

DEC-12-UW5A-D
June, 1970

NMR SIM(E)

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1.0 ABSTRACT

NMRSIM(E)¹ 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-DIAL² 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.

¹

NMRSIME utilizes the EAE option for the PDP-12.

²

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 10000. 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.¹

¹

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 α or β . 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 β spin and $+1/2$ for α spin, ν_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 α and β 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 α and β 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

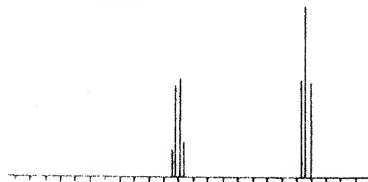
NO. OF SPINS= 5

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
189.00	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

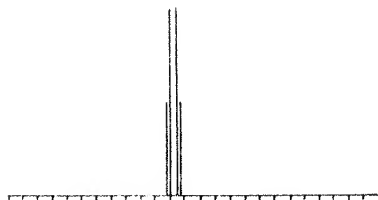
NO. OF SPINS= 2

OFFSET & WIDTH: 0,500

CHEMICAL SHIFTS: 265,280

COUPLING CONSTANTS: 5

BLOCK, U: 440,3



C:

COUPLING CONSTANTS: 10

BLOCK, U: 440,3

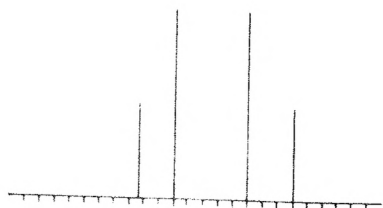
G:

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.

```
00000  
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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Spins, 2

Width, 2, 4


```

00000
00001
00002
00003
00004
00005
00006
00007
00008
00009
00010
00011
00012
00013
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```

/NMR SPECTRAL SIMULATOR!
/ORIGINALLY IN DECUS LIBRARY AS -194
/AS SUBMITTED BY D.F. JUERS, R.J. BOETTCHER, V.J. HULL
/AND H.E. ZIMMERMAN OF UNIV. OF WISC., MADISON, WISC.
/MODIFICATIONS MADE BY G.W. DULANEY OF DEC., MAYNARD, MASS.
/TO ALLOW OPERATION ON THE PDP-12.

PMODE
LODSYM
LISTAP =1
FEXT=0000
FADD=1000
FSUB=2000
FMPY=3000
FDIV=4000
FCGT=5000
FPUT=6000
FNOR=7000

SQUARE=1
SQRROOT=2
FMPY2=3
FDIV2=4
NEGATE=5
FLOIN=6
EXP=44
HORD=45
LORD=46

*5
INPUT, 0760
OUTPUT, 7200
INTERP, 5600

*20
PMODE
JMP I, +1
BEGIN
HIRED
HPUN,
TABLE,
READ,
KSF
JMP
KRB
JMP I READ
TYPE,
TSF
JMP
TLS
JMP I TYPE
*62
10
DECIMAL
IFZB, 16
NUSEB, 23
CPSB, 87
CUPB, 105
BOLD, 710
ENB, 650
SPECB, 150
UB, 1910
HB, 3110
OCTAL
PRINT,
PRINTL

```

```

0005 0760
0006 7200
0007 5600

0020 5421
0021 0202
0022 0354
0023 0361
0024 2145
0025 0000
0026 6031
0027 5026
0030 6036
0031 5425
0032 0000
0033 6041
0034 5033
0035 6046
0036 5432
0062 0010

