines than are displayed on the scope because the scope cannot resolve closely adjacent lines.<sup>1</sup>

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If the Teletype punch is turned on during a List operation, a binary coded decimal paper tape is produced which may be used as input to CATAL (DEC-12-UW1A-D) to produce a spectrum consisting of peaks instead of lines.



## 5.6 P (PUNCH)

The accumulated spectrum can be punched on the high-speed reader/punch by issuing the punch command.

## 6.0 OPERATING SUGGESTIONS

A useful starting point for many 60 MHz NMR (hydrogen) spectra of organic molecules is a sweep offset of 0 Hz and a sweep width of 500 Hz. For best results, however, all peaks should eventually be examined at a considerably smaller sweep width, since rounding errors may give misleading scope displays with large sweep widths. It should be noted that increasing the sweep offset moves peaks to the right, and decreasing the sweep offset moves peaks to the left. Once the peaks are observed, the proper sweep offset and width can be determined from the 25 calibration marks placed across the X axis.

For purposes of estimating a logical minimum intensity, remember that the calibration on the scope on the Y axis is always 0 to 1000.

## 7.0 NMR BACKGROUND

The discussion below assumes that the nuclei being studied are hydrogen, fluorine, carbon-13 or other nuclei of spin 1/2.

Each nucleus in a molecule can be assigned a spin of either  $\alpha$  or  $\beta$ . For a system containing  $n$  nuclei, there are  $2^n$  spin states possible. Each of these states is called a basic product function. The energy of a basic product function can be calculated from equation 1 below where  $s_i = -1/2$  for  $\beta$  spin and  $+1/2$  for  $\alpha$  spin,  $\nu_i$  is the frequency of absorption in Hz,  $T_{ij} = +1/4$  if  $i$  and  $j$  have the same spin and  $-1/4$  if  $i$  and  $j$  have opposite spin, and  $J_{ij}$  is the coupling constant between  $i$  and  $j$  in cps.

$$1 \quad H_{uu} = \sum_{i=1}^n (s_i \nu_i + \sum_{j>i} T_{ij} J_{ij})$$

The energy of interaction between two basic product functions is 0 unless both have the same number of  $\alpha$  and  $\beta$  spins. When this condition is fulfilled, the interaction energy is calculated from equation 2 where  $U=1$  if the basic product functions differ only in the interchange of spins  $i$  and  $j$  ( $J_{ij}$  as defined above). Otherwise,  $U=0$ .

$$2 \quad H_{uv} = 1/2 U J_{ij}$$

Thus, to calculate an NMR spectrum, one constructs all of the possible basic product functions and sorts them into groups, each member of a group containing the same number of  $\alpha$  and  $\beta$  spins. The energy of each of them is determined and used as the diagonal element in a square matrix. The off-diagonal elements of this matrix (H matrix) are energies of interaction between the members of the group. This matrix is diagonalized and these elements then contain the energies of the final spin functions. These final spin eigenfunctions are the columns of the matrix (U matrix) required to diagonalize the H matrix. Each element in a spin function represents the contribution of a basic product function to that spin function.

Before continuing, it is necessary to define the  $F_z$  value of a spin function, as shown in equation 3, where  $s_i$  is as previously defined.

$$3 \quad F_z = \sum_{i=1}^n s_i$$

Now the peaks observed in NMR spectra are transitions from one spin function to another. These transition energies and their intensities can be calculated as outlined below. Transitions are allowed between spin functions whose  $F_z$  values differ only by 1. If this holds, the energy of the transition is the difference in energy of the final spin eigenfunctions, and the intensity of the transition is given by equation 4 where  $C_u$  is the  $u$ th element in one spin function,  $C'_v$  is the  $v$ th element in the other spin function, and  $A=1$  if the basic product functions represented by  $C_u$  and  $C'_v$  differ by one spin. Otherwise,  $A=0$ .

$$4 \quad I = \left( \sum_u \sum_v C_u C'_v A \right)^2$$

## 8.0 EXAMPLE

The following pages represent an actual printout. The spectra are representations of those displayed on the scope. The underlined data is that typed by the user.

LO NMRSIME, 2

NMRSIM

COMMENTS: DEMO 1

WANT PAPER TAPE I/O?Y

WANT HIGH SPEED READER-PUNCH?Y

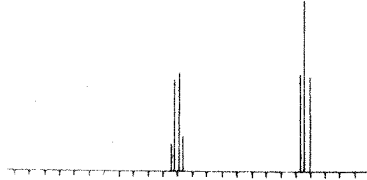
NO. OF SPINS= 5

OFFSET & WIDTH: 0, 500

CHEMICAL SHIFTS: 90, 90, 90, 260, 260

COUPLING CONSTANTS: 0, 0, 8, 8, 0, 8, 8, 8, 8, 0,

BLOCK, U: 400, 3



L:

MIN. INTENSITY: 0

DISPLAY LIST?Y

INTENSITY	ENERGY
27.00	272.00
90.00	264.00
99.00	256.00
36.00	248.00
104.00	97.00
109.00	90.00
86.00	81.00

P:  
Q:

OFFSET & WIDTH: 0,300

TAPE INPUT? Y

BLOCK, U: 420,3,

MORE? N

P:

NMRSIM

COMMENTS: DEMO 1 CONT

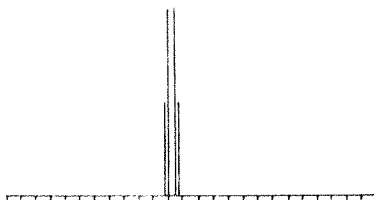
NO. OF SPINS= 2

OFFSET & WIDTH: 0,500

CHEMICAL SHIFTS: 265,280

COUPLING CONSTANTS: 5

BLOCK, U: 440,3



C:

COUPLING CONSTANTS: 10

BLOCK, U: 440,3

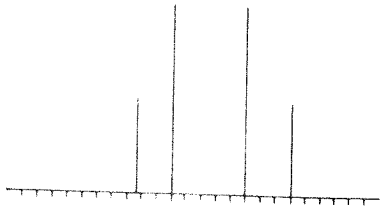
G:

OFFSET & WIDTH: 250,50

TAPE INPUT? N

BLOCK, U: 440,3

MORE?N



D:

## 9.0 ASSEMBLING NMRSIM

The NMRSIM program is supplied to the user in both source and binary on the tape. To generate a new binary file if the source program is modified, use the following procedure.

1. Load a DIAL-MS tape on unit 0. Load unit 1 with either a DIAL-V2 or DIAL-MS system tape. If another tape unit is available, mount the tape containing the CLEARSYM and NMRSIM source programs there. If only two tape units are available, place the source programs on unit 0 (with PIP if necessary), in order to reduce the assembly time.

2. Type →ZE↵ to clear the binary Working Area of unit 1.
3. Type →AS CLEARSYM↵. CLEARSYM is a two word program which produces a clean symbol table.

```
0000  
SAVSYM 1
```

4. Type →AS NMR2,0↵. Error messages generated at this time should be ignored. Press the RETURN key to terminate the assembly after the errors have all been printed to suppress printing of the symbol table.
5. Type →ZE↵. This clears the binary Working Area on unit 1.
6. Type →LI NMR3,0↵. If no listing is desired, use the AS command. Any errors generated now are real and must be corrected.
7. Type →LI NMR2,0↵. Because the symbol table produced is the same as the one generated in step 6, printing may be suppressed with the RETURN key after it has started to be printed.
8. Type →SB NMR23,0↵. This saves the binary output from the two previous assemblies
9. Type →ZE↵.
10. Two versions of the Floating Point Package are applied. If the machine has the FAE option, NMR1F should be used in the following steps and NMRSIME will be generated. If the machine does not have this option, NMR1 should be used to generate NMRSIM.

11. Type `+AB NMRL,Ø`.
12. Type `+AB NMR23,Ø`.
13. Type `+SB NMRSIM,ØP`. A binary file of NMRSIM(E) has now been generated and the command `+LO NMRSIM,Ø` will cause load and execute.

#### 10.0 INTERNAL DESCRIPTION

The complete program listings are contained at the back of the manual. The following is a brief outline of the program; capital letters below refer to variables.

1. Begins with text mode for input of commentary.
2. Enter the number of spins and store in N.
3. Set "switch" for punched output.
4. Set up basic produce functions (BPFs).
  - A. Calculate NARRY array which contains relative addresses of the BPFs of different  $F_z$  value.
  - B. Calculate NUSE array. This array actually contains the BPFs. They are stored in groups, each group having an  $F_z$  value one greater than the preceding group.
5. Get sweep offset and sweep width.
6. Get chemical shifts.
7. Get coupling constants.
8. Initialize SPEC array.
  - A. This array eventually contains the displayed spectrum.
  - B. It is initialized to Ø except for calibration points where it is set to 4ØØØØ.
9. Calculate first H and U matrices.
  - A. First H matrix is always a 1 X 1 which does not require diagonalization.
  - B. First U matrix is always a 1 X 1 with its only element equal to 1.
10. Set FLAG which is the negative of the number of times the loop from 11 to 17 must be executed.

11. Set N2, calculate EN and UOLD arrays.
  - A. Copy the trace of the H matrix into the EN array.
  - B. Copy the U matrix into the UOLD array.
  - C. Set N2 equal to the size of the H matrix just copied.
12. Calculate the size of the next H matrix and put in into N1.
13. Determine which transitions will be allowed between the BPFs represented by UOLD and those that will be represented by U. This is stored in the array called TABLE.
14. Initialize H and U matrixes.
  - A. Diagonal H elements are calculated by equation 1.
  - B. Off-diagonal H elements are calculated by equation 2.
  - C. The U matrix is initialized to all zeros except for ones on the diagonal.
15. Diagonalize the H matrix and calculate the U matrix by the Jacobi method.
16. Calculate transitions.
  - A. Calculate transition energies by forming the differences between the elements of the trace of the H matrix and the elements in the EN array.
  - B. Calculate transition intensities from equation 4.
  - C. Store appropriate values in SPEC array.
17. Test FLAG to see if the loop is done.
  - A. If loop is not done, go to 11.
  - B. If loop is done, display spectrum.
18. If ALT MODE is typed, interpret mnemonic and execute option.



