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EUROPEAN ATOMIC ENERGY COMMUNITY - EURATOM

COMPUTER PROGRAM FOR ACTIVATION
ANALYSIS WITH GERMANIUM LITHIUM
DRIFTED DETECTORS

by

G. GUZZI, J. PAULY, F. GIRARDI and B. DORPEMA

1967



Joint Nuclear Research Center
Ispra Establishment - Italy
Chemistry Department - Nuclear Chemistry
and
Scientific Data Processing Center - CETIS

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The program has been used routinely since a few months for the determination of radioelements in biological specimens.

The principles on which the program is based are given, and in appendices the necessary instructions for its use and the complete list are added.

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SUMMARY

A computer program especially developed for activation analysis problems is presented. This program is based on the measurement of photopeak surfaces of complex gamma spectra obtained by means of Ge(Li) detectors. Possible interferences from radioisotopes which give photopeaks which can be superimposed to that measured are evaluated, but not corrected.

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The principles on which the program is based are given, and in appendices the necessary instructions for its use and the complete list are added.

Gamma spectra obtained with high resolution Ge-Li drifted detectors require multichannel analyzers with a large memory if a wide range of gamma energies (from 0 to 2 Mev, e.g.) needs to be analyzed without loss of resolution due to the finite width of the channels.

The use of an electronic computer for processing the output data is almost a necessity in this case, particularly when a high number of spectra is obtained in routine applications, such as activation analysis.

Although many computer programs are available for the unscrambling of scintillation gamma spectra, only a few were developed up to now for the Ge-Li drifted spectra (1,2) and none of them was especially developed for activation analysis problems.

We have set up a Fortran program called ANGIR for the IBM 7090 computer, which was especially studied for qualitative and quantitative activation analysis. This program has been used routinely since a few months with satisfactory results.

The gamma spectra are presently obtained with an 18 cc Ge-Li drifted detector, developed in this laboratory, coupled with a 512 channels analyzer, and recorded on punched tape. The range of energies analyzed can be restricted to that of interest for the application done, by means of a threshold amplifier.

The program does not attempt to make a complete qualitative and quantitative analysis of all the peaks in the spectrum, but only determines radioelements and checks for interferences according to the instructions contained in libraries which are especially prepared for the different routine problems of the laboratory. All the libraries are loaded with the reading statements of the program, and the requester simply refers to them by numbers.

TABLE I

Program library for the determination of trace elements in biological materials.

Isotopes (xx)	Analytical peak energy in kev	Specific activity in cpm (^{oo})	Decay constants (minutes)	Control peaks energy in kev	Ratios
Co	1332	1.130x10 ⁵	2.496x10 ⁻⁷		
Cs	796	6.407x10 ⁴	5.980x10 ⁻⁷		
Sc*	885	1.490x10 ⁵	5.675x10 ⁻⁶		
*Ag	885	2.586x10 ³	1.850x10 ⁻⁶	1384	0.217
Fe	1098	0.750x10	1.060x10 ⁻⁵		
Rb	1079	8.430x10	3.320x10 ⁻⁵		
Zn**	1114	1.410x10 ²	1.965x10 ⁻⁶		
**Sc	1119	1.130x10 ⁵	5.675x10 ⁻⁶	885	1.320
Sr***	513	5.430x10	7.400x10 ⁻⁶		
***Zn	511	2.637x10	1.965x10 ⁻⁶	1114	5.55

(xx) The elements followed by asterisks are those having peaks not completely free from interferences. The related interfering peaks are preceded by the same number of asterisks.

(^{oo}) This factor is calculated from irradiation of one μgm of element in a thermal flux of 10^{13} neutrons/cm², at saturation.

Table I shows a typical library for the determination of trace elements giving raise to long lived radioisotopes in biological materials of interest in radioecology. In each library the elements which are called for analysis are listed and for each of them the energy of one or more "analytical peaks" is given. Analytical peaks are chosen as those giving the best sensitivity and the highest chance of being free from interfering activities, within a range of energy which depends on the resolution of the detector for that energy, and on the stability of the gamma spectrometer. The range chosen for our spectrometer is 1.5 times the full width at half maximum. The resolution of the detector vs. energy is tabulated as one of the libraries of the program. The actions of the program for each analytical peak are the following:

1) Scan the experimental spectrum and determine all peaks present. For each of them determine the energy and the counting rate. A first selection of possible photopeaks is done by considering a possible maximum in channel n when its content c_n satisfy the following condition:

$$c_{n-2} < c_n - P\sqrt{c_n} > c_{n+2}$$

where P is chosen empirically (presently $P = 1$).