0063 0020
0064 0027
0065 0127
0066 0151
0067 1306
0070 1212
0071 0226
0072 3566
0073 6046
0074 2676
0075

```

0076	0075	3600	DISPLAY,	STDIS
0077	0076	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	TPGT, 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	N1, 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	*200	CLA	
0146	0201	3055	DCA 55	
0147	0202	6032	KCC	/SA OF PROGRAM
0150	0203	6046	TLS	
0151	0204	6014	RFC	
0152	0205	4474	JMS I	/NMR SIMULATOR COMMENTS:
0153	0206	3747	HD1	
0154	0207	4025	JMS	/ROUTINE ALLOWS USER TO TYPE ANY AMOUNT
0155	0210	4232	JMS	
0156	0211	1332	TAD	/OF COMMENTARY AT BEGINNING OF PROGRAM,
0157	0212	7640	SZA CLA	/EXIT IS ACHIEVED BY TYPING CTRL/A,
0158	0213	5207	JMP	/GET MORE
0159	0214	4720	JMS I	/GET HSR/P AND TAPE SETUP
0161	0215	5214	DCA	/RETURNED WITH SKP IN AC; NO FURTHER CALLS
0162	0216	5222	JMP	
0163	0217	7200	CLA	
0164	0220	1530	TAD	
0165	0221	4032	JMS	
0166	0222	4474	JMS I	/NO, OF SPINS=
0167	0223	3764	HD2	
0168	0224	4405	JMS I	
0169	0225	4712	JMS I	
0170	0226	7110	CLL RAR	
0171	0227	7110	CLL RAR	
0172	0228	7110	CLL RAR	
0173	0229	7110	CLL RAR	

0170	0231	7004	RAL	M7	/NO
0177	0232	1331	TAD		/WAS IT >6?
0200	J233	7500	SMA		/YES, NO GOOD
0201	0234	5217	JMP	ERROR	
0202	0235	1333	TAD	P7	
0203	0236	3106	DCA	N	/STORE
0204	0237	4711	JMS	I	/INITIALIZE NARRAY & NUSE
0205	0240	4715	JMS	I	/GET UPPER SPECTRAL LIMIT
0206	0241	4474	JMS	I	/CHEM SHIFTS:
0207	0242	1744	HD5		
0210	0243	4714	JMS	I	/GET CHEMICAL SHIFTS
0211	0244	4474	JMS	I	/COUPLING CONSTANTS:
0212	0245	1755	HD6		
0213	0246	4716	JMS	I	/GET COUPLING CONSTANTS
0214	0247	4334	JMS	I	GTTP
0215	0250	4717	JMS	I	INPEC
0216	0251	1100	TAD	STBLK	
0217	0252	3101	DCA	BLK1	/RESET TAPE BLOCK
0220	0253	7201	CLA	IAC	
0221	0254	3133	DCA	JTEMP	
0222	0255	7001	IAC		
0223	0256	3115	DCA	N1	/READY TO INITIALIZE EN & BOLD
0224	0257	1106	TAD	N	
0225	0260	7041	CIA		
0226	0261	3326	DCA	FLAGO	/SET LOOP
0227	0262	1063	TAD	IFZB	
0230	0263	3327	DCA	ADRO	/SET UP TO FIND BPFS
0231	0264	4721	JMS	I	/H(1,1) HAS EN(1) & U(1,1) HAS UOLD(1,1)
0232	0265	4723	JMS	I	/COPY TRACE OF H INTO EN & U INTO UOLD
0233	0266	1727	TAD	I	/GET NEW JTEMP
0234	0267	3133	DCA	JTEMP	
0235	0270	2327	ISZ	ADRO	/SET TO GET NEW JTEMP
0236	0271	1133	TAD	JTEMP	
0237	0272	7041	CIA		
0240	0273	1727	TAD	I	ADRO
0241	0274	3115	DCA	N1	/NEW N1
0242	0275	4722	JMS	I	ALLOWO
0243	0276	4721	JMS	I	/INITIALIZE H & U MATRICES
0244	0277	4724	JMS	I	/DIAGNALIZE
0245	0300	4725	JMS	I	TRANSO
0246	0301	2326	ISZ	FLAGO	/DONE?
0247	0302	5265	JMP	RPTO	/NO, LOOP AGAIN
0250	0303	6201	COF	0	
0251	0304	7333	STL	CLA	/PUT TAG WORD IN CORE ARRAY
0252	0305	3411	DCA	I	11
0253	0306	4476	JMS	I	TAPTRN
0254	0307	5475	JMP	I	/WRITE OUT LAST PART OF BUFFER
0255	0310	2663	CRLF		DISPLAY
0256	0311	3400	INITB		/DISPLAY SPECTRUM
0257	0312	3127	FIX		
0260	0313	4315	ASKM		
0261	0314	0600	W,		
0262	0315	3554	ULIM		
0263	0316	0610	JO,		
0264	0317	1121	INPEC		
0265	0320	4400	INDIL		
0266	0321	2200	HUGET		
0267	0322	2000	ALLOWO		
0270	0323	2320	COPYO		
0271	0324	1200	JAKEO		
0272	0325	2400	TRANSO		
0273	0326	0000	FLAGO,		
			0		

ADDRESS	DATA	COMMENT
0274	0327 0000	ADDR0, 0
0275	0330 0277	QUEST, 0277
0276	0331 7771	-7
0277	0332 7577	M2010, 7
0300	0333 0007	P7, 0
0301	0334 0000	GTTP, 0
0302	0335 4474	JMS I PRINT
0303	0336 1736	HD4
0304	0337 4753	JMS I OCIN
0305	0340 5337	JMP
0306	0341 7450	SNA
0307	0342 5337	JMP
0310	0343 5100	DCA
0311	0344 4405	JMS I STBLK
0312	0345 4712	JMS I INPUT
0313	0346 0352	AND
0314	0347 5077	MSK7
0315	0350 4710	DCA UNIT
0316	0351 5734	JMS I CARIN
0317	0352 0007	JMP I GTTP
0320	0353 4200	7
0321	0354 0000	OCIN
0322	0355 6011	HIRED, 0
0323	0356 5355	RSF
0324	0357 6016	JMP
0325	0360 5754	RRB RFC
0326	0361 0000	JMP I HIRED
0327	0362 6026	0
0330	0363 6021	PLS
0331	0364 5363	PSF
0332	0365 5761	JMP
0333	0400 0002	JMP I HIPUN
0334	0401 6046	*400
0335	0402 4717	2
0336	0403 4474	TLS
0337	0404 1770	JMS I AULIM
0340	0405 4713	JMS I PRINT
0341	0406 5102	HD8
0342	0407 4505	JMS I ASKMX
0343	0410 4716	OCA
0345	0411 1102	JMS I INSWT
0346	0412 7640	JMS I TPOT
0347	0413 5222	JMS I INSPA
0350	0414 1100	TAD
0351	0415 3101	SZA CLA
0352	0416 5014	JMP
0353	0417 4422	TAD
0354	0420 7450	CCA
0355	0421 5217	RFC
0356	0422 4327	JMS I HRED
0357	0423 5267	SNA
0360	0424 4407	JMP
0361	0425 1110	JMS I
0362	0426 5134	FADD
0363	0427 1320	EMPTY
0364	0430 0000	FADD
0365	0431 4723	FEXT
0366	0432 3324	JMS I
0367	0433 4327	DCA
0370	0434 7402	JMS
0371	0435 4723	HLT
0372	0436 7700	JMS I
0373	0437 7700	CCA

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		/IN RIGHT RANGE?
0400	0444	5222	JMP	GET	/NO, LOOK NEXT CASE
0401	0445	1324	TAD	SPECAD	/YES, ADDRESS IN SPEC ARRAY
0402	0446	1071	TAD	SPECB	
0403	0447	3324	DCA	SPECAD	
0404	0450	6211	CDF 10		
0405	0451	1724	TAD I	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	TAD I	SPECAD	
0413	0457	1724	RAL	CMA RAR	
0414	0460	7004	CLA	DCA I	/STORE
0415	0461	7250	DCA I	GET	/LOOK NEXT CASE
0416	0462	3724	JMP	TAD I	SPECAD
0417	0463	5222	TAD	APROB	:-4
0420	0464	1724	TAD	JMP	I PRINT
0421	0465	1325	JMS I	HD3	
0422	0466	5262	JMS I	ASKMX	
0423	0467	4474	JMS I	SZA CLA	NMRE
0424	0470	3761	JMS I	TAD	INSWT
0425	0471	4713	JMS I	SNA CLA	GET-4
0426	0472	7640	JMP	JMS I	TPGT
0427	0473	5302	JMP	JMS I	TPSIR
0430	0474	1102	TAD	JMP	GET
0431	0475	7650	SNA CLA	JMS I	CARLFD
0432	0476	5216	JMP	TAD	INSWT
0433	0477	4505	JMS I	SZA CLA	
0434	0500	4715	JMS I	JMP I	DISPLAY
0435	0501	5222	JMP	STL IAC RTR	
0436	0502	4714	JMS I	CDF 0	
0437	0503	1102	TAD	DCA I	11
0440	0504	7640	JMP	JMS I	TAPTRN
0441	0505	5475	JMP I	JMP I	DISPLAY
0442	0506	7133	STL IAC RTR	ASKMX,	
0443	0507	6201	CDF 0	CARLFD,	
0444	0510	3411	DCA I	TPSTR,	
0445	0511	4476	JMS I	STRTP	
0446	0512	5475	JMP I	TPSTR,	
0447	0513	4315	ASKMX,	INSPE	
0450	0514	2663	CARLFD,	AULIM,	
0451	0515	3317	TPSTR,	HALFA,	
0452	0516	1121	INSPE,	2000	
0453	0517	3554	AULIM,	0	
0454	0520	0000	HALFA,	0	
0455	0521	2000	0	FIXA,	
0456	0522	0000	0	SPECAD,	
0457	0523	3127	FIXA,	APROB,	
0460	0524	0000	SPECAD,	DECIMAL	
0461	0525	0000	APROB,	M500,	
0462	0526	7014	DECIMAL	OCTAL	
0463	0527	0000	M500,	RDWD,	
0464	0528	7200	OCTAL	CLA	
0465	0529	0000	RDWD,	CDF 0	
0466	0530	7200	CLA	TAD	
0467	0531	6201	CDF 0	INSWT	
0470	0532	1102	TAD		

0472	0534	5340	JMP	STPE	
0473	0535	4773	JMS I	FACLOD	
0474	0536	5366	JMP	RDEX	/NORMAL RETURN
0475	0537	5727	JMP I	RWD	
0476	0540	7346	STA CLL	RTL	/-3
0477	0541	3372	DCA	FLAG	/INITIALIZE TO READ THREE WORDS
0500	0542	1370	TAD	P44	
0501	0543	5113	DCA	ADD0	
0502	0544	4771	JMS I	CKEND	/CHECK FOR END OF BUFFER
0503	0545	7300	CLA CLL		
0504	0546	4422	JMS I	HRED	
0505	0547	7006	RTL		/SHIFT TO BITS 2-7
0506	0550	7006	RTL		
0507	0551	7004	RAL		/IS THIS A STARTING MARK?
0510	0552	7510	SPA		/YES
0511	0553	5345	JMP	BACK0	/NO, IS IT AN END MARK?
0512	0554	7430	SZL		/YES, EXIT W/O INCRD RETURN
0513	0555	5727	JMP I	RWD	/NO, SHIFT TO BITS 0-5
0514	0556	7004	RAL		/STORE COMPLETE WORD
0515	0557	4422	JMS I	HRED	/STICK IT IN CORE BUFFER
0516	0560	5513	DCA I	ADD0	/IS WHOLE F.P. READ?
0517	0561	1513	TAD I	ADD0	/NO, READ NEXT WORD
0520	0562	5411	DCA I	11	/NORMALLY INCR, RETURN
0521	0563	2113	ISZ	ADD0	/YES, RETURN
0522	0564	2372	ISZ	FLAGR	
0523	0565	5345	JMP	BACK0	
0524	0566	2327	ISZ	RWD	
0525	0567	5727	JMP I	RWD	
0526	0570	0044	P44,		
0527	0571	1161	CKEND,	ENDCHK	
0530	0572	0000	FLAGR,		
0531	0573	3250	FACLOD,	LODFAC	
0532			*600		