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```

0076 3600 DISPLAY, STDIS
0077 4103 TAPTRN, LNCTAP
0100 0077 0010 UNIT, 10
0101 0100 0110 STBLK, 110
0102 0101 0000 BLK1, 0
0103 0102 0000 INSWT, 0
0104 0103 3051 AREND, -DATBUF+1=371
0105 0104 4536 CORBUF, DATBUF=1
0106 0105 0534 TPGI, GTTP
0107 0106 0000 N, 0
0110 0107 0000 TEMP, 0
0111 0110 0000 LIMIT, 0
0112 0111 0000 0
0113 0112 0000 0
0114 0113 0000 ADD0, 0
0115 0114 0000 TEMP1, 0
0116 0115 0000 NI, 0
0117 0116 0000 A, 0
0120 0117 0000 0
0121 0120 0000 0
0122 0121 0000 B, 0
0123 0122 0000 0
0124 0123 0000 0
0125 0124 0000 FSIN, 0
0126 0125 0000 0
0127 0126 0000 0
0130 0127 0000 FCOS, 0
0131 0130 0000 0
0132 0131 0000 0
0133 0132 0000 N2, 0
0134 0133 0000 JTEMP, 0
0135 0134 0000 FACTOR, 0
0136 0135 0000 0
0137 0136 0000 0
0140 0137 0000 OFFSET, 0
0141 0140 0000 0
0142 0141 0000 0
0143 0142 0000 0
0144 0143 0000 POND=, /MARK END P0
0145 0144 0000 *200
0146 0200 CLA
0147 0201 3055 DCA 55
0148 0202 6032 KCC
0149 0203 6046 TLS
0150 0204 6014 RFC
0151 0205 4474 JMS I PRINT
0152 0206 3747 HD1
0153 0207 4025 JMS READ
0154 0210 4232 JMS TYPE
0155 0211 1332 TAD M2010
0156 0212 7640 SZA CLA
0157 0213 5207 JMP OVERO
0158 0214 4720 JMS I INDIL
0159 0215 3214 DCA .=1
0160 0216 5222 JMP GTSPN
0161 0217 7200 ERROH0, CLA
0162 0220 1530 TAD QUEST
0163 0221 4032 JMS TYPE
0164 0222 4474 JMS I PRINT
0165 0223 3764 HD2
0166 0224 4405 JMS I INPUT
0167 0225 4712 JMS I FIXM
0168 0226 7110 CLL RAR
0169 0227 7110 0
0170 0228 7110 0
0171 0229 7110 0
0172 0230 7110 0
0173 0231 7110 0
0174 0232 7110 0
0175 0233 7110 0
0176 0234 7110 0
0177 0235 7110 0
0178 0236 7110 0
0179 0237 7110 0
0180 0238 7110 0
0181 0239 7110 0
0182 0240 7110 0
0183 0241 7110 0
0184 0242 7110 0
0185 0243 7110 0
0186 0244 7110 0
0187 0245 7110 0
0188 0246 7110 0
0189 0247 7110 0
0190 0248 7110 0
0191 0249 7110 0
0192 0250 7110 0
0193 0251 7110 0
0194 0252 7110 0
0195 0253 7110 0
0196 0254 7110 0
0197 0255 7110 0
0198 0256 7110 0
0199 0257 7110 0
0200 0258 7110 0
0201 0259 7110 0
0202 0260 7110 0
0203 0261 7110 0
0204 0262 7110 0
0205 0263 7110 0
0206 0264 7110 0
0207 0265 7110 0
0208 0266 7110 0
0209 0267 7110 0
0210 0268 7110 0
0211 0269 7110 0
0212 0270 7110 0
0213 0271 7110 0
0214 0272 7110 0
0215 0273 7110 0
0216 0274 7110 0
0217 0275 7110 0
0218 0276 7110 0
0219 0277 7110 0
0220 0278 7110 0
0221 0279 7110 0
0222 0280 7110 0
0223 0281 7110 0
0224 0282 7110 0
0225 0283 7110 0
0226 0284 7110 0
0227 0285 7110 0
0228 0286 7110 0
0229 0287 7110 0
0230 0288 7110 0
0231 0289 7110 0
0232 0290 7110 0
0233 0291 7110 0
0234 0292 7110 0
0235 0293 7110 0
0236 0294 7110 0
0237 0295 7110 0
0238 0296 7110 0
0239 0297 7110 0
0240 0298 7110 0
0241 0299 7110 0
0242 0300 7110 0
0243 0301 7110 0
0244 0302 7110 0
0245 0303 7110 0
0246 0304 7110 0
0247 0305 7110 0
0248 0306 7110 0
0249 0307 7110 0
0250 0308 7110 0
0251 0309 7110 0
0252 0310 7110 0
0253 0311 7110 0
0254 0312 7110 0
0255 0313 7110 0
0256 0314 7110 0
0257 0315 7110 0
0258 0316 7110 0
0259 0317 7110 0
0260 0318 7110 0
0261 0319 7110 0
0262 0320 7110 0
0263 0321 7110 0
0264 0322 7110 0
0265 0323 7110 0
0266 0324 7110 0
0267 0325 7110 0
0268 0326 7110 0
0269 0327 7110 0
0270 0328 7110 0
0271 0329 7110 0
0272 0330 7110 0
0273 0331 7110 0
0274 0332 7110 0
0275 0333 7110 0
0276 0334 7110 0
0277 0335 7110 0
0278 0336 7110 0
0279 0337 7110 0
0280 0338 7110 0
0281 0339 7110 0
0282 0340 7110 0
0283 0341 7110 0
0284 0342 7110 0
0285 0343 7110 0
0286 0344 7110 0
0287 0345 7110 0
0288 0346 7110 0
0289 0347 7110 0
0290 0348 7110 0
0291 0349 7110 0
0292 0350 7110 0
0293 0351 7110 0
0294 0352 7110 0
0295 0353 7110 0
0296 0354 7110 0
0297 0355 7110 0
0298 0356 7110 0
0299 0357 7110 0
0300 0358 7110 0
0301 0359 7110 0
0302 0360 7110 0
0303 0361 7110 0
0304 0362 7110 0
0305 0363 7110 0
0306 0364 7110 0
0307 0365 7110 0
0308 0366 7110 0
0309 0367 7110 0
0310 0368 7110 0
0311 0369 7110 0
0312 0370 7110 0
0313 0371 7110 0
0314 0372 7110 0
0315 0373 7110 0
0316 0374 7110 0
0317 0375 7110 0
0318 0376 7110 0
0319 0377 7110 0
0320 0378 7110 0
0321 0379 7110 0
0322 0380 7110 0
0323 0381 7110 0
0324 0382 7110 0
0325 0383 7110 0
0326 0384 7110 0
0327 0385 7110 0
0328 0386 7110 0
0329 0387 7110 0
0330 0388 7110 0
0331 0389 7110 0
0332 0390 7110 0
0333 0391 7110 0
0334 0392 7110 0
0335 0393 7110 0
0336 0394 7110 0
0337 0395 7110 0
0338 0396 7110 0
0339 0397 7110 0
0340 0398 7110 0
0341 0399 7110 0
0342 0400 7110 0
0343 0401 7110 0
0344 0402 7110 0
0345 0403 7110 0
0346 0404 7110 0
0347 0405 7110 0
0348 0406 7110 0
0349 0407 7110 0
0350 0408 7110 0
0351 0409 7110 0
0352 0410 7110 0
0353 0411 7110 0
0354 0412 7110 0
0355 0413 7110 0
0356 0414 7110 0
0357 0415 7110 0
0358 0416 7110 0
0359 0417 7110 0
0360 0418 7110 0
0361 0419 7110 0
0362 0420 7110 0
0363 0421 7110 0
0364 0422 7110 0
0365 0423 7110 0
0366 0424 7110 0
0367 0425 7110 0
0368 0426 7110 0
0369 0427 7110 0
0370 0428 7110 0
0371 0429 7110 0
0372 0430 7110 0
0373 0431 7110 0
0374 0432 7110 0
0375 0433 7110 0
0376 0434 7110 0
0377 0435 7110 0
0378 0436 7110 0
0379 0437 7110 0
0380 0438 7110 0
0381 0439 7110 0
0382 0440 7110 0
0383 0441 7110 0
0384 0442 7110 0
0385 0443 7110 0
0386 0444 7110 0
0387 0445 7110 0
0388 0446 7110 0
0389 0447 7110 0
0390 0448 7110 0
0391 0449 7110 0
0392 0450 7110 0
0393 0451 7110 0
0394 0452 7110 0
0395 0453 7110 0
0396 0454 7110 0
0397 0455 7110 0
0398 0456 7110 0
0399 0457 7110 0
0400 0458 7110 0
0401 0459 7110 0
0402 0460 7110 0
0403 0461 7110 0
0404 0462 7110 0
0405 0463 7110 0
0406 0464 7110 0
0407 0465 7110 0
0408 0466 7110 0
0409 0467 7110 0
0410 0468 7110 0
0411 0469 7110 0
0412 0470 7110 0
0413 0471 7110 0
0414 0472 7110 0
0415 0473 7110 0
0416 0474 7110 0
0417 0475 7110 0
0418 0476 7110 0
0419 0477 7110 0
0420 0478 7110 0
0421 0479 7110 0
0422 0480 7110 0
0423 0481 7110 0
0424 0482 7110 0
0425 0483 7110 0
0426 0484 7110 0
0427 0485 7110 0
0428 0486 7110 0
0429 0487 7110 0
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0275 0330 0277  QUEST, 0277  /ERROR RETURN
0276 0331 7771  M7, -7  /BLOCK 0 NOT ALLOWED
0277 0332 7577  M2010, -201  /
0300 0333 0007  P7, 7  /
0301 0334 0000  GTTP, 0  JMS I PRINT
0302 0335 4474  HD4  HD4  JMS I OCIN
0303 0336 1736  JMS I 0CIN
0304 0337 4753  JMP 0-1
0305 0340 5337  SNA 0-3
0306 0341 7450  JMP 03
0307 0342 5337  DCA STBLK
0308 0343 5100  JMS I INPUT
0309 0344 4405  JMS I FIXM
0310 0345 4712  AND MSK7
0311 0346 0352  DCA UNIT
0312 0347 5077  JMS I CARIN
0313 0350 4710  JMP I GTTP
0314 0351 7734 7
0315 0352 0007  MSK7,
0316 0353 4200  OCIN,
0317 0354 0000  HIRED,
0318 0355 6011  RSF
0319 0356 5355  JMP 0-1
0320 0357 6016  RRB RFC
0321 0360 5754  JMP I HIRED
0322 0361 0000 0
0323 0362 6026  PLS
0324 0363 6021  PSF
0325 0364 5363  JMP 0-1
0326 0365 5761  JMP I HIPUN
0327 0366 0002  *400
0328 0367 6046  TLS
0329 0368 4717  OFFS,
0330 0369 4474  JMS I AULIM
0331 0370 1770  HD8  JMS I PRINT
0332 0371 4713  JMS I ASKMX
0333 0372 5102  OCA INSWT
0334 0373 4505  JMS I TPGT
0335 0374 4716  JMS I INSPA
0336 0375 1102  TAD INSWT