The minima on both sides of the maxima are chosen as the channels $n-k$ and $n+k'$ for which:

$$c_{n-k-1} \geq c_{n-k} - P\sqrt{c_{n-k}}$$

$$c_{n+k'+1} \geq c_{n+k'} - P\sqrt{c_{n+k'}}$$

The area S of the photopeak is then determined as:

$$S = \sum_{n=n-k}^{n+k'} c_n - \frac{c_{n-k} + c_{n+k'}}{2} (k + k' + 1)$$

and its standard deviation σ_s :

$$\sigma_s = \sqrt{s + \frac{c_{n-k} + c_{n+k}}{4} n^2}$$

A peak is retained as a true peak if

$$\sigma_s < s/2$$

The energy corresponding to the peak is measured by determining the symmetry axis A of the peak, after subtracting the underlying background, by means of the equation:

$$A = \frac{\sum_{k_1}^{k_2} k(c_k)}{\sum_{k_1}^{k_2} c_k}$$

where the limits k_1 and k_2 are chosen so that the corrected channel contents c_k are all larger than half the channel content of the maximum.

All the preceding operations are performed by the Subroutine PIKAR.

2) Calculate the concentration of the stable element and the associate error, by correcting for decay (Function TDEC), and using auxiliary input data (weight of sample, irradiation data, etc) loaded together with the gamma spectra (Subroutine DETER). This subroutine uses the already described Single Comparator Technique (3).

Those elements which do not have peaks completely free from the danger of interfering radioactivities are marked by asterisks and the possible interferences are listed. Other peaks of the interfering radioisotopes and peaks ratios are also listed as a means of controlling the presence and the amount of the interference.

The program in this case also uses the Subroutine DETER and acts as follows:

1) measure the concentration of the wanted element in the way already indicated, and report it, as if no interference would occur.

2) check for the presence of the control peaks of the interfering element, and measure their counting rate. If control peaks are not found, determine with the Subroutine IPOL the minimum counting rates that would have had a photopeak to be detected over the existing background, and assume this as the counting rate of the control peak.

3) measure, on the bases of photopeak ratios, what is the highest fraction of the analytical peak which could be due to the interfering element, and report it in percent.

4) calculate the corresponding concentration of interfering stable element, and report it in parts per million.

The knowledge of these three figures (ppm in case of no interference, maximum interference possible, corresponding concentration of interfering element) are generally sufficient for the analyst who controls the output of the computer, to decide whether the determined concentration is reliable or if another technique (e.g. chemical separation) must be employed. A further control to see if the program has taken into consideration the correct peaks is the plotting of each spectrum, performed by the Subroutine GRAPH, after the numerical results. It is of course essential to assure that the detector is carefully calibrated. Thus a mixture of radioisotopes with gamma peaks of known energy is measured as the first of a set of spectra, for calibrating the detector. The calibration curve is calculated by the Subroutines KALIP and FITN and it is used to calibrate all the spectra which follow.

The preparation of the libraries for each kind of problems which becomes a routine task of the laboratory is a responsibility of the analyst, as the choice of the analytical peaks, possible interferences, and control peaks is fully based on his experience. It is nevertheless true that the selectivity of the detector is such that the cases of interferences are not many. The energy range in which the interfering peaks are searched could perhaps be restricted considerably by using a preamplifier with a high resolving power (preamplifier based on field-effect transistors instead of our present vacuum-tube charge sensitive preamplifier) and by studying more carefully the drifts of the analyzer.