0533	0600	0000	0		/INPUT OF CPS AND CUP
0534	0601	7200	CLA		
0535	0602	1065	TAD	CPSB	
0536	0603	3356	DCA	ADDRC	/START OF CPS ARRAY
0537	0604	1106	TAD	N	
0540	0605	7041	CIA		
0541	0606	3352	DCA	FLAG	/SET OF CHEMICAL SHIFTS
0542	0607	5226	JMP	RPTC	/GET CHEMICAL SHIFTS
0543	0610	0000	0		
0544	0611	7200	CLA		
0545	0612	1210	TAD	JC	
0546	0613	3200	DCA	WC	
0547	0614	1066	TAD	CUPB	
0550	0615	3356	DCA	ADDRC	/START OF CUP ARRAY
0551	0616	1106	TAD	N	
0552	0617	7041	CIA		
0553	0620	7001	IAC		
0554	0621	3352	DCA	FLAG	/SET TO CALCULATE OF JS
0555	0622	1352	TAD	FLAG	
0556	0623	2352	ISZ	FLAG	
0557	0624	5222	JMP	-2	
0560	0625	3352	DCA	FLAG	/FLAG CONTAINS - OF JS
0561	0626	4405	JMS I	INPUT	/GET A VALUE
0562	0627	4407	JMS I	INTERP	
0563	0630	0004	FDIV2		
0564	0631	6756	FPUT I	ADDRC	/STORE
0565	0632	0000	FEXT		
0566	0633	7325	CLA IAC	STL RAL	
0567	0634	1356	TAD	ADDRC	

0571	0636	2352	ISZ	FLAG	/DONE?
0572	0637	5226	JMP	RPTC	/NO; GET NEXT
0573	0640	6211	CDF 10		MENT
0574	0641	5600	JMP I	WC	/YES; RETURN
0575	0642	0000	DIAGC, 0		
0576	0643	4751	JMS I	KLAEL	/CLEAR ADD0 (3 WORDS)
0577	0644	1065	TAD	CPSB	
0600	0645	3356	DCA	ADDRC	/ADDRC INITIALIZED TO CPS
0601	0646	1066	TAD	CUPB	
0602	0647	3357	DCA	ADDRC1	/ADDRC1 INITIALIZED TO CUP
0603	0650	1106	TAD	N	
0604	0651	7041	CIA		
0605	0652	5352	DCA	FLAG	/SET CPS DO LOOP
0606	0653	1107	TAD	TEMP	/GET BPF
0607	0654	5354	DCA	TEMP	/STORE IN TEMP
0610	0655	7300	RPTC1, CLA CLL		
0611	0656	1354	TAD	TEMP	
0612	0657	7010	RAR		/GET RIGHTMOST BIT
0613	0660	3354	DCA	TEMP	/STORE REDUCED BPF
0614	0661	1354	TAD	TEMP	
0615	0662	5355	DCA	TEMP1	/STORE FOR J USE
0616	0663	7430	SEL		/ALPHA OR BETA?
0617	0664	5272	JMP	.*6	/ALPHA
0620	0665	1346	TAD	BETA	/BETA SPIN
0621	0666	5300	DCA	ORDER	/SET DIRECTIONS
0622	0667	1350	TAD	CASE1	
0623	0670	5320	DCA	DIRC	/SET DIRECTIONS FOR JS
0624	0671	5276	JMP	.*5	
0625	0672	1344	TAD	ALPHA	
0626	0673	3300	DCA	ORDER	/SET DIRECTIONS
0627	0674	1263	TAD	CASE2	
0630	0675	5320	DCA	DIRC	/SET DIRECTIONS
0631	0676	4407	JMS I	INTERP	
0632	0677	5513	FGET I	ADD0	
0633	0700	0000	ORDER, 0		/INCREMENT ELEMENT DEPENDING ON DIRECTIONS
0634	0701	6513	FPUT I	ADD0	
0635	0702	0000	FEXT		
0636	0703	7525	CLA IAC	STL RAL	
0637	0704	1356	TAD	ADDRC	
0640	0705	3356	DCA	ADDRC	/INCREMENT ADDR
0641	0706	2352	ISZ	FLAG	/DONE?
0642	0707	5312	JMP	.*3	/NO; CONTINUE
0643	0710	6211	CDF 10		
0644	0711	5642	JMP I	DIAGC	/YES; RETURN
0645	0712	1352	TAD	FLAG	
0646	0713	3353	DCA	FLAGC1	/SET J DO LOOP
0647	0714	7300	RPTC2, CLA CLL		
0650	0715	1355	TAD	TEMP1	/GET PARTIALLY ROTATED BPF
0651	0716	7010	RAR		/ROTATE
0652	0717	3355	DCA	TEMP1	/STORE ROTATED VALUE
0653	0720	2000	DIRC, 0		/DEPENDS ON SPIN
0654	0721	5325	JMP	.*4	/SAME AS REFERENCE
0655	0722	1347	TAD	BETA1	/DIFFERENT THAN REFERENCE
0656	0723	5332	DCA	CONTROL	/SET INSTRUCTION
0657	0724	5327	JMP	.*3	
0660	0725	1345	TAD	ALPH1	
0661	0726	5332	DCA	CONTROL	/SET INSTRUCTION
0662	0727	4407	JMS I	INTERP	
0663	0730	5513	FGET I	ADD0	
0664	0731	1513	FADD I	ADD0	/DEPENDS ON SPIN
0665	0732	0000	CONTROL, 0		
0666	0733	0004	FDIV2		

[illegible]

0767	1043	1106	TAD	N		
0770	1044	1320	TAD	FLAGD	/POSITION OF T	DIFFERENCE
0771	1045	2313	ISZ	INDD1	/WHERE TO STORE	
0772	1046	5251	JMP	.+3	/INDD1 HAS A VALUE, STORE INDD2	
0773	1047	5313	DCA	INDD1	/STORE IN INDD1	
0774	1050	5252	JMP	.+2		
0775	1051	5314	DCA	INDD2		
0776	1052	2520	ISZ	FLAGD	/WHOLE BPF EXAMINED?	
0777	1053	5216	JMP	RPTD	/NO, ROTATE AGAIN	
1000	1054	1313	TAD	INDD1	/YES, GET ADDRESS OF RELEVANT J	
1001	1055	7041	CIA			
1002	1056	1314	TAD	INDD2		
1003	1057	5314	DCA	INDD2		
1004	1060	1313	TAD	INDD1		
1005	1061	7041	CIA			
1006	1062	3313	DCA	INDD1		
1007	1063	7040	CMA			
1010	1064	1106	TAD	N		
1011	1065	7041	CIA			
1012	1066	3320	DCA	FLAGD		
1013	1067	2313	ISZ	INDD1		
1014	1070	5272	JMP	.+2		
1015	1071	5275	JMP	.+4		
1016	1072	1320	TAD	FLAGD		
1017	1073	2320	ISZ	FLAGD		
1020	1074	5267	JMP	.+5		
1021	1075	7041	CIA			
1022	1076	1314	TAD	INDD2		
1023	1077	5312	DCA	CTRDD		
1024	1100	1312	TAD	CTRDD		
1025	1101	1312	TAD	CTRDD		
1026	1102	1312	TAD	CTRDD		
1027	1103	1066	TAD	CUPB		
1030	1104	3312	DCA	CTRDD	/CTRDD CONTAINS PROPER ADDRESS	
1031	1105	4407	JMS I	INTERP		
1032	1106	5712	FGET I	CTRDD	/GET J VALUE	
1033	1107	6513	FPUT I	ADD0	/PUT IN H ARRAY	
1034	1110	0000	FEXT			
1035	1111	5241	JMP	RET	/RETURN	
1036	1112	0000	CTRDD,			
1037	1113	0000	INDD1,			
1040	1114	0000	INDD2,			
1041	1115	0000	TEM,			
1042	1116	0000	TEM1,			
1043	1117	7420	INSTD1,	SNL		
1044	1120	0000	FLAGD,			
1045	1121	0000	INSPEC,			
1046	1122	6211	CDF	10	/INITIALIZE SPEC ARRAY	
1047	1123	7240	STA			
1050	1124	5315	DCA	TEM	/INITIALIZE CALIBRATION COUNTER	
1051	1125	1346	TAD	N500D		
1052	1126	5320	DCA	FLAGD		
1053	1127	1071	TAD	SPECB		
1054	1130	5312	DCA	CTRDD		
1055	1131	2315	ISZ	TEM	/INITIALIZE ADDRESS	
1056	1132	5336	JMP	.+4	/NEED A CALIBRATION?	
1057	1133	1345	TAD	M20	/NO, DEPOSIT A 0	
1060	1134	3315	DCA	TEM	/YES	
1061	1135	7130	STL	RAR	/REINITIALIZE CALIBRATION COUNTER	
1062	1136	3712	DCA I		/PUT IN CALIBRATION	
1063	1137	2312	ISZ	CTRDD	/PUT VALUE IN SPEC ARRAY	
1064	1140	2320	ISZ	FLAGD	/DONE?	

1066	1142	4744	JMS I	INTAP	
1067	1143	5721	JMP I	INSPEC	/RETURN
1070	1144	5317	STRYP		
1071	1145	7754			
1072	1146	7014			
1073	1147	0000			
1074	1150	6211	COF 10		
1075	1151	7240	STA		
1076	1152	1113	TAD	ADD0	
1077	1153	3010	OCA	10	
1100	1154	3410	OCA I	10	
1101	1155	3410	OCA I	10	
1102	1156	3410	OCA I	10	
1103	1157	6201	COF 0		
1104	1160	5747	JMP I	CLAEI	
1105	1161	0000			
1106	1162	7300	CLA CLL		
1107	1163	1011	TAD	11	
1110	1164	1103	TAD	AREND	
1111	1165	7710	SPA CLA		/REACHED END OF TAPE BUFFER?
1112	1166	5761	JMP I	ENDCHK	/NO
1113	1167	4476	JMS I	TAPTRN	/YES, WRITE OUT THE BUFFER
1114	1170	1104	TAD	CORBUF	
1115	1171	3011	OCA	11	
1116	1172	5761	JMP I	ENDCHK	
1117					
1120	1200	0000	*1200		
1121	1201	7200	JAKE,		
1122	1202	1115	RPTE,		
1123	1203	7041	CIA	N1	
1124	1204	5365	OCA	FLAGE	/SET DO LOOP
1125	1205	7040	CMA		
1126	1206	1115	TAD	N1	
1127	1207	3267	DCA	CTRE	/CTRE=N1-1
1130	1210	3270	OCA	IS	/IS=0
1131	1211	7200	CLA	FLAGE	/LOOP DONE?
1132	1212	2365	ISZ	1-5	/NO, CONTINUE
1133	1213	5220	JMP	IS	/YES
1134	1214	1270	TAD		/MATRIX DIAGONALIZED?
1135	1215	7450	SNA		
1136	1216	5600	JMP I	JAKE	/YES, RETURN
1137	1217	5201	JMP	RPTE	/NO, GO THROUGH AGAIN
1140	1220	1267	TAD	CTRE	
1141	1221	7041	CIA	FLAGE1	/SET INNER DO LOOP
1142	1222	5265	DCA	R2	
1143	1223	1367	TAD	INSTE	
1144	1224	5364	OCA	FLAGE1	/DONE WITH INNER LOOP?
1145	1225	2265	ISZ	1-6	/NO, CONTINUE
1146	1226	5234	JMP	CMA	/YES, INCREMENT CTRE AND OUTER DO LOOP
1147	1227	7240	CLA	CTRE	
1150	1230	1267	TAD	CTRE	/CTRE=CTRE-1
1151	1231	3267	OCA	R1	
1152	1232	1366	TAD	INSTE	
1153	1233	3364	DCA		
1154	1234	7200	CLA		
1155	1235	1115	TAD	N1	
1156	1236	1365	TAD	FLAGE	
1157	1237	5107	DCA	TEMP	
1160	1240	1115	TAD	N1	
1161	1241	1265	TAD	FLAGE1	/TEMP AND TEMP1 HAVE SUBSCRIPTS
1162	1242	5114	DCA	TEMP1	
1163	1243	4273	JMS	HSUBE	
1164	1244	1414	TAD		

1165	1245	1266	TAD	TESTE	/ADD 13 TO EXPONENT
1166	1246	7510	SPA		/ELEMENT SMALL, ENOUGH?
1167	1247	5764	JMP I	INSTE	/YES, LOOK FOR OTHER
1170	1250	2113	ISZ	ADD0	/IS IT 0?
1171	1251	7300	CLA CLL		
1172	1252	1513	TAD I	ADD0	
1173	1253	7004	RAL		
1174	1254	7450	SNA		
1175	1255	5764	JMP I	INSTE	/ITS 0
1176	1256	7240	STA		/RESTORE ADD0
1177	1257	1113	TAD	ADD0	
1200	1260	3113	DCA	ADD0	
1201	1261	2270	ISZ	IS	/SHOW THAT A LARGE ELEMENT IS FOUND