0337 0376 7640  SZA CLA
0338 0377 5222  JMP GET
0339 0378 1100  TAD STBLK
0340 0379 3101  OCA BLK1
0341 0380 6014  RFC  JMS I HRED
0342 0381 4422  SNA 0-2
0343 0382 7450  JMP ROWD
0344 0383 5217  JMS DONIN
0345 0384 5267  JMP INTERP
0346 0385 4407  JMS I LIMIT
0347 0386 1110  FADD FACTOR
0348 0387 5134  EMPY HALFA
0349 0388 1320  FEXT
0350 0389 0000  JMS I FIXA
0351 0390 4723  DCA SPECAD
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0703 0742 4723  *400
0704 0743 3334  *400
0705 0744 6046  *400
0706 0745 4717  *400
0707 0746 4474  *400
0708 0747 1770  *400
0709 0748 4713  *400
0710 0749 5102  *400
0711 0750 4505  *400
0712 0751 4716  *400
0713 0752 1102  *400
0714 0753 7640  *400
0715 0754 5222  *400
0716 0755 1100  *400
0717 0756 3101  *400
0718 0757 6014  *400
0719 0758 4422  *400
0720 0759 7450  *400
0721 0760 5217  *400
0722 0761 5267  *400
0723 0762 4407  *400
0724 0763 1110  *400
0725 0764 5134  *400
0726 0765 1320  *400
0727 0766 0000  *400
0728 0767 4723  *400
0729 0768 3324  *400
0730 0769 4327  *400
0731 0770 7402  *400
0732 0771 4723  *400
0733 0772 3334  *400
0734 0773 6046  *400
0735 0774 4717  *400
0736 0775 4474  *400
0737 0776 1770  *400
0738 0777 4713  *400
0739 0778 5102  *400
0740 0779 4505  *400
0741 0780 4716  *400
0742 0781 1102  *400
0743 0782 7640  *400
0744 0783 5222  *400
0745 0784 1100  *400
0746 0785 3101  *400
0747 0786 6014  *400
0748 0787 4422  *400
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0750 0789 5217  *400
0751 0790 5267  *400
0752 0791 4407  *400
0753 0792 1110  *400
0754 0793 5134  *400
0755 0794 1320  *400
0756 0795 0000  *400
0757 0796 4723  *400
0758 0797 3324  *400
0759 0798 4327  *400
0760 0799 7402  *400
0761 0800 4723  *400
0762 0801 3334  *400
0763 0802 6046  *400
0764 0803 4717  *400
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0783 0822 5134  *400
0784 0823 1320  *400
0785 0824 0000  *400
0786 0825 4723  *400
0787 0826 3324  *400
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0790 0829 4723  *400
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0804 0843 3101  *400
0805 0844 6014  *400
0806 0845 4422  *400
0807 0846 7450  *400
0808 0847 5217  *400
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0827 0866 4505  *400
0828 0867 4716  *400
0829 0868 1102  *400
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0831 0870 5222  *400
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0833 0872 3101  *400
0834 0873 6014  *400
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0842 0881 1320  *400
0843 0882 0000  *400
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0850 0889 6046  *400
0851 0890 4717  *400
0852 0891 4474  *400
0853 0892 1770  *400
0854 0893 4713  *400
0855 0894 5102  *400
0856 0895 4505  *400
0857 0896 4716  *400
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0859 0898 7640  *400
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0861 0900 1100  *400
0862 0901 3101  *400
0863 0902 6014  *400
0864 0903 4422  *400
0865 0904 7450  *400
0866 0905 5217  *400
0867 0906 5267  *400
0868 0907 4407  *400
0869 0908 1110  *400
0870 0909 5134  *400
0871 0910 1320  *400
0872 0911 0000  *400
0873 0912 4723  *400
0874 0913 3324  *400
0875 0914 4327  *400
0876 0915 7402  *400
0877 0916 4723  *400
0878 0917 3334  *400
0879 0918 6046  *400
0880 0919 4717  *400
0881 0920 4474  *400
0882 0921 1770  *400
0883 0922 4713  *400
0884 0923 5102  *400
0885 0924 4505  *400
0886 0925 4716  *400
0887 0926 1102  *400
0888 0927 7640  *400
0889 0928 5222  *400
0890 0929 1100  *400
0891 0930 3101  *400
0892 0931 6014  *400
0893 0932 4422  *400
0894 0933 7450  *400
0895 0934 5217  *400
0896 0935 5267  *400
0897 0936 4407  *400
0898 0937 1110  *400
0899 0938 5134  *400
0900 0939 1320  *400
0901 0940 0000  *400
0902 0941 4723  *400
0903 0942 3324  *400
0904 0943 4327  *400
0905 0944 7402  *400
0906 0945 4723  *400
0907 0946 3334  *400
0908 0947 6046  *400
0909 0948 4717  *400
0910 0949 4474  *400
0911 0
```

0373	0437	1324	TAD	SPECAD	
0374	0440	7510	SPA		/IN RIGHT RANG
0375	0441	5222	JMP	GET	/NO, LOOK AT NL, ONE
0376	0442	1326	TAD	M500	/MAYBE
0377	0443	7700	SMA CLA	GET	/IN RIGHT RANGE?
0400	0444	5222	JMP	SPECAD	/NO, LOOK NEXT CASE
0401	0445	1324	TAD	SPECB	/YES, ADDRESS IN SPEC ARRAY
0402	0446	1071	TAD	SPECAD	
0403	0447	3324	DCA	10	
0404	0450	6211	CDF	I	
0405	0451	1724	TAD	SPECAD	
0406	0452	7004	RAL		/SET BIT 0 TO 0
0407	0453	7110	CLL RAR	APROB	/OVERFLOW?
0410	0454	1325	TAD	SMA CLA	/NO
0411	0455	7700	JMP	6	/YES, SET TO MAX
0412	0456	5264	JMP	I	
0413	0457	1724	TAD	SPECAD	
0414	0460	7004	RAL		
0415	0461	7250	CLA CMA	RAR	
0416	0462	3724	DCA I	SPECAD	/STORE
0417	0463	5222	JMP	GET	/LOOK NEXT CASE
0420	0464	1724	TAD	I	
0421	0465	1325	TAD	APROB	/INCREMENT CURRENT VALUE
0422	0466	5262	JMP	4	
0423	0467	4474	JMS I	PRINT	/MORE?
0424	0470	3761	HD3		
0425	0471	4713	JMS I	ASKMX	
0426	0472	7640	SZA CLA		
0427	0473	5302	JMP	NMRE	
0430	0474	1102	TAD	INSWT	/YES
0431	0475	7650	SNA CLA		/PAPER?
0432	0476	5216	JMP	GET-4	/YES
0433	0477	4505	JMS I	TPGT	/NO, LINCTAPE; GET BLOCK, UNIT
0434	0500	4715	JMS I	TPSIR	/INIT. TAPE AND BUFFER
0435	0501	5222	JMP	GET	
0436	0502	4714	JMS I	CARLFD	
0437	0503	1102	TAD	INSWT	
0440	0504	7640	SZA CLA		
0441	0505	5475	JMP I	DISPLAY	
0442	0506	7133	STL IAC	RTR	/INSERT TAG WORD
0443	0507	6201	COF 0		
0444	0510	3411	DCA I	11	
0445	0511	4476	JMS I	TAPTRN	/WRITE OUT LAST BUFFER
0446	0512	5475	JMP I	DISPLAY	
0447	0513	4315	ASKMX,	ASKM	
0450	0514	2663	CARLFD,	CRLFD	
0451	0515	3317	TPSTR,	STRTP	
0452	0516	1121	INSPA,	INSPEC	
0453	0517	3554	AULIM,	ULIMP	
0454	0520	0000	HALFA,	0	
0455	0521	2000	0	2000	
0456	0522	0000	0	0	
0457	0523	3127	FIXA,	FIX	
0460	0524	0000	SPECAD,	0	
0461	0525	0000	APROB,	0	
0462			DECIMAL		
0463	0526	7014	M500,	-500	
0464			OCIAL		
0465	0527	0000	RWD,	0	
0466	0530	7200	CLA	CLA	
0467	0531	6201	COF 0		
0470	0532	1102	TAD	INSWT	

0472	JMP	STPE	
0534	JMS I	FACLOD	
0535	JMP	RDEX	/NORMAL RETURN
0474	JMP I	RWD	
0475	STA CLL	RTL	/-3
0476	DCA	FLAG	/INITIALIZE TO READ THREE WORDS
0477	TAD	P44	
0500	DCA	ADD0	
0501	JMS I	CKEND	/CHECK FOR END OF BUFFER
0502	CLA CLL		
0503	JMS I	HRED	
0504	RTL		/SHIFT TO BITS 2-7
0505	RTL		
0506	RTL		
0507	RAL		
0510	SPA		
0511	JMP	BACK0	/IS THIS A STARTING MARK?
0512	SZL		/YES
0513	JMP I	RWD	/NO, IS IT AN END MARK?
0514	RAL		/YES, EXIT W/O INCRD RETURN
0515	JMS I	HRED	/NO, SHIFT TO BITS 0-5
0516	DCA I	ADD0	/STORE COMPLETE WORD
0517	TAD I	ADD0	/STICK IT IN CORE BUFFER
0518	DCA I	I1	
0520	ISZ	ADD0	
0521	ISZ	FLAG	/IS WHOLE F.P. READ?
0522	ISZ	BACK0	/NO, READ NEXT WORD
0523	JMP	RWD	/NORMALLY INCR, RETURN
0524	ISZ	RWD	/YES, RETURN
0525	JMP I	RWD	
0526	P44,	0044	
0527	ENDCHK		
0530	FLAGR,	0	
0531	FACLOD,	LODFAC	
0532	*600		
0533	WC,		
0534	CLA		/INPUT OF CPS AND CUP
0535	TAD		
0536	DCA	CPSB	
0537	TAD	ADDR	/START OF CPS ARRAY
0540	CIA	N	
0541	DCA	FLAG	/SET OF CHEMICAL SHIFTS
0542	JMP	RPTC	/GET CHEMICAL SHIFTS
0543	0		
0544	CLA		
0545	TAD	JC	
0546	DCA	WC	
0547	TAD	CUPB	
0550	DCA	ADDR	/START OF CUP ARRAY
0551	TAD	N	
0552	CIA		
0553	IAC		
0554	DCA	FLAG	/SET TO CALCULATE OF JS
0555	TAD	FLAG	
0556	ISZ	FLAG	
0557	JMP	,-2	
0560	DCA	FLAG	/FLAG CONTAINS - OF JS
0561	JMS I	INPUT	/GET A VALUE
0562	JMS I	INTERP	
0563	FDIV2		
0564	FPUT I	ADDR	/STORE
0565	FEXT		
0566	CLA IAC	STL RAL	
0567	TAD	ADDR	



ISZ	FLAG	/DONE?
0571	RPTC	/NO; GET NEXT
0572	WC	/YES; RETURN
0573	KLAEL	/CLEAR ADD0 (3 WORDS)
0574	CPSB	
0575	ADDRC	/ADDRC INITIALIZED TO CPS
0576	CUPB	
0577	ADDRC1	/ADDRC1 INITIALIZED TO CUP
0578	N	
0579	FLAG	/SET CPS DO LOOP
0580	TEMP	/GET BPF
0581	TEMC	/STORE IN TEMC
0582	TEMC	
0583	TEMC1	/GET RIGHTMOST BIT
0584	TEMC1	/STORE REDUCED BPF
0585	TEMC1	
0586	TEMC1	/STORE FOR J USE
0587	TEMC1	/ALPHA OR BETA?
0588	TEMC1	/ALPHA
0589	TEMC1	/BETA SPIN
0590	TEMC1	/SET DIRECTIONS
0591	TEMC1	
0592	TEMC1	/SET DIRECTIONS FOR JS
0593	TEMC1	
0594	TEMC1	
0595	TEMC1	
0596	TEMC1	
0597	TEMC1	
0598	TEMC1	
0599	TEMC1	
0600	TEMC1	
0601	TEMC1	
0602	TEMC1	
0603	TEMC1	
0604	TEMC1	
0605	TEMC1	
0606	TEMC1	
0607	TEMC1	
0608	TEMC1	
0609	TEMC1	
0610	TEMC1	
0611	TEMC1	
0612	TEMC1	
0613	TEMC1	
0614	TEMC1	
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0616	TEMC1	
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0618	TEMC1	
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0646	TEMC1	
0647	TEMC1	
0648	TEMC1	
0649	TEMC1	
0650	TEMC1	
0651	TEMC1	
0652	TEMC1	
0653	TEMC1	
0654	TEMC1	
0655	TEMC1	
0656	TEMC1	
0657	TEMC1	
0658	TEMC1	
0659	TEMC1	
0660	TEMC1	
0661	TEMC1	
0662	TEMC1	
0663	TEMC1	
0664	TEMC1	
0665	TEMC1	
0666	TEMC1	

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0670 0735 0000 FEXT
0671 0736 7325 CLA IAC STL RAL
0672 0737 1357 TAD ADDR1
0673 0740 3357 DCA ADDR1 /INCREMENT ADDR1
0674 0741 2353 ISZ FLAG1 /DONE WITH J LOOP?
0675 0742 5314 JMP RPTC2 /NO! REPEAT
0676 0743 5255 JMP RPTC1 /CONTINUE CPS LOOP
0677 0744 1756 FADD I ADDR1 ALPHA,
0678 0745 1757 FADD I ADDR1 ALPH1,
0679 0746 2756 BETAI, FSUB I ADDR1 BETA,
0680 0747 2757 BETAI, FSUB I ADDR1 BETAI,
0681 0750 7420 SNL CASE1, SNL
0682 0751 1147 KLAEL, CLAE1 KLAEL,
0683 0752 0000 FLAGC, 0 FLAGC,
0684 0753 0000 FLAGC1, 0 FLAGC1,
0685 0754 0000 TEMC, 0 TEMC,
0686 0755 0000 TEMC1, 0 TEMC1,
0687 0756 0000 ADDR, 0 ADDR,
0688 0757 0000 ADDR1, 0 ADDR1,
0689 0760 0000 FPINP, 0 FPINP,
0690 0761 6201 CDF 0
0691 0762 4767 JMS I FLIN JMS I FLIN
0692 0763 1060 TAD 60
0693 0764 7650 SNA CLA
0694 0765 5362 JMP *-3
0695 0766 5760 JMP I FPINP
0696 0767 7400 FLIN,
0697 7400 *1000
0698 XTERM,
0699 1000 0000
0700 1001 4347 JMS CLAE1 /3 WORD CLEAR OF ADD0
0701 1002 7240 STA INDD1
0702 1003 3313 DCA INDD2 /INITIALIZE VARIABLES
0703 1004 5314 OCA INDD2
0704 1005 7346 CLL STA RTL
0705 1006 3312 DCA CTRDD
0706 1007 1107 YAD TEMP /GET BPFs TO BE COMPARED
0707 1010 3315 DCA TEM
0708 1011 1114 TAD TEMP1
0709 1012 3316 DCA TEM1
0710 1015 1106 TAD N
0711 1014 7041 CIA
0712 1015 3320 DCA CLL /SET DO LOOP
0713 1016 7300 CLA CLL /EXAMINE 1ST BPF
0714 1017 1315 TAD TEM /STORE REDUCED VALUE
0715 1020 7010 RAR /TEST LINK
0716 1021 3315 DCA TEM
0717 1022 7430 SZL INSTD1 BE SNL
0718 1023 5227 JMP INSTD1
0719 1024 1317 TAD DIRD /DIRD SHOULD BE SZL
0720 1025 3235 DCA JMP *-3
0721 1026 2231 JMP INSTD1
0722 1027 1222 TAD DIRD /DIRD SHOULD BE SZL
0723 1030 3235 DCA JMP *-3
0724 1031 7100 CLL TEM1 /EXAMINE CORRESPONDING BIT OF OTHER BPF
0725 1032 1316 TAD RAR /STORE REDUCED VALUE
0726 1033 7010 RAR TEM1
0727 1034 3316 DCA DIRD /SPINS THE SAME, ROTATE AGAIN
0728 1035 0000 0 /HOW MANY DIFFERENCES?
0729 1036 2252 JMP *-3
0730 1037 2312 ISZ CTRDD
0731 1038 5243 JMP *-3
0732 1041 6211 CUF 10 /T00 MANY, RETURN
0733 1042 5243 RET,
0734 1043 5243
0735 1044 5243
0736 1045 5243
0737 1046 5243
0738 1047 5243
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0771 1080 5243
0772 1081 5243
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0789 1098 5243
0790 1099 5243
0791 1100 5243
0792 1101 5243
0793 1102 5243
0794 1103 5243
0795 1104 5243
0796 1105 5243
0797 1106 5243
0798 1107 5243
0799 1108 5243
0800 1109 5243

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1165 1245 1266 1165 1245 1266 /ADD 13 TO EXPONENT
1166 1246 7510 1166 1246 7510 /ELEMENT SMALL ENOUGH?
1167 1247 5764 1167 1247 5764 /YES, LOOK FOR OTHER
1170 1250 2113 1170 1250 2113 /IS IT 0?
1171 1251 7300 1171 1251 7300
1172 1252 1513 1172 1252 1513
1173 1253 7004 1173 1253 7004
1174 1254 7450 1174 1254 7450
1175 1255 5764 1175 1255 5764 /ITS 0
1176 1256 7240 1176 1256 7240 /RESTORE ADD0
1177 1257 1113 1177 1257 1113
1200 1260 3113 1200 1260 3113
1201 1261 2270 1201 1261 2270
1202 1262 4671 1202 1262 4671 /SHOW THAT A LARGE ELEMENT IS FOUND
1203 1263 4672 1203 1263 4672 /0 THE ELEMENT
1204 1264 5764 1204 1264 5764 /CONTINUE
1205 1265 0000 1205 1265 0000
1206 1266 0015 1206 1266 0015
1207 1267 0000 1207 1267 0000
1210 1270 0000 1210 1270 0000
1211 1271 1400 1211 1271 1400 IS,
1212 1272 1600 1212 1272 1600 TRIGE, TRIG VALUE,
1213 1273 0000 1213 1273 0000 HSUBE, 0
1214 1274 7200 1214 1274 7200
1215 1275 1107 1215 1275 1107
1216 1276 7041 1216 1276 7041
1217 1277 1114 1217 1277 1114
1220 1300 7500 1220 1300 7500
1221 1301 5310 1221 1301 5310
1222 1302 7041 1222 1302 7041
1223 1303 5340 1223 1303 5340
1224 1304 1114 1224 1304 1114
1225 1305 7041 1225 1305 7041
1226 1306 3336 1226 1306 3336
1227 1307 5314 1227 1307 5314
1230 1310 3340 1230 1310 3340
1231 1311 1107 1231 1311 1107
1232 1312 7041 1232 1312 7041
1233 1313 5336 1233 1313 5336
1234 1314 1115 1234 1314 1115
1235 1315 7041 1235 1315 7041
1236 1316 5337 1236 1316 5337
1237 1317 2336 1237 1317 2336
1240 1320 5322 1240 1320 5322
1241 1321 5325 1241 1321 5325
1242 1322 1337 1242 1322 1337
1243 1323 2337 1243 1323 2337
1244 1324 5317 1244 1324 5317
1245 1325 7041 1245 1325 7041
1246 1326 1340 1246 1326 1340
1247 1327 3113 1247 1327 3113
1250 1330 1113 1250 1330 1113
1251 1331 1113 1251 1331 1113
1252 1332 1113 1252 1332 1113
1253 1333 1073 1253 1333 1073
1254 1334 3113 1254 1334 3113
1255 1335 5673 1255 1335 5673
1256 1336 0000 1256 1336 0000
1257 1337 0000 1257 1337 0000
1260 1340 0000 1260 1340 0000
1261 1341 0000 1261 1341 0000
1262 1342 7240 1262 1342 7240

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TESTE /ADD 13 TO EXPONENT
INSTE /ELEMENT SMALL ENOUGH?
ADD0 /YES, LOOK FOR OTHER
ADD0 /IS IT 0?
INSTE /ITS 0
RESTORE ADD0 /RESTORE ADD0
INSTE /SHOW THAT A LARGE ELEMENT IS FOUND
ADD0 /0 THE ELEMENT
INSTE /CONTINUE
TEMP /FIND ADDRESS OF H ELEMENT
TEMP1 /TEMP1-TEMP
+7 /WHICH IS BIGGEST?
DIFF /TEMP1
TEMP1 /TEMP
IND1 / FROM DIAGONAL ELEMENT
+5 /SET DO LOOP
DIFF /TEMP1
TEMP /SET DO LOOP
IND1 /SET UP REGISTER
N1 /ENOUGH ADDITIONS?
IND2 /NO, CONTINUE
+4 /YES, GET OUT OF LOOP
IND2 /AC CONTAINS OF ELEMENTS IN SKIPPED ROWS
DIFF / OF ELEMENTS TO SKIP
ADD0 /ADD0 CONTAINS ADDRESS
HSUBE /GETS ADDRESS IN U MATRIX

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TAD SPA
JMP I
ISZ ADD0
CLA CLL
TAD I
RAL
SNA
JMP I
STA
TAD
DCA ADD0
ISZ IS
JMS I TRIGE
JMS I VALUE
JMP I
0
15
0
0
TRIG
VALUEG
0
CLA
TAD
CIA
TAD
SMA
JMP
CIA
DCA
TAD
CIA
DCA
JMP
DCA
TAD
CIA
DCA
ISZ
JMP
JMP
TAD
ISZ
JMP
CIA
TAD
CIA
ISZ
JMP
TAD
DCA
JMP I
0
0
0
IND1,
IND2,
DIFF,
USUB,
STA