1202	1262	4671	JMS I	TRIGE	/0 THE ELEMENT
1203	1263	4672	JMS I	VALUE	
1204	1264	5764	JMP I	INSTE	/CONTINUE
1205	1265	0000	FLAGE1, 0		
1206	1266	0015	TESTE, 15		
1207	1267	0000	CTRE, 0		
1210	1270	0000	IS, 0		
1211	1271	1400	TRIGE, TRIG		
1212	1272	1600	VALUE, VALUEG		
1213	1273	0000	HSUBE, 0		
1214	1274	7200	CLA		/FIND ADDRESS OF H ELEMENT
1215	1275	1107	TAD	TEMP	
1216	1276	7041	CIA		
1217	1277	1114	TAD	TEMP1	/TEMP1-TEMP
1220	1300	7500	SMA		/WHICH IS BIGGEST?
1221	1301	5310	JMP	.+7	/TEMP1
1222	1302	7041	CIA		/TEMP
1223	1303	5340	DCA	DIFF	/ FROM DIAGONAL ELEMENT
1224	1304	1114	TAD	TEMP1	
1225	1305	7041	CIA		
1226	1306	3336	DCA	IND1	/SET DO LOOP
1227	1307	5314	JMP	.+5	
1230	1310	3340	DCA	DIFF	
1231	1311	1107	TAD	TEMP	
1232	1312	7041	CIA		
1233	1313	5336	DCA	IND1	
1234	1314	1115	TAD	N1	
1235	1315	7041	CIA		
1236	1316	3337	DCA	IND2	/SET UP REGISTER
1237	1317	2336	ISZ	IND1	/ENOUGH ADDITIONS?
1240	1320	5322	JMP	.+2	/NO, CONTINUE
1241	1321	5325	JMP	.+4	/YES, GET OUT OF LOOP
1242	1322	1337	TAD	IND2	
1243	1323	2337	ISZ	IND2	
1244	1324	5317	JMP	.-5	
1245	1325	7041	CIA		/AC CONTAINS OF ELEMENTS IN SKIPPED ROWS
1246	1326	1340	TAD	DIFF	/ OF ELEMENTS TO SKIP
1247	1327	3113	DCA	ADD0	
1250	1330	1113	TAD	ADD0	
1251	1331	1113	TAD	ADD0	
1252	1332	1113	TAD	ADD0	
1253	1333	1073	TAD	HB	
1254	1334	3113	DCA	ADD0	/ADD0 CONTAINS ADDRESS
1255	1335	5673	JMP I	HSUBE	
1256	1336	0000	IND1, 0		
1257	1337	0000	IND2, 0		
1260	1340	0000	DIFF, 0		
1261	1341	0000	USUB, 0		/GETS ADDRESS IN U MATRIX
1262	1342	7240	STA		

1204	1344	1420	JNA		/IS HIS 0	
1265	1345	5353	JMP	+6	/YES	
1266	1346	7041	CIA		/NO	
1267	1347	3336	DCA	IND1	/SET DO LOOP	
1270	1350	1115	TAD	N1		
1271	1351	2336	ISZ	IND1	/DONE WITH LOOP?	
1272	1352	5350	JMP	-2	/NO CONTINUE	
1273	1353	1107	TAD	TEMP	/AC CONTAINS OF ELEMENTS TO BE SKIPPED	
1274	1354	3113	DCA	ADD0		
1275	1355	7346	CLL	STA		
1276	1356	1113	TAD	ADD0		
1277	1357	1113	TAC	ADD0		
1300	1360	1113	TAD	ADD0		
1301	1361	1072	TAD	UB	/ADD0 CONTAINS ADDRESS	
1302	1362	3113	DCA	ADD0		
1303	1363	5741	JMP	I		
1334	1364	0000				
1305	1365	0000				
1306	1366	1211	RPT1			
1307	1367	1225	RPT2			
1310						
1311	1400	0000				
1312	1401	4407	JMS	I	/GET H(JF,K)	
1313	1402	5513	FGET	I		
1314	1403	6337	FPUT	HJK		
1315	1404	0000	FEXT			
1316	1405	1107	TAD	TEMP		
1317	1406	3327	DCA	JF		
1320	1407	1114	TAD	TEMP1		
1321	1410	3330	DCA	KF		
1322	1411	1327	TAD	JF		
1323	1412	3114	DCA	TEMP1		
1324	1413	4742	JMS	I	/GET ADDRESS OF H(J,J)	
1325	1414	4407	JMS	I		
1326	1415	5513	FGET	I		
1327	1416	6331	FPUT	HJJ	/HJJ=H(J,J)	
1330	1417	0000	FEXT			
1331	1420	1330	TAD	KF		
1332	1421	3107	DCA	TEMP		
1333	1422	1330	TAD	KF		
1334	1423	3114	DCA	TEMP1		
1335	1424	4742	JMS	I	/GET ADDRESS OF H(K,K)	
1336	1425	4407	JMS	I		
1337	1426	5513	FGET	I		
1340	1427	6334	FPUT	HKK	/HKK=H(K,K)	
1341	1430	2331	FPUT	HJJ	/Y=HKK=HJJ	
1342	1431	6321	FPUT	Y	/R=Y**2	
1343	1432	3321	FPUT	Y		
1344	1433	6324	FPUT	R		
1345	1434	5337	FGET	HJK		
1346	1435	0003	FPUT			
1347	1436	0003	FPUT			
1350	1437	3337	FPUT	HJK		
1351	1440	1324	FADD	R		
1352	1441	0002	SUB001		/R=(Y**2+4*HJK**2)**.5	
1353	1442	5324	FPUT			
1354	1443	0000	FEXT			
1355	1444	1322	TAD	Y1	/IS Y NEGATIVE?	
1356	1445	7500	SMA		/NO	
1357	1446	5253	JMP	TR1	/YES	
1360	1447	4407	JMS	I	/THEN SET R=R	
1361	1448	0005	NEGATE			
1362	1451	6324	FPUT	R		

1363	1452	0000	FEXT	JMS I	INTERP	
1364	453	4407	JMS I	Y		
1365	454	5321	FGET	R		
1366	1455	4324	FDIV	Y		/Y(FCOS2)=Y/R
1367	1456	6321	FPUT	HJK		
1370	1457	5337	FGET	R		
1371	1460	0003	FMPLY2			
1372	1461	4524	FDIV	R		
1373	1462	6324	FPUT	R		/R(FSIN2)=2*HJK/R
1374	1463	5316	FGET	ONEF		
1375	1464	1321	FADD	Y		
1376	1465	0004	FDIV2			
1377	1466	0002	SQR00T			
1400	1467	6127	FPUT	FCOS		/FCOS=((1+FCOS2)/)**.5
1401	1470	5324	FGET	R		
1402	1471	4127	FDIV	FCOS		
1403	1472	0004	FDIV2			
1404	1473	6124	FPUT	FSIN		/FSIN=FSIN2/FCOS/2
1405	1474	5331	FGET	HJJ		
1406	1475	1334	FADD	HKK		
1407	1476	0004	FDIV2			
1410	1477	6116	FPUT	A		/A=(HJJ+HKK)/2
1411	1500	5337	FGET	HJK		
1412	1501	3324	FMPLY	R		
1413	1502	6121	FPUT	B		/B=HJK*FSIN2
1414	1503	5331	FGET	HJJ		
1415	1504	2334	FSUB	HKK		
1416	1505	0004	FDIV2			
1417	1506	3321	FMPLY	Y		
1420	1507	2121	FSUB	B		
1421	1510	6121	FPUT	B		/B=(HJJ+HKK)*FCOS2/2-HJK*FSIN2
1422	1511	0000	FEXT			
1423	1512	1327	TAD	JF		/RESTORE TEMP AND TEMPI
1424	1513	3107	DCA	TEMP		
1425	1514	6211	CDF 10	TRIG		
1426	1515	5600	JMP I			/RETURN
1427	1516	0001	ONEF,	1		
1430	1517	2000	2000			
1431	1520	0000	0			
1432	1521	0000	0			
1433	1522	0000	Y,			
1434	1523	0000	Y1,			
1435	1524	0000	R,			
1436	1525	0000				
1437	1526	0000	0			
1440	1527	0000	JF,			
1441	1530	0000	KF,			
1442	1531	0000	HJJ,			
1443	1532	0000	0			
1444	1533	0000	0			
1445	1534	0000	HKK,			
1446	1535	0000	0			
1447	1536	0000	0			
1450	1537	0000	HJK,			
1451	1540	0000	0			
1452	1541	0000	0			
1453	1542	1273	HSUBF,	HSUBE		
1454	1543	0000	ONESET,	0		
1455	1544	7240	STA			
1456	1545	1113	TAD	ADD0		
1457	1546	5010	DCA	10		
1460	1547	6211	CDF 10			

1462	1551	3410	DCA I	10
1463	1552	7132	STL RTR	
1464	1553	3410	DCA I	10
1465	1554	3410	DCA I	10
1466	1555	6201	CDF 0	
1467	1556	5743	JMP I	ONESET
1472			TEXT4=,	/TEXT4 LOADS
1471		*1600		/CHANGES H AND U MATRICES
1472	1600	0000	VALUEG, 0	
1473	1601	7200	CLA	
1474	1602	1107	TAD	TEMP
1475	1603	3262	DCA	JG
1476	1604	1114	TAD	TEMP1
1477	1605	3263	DCA	K
1500	1606	1115	TAD	N1
1501	1607	7041	CIA	
1502	1610	9264	DCA	FLAGG
1503	1611	6201	CDF 0	/SET UP DO LOOP
1504	1612	7201	CLA IAC	
1505	1613	1264	TAD	FLAGG
1506	1614	1115	TAD	N1
1507	1615	3107	DCA	TEMP
1510	1616	1261	TAD	USUBG
1511	1617	3256	DCA	SUBG
1512	1620	4273	JMS	EL
1513	1621	1260	TAD	HSUBG
1514	1622	9256	DCA	SUBG
1515	1623	4273	JMS	EL
1516	1624	2264	ISZ	FLAGG
1517	1625	5212	JMP	RPTG
1520	1626	1263	TAD	K
1521	1627	5107	DCA	TEMP
1522	1630	4660	JMS I	HSUBG
1523	1631	4807	JMS I	INTERP
1524	1632	5116	FGET A	
1525	1633	2121	FSUB B	
1526	1634	6513	FPUT I	ADD0
1527	1635	0002	FEXT	/H(K,K)=A*B
1530	1636	1262	TAD	JG
1531	1637	3107	DCA	TEMP
1532	1640	1262	TAD	JG
1533	1641	3114	DCA	TEMP1
1534	1642	4660	JMS I	HSUBG
1535	1643	4427	JMS I	INTERP
1536	1644	5116	FGET A	
1537	1645	1121	FADD B	
1540	1646	6513	FPUT I	ADD0
1541	1647	0000	FEXT	/H(J,J)=A*B
1542	1652	1263	TAD	K
1543	1651	3114	DCA	TEMP1
1544	1652	4660	JMS I	HSUBG
1545	1653	4657	JMS I	KLREL
1546	1654	6211	CDF 10	
1547	1655	5000	JMP I	VALUEG
1550	1656	4000	SUBG,	/RETURN
1551	1657	1147	KLREL,	
1552	1660	1273	HSUBG,	
1553	1661	1341	USUBG,	
1554	1662	0000	JG,	
1555	1663	0000	K,	
1556	1664	0000	FLAGG,	
1557	1665	0000	LK,	
1558	1666	0000		

ADDRESS	DATA	INSTR	COMMENT
1561	0000		
1562	0000	LJ	
1563	0000		
1564	0000		
1565	0000	EL	
1566	1263		
1567	3114		
1568	4656		
1569	4407		
1570	5513		
1571	6265		
1572	0000		
1573	1262		
1574	3114		
1575	4656		
1576	4407		
1577	5513		
1578	6265		
1579	0000		
1580	1262		
1581	3114		
1582	4656		
1583	4407		
1584	5513		
1585	6265		
1586	0000		
1587	1262		
1588	3114		
1589	4656		
1590	4407		
1591	5513		
1592	6265		
1593	0000		
1594	1262		
1595	3114		
1596	4656		
1597	4407		
1598	5513		
1599	6265		
1600	0000		
1601	1262		
1602	3114		
1603	4656		
1604	4407		
1605	5513		
1606	6265		
1607	0000		
1608	1262		
1609	3114		
1610	4656		
1611	4407		
1612	5513		
1613	6265		
1614	0000		
1615	1262		
1616	3114		
1617	4656		
1618	4407		
1619	5513		
1620	6265		
1621	0000		
1622	1262		
1623	3114		
1624	4656		
1625	4407		