```

```

1204 1344 /420 /IS THIS 0
1265 JMP +6 /YES
1266 CIA 7041 /NO
1267 1347 3336 /SET DO LOOP
1270 TAD DCA IND1
1271 1351 2336 N1
1272 1352 5350 IND1 /DONE WITH LOOP?
1273 1353 1107 JMP -2 /NO CONTINUE
1274 1354 3113 TAD TEMP /AC CONTAINS OF ELEMENTS TO BE SKIPPED
1275 1355 7346 CLL STA RTL
1276 1356 1113 TAD ADD0
1277 1357 1113 TAD ADD0
1300 1360 1113 TAD ADD0
1301 1361 1072 TAD UB
1302 1362 3113 DCA ADD0 /ADD0 CONTAINS ADDRESS
1303 1363 5741 JMP I USUB
1304 1364 0000 INSTE,
1305 1365 0000 FLAGE,
1306 1366 1211 R1,
1307 1367 1225 R2,
1310 *1400
1311 1400 0000 TRIG,
1312 1401 4407 JMS I INTERP /GET H(JF,K)
1313 1402 5513 FGET I ADD0
1314 1403 6337 FPUT HJK
1315 1404 0000 FEXT
1316 1405 1107 TAD TEMP
1317 1406 3527 DCA JF
1320 1407 1114 TAD TEMPI
1321 1410 3330 DCA KF
1322 1411 1527 TAD JF
1323 1412 3114 DCA TEMPI
1324 1413 4742 JMS I HSUBF /GET ADDRESS OF H(J,J)
1325 1414 4407 JMS I INTERP
1326 1415 5513 FGET I ADD0
1327 1416 6531 FPUT HJJ /HJJ=H(J,J)
1330 1417 0000 FEXT
1331 1420 1530 TAD KF
1332 1421 3107 DCA TEMP
1333 1422 1530 TAD KF
1334 1423 3114 DCA TEMPI
1335 1424 4742 JMS I HSUBF /GET ADDRESS OF H(K,K)
1336 1425 4407 JMS I INTERP
1337 1426 5513 FGET I ADD0
1340 1427 6334 FPUT HKK /HKK=H(K,K)
1341 1430 2331 FSUB HJJ
1342 1431 6321 FPUT Y /Y=HKK=HJJ
1343 1432 3321 FMPY Y /R=Y**2
1344 1433 6324 FPUT R
1345 1434 5337 FGET HJK
1346 1435 0003 FMPY2
1347 1436 0003 FMPY2
1350 1437 3337 FMPY HJK
1351 1440 1324 FADD R
1352 1441 0002 SUBR00T R
1353 1442 6324 FPUT Y1
1354 1443 0000 FEXT
1355 1444 1522 TAD SMA
1356 1445 7500 JMS I INTERP /IS Y NEGATIVE?
1357 1446 5253 JMP TRI /NO
1360 1447 4407 JMS I INTERP /YES
1361 1448 0005 NEGATE /THEN SET R=R
1362 1451 6324 FPUT R

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1363 1452 0000 FEXT INTERP
1364 4407 JMS I Y
1365 454 5321 FGET Y
1366 4324 FDIV R
1367 6321 FPUT Y
1370 5337 FGET HJK
1371 0003 FMPY2
1372 4524 FDIV R
1373 6524 FPUT R
1374 5316 FGET ONEF
1375 1521 FADD Y
1376 0004 FDIV2
1377 0002 SQR00T
1400 6127 FPUT
1401 5324 FGET
1402 4127 FDIV
1403 0004 FDIV2
1404 6124 FPUT
1405 474 5331 FGET HJJ
1406 1334 FADD HJK
1407 0004 FDIV2
1410 1477 6116 FPUT A
1411 1500 5337 FGET HJK
1412 1501 3324 FMPY R
1413 1502 6121 FPUT B
1414 1503 5331 FGET HJJ
1415 1504 2334 FSUB HJK
1416 1505 0004 FDIV2
1417 1506 3321 FMPY Y
1420 1507 2121 FSUB B
1421 1510 6121 FPUT B
1422 1511 0000 FEXT
1423 1512 1327 TAD
1424 1513 3107 DCA
1425 1514 6211 CDF 10
1426 1515 5600 JMP I
1427 1516 0001 ONEF,
1430 1517 2000 1
1431 1520 0000 0
1432 1521 0000 Y,
1433 1522 0000 Y1,
1434 1523 0000 R,
1435 1524 0000 R,
1436 1525 0000
1437 1526 0000
1440 1527 0000 JF,
1441 1530 0000 KF,
1442 1531 0000 HJJ,
1443 1532 0000
1444 1533 0000
1445 1534 0000 HKK,
1446 1535 0000
1447 1536 0000
1450 1537 0000 HJK,
1451 1540 0000
1452 1541 0000
1453 1542 1273 HSUBF, HSUBE
1454 1543 0000 ONESET,
1455 1544 7240 STA
1456 1545 1113 TAD ADD0
1457 1546 5010 DCA 10
1460 1547 6211 CDF 10

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/Y(FCOS2)=Y/R

/R(FSIN2)=2\*HJK/R

/FCOS=((1+FCOS2)/)\*\*.5

/FSIN=FSIN2/FCOS/2

/A=(HJJ+HKK)/2

/B=HJK\*FSIN2

/B=(HJJ-HKK)\*FCOS2/2-HJK\*FSIN2

/RESTORE TEMP AND TEMPI

/RETURN







1660	1734	IAU I	ADDZ	
1661	3340	DCA	BPF2	/GET BPF2
1662	2030	TAD I	ADD1	
1663	3337	OCA	BPF1	/GET BPF1
1664	2032	COF 0		
1665	2033	ISZ	ADD1	
1666	2034	JMS	TEST	/FIND OUT IF ALLOWED TRANSITION
1667	2035	ISZ	FLAGH1	/DONE WITH INNER LOOP?
1670	2036	JMP	RPTH1	/NO, CONTINUE
1671	2037	ISZ	FLAGH	/YES, DONE WITH OUTER LOOP?
1672	2040	JMP	INC	/NO, CONTINUE
1673	2041	TAD	CTRH3	/IS LAST TABLE ENTRY NORMALIZED?
1674	2042	CIA		
1675	2043	TAD	M12H	
1676	2044	SNA	CLA	
1677	2045	JMP	RETH	/YES, RETURN
1700	2046	TAD I	TABADH	/NO, NORMALIZE IT
1701	2047	CLL	RAR	
1702	2050	ISZ	CTRH3	/NORMALIZED?
1703	2051	JMP	:2	/NO, ROTATE AGAIN
1704	2052	OCA I	TABADH	/YES, STORE IT
1705	2053	COF 10		
1706	2054	JMP I	ALLOW	/RETURN
1707	2055	ISZ	ADD2	
1710	2056	JMP	RPTH	
1711	2057	0		
1712	2060	TAD	N	
1713	2061	CIA		
1714	2062	DCA	CTRH	/- OF ROTATIONS
1715	2063	IAC		
1716	2064	CMA		
1717	2065	DCA	CTRH1	/INITIALIZED TO -2
1720	2066	CLA	CLL	
1721	2067	TAD	BPF1	
1722	2070	RAR		
1723	2071	OCA	BPF1	/STORE ROTATED VALUE
1724	2072	SEL		/TEST LINK AND SET UP LATER TEST
1725	2073	JMP	:4	
1726	2074	TAD	NLINK	
1727	2075	OCA	INSTH	
1730	2076	JMP	:3	
1731	2077	TAD	ZLINK	
1732	2100	OCA	INSTH	
1733	2101	CLL		
1734	2102	TAD	BPF2	
1735	2103	RAR		
1736	2104	OCA	BPF2	/STORE ROTATED VALUE
1737	2105	0		
1740	2106	JMP	:5	/SPINS THE SAME
1741	2107	ISZ	CTRH1	/DIFFERENT
1742	2110	JMP	:3	
1743	2111	CLA	CLL	/TOO MANY DIFFERENCES
1744	2112	JMP	:5	
1745	2113	ISZ	CTRH	/DONE ROTATING?
1746	2114	JMP	OVER	/NO, ROTATE AGAIN
1747	2115	CLA		/YES, ALLOWED TRANSITION
1750	2116	STL		
1751	2117	TAD I	TABADH	/STORES ALLOWEDNESS
1752	2120	RAR		
1753	2121	OCA I	TABADH	
1754	2122	ISZ	CTRH3	/NEED TO INCREMENT ABAD?
1755	2123	JMP I	TEST	/NO
1756	2124	ICZ	TARION	

/REINIT CTRH3

1757	2125	1531	TAD M12H
1760	2126	3532	DCA CTRH3
1761	2127	5657	JMP I TEST
1762	2130	0000	TABADH, 0
1763	2131	7764	M12H, 7764
1764	2132	0000	CTRH3, 0
1765	2133	0000	ADD1, 0
1766	2134	0000	ADD2, 0
1767	2135	0000	FLAGH, 0
1770	2136	0000	FLAGH1, 2
1771	2137	0000	BPF1, 0
1772	2140	0000	BPF2, 0
1773	2141	0000	CTRH, 0
1774	2142	0000	CTRH1, 0
1775	2143	7420	NLINK, SNL
1776	2144	0000	TABL, 0
1777	2145	0000	SAVSYM 2
2000			



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0076 2271 5113 DCA ADD0 /ADDRESS IN U MATRIX
0077 2272 5513 DCA I ADD0 /LOOP ZEROES A OF U MATRIX
0100 2273 2113 ISZ ADD0
0101 2274 2246 ISZ CTRI /LOOP DONE?
0102 2275 5272 JMP ,=3 /NO
0123 2276 1115 TAD N1 /YES, PUT 1S ON DIAGONAL
0124 2277 7041 CIA /SET LOOP
0109 2500 3246 DCA CTRI
0126 2501 6201 CDF 0
0127 2502 7201 CLA IAC
0110 2503 1246 TAD CTRI
0111 2504 1115 TAD N1
0112 2505 3107 DCA TEMP
0113 2506 1107 TAD TEMP
0114 2507 3114 DCA TEMPI
0115 2510 4717 JMS I USUBI /INDICES OF DIAGONAL U ELEMENT
0116 2511 4716 JMS I SETONE /GET ADDRESS OF DIAGONAL ELEMENT
0117 2512 2246 ISZ CTRI /LOOP DONE?
0120 2513 5302 JMP OVERI /NO
0121 2514 6211 CDF 10 /YES
0122 2515 5600 JMP I HUGET /RETURN
0123 2516 1543 SETONE, ONESET
0124 2517 1341 USUBI, USUB
0125 2520 0200 COPY, 0
0126 2521 7200 CLA
0127 2522 1072 TAD UB
0130 2523 3247 DCA ADDR0
0131 2524 1067 TAD BOLD
0132 2525 3072 DCA UB
0133 2526 1247 TAD ADDR0
0134 2527 3067 DCA BOLD
0135 2530 6201 CDF 0
0136 2531 1115 TAD N1
0137 2532 7041 CIA
0140 2533 5246 DCA CTRI /SET LOOP
0141 2534 1070 TAD ENB
0142 2535 5247 DCA ADDR0 /ADDRESS IN EN
0143 2536 7201 AGAINI, CLA IAC
0144 2537 1246 TAD CTRI
0145 2540 1115 TAD N1
0146 2541 3107 DCA TEMP
0147 2542 1107 TAD TEMP
0150 2543 3114 DCA TEMPI /INDICES OF DIAGONAL H ELEMENT
0151 2544 4703 JMS I HSUBI /ADDRESS OF DIAGONAL H ELEMENT
0152 2545 4407 JMS I INTERP
0153 2546 5513 FGET I ADDR0 /GET H ELEMENT
0154 2547 6647 FPUT I ADDR0 /STORE IT
0155 2550 0000 FEXT
0156 2551 2247 ISZ ADDR0
0157 2552 2247 ISZ ADDR0
0160 2553 2247 ISZ ADDR0
0161 2554 2246 ISZ CTRI /DONE?
0162 2555 5336 JMP AGAINI /NO
0163 2556 7200 CLA
0164 2557 1115 TAD N1
0165 2560 3132 DCA N2 /SET N2=N1
0166 2561 5211 CDF 10
0167 2562 5720 JMP I COPY /RETURN
0170 2563 1273 HSUBI,
0171 2400 *2400 TRANS, 0
0172 0000
0173 6201

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0175 2403 1067 TAD DCA /ADDRESS OF 1ST ELEMENT IN CURRENT OLD
2176 2404 3336 DCA IN2ADD /EIGENVECTOR
0177 2405 1070 TAD ENB /ADDRESS OF OLD EIGENVALUE
0200 2406 3121 DCA B
0201 2407 1132 TAD N2
0202 2410 7041 CIA
0203 2411 3337 DCA FLAGJ1 /SET 1ST ORDER LOOP
0204 2412 5224 JMP UP
0205 2413 7200 RPT1, CLA
0206 2414 2121 ISZ B
0207 2415 2121 ISZ B
0210 2416 2121 ISZ B
0211 2417 1132 TAD N2
0212 2420 1132 TAD N2
0213 2421 1132 TAD N2
0214 2422 1336 TAD IN2ADD /INCREMENT IN2 ADD
0215 2423 3336 DCA IN2ADD
0216 2424 1072 TAD UB
0217 2425 3340 DCA IN1ADD /ADDRESS OF 1ST ELEMENT IN CURRENT
0220 2426 1115 TAD N1 /NEW EIGENVECTOR
0221 2427 7041 CIA FLAGJ2 /SET 2ND ORDER LOOP
0222 2430 3341 DCA ,+7
0223 2431 5240 JMP
0224 2432 7200 RPT2, CLA
0225 2433 1115 TAD N1
0226 2434 1115 TAD N1
0227 2435 1115 TAD N1
0230 2436 1340 TAD IN1ADD
0231 2437 3340 DCA IN1ADD /INCREMENT IN1ADD
0232 2440 7001 IAC
0233 2441 1341 TAD FLAGJ2
0234 2442 1115 TAD N1
0235 2443 5107 DCA TEMP
0236 2444 1107 TAD TEMP
0237 2445 5114 DCA TEMP1 /SET SUBSCRIPTS FOR NEW EIGENVALUE
0240 2446 3116 DCA A
0241 2447 3117 DCA A+1
0242 2450 3120 DCA A+2
0243 2451 1336 TAD IN2ADD
0244 2452 3342 DCA N2ADD /INITIALIZE TRANSITION PROBABILITY
0245 2453 7040 CMA /ADDRESS IN OLD EIGENVECTOR
0246 2454 3343 DCA CTR /INITIALIZE CTR
0247 2455 7040 CMA
0250 2456 1024 TAD TABLE /ADDRESS OF CHECK WORD
0251 2457 3344 DCA TABAD
0252 2460 1132 TAD N2
0253 2461 7041 CIA FLAGJ3 /SET 3RD ORDER LOOP
0254 2462 3345 DCA CALC1 /CALCULATE TRANSITION ENERGY
0255 2463 4746 JMS I
0256 2464 7200 RPT3, CLA
0257 2465 1340 TAD IN1ADD
0258 2466 3347 DCA N1ADD /ADDRESS IN NEW EIGENVECTOR
0259 2467 1115 TAD N1
0262 2470 7041 CIA FLAGJ4 /SET 4TH ORDER LOOP
0263 2471 3350 DCA
0264 2472 7200 RPT4, CLA
0265 2473 2343 ISZ CTR /NEED A NEW CHECK WORD?
0266 2474 5302 JMP +6 /NO, GO ON
0267 2475 2344 ISZ TABAD /YES, INCREMENT ADDRESS
0270 2476 1351 TAD M12
0271 2477 3343 DCA CTR /REINITIALIZE CTR
0272 2480 1744 TAD I
0273 2481 3343 DCA

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0274	2502	1352	TAD	CHECK	/GET CHECK WORD
0275	2503	7210	RAR	CHECK	/PUT CURRENT BY INTO LINK
0276	2504	3352	DCA	CHECK	/STORE BALANCE
0277	2505	7420	SNL	.+7	/ALLOWED TRANSITION?
0300	2506	5315	JMP	INTERP	/NO, SKIP CALCULATION
0301	2507	4407	JMS I	N2ADD	/YES, CALCULATE PROBABILITY
0302	2510	5742	FGET I	N1ADD	
0303	2511	5747	FMPI I	A	
0304	2512	1116	FADD	A	/INCREMENT PROBABILITY
0305	2513	6116	FPUT		
0306	2514	0000	FEXT		
0307	2515	2347	ISZ	N1ADD	
0310	2516	2347	ISZ	N1ADD	
0311	2517	2347	ISZ	N1ADD	/INCREMENT NEW EIGENFUNCTION
0312	2520	2350	ISZ	FLAGJ4	/4TH ORDER LOOP DONE?
0313	2521	5272	JMP	RPT4	/NO, CONTINUE
0314	2522	2342	ISZ	N2ADD	/YES
0315	2523	2342	ISZ	N2ADD	
0316	2524	2342	ISZ	N2ADD	
0317	2525	2345	ISZ	FLAGJ3	/INCREMENT OLD EIGEN FUNCTION
0320	2526	5264	JMP	RPT3	/3RD ORDER LOOP DONE?
0321	2527	4753	JMS I	CALC2	/NO, CONTINUE
0322	2530	2341	ISZ	FLAGJ2	/YES, COMPUTE TOTAL PROBABILITY
0323	2531	5232	JMP	RPT2	/2ND ORDER LOOP DONE?
0325	2532	2337	ISZ	FLAGJ1	/NO, CONTINUE
0325	2533	5213	JMP	RPT1	/1ST ORDER LOOP DONE?
0326	2534	6211	CDF 10	YES	/NO, CONTINUE
0327	2535	5600	JMP I	TRANS	/YES
0328	2536	0000	IN2ADD, 0	/RETURN	
0331	2537	0000	FLAGJ1, 0		
0332	2540	0000	IN1ADD, 0		
0333	2541	0000	FLAGJ2, 0		
0334	2542	0000	N2ADD, 0		
0335	2543	0000	CTR, 0		
0336	2544	0000	TABAD, 0		
0337	2545	0000	FLAGJ3, 0		
0340	2546	3000	CALC1, CALCM1		
0341	2547	0000	N1ADD, 0		
0342	2550	0000	FLAGJ4, 0		
0343	2551	7764	M12, =14		
0344	2552	0000	CHECK, 0		
0345	2553	5042	CALC2, CALCM2		
0346	2554	0000	ARRLD, 0		
0347	2555	4765	JMS I	CHKEND	/CHECK FOR END OF TAPE BUFFER
0348	2556	1044	TAD	EXP	
0351	2557	5411	DCA I	11	
0352	2560	1045	TAD	HORD	
0353	2561	5411	DCA I	11	
0354	2562	1046	TAD	LORD	
0355	2563	5411	DCA I	11	
0356	2564	5754	JMP I	ARRLD	
0357	2565	1161	CHKEND, ENDCBK		
0358	2600	6036	INTRUP, KRB		
0359	2601	4032	JMS	TYPE	/GET A CHARACTER
0360	2602	7041	CIA		
0361	2603	5127	DCA	TEMP	
0362	2604	5114	DCA	TEMP1	
0363	2605	1244	TAD	CHTB	
0364	2606	5010	DCA	10	
0365	2607	4025	JMS	READ	
0366	2610	4032	JMS	TYPE	
0367	2611	4032	JMS	TYPE	
0368	2612	4032	JMS	TYPE	
0369	2613	4032	JMS	TYPE	
0370	2614	4032	JMS	TYPE	
0371	2615	4032	JMS	TYPE	
0372	2616	4032	JMS	TYPE	
0373	2617	4032	JMS	TYPE	
0374	2618	4032	JMS	TYPE	
0375	2619	4032	JMS	TYPE	
0376	2620	4032	JMS	TYPE	
0377	2621	4032	JMS	TYPE	
0378	2622	4032	JMS	TYPE	
0379	2623	4032	JMS	TYPE	
0380	2624	4032	JMS	TYPE	
0381	2625	4032	JMS	TYPE	
0382	2626	4032	JMS	TYPE	
0383	2627	4032	JMS	TYPE	
0384	2628	4032	JMS	TYPE	
0385	2629	4032	JMS	TYPE	
0386	2630	4032	JMS	TYPE	
0387	2631	4032	JMS	TYPE	
0388	2632	4032	JMS	TYPE	
0389	2633	4032	JMS	TYPE	
0390	2634	4032	JMS	TYPE	
0391	2635	4032	JMS	TYPE	
0392	2636	4032	JMS	TYPE	
0393	2637	4032	JMS	TYPE	
0394	2638	4032	JMS	TYPE	
0395	2639	4032	JMS	TYPE	
0396	2640	4032	JMS	TYPE	
0397	2641	4032	JMS	TYPE	
0398	2642	4032	JMS	TYPE	
0399	2643	4032	JMS	TYPE	
0400	2644	4032	JMS	TYPE	





0476	CALL	WRITE	/TYPE LEFT 6 BITS
0475	JMS	WRITE	
0474	CLA	JUMP	
0473	TAD I	JUMP	
0472	ISZ	JUMP	
0471	JMS	WRITE	/TYPE RIGHT 6 BITS
0470	JMP	AGAINL	
0469	0		
0468	AND	MASK1	/MASK OUT LEFT 6 BITS
0467	SNA	EXITT	/EITHER HALF =0?
0466	JMP	M36	/YES, EXIT
0465	TAD		/NO
0464	SPA SNA		/200 OR 300 SERIES?
0463	JMP	+4	/300 SERIES
0462	TAD	P236	/200 SERIES
0461	JMS	TYPE	/TYPE IT
0460	JMP I	WRITE	
0459	SZA		/SPECIAL CODE 36?
0458	JMS	+3	/NO
0457	JMP	CRLFD	
0456	JMP I	WRITE	
0455	TAD	P336	
0454	JMS	TYPE	/TYPE IT
0453	JMP I	WRITE	
0452	CDF 10		
0451	JMP I	PRINTL	
0450	0		
0449	=36		
0448	336		
0447	336		
0446	0077		
0445	TEXT3=.		/TEXT3 LOADS
0444	*3000		
0443	0		
0442	CALCM1,		/GET ADDRESS OF OLD EIGENVALUE
0441	JMS I	HSUBM	
0440	JMS I	INTERP	
0439	FCGT I	B	/EN=HII
0438	FSUB I	ADD0	
0437	FEXT		
0436	JMS I	LOARR	/LOAD ARRAY W/ -CHEMICAL SHIFT
0435	JMS I	INTERP	
0434	FADD	LIMIT	/LIMIT -CHEMICAL SHIFT
0433	FMPY	FACTOR	
0432	FADD	HALFM	/SET TO FIX AND ROUND
0431	FEXT		
0430	JMS	FIX	/FIX IT
0429	SPA		/IN RIGHT RANGE?
0428	JMP	AHEAD	/NO, TOO SMALL
0427	TAD	M500M	/MAYBE
0426	SMA		/IN RIGHT RANGE?
0425	JMP	AHEAD	/NO, TOO BIG
0424	TAD	P500M	/YES
0423	TAD	SPECB	
0422	DCA	ADSPEC	/ADDRESS FOR STORING PROBABILITY
0421	JMP I	CALCM1	
0420	CLA CLL		
0419	TAD	M500M	
0418	DCA	ADSPEC	
0417	JMP I	CALCM1	
0416	ARRLD		
0415	LDARR,		
0414	HSUBM,		
0413	HALFM,		
0412	0		
0411	2000		
0410	2000		
0409	2000		
0408	2000		
0407	2000		
0406	2000		
0405	2000		
0404	2000		
0403	2000		
0402	2000		
0401	2000		
0400	2000		
0399	2000		
0398	2000		
0397	2000		
0396	2000		
0395	2000		
0394	2000		
0393	2000		
0392	2000		
0391	2000		
0390	2000		
0389	2000		
0388	2000		
0387	2000		
0386	2000		
0385	2000		
0384	2000		
0383	2000		
0382	2000		
0381	2000		
0380	2000		
0379	2000		
0378	2000		
0377	2000		
0376	2000		
0375	2000		
0374	2000		
0373	2000		
0372	2000		
0371	2000		
0370	2000		
0369	2000		
0368	2000		
0367	2000		
0366	2000		
0365	2000		
0364	2000		
0363	2000		
0362	2000		
0361	2000		
0360	2000		
0359	2000		
0358	2000		
0357	2000		
0356	2000		
0355	2000		
0354	2000		
0353	2000		
0352	2000		
0351	2000		
0350	2000		
0349	2000		
0348	2000		
0347	2000		
0346	2000		
0345	2000		
0344	2000		
0343	2000		
0342	2000		
0341	2000		
0340	2000		
0339	2000		
0338	2000		
0337	2000		
0336	2000		
0335	2000		
0334	2000		
0333	2000		
0332	2000		
0331	2000		
0330	2000		
0329	2000		
0328	2000		
0327	2000		
0326	2000		
0325	2000		
0324	2000		
0323	2000		
0322	2000		
0321	2000		
0320	2000		
0319	2000		
0318	2000		
0317	2000		
0316	2000		
0315	2000		
0314	2000		
0313	2000		
0312	2000		
0311	2000		
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0305	2000		
0304	2000		
0303	2000		
0302	2000		
0301	2000		
0300	2000		

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0571 3036 0000
0572 3037 7014 M500M,
0573 3040 0764 P5000M,
0574 3041 0000 ADSPEC, 0
0575 3042 0000 CALCM2, 0
0576 3043 6211 CDF 10
0577 3044 7200 CLA
0600 3045 1641 TAD I ADSPEC
0601 3046 0305 AND MASKM /ERASE CALIBRATION MARK
0602 3047 3024 DCA SIGN /STORE
0603 3050 4407 JMS I INTERP
0604 3051 5116 FGET A
0605 3052 3116 FMPY A /SQUARE TO GET PROBABILITY
0606 3053 0000 FEXT /SCREEN OUT LOW INTENSITIES
0607 3054 1306 TAD PL6
0610 3055 1044 TAD EXP
0611 3056 3044 DCA EXP
0612 3057 4632 JMS I LDARR
0613 3060 4327 JMS FIX /FIX
0614 3061 3303 DCA PROB /STORE CURRENT PROBABILITY
0615 3062 1241 TAD ADSPEC
0616 3063 7710 SPA CLA
0617 3064 5642 JMP I CALCM2
0620 3065 6211 CDF 10
0621 3066 1303 TAD PROB
0622 3067 1304 TAD SIGN
0623 3070 7700 SMA CLA
0624 3071 5276 JMP ,+5 /NOT TOO BIG
0625 3072 1641 TAD I ADSPEC /TOO BIG, SET TO MAX
0626 3073 7004 RAL
0627 3074 7250 STA RAR
0630 3075 5300 JMP ,+3
0631 3076 1641 TAD I ADSPEC /GET OLD SPEC ELEMENT
0632 3077 1303 TAD PROB /INCREMENT IT
0633 3100 5641 DCA I ADSPEC /STORE IT
0634 3101 6201 CDF 0
0635 3102 5642 JMP I CALCM2 /RETURN
0636 3103 0000 PROB,
0637 3124 0000 SIGN,
0640 3105 3777 MASKM,
0641 3106 0026 PL6,
0642 3107 0000 SETUP,
0643 3110 3325 DCA HOLD
0644 3111 1325 TAD HOLD
0645 3112 7012 RTR
0646 3113 7012 RTR
0647 3114 7012 RTR
0650 3115 0326 AND BLIND /MASK OUT BITS 0-5
0651 3116 4423 JMS I HPUN /PUNCH FIRST 6 BITS
0652 3117 7200 CLA
0653 3120 1325 TAD HOLD
0654 3121 0326 AND BLIND /PUNCH LST 6 BITS
0655 3122 4423 JMS I HPUN
0656 3123 7200 CLA
0657 3124 5707 JMP I SETUP /RETURN
0660 3125 0000 HOLD,
0661 3126 0377 BLIND,
0662 3127 0000 FIX,
0663 3150 7200 CLA
0664 3151 1044 TAD EXP
0665 3152 7540 SMA SZA
0666 3153 5336 JMP ,+3

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/SUBROUTINE INCREMENTS PROPER ELEMENT  
/IN SPEC ARRAY

/ERASE CALIBRATION MARK  
/STORE

/SQUARE TO GET PROBABILITY

/SCREEN OUT LOW INTENSITIES

/FIX  
/STORE CURRENT PROBABILITY

/GET - AC IF SUM IS TOO BIG

/NOT TOO BIG  
/TOO BIG, SET TO MAX

/GET OLD SPEC ELEMENT  
/INCREMENT IT  
/STORE IT

/RETURN

HOLD  
HOLD

BLIND  
HPUN

HOLD  
BLIND  
HPUN

SETUP  
RETURN

ROUTINE FIXES A F, P.

EXP  
SMA SZA  
JMP ,+3

IS <1  
NO GO ON

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0671 0671 JMP I PIA /RETURN
0672 0672 TAD M11 /IS HORD ALREADY RIGHT?
0673 0673 SZA +3 /NO
0674 0674 TAD HORD /YES, GET HORD
0675 0675 JMP I FIX /RETURN
0676 0676 SMA /IS TOO BIG TO FIX?
0677 0677 JMP /YES, SET TO 3777
0678 0678 DCA HOLD /NO, SET FIXING LOOP
0679 0679 TAD HORD /ROTATE RIGHT FILLING WITH 1S IF NEG
0680 0680 CLL /FOR 0S IF POS
0681 0681 SPA /LOOP DONE?
0682 0682 STL /NO
0683 0683 RAR /YES RETURN
0684 0684 ISZ *5
0685 0685 JMP /FIX
0686 0686 JMP I MASKM
0687 0687 TAD /FIX
0688 0688 CLA /MIN INTENSITY=
0689 0689 TAD *3200
0690 0690 JMP I H010
0691 0691 SZA H010
0692 0692 TAD H010
0693 0693 JMP I INPUT
0694 0694 SZA H010
0695 0695 TAD H010
0696 0696 JMP I INTERP
0697 0697 SZA H010
0698 0698 TAD H010
0699 0699 JMP I A
0700 0700 SZA H010
0701 0701 TAD H010
0702 0702 JMP I PRINT /DISPLAY LISTING?
0703 0703 SZA H010
0704 0704 TAD H010
0705 0705 JMP I ASKRX
0706 0706 SZA H010
0707 0707 TAD H010
0708 0708 JMP I DSLST /YES
0709 0709 SZA H010
0710 0710 TAD H010