1626	5513		
1627	6265		
1628	0000		
1629	1262		
1630	3114		
1631	4656		
1632	4407		
1633	5513		
1634	6265		
1635	0000		
1636	1262		
1637	3114		
1638	4656		
1639	4407		
1640	5513		
1641	6265		
1642	0000		
1643	1262		
1644	3114		
1645	4656		
1646	4407		
1647	5513		
1648	6265		
1649	0000		
1650	1262		
1651	3114		
1652	4656		
1653	4407		
1654	5513		
1655	6265		
1656	0000		
1657	1262		
1658	3114		
1659	4656		
1660	4407		
1661	5513		
1662	6265		
1663	0000		
1664	1262		
1665	3114		
1666	4656		
1667	4407		
1668	5513		
1669	6265		
1670	0000		
1671	1262		
1672	3114		
1673	4656		
1674	4407		
1675	5513		
1676	6265		
1677	0000		
1678	1262		
1679	3114		
1680	4656		
1681	4407		
1682	5513		
1683	6265		
1684	0000		
1685	1262		
1686	3114		
1687	4656		
1688	4407		
1689	5513		
1690	6265		
1691			

1660	2026	IAU I	ADD2	
1661	2027	DCA	BPF2	/GET BPF2
1662	2030	TAD I	ADD1	
1663	2031	DCA	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	DCA 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	DCA	BPF1	/STORE ROTATED VALUE
1724	2072	SEL		/TEST LINK AND SET UP LATER TEST
1725	2073	JMP	*4	
1726	2074	TAD	NLINK	
1727	2075	DCA	INSTH	
1730	2076	JMP	*3	
1731	2077	TAD	ZLINK	
1732	2100	DCA	INSTH	
1733	2101	CLL		
1734	2102	TAD	BPF2	
1735	2103	RAR		
1736	2104	DCA	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	DCA I	TABADH	
1754	2122	ISZ	CTRH3	/NEED TO INCREMENT ABAD?
1755	2123	JMP I	TEST	/NO
1756	2124	103	TABADH	

/REINIT CTRH3

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

ADDRESS	DATA	INSTR	COMMENT
0000			
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0070			
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0075			

2076	2271	5113	DCA	ADD	/ADDRESS IN U MATRIX
0077	2272	5513	DCA I	ADD	/LOOP ZEROES A OF U MATRIX
0100	2273	2113	ISZ	ADD	
0101	2274	2246	ISZ	CTRI	/LOOP DONE?
0102	2275	5272	JMP	.-3	/NO
2123	2276	1115	TAD	N1	/YES. PUT 1S ON DIAGONAL
0124	2277	7041	CIA		
0105	2320	3246	DCA	CTRI	/SET LOOP
2126	2301	6201	CONF		
2127	2322	7201	CLA	IAC	
0110	2323	1246	TAD	CTRI	
2111	2304	1115	TAD	N1	
0112	2305	5107	DCA	TEMP	
2113	2306	1107	TAD	TEMP	
2114	2307	5114	DCA	TEMP1	
2115	2310	4717	JMS I	USUBI	/INDICES OF DIAGONAL U ELEMENT
2116	2311	4716	JMS I	SETONE	/GET ADDRESS OF DIAGONAL ELEMENT
2117	2312	2246	ISZ	CTRI	/LOOP DONE?
2120	2313	5302	JMP	OVERI	/NO
2121	2314	6211	CONF		/YES
2122	2315	5600	JMP I	HUGET	/RETURN
2123	2316	1543	SETONE,	ONESET	
0124	2317	1341	USUBI,	USUB	
2125	2320	0200	COPY,		
2126	2321	7200	CLA		/COPY U MATRIX
2127	2322	1072	TAD	UB	
0130	2323	3247	DCA	ADDR	
2131	2324	1067	TAD	BOLD	
2132	2325	3072	DCA	UB	
2133	2326	1247	TAD	ADDR	
2134	2327	5067	DCA	BOLD	
2135	2330	6201	CONF		/YES. COPY DIAGONAL H ELEMENTS INTO EN
2136	2331	1115	TAD	N1	
2137	2332	7041	CIA		
2143	2333	5246	DCA	CTRI	/SET LOOP
2141	2334	1070	TAD	ENB	
2142	2335	5247	DCA	ADDR	/ADDRESS IN EN
2143	2336	7221	AGAINI,	CLA	
2144	2337	1246	TAD	CTRI	
2145	2340	1115	TAD	N1	
2146	2341	3107	DCA	TEMP	
2147	2342	1107	TAD	TEMP	
2150	2343	5114	DCA	TEMP1	
2151	2344	4763	JMS I	HSUBI	/INDICES OF DIAGONAL H ELEMENT
2152	2345	4407	JMS I	INTERP	/ADDRESS OF DIAGONAL H ELEMENT
2153	2346	5513	FGET I	ADDR	/GET H ELEMENT
2154	2347	6647	FPUT I	ADDR	/STORE IT
2155	2350	0000	FEXT		
2156	2351	2247	ISZ	ADDR	
2157	2352	2247	ISZ	ADDR	
2158	2353	2247	ISZ	ADDR	
2159	2354	2246	ISZ	CTRI	/DONE?
2162	2355	5336	JMP	AGAINI	/NO
2163	2356	7200	CLA		
2164	2357	1115	TAD	N1	
2165	2360	3132	DCA	N2	/SET N2=N1
2166	2361	6211	CONF		
2167	2362	5720	JMP I	COPY	/RETURN
0170	2363	1273	HSUBI,	HSUBE	
0171	2400		TRANS,		
0172	2400	0000	CONF		
0173	2401	6201			
2442	2442	2442			

0175	2403	1067	TAD	BOLD	/ADDRESS OF 1ST ELEMENT IN CURRENT OLD
0176	2404	3336	OCA	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	5337	OCA	FLAGJ1	/SET 1ST ORDER LOOP
0204	2412	5224	JMP	UP	
0205	2413	7200	CLA		/INCREMENT ADDRESS IN EN
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	OCA	IN2ADD	
0216	2424	1072	TAD	UB	
0217	2425	3340	OCA	IN1ADD	/ADDRESS OF 1ST ELEMENT IN CURRENT
0220	2426	1115	TAD	N1	/NEW EIGENVECTOR
0221	2427	7041	CIA		
0222	2430	3341	OCA	FLAGJ2	/SET 2ND ORDER LOOP
0223	2431	5240	JMP	.+7	
0224	2432	7200	CLA		
0225	2433	1115	TAD	N1	
0226	2434	1115	TAD	N1	
0227	2435	1115	TAD	N1	
0230	2436	1340	TAD	IN1ADD	
0231	2437	3340	OCA	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	OCA	A+2	/INITIALIZE TRANSITION PROBABILITY
0243	2451	1336	TAD	IN2ADD	
0244	2452	3342	DCA	N2ADD	/ADDRESS IN OLD EIGENVECTOR
0245	2453	7240	CMA		
0246	2454	3343	DCA	CTR	/INITIALIZE CTR
0247	2455	7040	CMA		
0250	2456	1024	TAD	TABLE	
0251	2457	3344	DCA	TABAD	/ADDRESS OF CHECK WORD
0252	2460	1132	TAD	N2	
0253	2461	7041	CIA		
0254	2462	3345	OCA	FLAGJ3	/SET 3RD ORDER LOOP
0255	2463	4746	JMS	CALC1	/CALCULATE TRANSITION ENERGY
0256	2464	7200	CLA		
0257	2465	1340	TAD	IN1ADD	
0258	2466	3347	DCA	N1ADD	/ADDRESS IN NEW EIGENVECTOR
0261	2467	1115	TAD	N1	
0262	2470	7041	CIA		
0263	2471	3350	OCA	FLAGJ4	/SET 4TH ORDER LOOP
0264	2472	7200	CLA		
0265	2473	3343	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	2478	1744	TAD	TABAD	
0273	2479	3344	OCA		

0274	2502	1352	TAD	CHECK	/GET CHECK WORD
0275	2503	7210	RAR	CHECK	/PUT CURRENT B INTO LINK
0276	2504	3352	DCA	CHECK	/STORE BALANCE
0277	2505	7420	SNL		/ALLOWED TRANSITION?
0300	2506	5315	JMP	.+7	/NO, SKIP CALCULATION
0301	2507	4407	JMS I	INTERP	/YES, CALCULATE PROBABILITY
0302	2510	5742	FGT I	N2ADD	
0303	2511	5747	FMPY I	N1ADD	
0304	2512	1116	FADD	A	/INCREMENT PROBABILITY
0305	2513	6116	FPUT	A	
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	/INCREMENT OLD EIGEN FUNCTION
0317	2525	2345	ISZ	FLAGJ3	/3RD ORDER LOOP DONE?
0320	2526	5264	JMP	RPT3	/NO, CONTINUE
0321	2527	4753	JMS I	CALC2	/YES, COMPUTE TOTAL PROBABILITY
0322	2530	2341	ISZ	FLAGJ2	/2ND ORDER LOOP DONE?
0323	2531	5232	JMP	RPT2	/NO, CONTINUE
0324	2532	2337	ISZ	FLAGJ1	/1ST ORDER LOOP DONE?
0325	2533	5213	JMP	RPT1	/NO, CONTINUE
0326	2534	6211	CCF 10		/YES
0327	2535	5600	JMP I	TRANS	/RETURN
0330	2536	0000	IN2ADD, 0		
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	KRB		/GET A CHARACTER
0359	2601	4032	INTRUP, JMS	TYPE	
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	RDMOR, JMS	TYPE	

2373	2612	SNA	LOKUP	
0374	5221	JMP	MR377	
0375	2614	TAD		
0376	2615	SHA CLA		
0377	2616	JMP	ROMOR	
0400	2617	JMS	CRLF	
2421	2620	JMP	DSPL	
2422	2621	COF	0	
2423	2622	TAD	1	
2424	2623	SNA		
2425	2624	JMP	LOKUP-2	
2426	2625	ISZ	TEMP1	
0407	2626	TAD	TEMP	
0410	2627	SHA CLA		
0411	2630	JMP	LOKUP+1	
0412	2631	TAD	TEMP1	
2413	2632	TAD	ADDR	
0414	2633	DCA	TEMP	
0415	2634	TAD	TEMP	
0416	2635	DCA	TEMP	
0417	2636	COF	10	
2420	2637	JMS	CRLF	
0421	2640	JMP	TEMP	
0422	2641	START		
2423	2642	DSPL,		
2424	2643	MR272,		
0425	2644	MR377,		
2426	2645	CHTB,		
2427	2645	ADDR,		
2428	2646	CHTB,		
2431	2650	322	/P-UNCH	
2432	2651	323	/R-ESTART	
2433	2652	317	/C-OUPLING CONSTANTS	
2434	2653	304	/O-FFSET	
2435	2654	314	/D-IAL EXIT	
0436	2655	0	/L-IST	
0437	2656	0		
2440	2657	TABADL,		
2441	2660	BPNCB		
2442	2661	BEGIN+3		
2443	2662	NEWJ		
2444	2663	OFFS		
2445	2664	DIALEX		
2446	2665	LISP		
2447	2666	0		
2448	2667	CLA		
2449	2668	TAD	P215	
2450	2669	JMS	TYPE	
2451	2670	CLA		
2452	2671	TAD	LF	
2453	2672	JMS	TYPE	
2454	2673	CLA		
2455	2674	JMP	I	
2456	2675	215	CRLF	
2457	2676	212		
2458	2677	PRINTL,		
2459	2678	COF	0	
2460	2679	JMS		
2461	2680	JMS	CRLF	
2462	2681	TAD	CRLF	
2463	2682	ISZ	PRINTL	
2464	2683	2276	PRINTL	
2465	2684	DCA	JUMP	
2466	2685	AGAINL,		
2467	2686	CLA	CLL	
0470	2687	TAD	I	
2471	2688	RIP		
2472	2689	2689		
2473	2690	2690		
2474	2691	2691		
2475	2692	2692		
2476	2693	2693		
2477	2694	2694		
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2581	2798	2798		
2582	2799	2799		
2583	2800	2800		
2584	2801	2801		
2585	2802	2802		
2586	2803	2803		
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2589	2806	2806		
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2591	2808	2808		
2592	2809	2809		
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2640	2857	2857		
2641	2858	2858		
2642	2859	2859		
2643	2860	2860		
2644	2861	2861		
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2646	2863	2863		
2647	2864	2864		
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2710	2927	2927		
2711	2928	2928		
2712	2929	2929		
2713	2930	2930		
2714	2931	2931		

0476	2711	WRITE	/TYPE LEFT 6 BITS
0473	2712	WRITE	
0474	2713	JUMP	
0475	2714	JUMP	
0476	2715	JUMP	
0477	2716	WRITE	/TYPE RIGHT 6 BITS
0500	2717	AGAINL	
0501	2720	WRITE,	
0502	2721	MASK1	/MASK OUT LEFT 6 BITS
0503	2722	SNA	/EITHER HALF =0?
0504	2723	JMP	/YES, EXIT
0505	2724	M36	/NO
0506	2725	SPA SNA	/200 OR 300 SERIES?
0507	2726	JMP	/300 SERIES
0510	2727	TAD	/200 SERIES
0511	2730	JMS	/TYPE IT
0512	2731	JMP I	
0513	2732	SZA	/SPECIAL CODE 36?
0514	2733	JMP	/NO
0515	2734	JMS	
0516	2735	JMP I	
0517	2736	TAD	
0520	2737	JMS	/TYPE IT
0521	2740	JMP I	
0522	2741	CDF 10	
0523	2742	JMP I	
0524	2743	JUMP,	
0525	2744	M36,	
0526	2745	P236,	
0527	2746	P336,	
0532	2747	MASK1,	
0531		EXITT,	
0532		JMP I	
0533		PRINTL	
0534		JUMP,	
0535		M36,	
0536		P236,	
0537		P336,	
0540		MASK1,	
0541		TEXT3=,	
0542		*3000	
0543		TEXT3 LOADS	
0544		GET ADDRESS OF OLD EIGENVALUE	
0545		EN=HI	
0546		LOAD ARRAY W/ -CHEMICAL SHIFT	
0547		LIMIT -CHEMICAL SHIFT	
0548		SET TO FIX AND ROUND	
0549		FIX IT	
0550		IN RIGHT RANGE?	
0551		NO, TOO SMALL	
0552		MAYBE	
0553		IN RIGHT RANGE?	
0554		NO, TOO BIG	
0555		YES	
0556		ADDRESS FOR STORING PROBABILITY	
0557		ADSPCL	
0558		ADSPCL	
0559		ADSPCL	
0560		ADSPCL	
0561		ADSPCL	
0562		ADSPCL	
0563		ADSPCL	
0564		ADSPCL	
0565		ADSPCL	
0566		ADSPCL	
0567		ADSPCL	
0568		ADSPCL	
0569		ADSPCL	
0570		ADSPCL	
0571		ADSPCL	
0572		ADSPCL	
0573		ADSPCL	
0574		ADSPCL	
0575		ADSPCL	
0576		ADSPCL	
0577		ADSPCL	
0578		ADSPCL	
0579		ADSPCL	
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0585		ADSPCL	
0586		ADSPCL	
0587		ADSPCL	
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0589		ADSPCL	
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0593		ADSPCL	
0594		ADSPCL	
0595		ADSPCL	
0596		ADSPCL	
0597		ADSPCL	
0598		ADSPCL	
0599		ADSPCL	
0600		ADSPCL	

Address	Hex	Assembly	Comment
0571	3036	0000	
0572	3037	7014	
0573	3040	0764	
0574	3041	0000	
0575	3042	0000	
0576	3043	6211	COF 10
0577	3044	7200	CLA
0578	3045	1641	TAD I
0579	3046	0305	AND
0580	3047	3304	DCA
0581	3048	4407	JMS I
0582	3049	5116	FGET A
0583	3050	5116	FMPY A
0584	3051	0000	FEXT
0585	3052	1306	TAD
0586	3053	1044	TAD
0587	3054	3044	DCA
0588	3055	4632	JMS I
0589	3056	4327	JMS
0590	3057	3303	DCA
0591	3058	1241	TAD
0592	3059	7710	SPA CLA
0593	3060	5642	JMP I
0594	3061	6211	COF 10
0595	3062	1303	TAD
0596	3063	1304	TAD
0597	3064	7700	SMA CLA
0598	3065	5276	JMP
0599	3066	1641	TAD I
0600	3067	7004	RAL
0601	3068	7250	STA RAR
0602	3069	5300	JMP
0603	3070	1641	TAD I
0604	3071	1303	TAD
0605	3072	3641	DCA I
0606	3073	6201	COF 0
0607	3074	5642	JMP I
0608	3075	0000	PROB,
0609	3076	0000	SIGN,
0610	3077	3777	PL6,
0611	3078	0000	SETUP,
0612	3079	3325	DCA
0613	3080	1325	TAD
0614	3081	7012	RTR
0615	3082	7012	RTR
0616	3083	0326	AND
0617	3084	4423	JMS I
0618	3085	7200	CLA
0619	3086	1325	TAD
0620	3087	0326	AND
0621	3088	4423	JMS I
0622	3089	7200	CLA
0623	3090	5707	JMP I
0624	3091	0000	HOLD,
0625	3092	0377	BLIND,
0626	3093	0000	FIX,
0627	3094	7200	CLA
0628	3095	1044	TAD
0629	3096	7540	SMA SZA
0630	3097	5336	JMP
0631	3098	0000	
0632	3099	0000	
0633	3100	0000	
0634	3101	0000	
0635	3102	0000	
0636	3103	0000	
0637	3104	0000	
0638	3105	3777	PL6,
0639	3106	0000	SETUP,
0640	3107	0000	
0641	3108	0000	
0642	3109	0000	
0643	3110	0000	
0644	3111	0000	
0645	3112	0000	
0646	3113	0000	
0647	3114	0000	
0648	3115	0000	
0649	3116	0000	
0650	3117	0000	
0651	3118	0000	
0652	3119	0000	
0653	3120	0000	
0654	3121	0000	
0655	3122	0000	
0656	3123	0000	
0657	3124	0000	
0658	3125	0000	
0659	3126	0000	
0660	3127	0000	
0661	3128	0000	
0662	3129	0000	
0663	3130	0000	
0664	3131	0000	
0665	3132	0000	
0666	3133	0000	

ADDR	PC	OP	DATA	COMMENT
0671	3136	TAD	M11	/RETURN
0672	3137	SZA		/IS HORD ALREADY RIGHT?
0673	3140	JMP	+3	/NO
0674	3141	TAD	HORD	/YES, GET HORD
0675	3142	JMP	FIX	/RETURN
0676	3143	SMA		/IS TOO BIG TO FIX?
0677	3144	JMP	ERROR	/YES, SET TO 3777
0678	3145	DCA	HOLD	/NO, SET FIXING LOOP
0679	3146	TAD	HORD	
0680	3147	CLL		/ROTATE RIGHT FILLING WITH 1S IF NEG
0681	3150	SPA		/OR 0S IF POS
0682	3151	STL		
0683	3152	RAR		
0684	3153	ISZ	HOLD	/LOOP DONE?
0685	3154	JMP	=5	/NO
0686	3155	JMP	FIX	/YES RETURN
0687	3156	CLA		
0688	3157	TAD	MASKM	
0689	3160	JMP	FIX	
0690	3161		7765	
0691			*3200	
0692	3200	JMS	I	/MIN INTENSITY=
0693	3201	HDI		
0694	3202	JMS	I	INPUT
0695	3203	JMS	I	INTERP
0696	3204	FPUT	A	
0697	3205	FEXT		
0698	3206	JMS	I	PRINT
0699	3207	HDI		/DISPLAY LISTING?
0700	3210	JMS	I	ASKRX
0701	3211	SNA	CLA	
0702	3212	JMP	I	DSLST
0703	3213	JMS	I	STRIP
0704	3214	JMS	I	PRINT
0705	3215	HDI		/INIT, TAPE READ
0706	3216	ODF	0	/INTENSITY ENERGY
0707	3217	JMS		
0708	3220	SKP		LODFAC
0709	3221	JMP	I	/NORMAL RETURN
0710	3222	JMS	I	/FOUND TERMINATOR
0711	3223	JMS	I	INTERP
0712	3224	FPUT		FSIN
0713	3225	FEXT		
0714	3226	JMS		LODFAC
0715	3227	SKP		/GET CORRESPONDING INTENSITY
0716	3230	HLT		/GOT HERE ONLY BY BAD FILE!
0717	3231	JMS		EIPRNT
0718	3232	JMP	BACK	
0719	3233	DSLST,		
0720	3234	ASKRX,		
0721	3235	LOCHK,		
0722	3236	CLA		
0723	3237	TAD	AREND	
0724	3240	SPA	CLA	/NEED NEW BUFFER LOAD?
0725	3242	JMP	I	/NO
0726	3243	TAD	LOCHK	/YES
0727	3244	DCA		
0728	3245	IAC	11	
0729	3246	JMS	I	TAPTRN
0730	3247	JMP	I	LOCHK
0731	3250	LODFAC,	0	

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0767 JMS LDCHK
0770 TAD I 11
0771 DCA EXP
0772 STL RTR
0773 TAD EXP
0774 SNA CLA
0775 ISZ LODFAC
0776 TAD I 11
0777 DCA HORD
0778 TAD I 11
0779 DCA LORD
0780 JMP I LODFAC
0781
0782 EIPRNT,
0783
0784 JMS I INTERP
0785 FPUT FCOS
0786 FSUB A
0787 FEXT
0788 TAD HORD
0789 SPA CLA
0790 JMP I EIPRNT
0791 JMS I INTERP
0792 FGET FCOS
0793 FEXT
0794 CLL IAC RAL
0795 JMS I OUTPUT
0796 TAD SPACE
0797 JMS TYPE
0798 JMS TYPE
0799 JMS I INTERP
0800 FGET FSIN
0801 FEXT
0802 IAC CLL RAL
0803 JMS I OUTPUT
0804 JMS I CARLF
0805 JMP I EIPRNT
0806
0807 CARLF,
0808 ASKN,
0809 SPACE,
0810 STRTP,
0811
0812 CLA
0813 TAD CORBUF
0814 DCA 11
0815 TAD STBLK
0816 DCA BLK1
0817 IAC
0818 JMS I TAPTRN
0819 JMP I STRTP
0820 JMS STRTP
0821 CDF
0822 JMS LEDR
0823 TAD KK300
0824 JMS HPUN
0825 JMS LDCHK
0826 TAD I 11
0827 DCA TTT
0828 STL RTR
0829 TAD TTT
0830 SNA CLA
0831 JMP PEX
0832 TAD TTT
0833 JMS I BPUN
0834 TAD I 11
0835
0836 /GET 6000, I.E., END WORD?
0837 /YES, INCR, RETURN
0838
0839 /INTENSITY TOO SMALL?
0840 /YES, GET NEXT VALUES
0841 /NO, OUTPUT
0842
0843 /OUTPUT INTENSITY
0844
0845 /OUTPUT CHEM SHIFT
0846
0847 /INITIALIZE TO READ FROM TAPE
0848
0849 /READ FIRST BLOCK
0850
0851 BPNCH,
0852
0853 PNOUT,
0854
0855 /GET 6000 FOR END?
0856 /YES