0711 0711 JMP I STRIP /INIT, TAPE READ
0712 0712 SZA H010
0713 0713 TAD H010
0714 0714 JMP I PRINT /INTENSITY ENERGY
0715 0715 SZA H010
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0718 0718 SZA H010
0719 0719 TAD H010
0720 0720 JMP I LODFAC /NORMAL RETURN
0721 0721 SZA H010
0722 0722 TAD H010
0723 0723 JMP I DISPLAY /FOUND TERMINATOR
0724 0724 SZA H010
0725 0725 TAD H010
0726 0726 JMP I INTERP
0727 0727 SZA H010
0728 0728 TAD H010
0729 0729 JMP I FSIN
0730 0730 SZA H010
0731 0731 TAD H010
0732 0732 JMP I LODFAC /GET CORRESPONDING INTENSITY
0733 0733 SZA H010
0734 0734 TAD H010
0735 0735 JMP I EIPRNT /GOT HERE ONLY BY BAD FILE:
0736 0736 SZA H010
0737 0737 TAD H010
0738 0738 JMP I BACK
0739 0739 SZA H010
0740 0740 TAD H010
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1342 1342 JMP I JMS I
1343 1343 SZA H010
1344 1344 TAD H010
1345 1345 JMP I JMP I
1346 1346 SZA H010
1347 1347 TAD H010
1348 1348 JMP I JMS I
1349 1349 SZA H010
1350 1350 TAD H010
1351 1351 JMP I JMP I
1352 1352 SZA H010
1353 1353 TAD H010
1354 1354 JMP I JMS I
1355 1355 SZA H010
1356 1356 TAD H010
1357 1357 JMP I JMP I
1358 1358 SZA H010
1359 1359 TAD H010
1360 1360 JMP I JMS I
1361 1361 SZA H010
1362 1362 TAD H010
1363 1363 JMP I JMP I
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1365 1365 TAD H010
1366 1366 JMP I JMS I
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1459 1459 JMP I JMP I
1460 1460 SZA H010
1461 1461 TAD H010
1462 1462 JMP I JMS I
1463 1463
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0767 JMS LDCHK
0770 TAD I 11
0771 DCA EXP
0772 STL RTR
0773 TAD EXP
0774 SNA CLA /GET 6000, I.E., END WORD?
0775 ISE LODFAC /YES, INCR, RETURN
0776 TAD I 11
0777 DCA HORD
1000 TAD I 11
1001 DCA LORD
1002 JMP I LODFAC
1003 EIPRNT,
1004 JMS I INTERP
1005 FPUT FCOS
1006 FSUB A
1007 FEXT
1010 TAD HORD
1011 SPA CLA /INTENSITY TOO SMALL?
1012 JMP I EIPRNT /YES, GET NEXT VALUES
1013 JMS I INTERP /NO, OUTPUT
1014 FGET FCOS
1015 FEXT
1019 CLL IAC RAL /OUTPUT INTENSITY
1020 JMS I OUTPUT
1021 TAD SPACE
1022 JMS TYPE
1023 JMS TYPE
1024 JMS I INTERP /OUTPUT CHEM SHIFT
1025 FGET FSIN
1026 FEXT
1028 IAC CLL RAL
1029 JMS I OUTPUT /OUTPUT CHEM SHIFT
1030 JMS I CARLF
1031 JMP I EIPRNT
1032 CARLF,
1033 ASKN,
1034 SPACE,
1035 STRTP,
1036 CLA
1037 TAD CORBUF
1040 OCA 11
1041 TAD STBLK
1042 DCA BLK1
1043 JMS I TAPTRN /READ FIRST BLOCK
1044 JMP I STRTP
1045 JMS STRTP
1047 CDF 0
1050 JMS LEDR
1051 TAD KK300
1052 JMS I HPUN
1053 JMS LDCHK
1054 TAD I 11
1055 DCA TTT
1056 STL RTR TTT
1057 TAD TTT
1060 SNA CLA /GET 6000 FOR END?
1061 JMP PEX /YES
1062 TAD TTT
1063 JMS I BPUN
1064 TAD I 11
1065 JMS I 11

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1000	3520	1411	TAD I	11
1067	3551	4757	JMS I	BPUN
1070	3322	5335	JMP	PNOUT
1071	3355	1361	TAD	KK200
1072	3354	4423	JMS I	HPUN
1073	3355	4564	JMS	LEDR
1074	3356	5475	JMP I	DISPLAY
1075	3357	3107	SETUP	
1076	3360	7700	LCT,	-100
1077	3361	2400	KK200,	200
1100	3362	0500	KK300,	300
1101	3363	0000	TTT,	0
1102	3364	0000	LEDR,	0
1103	3365	7200	CLA	
1104	3366	1360	TAD	LCT
1105	3367	3563	DCA	TTT
1106	3370	4423	JMS I	HPUN
1107	3371	2363	ISZ	TTT
1110	3372	5370	JMP	*2
1111	3373	5764	JMP I	LEDR
1112				
1113	3400	0000	INITB,	
1114	3401	7200	CLA	
1115	3402	6211	COF 10	
1116	3403	1106	TAD	N
1117	3404	7041	CIA	
1120	3405	3334	DCA	FLAGB
1121	3406	7201	CLA	IAC
1122	3407	7104	CLL	RAL
1123	3410	2334	ISZ	FLAGB
1124	3411	5207	JMP	*2
1125	3412	5536	DCA	NTOT
1126	3413	1063	TAD	IFZB
1127	3414	3333	DCA	ADDRB
1130	3415	7001	IAC	
1131	3416	3733	DCA I	ADDRB
1132	3417	2333	ISZ	ADDRB
1133	3420	7105	CLL	IAC
1134	3421	3733	DCA I	ADDRB
1135	3422	2333	ISZ	ADDRB
1136	3423	7105	CLL	IAC
1137	3424	1106	TAD	N
1140	3425	3733	DCA I	ADDRB
1141	3426	2333	ISZ	ADDRB
1142	3427	7346	CLL	STA
1143	3430	1106	TAD	RTL
1144	3431	7510	SPA	N
1145	3432	5267	JMP	CONT3
1146	3433	7550	SPA	SNA
1147	3434	5264	JMP	CONT4
1148	3435	7041	CIA	
1151	3436	7001	IAC	
1152	3437	7001	IAC	
1153	3440	7540	SMA	SZA
1154	3441	2256	JMP	CONT2
1155	3442	7650	SNA	CLA
1156	3443	2253	JMP	CONT1
1157	3444	1340	TAD	P23
1160	3445	3733	DCA I	ADDRB
1161	3446	2333	ISZ	ADDRB
1162	3447	1341	TAD	P43
1163	3450	3733	DCA I	ADDRB
1164	3451	2333	ISZ	ADDRB

/GET OF BASIC PRODUCT FUNCTIONS

/INITIALIZE NARRAY

/FIRST 3 INITIALIZED

/N-3 IN AC

/DONE INITIALIZING

/JUST ONE TO CALCULATE

/3-N IN AC

/5-N IN AC

/JUST TWO TO CALCULATE

/3 TO CALCULATE

/4 TO GO

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1165 3452 JMP CONT2 /FOR N#6, 4 & 5 DONE
1166 3453 TAD P17
1167 3454 DCA I ADDR8
1170 3455 ISZ ADDR8 /FOR N#5, 4 DONE
1171 3456 CLA CONT2, N
1172 3457 TAD
1173 3460 CIA
1174 3461 TAD NTOT
1175 3462 DCA I ADDR8 /2ND LAST ELEMENT=NTOT-N
1176 3463 ISZ ADDR8
1177 3464 CLA CONT4, /CALCULATE FINAL ELEMENT
1200 3465 TAD NTOT
1201 3466 DCA I ADDR8 /INITIALIZE NUSE
1202 3467 CLA CONT3, /-NTOT IN FLAGB
1203 3470 TAD NTOT
1204 3471 CIA
1205 3472 DCA RPTB1, /-NTOT IN FLAGB
1206 3473 CLA
1207 3474 DCA CTRB
1210 3475 TAD N
1211 3476 CIA INDEX
1212 3477 DCA /-N IN INDEX
1213 3500 IAC
1214 3501 TAD FLAGB
1215 3502 CIA /BPF TO BE TESTED IN AC
1216 3503 GLL
1217 3504 RAR /EXAMINE BIT BY BIT
1220 3505 SZL
1221 3506 ISZ CTRB /INCREMENT CTRB ON NON-ZERO LINK
1222 3507 ISZ INDEX /DONE WITH THIS BPF?
1223 3510 JMP RPTB2 /NO; ROTATE AGAIN
1224 3511 CLA /YES; PUT IN PROPER IN NUSE ARRAY
1225 3512 TAD CTRB
1226 3513 TAD IFZB
1227 3514 DCA ADDR8
1230 3515 TAD I ADDR8
1231 3516 DCA TEMP /TEMP CONTAINS REL. ADDRESS
1232 3517 ISZ I ADDR8 /INCREMENT NARRAY ELEMENT
1233 3520 STA
1234 3521 TAD TEMP
1235 3522 TAD NUSEB
1236 3523 DCA ADDR8 /ADDR8 CONTAINS LOCATION IN NUSE
1237 3524 IAC FLAGB
1240 3525 TAD /VALUE IN NUSE
1241 3526 CIA /DONE?
1242 3527 DCA I ADDR8
1243 3530 ISZ FLAGB
1244 3531 JMP RPTB1 /NO; GET NEXT NUMBER
1245 3532 JMP I /YES; RETURN
1246 3533 ADDR8, 0
1247 3534 FLAGB, 0
1250 3535 INDEX, 0
1251 3536 NTOT, 0
1252 3537 P17, 21
1253 3540 P23, 27
1254 3541 P43, 53
1255 3542 CTRB, 0
1256 3543 MLPY2, 0
1257 3544 EXP
1260 3545 MLPY2
1261 3546 JMP I
1262 3547 DIVD2, 0
1263 3548

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1264 TAD EXP 1044
1265 DCA EXP 3044
1266 JMP I DIV02 5747
1267 0 ULIMP, 0000
1270 JMS I PRINT /SWEEP OFFSET AND WIDTH: 4474
1271 HD7 3554
1272 JMS I INPUT 3555
1273 JMS I INTERP 4405
1274 FPUT OFSET 4407
1275 FPUT LIMIT 6137
1276 FLOIN 3562
1277 FPUT 0006 6110
1278 FADD 3564
1279 FPUT LIMIT 1110 6134
1280 FPUT LIMIT 3565
1281 FGET P500 6110
1282 FDIV 3567
1283 FPUT FACTOR 4134 4134
1284 FEFT 3571
1285 CDF 10 0000 6134
1286 JMP I ULIMP 3573
1287 0011 6211
1288 3720 5754
1289 0000 P500, 0011
1290 /NMR DISPLAY ROUTINE PART A 3720
1291 *3600
1292 STDIS, 3600
1293 JMS 7200
1294 TAD I INITK 6211
1295 AND K3777 4526
1296 SNA 3603
1297 DCA HOLDK 1741
1298 ISZ YK 0334
1299 ISZ XCTRK 7450
1300 JMP *+2 5237
1301 TAD I ENDCOM 3606
1302 AND K3777 5344
1303 SNA 3610
1304 JMP NINCR 2541
1305 TAD HOLDK 3611
1306 AND K3777 2342
1307 DCA 5214
1308 ISZ *+2 2242
1309 JMP ENDCOM 1741
1310 TAD I YK 3615
1311 AND K3777 0334
1312 SNA 3616
1313 JMP NINCR 7450
1314 TAD HOLDK 3617
1315 AND K3777 5237
1316 DCA 1344
1317 ISZ YK 0334
1318 ISZ XCTRK 3621
1319 JMP *+2 3344
1320 TAD I YK 3622
1321 AND K4000 1741
1322 DCA HOLDK 3623
1323 TAD I YK 3624
1324 AND K4000 0335
1325 DCA I YK 3625
1326 CMA 3626
1327 TAD YK 3741
1328 DCA 7040
1329 TAD YK 3630
1330 DCA YK 1541
1331 TAD I YK 3631
1332 AND K4000 5341
1333 DCA I YK 1741
1334 ISZ YK 0335
1335 JMP NEXTK 3634
1336 ISZ YK 3741
1337 NINCR, 3635
1338 ISZ YK 5203
1339 ISZ XCTRK 3636
1340 JMP NEXTK 3637
1341 JMS INITK 2341
1342 TAD I YK 3641
1343 AND K3777 4326
1344 *ROUTINE TO FIND LARGEST ELEMENT 1741
1345 /IN ARRAY 3643
1346 3644
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2210 5203
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2214 4326
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2216 3643
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2218 0334
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2221 3741
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2240 4326
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2456 2341
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```

1360 3690 DCA
1364 3647 NEXTKV, ISZ
1365 3650 XCTRK
1366 3651 ,*2
1367 3652 JMP ROTATE
1370 3655 TAD, I
1371 3654 AND
1372 3655 TAD
1373 3656 SPA CLA
1374 3657 JMP
1375 3660 JMP
1376 3661 ROTATE, JMS
1377 3662 DCA
1400 3663 TAD
1401 3664 CIA
1402 3665 DCA
1403 3666 TAD
1404 3667 AND
1405 3670 SNA CLA
1406 3671 JMP
1407 3672 TAD
1410 3673 AND
1411 3674 RAR
1412 3675 DCA
1413 3676 ISZ
1414 3677 JMP
1415 3700 OK,
1416 3701 TAD
1417 3702 SNA
1420 3703 JMP I
1421 3704 CIA
1422 3705 DCA
1423 3706 TAD
1424 3707 DCA
1425 3710 TAD I
1426 3711 RAR
1427 3712 AND
1430 3713 ISZ
1431 3714 JMP
1432 3715 DCA
1433 3716 TAD I
1434 3717 AND
1435 3720 TAD
1436 3721 DCA I
1437 3722 ISZ
1440 3723 ISZ
1441 3724 JMP
1442 3725 JMP I
1443 3726 INITK,
1444 3727
1445 3730 DCA
1446 3731 TAD
1447 3732 DCA
1450 3733 JMP I
1451 3734 INITK,
1452 3735 K3777,
1453 3736 K4000,
1454 3737 K3400,
1455 3737 ARRLIK, =764
1456 3741 HGT,
1457 3741 YK,
1460 3743 XCTRK,
1461 3744 FLAG,

```

```

/ROUTINE TO CHECK FOR OVERSIZED
/ELEMENT AND COMPUTE NUMBER OF
/ROTATIONS REQUIRED TO PREVENT
/DISPLAY BUFFER OVERFLOW

```

```

/ROTATE ALL ELEMENTS IN ARRAY
/ANY ROTATIONS NEEDED?
/NO, EXIT TO DISPLAY

```

```

/SAVE CALIBRATION MARK

```

```

/NUMBER OF ELEMENTS IN ARRAY

```



```

1462 FLGR, 0
1463 XSTART, START
1464 TEXT1=,
1465 *4000 /TEXT1 LOADS
1466 /NMR DISPLAY ROUTINE PART B
1467 X, /OPEN FOR X VALUE FOR LINC DISPLAY
1468 START, CDF 10 /KEYBOARD INTERRUPT
1469 4001 0000 SKP CLA IRRPT
1470 4001 6211 DCA X
1471 4002 6031 TAD SPECB
1472 4003 7610 DCA YP
1473 4004 5702 JMP I RPX=2
1474 4005 3200 DCA X
1475 4006 1071 TAD SPECB
1476 4007 3300 DCA YP
1477 4010 5220 JMP RPX=2
1500 /THE FOLLOWING 7 WORD KLUDGE BOOTSTRAPS DIAL INTO CORE:
1501 DIALEX, LINC
1502 LMODE
1503 0012 1020 /LDA I 0
1504 0013 0020 20
1505 0014 0004 4
1506 0015 0643 /ESF TO GET I/O PRESET
1507 0016 0701 /SET LINC DF=3
1508 0017 7300 /READ TAPE GROUP
1509 /MUST BE IN LOCN 4017:
1510 PMODE
1511 TAD ARRLIM
1512 4020 1273 DCA XCTR
1513 4021 3277 DCA YP
1514 4022 1700 TAD I YP
1515 4023 7440 SZA AFMRK=2
1516 4024 5233 JMP M377
1517 4025 1274 TAD
1518 4026 6141 LINC
1520 LMODE
1521 DIS 0
1522 PDP
1523 PMODE
1524 CLA
1525 4031 7200 INCR
1526 4032 5252 JMP MRKR
1527 4033 7510 SPA
1528 4034 5257 JMP
1529 4035 7041 CIA AFMRK,
1530 4036 3301 DCA
1531 4037 1274 TAD
1532 4040 1276 RPY,
1533 4041 6141 LINC
1534 LMODE
1535 DIS 0
1536 PDP
1537 PMODE
1538 ISZ
1539 JMP
1540 LAS
1541 AND
1542 IAC
1543 DCA
1544 ISZ X
1545 ISZ YP
1546 JMP RPX
1547 INCR,
1548 4051 3276 DCA
1549 4052 2200 ISZ
1550 4053 2300 ISZ
1551 4054 2277 JMP
1552 4055 5222 JMP
1553 4056 5202 JMP
1554 4057 7346 CLL STA RTL
1555 4060 1274 TAD
1556 4061 6141 LINC
1557

```

/CHECK FOR CALIBRATION MARK

/GET Y INCREMENT

/DISPLAY CALIBRATION MARK

1561	0002	0140	DIS 0
1562	0063	0002	PDP
1563			PMODE
1564	4064	7200	CLA
1565	4065	1700	TAD I
1566	4066	0272	AND
1567	4067	7450	SNA
1570	4070	5252	JMP
1571	4071	0235	JMP
1572	4072	3777	K3777P, 3777
1573	4073	7014	ARRHLIM, -764
1574	4074	7404	M377, -374
1575	4075	0007	KK7, 7
1576	4076	0000	INKY, 0
1577	4077	0000	XCTR, 0
1600	4100	0000	YP, 0
1601	4101	0000	HGTP, 0
1602	4102	2600	INTRUP
1603	4103	0000	LNCTAP, 0
1604	4104	7640	SZA CLA
1605	4105	1342	TAD CRDC
1606	4106	1343	TAD CWRC
1607	4107	5332	DCA RWTI
1610	4110	1101	TAD BLK1
1611	4111	5333	DCA RWTI+1
1612	4112	2101	ISZ BLK1
1613	4113	1077	TAD UNIT
1614	4114	7110	CLL RAR
1615	4115	1344	TAD CXOB
1616	4116	5332	DCA XOBL
1617	4117	7026	RTL
1620	4120	7026	RTL
1621	4121	1332	TAD RWTI
1622	4122	5332	DCA RWTI
1623	4123	7001	IAC
1624	4124	1104	TAD CORBUF
1625	4125	6141	LINC
1626			LMODE
1627	0126	0023	23 /TMA
1630	0127	1020	1020 /LDA I 0
1631	0130	0020	XOBL, 20
1632	0131	0001	1 /AXO
1633	0132	0000	0 RWTI, 0
1634	0133	0000	2 /TAC
1635	0134	0003	3
1636	0135	0002	PDP
1637			PMODE
1640	4136	7001	IAC
1641	4137	7440	SZA
1642	4140	7402	HLT
1643	4141	5703	JMP I LNCTAP
1644	4142	7774	CROC, 7774
1645	4143	0704	CWRC, 724
1646	4144	0020	20 CXOB, 0
1647			*4200
1650	4200	0000	0 OCTIN, 0
1651	4201	7200	CLA VALU
1652	4202	3243	DCA READ
1653	4203	4025	JMS TYPE
1654	4204	4032	JMS TYPE
1655	4205	3245	DCA LSCHR
1656	4206	1245	TAD LSCHR

/GENERAL LINC TAPE I/O SUBR,  
/IF AC=0, WRITE; IF NOT, READ

/TRANSFER OK?  
/NO!!

/OCTAL INPUT ROUTINE  
/ANY NON OCTAL CHAR TERMINATES  
/GET A CHARACTER

2052 4445 2005  
2052 4446 2240  
2052 4447 2401  
2052 4450 2005  
2052 4451 4011  
2052 4452 5717  
2052 4453 7700

IHD1, TEXT \^\*WANT PAPER TAPE I/0? \

2052 4454 2701  
2053 4455 1624  
2053 4456 4010  
2053 4457 1107  
2053 4460 1040  
2053 4461 2320  
2053 4462 0505  
2053 4463 0440  
2053 4464 2205  
2053 4465 0104  
2053 4466 0522  
2053 4467 5520  
2053 4470 2516  
2053 4471 0310  
2053 4472 7700

IHD2, TEXT /WANT HIGH SPEED READER=PUNCH?/  
\*TEXT1

2054  
2055 3747 3616  
2055 3750 1522  
2055 3751 2311  
2055 3752 1536  
2055 3753 3603  
2055 3754 1715  
2055 3755 1505  
2055 3756 1624  
2055 3757 2372  
2055 3760 4000

HD1, TEXT /+NMRSIM+COMMENTS: /

2056 3761 1517  
2056 3762 2205  
2056 3763 7700

HD3, TEXT /MORE? /

2056 3764 1617  
2057 3765 5640  
2057 3766 1706  
2057 3767 4023  
2057 3770 2011  
2057 3771 1623  
2057 3772 7540  
2057 3773 4000

HD2, TEXT /NO. OF SPINS= /  
\*TEXT2

2060 1736 0214  
2061 1737 1703  
2061 1740 1554  
2061 1741 4025  
2061 1742 7240  
2061 1743 4000  
2061 1744 0310  
2062 1745 0515  
2062 1746 1103  
2062 1747 0114  
2062 1750 4023

HD4, TEXT /BLOCK, U: /

2062 1751 1000  
2062 1752 1000  
2062 1753 1000  
2062 1754 1000  
2062 1755 1000  
2062 1756 1000  
2062 1757 1000  
2062 1758 1000  
2062 1759 1000  
2062 1760 1000  
2062 1761 1000  
2062 1762 1000  
2062 1763 1000  
2062 1764 1000  
2062 1765 1000  
2062 1766 1000  
2062 1767 1000  
2062 1768 1000  
2062 1769 1000  
2062 1770 1000  
2062 1771 1000  
2062 1772 1000  
2062 1773 1000  
2062 1774 1000  
2062 1775 1000  
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2062 1779 1000  
2062 1780 1000  
2062 1781 1000  
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2062 1791 1000  
2062 1792 1000  
2062 1793 1000  
2062 1794 1000  
2062 1795 1000  
2062 1796 1000  
2062 1797 1000  
2062 1798 1000  
2062 1799 1000  
2062 1800 1000

2002	1754	4000	HD5,	TEXT /CHEMICAL SHIFTS: /
2062	1753	2372		
2062	1754	4000		
2062				
2063	1755	0317		
2063	1756	2520		
2063	1757	1411		
2063	1760	1607		
2063	1761	4003		
2063	1762	1716		
2063	1763	2324		
2063	1764	0116		
2063	1765	2423		
2063	1766	7240		
2063	1767	4000		
2063				
2064	1770	2401	HD6,	TEXT /COUPLING CONSTANTS: /
2064	1771	2005		
2064	1772	4011		
2064	1773	1620		
2064	1774	2524		
2064	1775	7700		
2064				
2065				
2066	2750	1706	HD8,	TEXT /TAPE INPUT?/ *TEXT3
2066	2751	0623		
2066	2752	0524		
2066	2753	4046		
2066	2754	4027		
2066	2755	1104		
2066	2756	2410		
2066	2757	7200		
2066				
2067	2760	0411	HD7,	TEXT /OFFSET & WIDTH: /
2067	2761	2320		
2067	2762	1401		
2067	2763	3140		
2067	2764	1411		
2067	2765	2324		
2067	2766	7700		
2067				
2070	2767	1511	HD9,	TEXT /DISPLAY LIST? /
2070	2770	1656		
2070	2771	4011		
2070	2772	1624		
2070	2773	0516		
2070	2774	2311		
2070	2775	2431		
2070	2776	7200		
2070				
2071			HD10,	TEXT /MIN. INTENSITY: / *TEXT4
2072	1557	3640		
2072	1560	4011		
2072	1561	1624		
2072	1562	0516		
2072	1563	2311		
2072	1564	2431		
2072	1565	4040		
2072	1566	4040		
2072	1567	4005		
2072	1568	1605		
2072	1571	2207		
2072	1573	3140		







2366	5501	1364	TAD TEMPX	/NO,
2367	5502	7001	IAC	
2370	5503	7710	SPA CLA	/ P > 1 ?
2371	5504	1360	TAD SPACX	/YES, TAKE SPACE; OTHERWISE 0
2372	5505	4323	JMS OUTX	/PRINT CHARACTER
2373	5506	2364	ISZ TEMPX	/P CHARACTERS PRINTED?
2374	5507	5275	JMP BACKX	/NO
2375	5510	1362	TAD POINT	/YES,
2376	5511	4757	JMS I OPUT	/PRINT DECIMAL POINT
2377	5512	5275	JMP BACKX	
2400	5513	7040	CMA	
2401	5514	1366	TAD PLCE	
2402	5515	3366	DCA PLCE	
2403	5516	5236	JMP RETX	
2404	5517	7200	CLA	
2405	5520	1363	TAD CHX	
2406	5521	4323	JMS OUTX	/PRINT "X"
2407	5522	5320	JMP ,=2	/AND REPEAT
2410	5523	0000	0	
2411	5524	4757	JMS I OPUT	/PRINT CHARACTER
2412	5525	2366	ISZ FCOUNT	/F CHARACTERS PRINTED?
2413	5526	5723	JMP I OUTX	/NO, RETURN
2414	5527	5600	JMP I FIXX	/YES, NUMBER FINISHED
2415	5530	7040	CMA	
2416	5531	1044	TAD 44	/REDUCE E BY 1
2417	5532	3044	DCA 44	
2420	5533	2365	ISZ SCOUNT	/6 SIG, FIGS, PRINTED?
2421	5534	5340	JMP ,+4	/NO
2422	5535	7040	CMA	/YES,
2423	5536	3365	DCA SCOUNT	/RESET COUNT TO -1
2424	5537	5305	JMP IN	/AND LEAVE C(IAC) = 0
2425	5540	1415	TAD I 15	/TAKE NEXT DIGIT FROM BUFFER
2426	5541	5305	JMP IN	
2427	5542	1354	TAD M6	/SET COUNT TO PRINT
2430	5543	3366	DCA FCOUNT	/6 DIGITS AFTER DECIMAL POINT
2431	5544	4757	JMS I OPUT	/PRINT "0"
2432	5545	1362	TAD POINT	
2433	5546	4757	JMS I OPUT	/PRINT " ,"
2434	5547	2200	ISZ FIXX	/INCREMENT RETURN ADDRESS
2435	5550	1415	TAD I 15	/TAKE NEXT DIGIT FROM BUFFER
2436	5551	4323	JMS OUTX	/PRINT IT
2437	5552	5350	JMP ,=2	/AND REPEAT
2440	5553	0007	7	
2441	5554	7772	M6,	-6
2442	5555	7766	M10,	=12
2443	5556	5566	BUFST,	BUFFER=1
2444	5557	7352	OPUT,	7352
2445	5560	7760	SPACX,	240=260
2446	5561	7771	M7X,	=7
2447	5562	7776	POINT,	256=260
2450	5563	0050	CHX,	330=260
2451	5564	0000	TEMPX,	0
2452	5565	0020	SCOUNT,	0
2453	5566	0000	FCOUNT,	0
2454	5567	0000	BUFFER,	2
2455			FACE=FCOUNT	
2456			FACE=SCOUNT	
2457			FACE=SYM	





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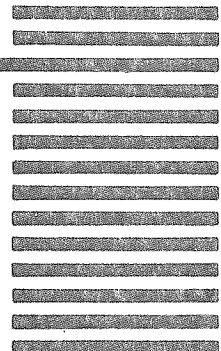
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