```

1000	3320	1411	TAD I	11
1067	3351	4757	JMS I	BPUN
1070	3352	5335	JMP	PNOUT
1071	3353	1361	TAD	KK200
1072	3354	4423	JMS I	HPUN
1073	3355	4364	JMS	LEDR
1074	3356	5475	JMP I	DISPLAY
1075	3357	3107	BPUN,	
1076	3360	7700	LCT,	
1077	3361	2020	KK200,	
1100	3362	0300	KK300,	
1101	3363	0000	TTT,	
1102	3364	0000	LEDR,	
1103	3365	7200	CLA	
1104	3366	1360	TAD	LCT
1105	3367	3663	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	5336	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	RAL
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	2267	JMP	CONT3
1146	3433	7550	SPA	SNA
1147	3434	2264	JMP	CONT4
1150	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

1165	3452	5256	JMP	CONT2	/FOR N=6, 4 & 5 DONE
1166	3453	1337	TAD	P17	
1167	3454	3733	DCA I	ADDRB	
1170	3455	2333	ISZ	ADDRB	/FOR N=5, 4 DONE
1171	3456	7200	CLA		
1172	3457	1106	TAD	N	
1173	3460	7041	CIA		
1174	3461	1336	TAD	NTOT	
1175	3462	3733	DCA I	ADDRB	/2ND LAST ELEMENT=NTOT-N
1176	3463	2333	ISZ	ADDRB	
1177	3464	7200	CLA		/CALCULATE FINAL ELEMENT
1200	3465	1336	TAD	NTOT	
1201	3466	3733	DCA I	ADDRB	/INITIALIZE NUSE
1202	3467	7200	CLA	NTOT	
1203	3470	1336	TAD		
1204	3471	7041	CIA		
1205	3472	3334	DCA	FLAGB	/-NTOT IN FLAGB
1206	3473	7200	CLA		
1207	3474	3342	DCA	CTRB	
1210	3475	1106	TAD	N	
1211	3476	7041	CIA		
1212	3477	3335	DCA	INDEX	/-N IN INDEX
1213	3500	7001	IAC		
1214	3501	1334	TAD	FLAGB	/BPF TO BE TESTED IN AC
1215	3502	7041	CIA		
1216	3503	7100	CLL		
1217	3504	7010	RAR		/EXAMINE BIT BY BIT
1220	3505	7430	SZL		
1221	3506	2342	ISZ	CTRB	/INCREMENT CTRB ON NON-ZERO LINK
1222	3507	2335	ISZ	INDEX	/DONE WITH THIS BPF?
1223	3510	5304	JMP	RPTB2	/NO: ROTATE AGAIN
1224	3511	7200	CLA		/YES: PUT IN PROPER IN NUSE ARRAY
1225	3512	1342	TAD	CTRB	
1226	3513	1063	TAD	IF2B	
1227	3514	3333	DCA	ADDRB	
1230	3515	1733	TAD I	ADDRB	
1231	3516	3107	UCA	TEMP	/TEMP CONTAINS REL, ADDRESS
1232	3517	2733	ISZ I	ADDRB	/INCREMENT NARRAY ELEMENT
1233	3520	7240	STA		
1234	3521	1107	TAD	TEMP	
1235	3522	1064	TAD	NUSEB	
1236	3523	3333	DCA	ADDRB	/ADDRB CONTAINS LOCATION IN NUSE
1237	3524	7001	IAC		
1240	3525	1334	TAD	FLAGB	
1241	3526	7041	CIA		
1242	3527	3733	DCA I	ADDRB	/VALUE IN NUSE
1243	3530	2334	ISZ	FLAGB	/DONE?
1244	3531	5273	JMP	RPTB1	/NO: GET NEXT NUMBER
1245	3532	5000	JMP I	INITB	/YES: RETURN
1246	3533	2000			
1247	3534	0000	ADDRB,		
1250	3535	0000	FLAGB,		
1251	3536	0000	INDEX,		
1252	3537	0021	NTOT,		
1253	3540	0027	P17,		
1254	3541	0053	P23,		
1255	3542	0000	P43,		
1256	3543	0000	CTRB,		
1257	3544	2044	MLPY2,		
1260	3545	5743	ISZ	EXP	
1261	3546	5743	JMP I	MLPY2	
1262	3547	0000	JMP I	MLPY2	
1263	3548	7000	DIVD2,		

1264	3551	1044	TAD EXP		
1265	3552	3044	DCA EXP		
1266	3553	5747	JMP I	DIV02	
1267	3554	0000	ULIMP,		
1270	3555	4474	JMS I	PRINT	/SWEEP OFFSET AND WIDTH:
1271	3556	2750	HD7		
1272	3557	4405	JMS I	INPUT	
1273	3558	4407	JMS I	INTERP	
1274	3561	6137	FPUT	OFFSET	
1275	3562	6110	FPUT	LIMIT	
1276	3563	0006	FLOIN		
1277	3564	6134	FPUT	FACTOR	
1300	3565	1110	FADD	LIMIT	
1301	3566	6110	FPUT	LIMIT	
1302	3567	5375	FGET	P500	
1303	3570	4134	FQIV	FACTOR	
1304	3571	6134	FPUT	FACTOR	
1305	3572	0000	FEXT		
1306	3573	6211	CONF 10		
1307	3574	5754	JMP I	ULIMP	
1310	3575	0011			
1311	3576	3720			
1312	3577	0000			
1313			/NMR DISPLAY ROUTINE PART A		
1314					
1315	3600	7200	CLA		
1316	3601	6211	CONF 10		
1317	3602	4526	JMS	INITK	
1320	3603	1741	TAD I	YK	/ROUTINE TO COMBINE ADJACENT
1321	3604	0334	AND	K3777	/ELEMENTS IN THE SPECS ARRAY
1322	3605	7450	SNA		/CHECK FOR NON-ZERO ELEMENT
1323	3606	5237	JMP	NINCR	
1324	3607	3344	DCA	HOLDK	
1325	3610	2541	ISZ	YK	
1326	3611	2342	ISZ	XCTRK	
1327	3612	5214	JMP	*+2	
1330	3613	2242	JMP	ENDCOM	
1331	3614	1741	TAD I	YK	/GET NEXT ELEMENT
1332	3615	0334	AND	K3777	
1333	3616	7450	SNA		
1334	3617	5237	JMP	NINCR	
1335	3620	1344	TAD	HOLDK	
1336	3621	0334	AND	K3777	/COMBINE ELEMENTS
1337	3622	3344	DCA	HOLDK	
1340	3623	1741	TAD I	YK	/SAVE CALIBRATION MARK
1341	3624	0335	AND	K4000	
1342	3625	1344	TAD	HOLDK	
1343	3626	3741	DCA I	YK	
1344	3627	7040	CMA		
1345	3630	1341	TAD	YK	
1346	3631	3341	DCA	YK	
1347	3632	1741	TAD I	YK	/ERASE PREVIOUS ELEMENT
1350	3633	0335	AND	K4000	
1351	3634	3741	DCA I	YK	
1352	3635	2341	ISZ	YK	
1353	3636	5203	JMP	NEXTK	/GO ON TO NEXT ELEMENT
1354	3637	2341	ISZ	YK	
1355	3640	2342	ISZ	XCTRK	
1356	3641	5203	JMP	NEXTK	
1357	3642	4326	JMS	INITK	/ROUTINE TO FIND LARGEST ELEMENT
1360	3643	1741	TAD I	YK	/IN ARRAY
1361	3644	0334	AND	K3777	

[illegible]

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1462 3745 0000 FLGR, 0
1463 3746 0001 XSTART, START
1464 TEXT1=,
1465 *4000 /TEXT1 LOADS
1466 /NMR DISPLAY ROUTINE PART B
1467 X, 0 /OPEN FOR X VALUE FOR LINC DISPLAY
1468 START, CDF 10 /KEYBOARD INTERRUPT
1469 0000 0000 SKP CLA
1470 0001 0211 JMP I IRRPT
1471 0002 0031 DCA X
1472 0003 7610 TAD SPECB
1473 0004 5702 DCA YP
1474 0005 3200 JMP RPX-2
1475 0006 1071 /THE FOLLOWING 7 WORD KLUDGE BOOTSTRAPS DIAL INTO CORE:
1476 0007 3300 DIALX, LINC
1477 0010 5220 LMODE
1478 0011 6141 1020
1479 0012 1020 20
1480 0013 0020 4
1481 0014 0004 643
1482 0015 0643 701
1483 0016 0701 7300
1484 0017 7300 PMODE
1485 0020 1273 TAD ARRLIM
1486 0021 3277 DCA XCTR
1487 0022 1700 RPX, TAD I YP
1488 0023 7440 SZA /GET ELEMENT FROM ARRAY
1489 0024 5233 JMP AFMRK-2 /CHECK FOR ZERO ELEMENT
1490 0025 1274 TAD M377
1491 0026 6141 LINC
1492 0027 0140 LMODE
1493 0030 0002 DIS 0
1494 0031 7200 PDP
1495 0032 5252 PMODE
1496 0033 7510 CLA
1497 0034 5257 JMP INCR
1498 0035 7041 MRKR
1499 0036 3301 CIA
1500 0037 1274 DCA HGIP
1501 0040 1276 TAD M377
1502 0041 6141 TAD INKY
1503 0042 0140 LINC
1504 0043 0002 LMODE
1505 0044 2301 ISZ
1506 0045 5240 JMP RPY
1507 0046 7604 LAS
1508 0047 0275 AND KK7
1509 0050 7001 IAC
1510 0051 3276 DCA INKY
1511 0052 2200 ISZ X
1512 0053 2300 ISZ YP
1513 0054 2277 ISZ XCTR
1514 0055 5222 JMP RPX
1515 0056 5202 JMP START+1
1516 0057 7346 MRKR, CLL STA RTL
1517 0060 1274 TAD M377
1518 0061 6141 LINC

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DIS	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99
DIS	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99
PDP	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99
PMODE	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99
CLA	0	1	2	3	4	5	6	7	8	9	10	11	12	13	14	15	16	17	18	19	20	21	22	23	24	25	26	27	28	29	30	31	32	33	34	35	36	37	38	39	40	41	42	43	44	45	46	47	48	49	50	51	52	53	54	55	56	57	58	59	60	61	62	63	64	65	66	67	68	69	70	71	72	73	74	75	76	77	78	79	80	81	82	83	84	85	86	87	88	89	90	91	92	93	94	95	96	97	98	99
TAD	0	1	2	3	4	5	6																																																																																													

2052	4445	2005			
2052	4446	2240			
2052	4447	2401			
2052	4450	2005			
2052	4451	4011			
2052	4452	5717			
2052	4453	7700			
2052			IHD1,	TEXT \^WANT PAPER TAPE I/O?\	
2053	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			
2053			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			
2055			HD1,	TEXT /NMRSIM*COMMENTS: /	
2056	3761	1517			
2056	3762	2205			
2056	3763	7700			
2056			HD3,	TEXT /MORE?/	
2057	3764	1617			
2057	3765	5640			
2057	3766	1706			
2057	3767	4023			
2057	3770	2011			
2057	3771	1623			
2057	3772	7540			
2057	3773	4000			
2057			HD2,	TEXT /NO. OF SPINS= / *TEXT2	
2060					
2061	1736	0214			
2061	1737	1703			
2061	1740	1554			
2061	1741	4025			
2061	1742	7240			
2061	1743	4000			
2061			HD4,	TEXT /BLOCK, U: /	
2062	1744	0310			
2062	1745	0515			
2062	1746	1103			
2062	1747	0114			
2062	1750	4023			
2062					

[illegible]

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2170 /IF (62)=0, OUTPUT FLOATING
2171 /OTHERWISE C(62) = NUMBER OF DIGITS
2172 /C(AC) = NUMBER OF DECIMAL PLACES
2173 /C(15) LOST DURING EXECUTION
2174 *55
2175 0
2176
2177 *7200
2178 FOUT,
2179
2200 DCA I SCAD /SAVE C(AC)
2201 TAD HORDER
2202 SPA CLA
2203 TAD SMINUS
2204 TAD SPLUS
2205 JMS ASCOUT
2206 TAD BFRST
2207 DCA 15
2208 /INITIALIZE AUTO-INDEX
2209 JMP 7234
2210 /CONVERT MANTISSA AND BUFFER THE DIGITS
2211 TAD BEXP
2212 DCA 44
2213 /STORE DECIMAL EXPONENT
2214 JMS I FXAD
2215 /GO TO OUTPUT THE NUMBER
2216 JMP CRLF
2217 /FIXED POINT RETURN
2218 TAD CHE
2219 /FLOATING POINT RETURN
2220 JMS ASCOUT
2221 /PRINT "E"
2222 NOP
2223 /GO TO OUTPUT EXPONENT
2224 TAD SWIT1
2225 SNA CLA
2226 /PRINT CR-LF?
2227 JMP I FOUT
2228 /NO, EXIT
2229 TAD CARRTN
2230 /YES
2231 JMS ASCOUT
2232 TAD LNFEED
2233 JMS ASCOUT
2234 JMP I FOUT /EXIT
2235
2236 *7375
2237 SCAD,
2238 BFRST,
2239 FXAD,
2240 *7301
2241 DCA I 15
2242 *7305
2243 CCA I 15
2244 *7310
2245 JMP RETN
2246 HORDER=45
2247 SMINUS=7332
2248 SPLUS=7327
2249 BEXP=7324
2250 CHE=7343
2251 EXPT=7337
2252 ASCOUT=7344
2253 SWIT1=55
2254 CARRTN=7341
2255 LNFEED=7342
2256 /IN THE COMMENTS BELOW:
2257 / F = NUMBER OF DIGITS TO BE OUTPUT
2258 / D = NUMBER OF DECIMAL PLACES
2259 / E = DECIMAL EXPONENT
2260 / P = NUMBER OF PLACES REMAINING TO BE
2261 / PRINTED BEFORE DECIMAL POINT
2262 *5400
2263 FIXX,
2264
2265 5400 0000

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2270	2402	1920	SNA	/FLOATING OUTPUT?
2271	5403	5225	JMP R6	/YES, ROUND OFF TO 6 PLACES
2272	5404	7041	CIA	
2273	5405	1365	TAD SAC	
2274	5406	7510	SPA	/ F-D > 0 ?
2275	5407	5214	JMP +5	/YES
2276	5410	7240	CLA CMA	
2277	5411	1062	TAD 62	
2278	5412	3365	DCA SAC	/MAKE D = F-1
2279	5413	7040	CMA	
2280	5414	1044	TAD 44	
2281	5415	7500	SMA	/ F-D > E ?
2282	5416	7200	CLA	/NO, ROUND OFF TO F PLACES
2283	5417	1062	TAD 62	/YES
2284	5420	7510	SPA	/ D+E < 0 ?
2285	5421	5250	JMP PRNT=1	/YES, NO ROUNDING NEEDED, GO TO PRINT
2286	5422	1354	TAD M6	/NO, ROUND TO D+E PLACES,
2287	5423	7500	SMA	/TO A MAXIMUM OF 6 PLACES
2288	5424	7200	CLA	
2289	5425	1353	TAD K7	
2290	5426	3364	DCA TEMPX	/SAVE NUMBER+1 OF PLACES TO ROUND TO
2291	5427	1356	TAD BUFST	
2292	5430	1364	TAD TEMPX	/SET UP BUFFER ADDRESS AT WHICH
2293	5431	3366	DCA PLCE	/ROUNDING OFF SHOULD START
2294	5432	1364	TAD TEMPX	
2295	5433	7041	CIA	/SET UP COUNT OF MAXIMUM NUMBER
2296	5434	3364	DCA TEMPX	/OF CARRIES ALLOWABLE
2297	5435	7107	CLL IAC RTL	/+4
2298	5436	2766	ISZ I PLCE	/ADD 1 TO DIGIT AT CURRENT POSITION
2299	5437	1766	TAD I PLCE	
2300	5440	1355	TAD M10	
2301	5441	7710	SPA CLA	/CARRY REQUIRED?
2302	5442	5251	JMP PRNT	/NO, GO TO OUTPUT
2303	5443	3766	DCA I PLCE	/YES, MAKE CURRENT DIGIT A ZERO
2304	5444	2364	ISZ TEMPX	/BEGINNING OF BUFFER REACHED?
2305	5445	5313	JMP DECR	/NO, DECREMENT BUFFER ADDRESS AND REPEAT
2306	5446	2766	ISZ I PLCE	/YES, SET MANTISSA TO 0.1
2307	5447	2044	ISZ 44	/COMPENSATE BY INCREMENTING EXPONENT
2308	5450	7200	CLA	
2309	5451	1356	TAD BUFST	
2310	5452	3015	DCA 15	/SET AUTO-INDEX REGISTER
2311	5453	1062	TAD 62	
2312	5454	7450	SNA	/ F = 0 ?
2313	5455	5342	JMP FLOP	/YES, OUTPUT AS FLOATING NUMBER
2314	5456	7041	CIA	/NO,
2315	5457	3366	DCA FCOUNT	/SET UP COUNT TO PRINT F PLACES
2316	5460	1366	TAD FCOUNT	
2317	5461	1044	TAD 44	
2318	5462	7540	SMA SZA	/ E > F ?
2319	5463	5317	JMP XXX	/YES, PRINT XS
2320	5464	1365	TAD SAC	
2321	5465	7500	SMA	/ E < F-D ?
2322	5466	7200	CLA	/NO, TAKE P = E
2323	5467	7041	CIA	/YES, TAKE P = F-D
2324	5470	1044	TAD 44	
2325	5471	7041	CIA	
2326	5472	3364	DCA TEMPX	/SET UP MINUS P
2327	5473	1361	TAD M7X	
2328	5474	3365	DCA SCOUNT	/SET COUNT OF MAX. NO. OF SIG. FIGS.
2329	5475	1044	TAD 44	
2330	5476	1364	TAD TEMPX	
2331	5477	7650	SNA CLA	/ P = E ?
2332	5500	5330	JMP R6	

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	
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