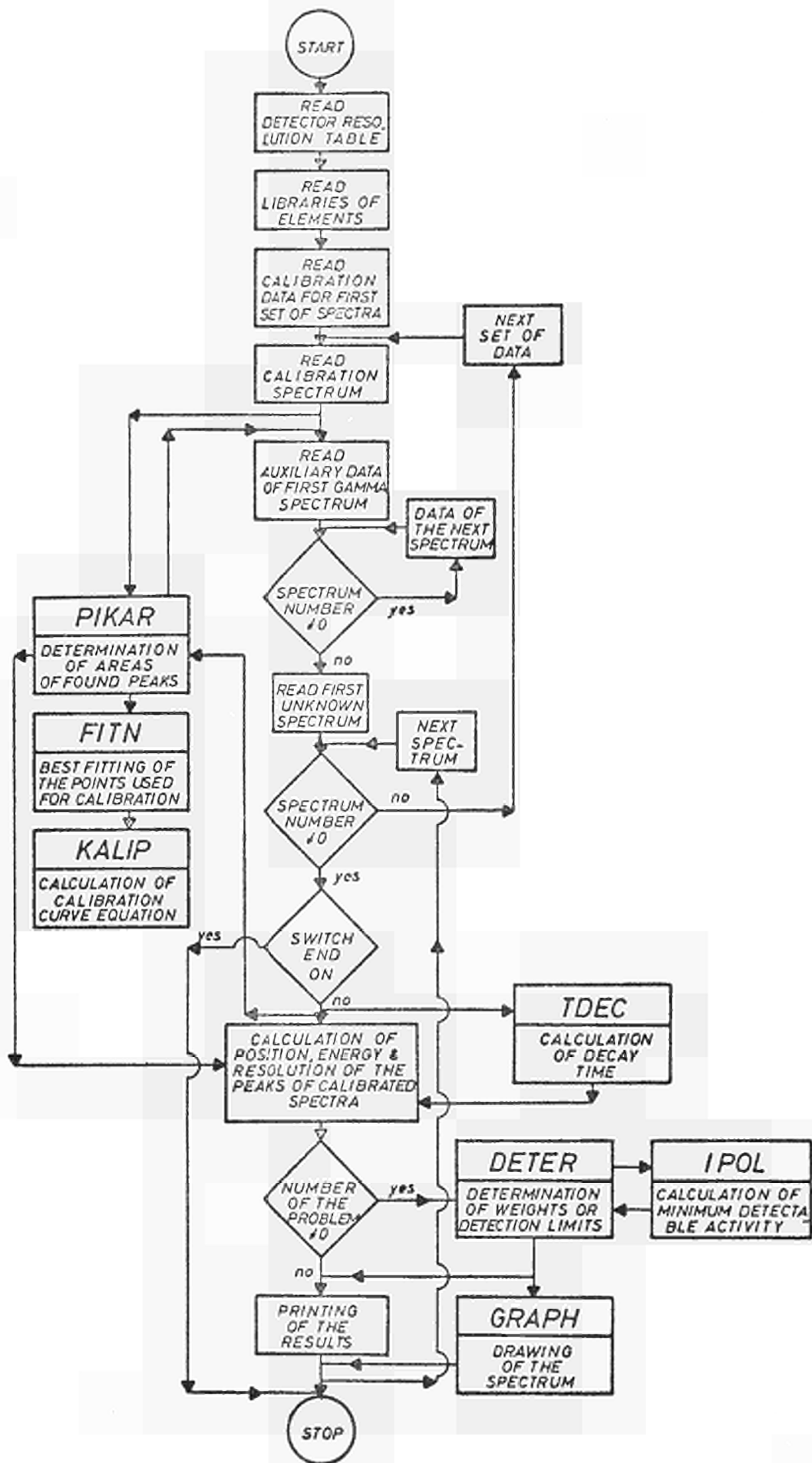


Figure 1. flow sheet of the program ANGRIR

The necessary data for the preparation of libraries are taken from a tabulation of gamma emitting radioelements formed by (n, γ) reactions, which is kept up to date for the detector used, by means of another computer program (4). In the tabulation all the possible gamma peaks are reported in order to increase energy, with the indication of the corresponding radioelement, half life, and the specific activity of all its peaks obtained under fixed irradiation conditions and counting geometry. When a new detector is obtained, the new tabulation is prepared by running the program with the new efficiency curves of the detector.

A flow-sheet of the program is reported in Figure 1. The full program listing and the instructions for its use are given in appendices.

REFERENCES:

- (1) R.L. Heath, W.W. Black and J.E. Cline, IEEE Trans. Nuclear Science, 455, June 1966.
- (2) J.M. Wyckoff, On Line Transformations of High Resolution Spectra, Nat. Bureau of Standards, 1966.
- (3) F. Girardi, G. Guzzi and J. Pauly, Anal. Chem. 37, 1085, 1965.
- (4) G. Guzzi, J. Pauly, F. Girardi and B. Dorpema, Report EUR 3154.e (1966)

Appendix 1 : Instructions for the use of the computer program : ANGIR

1. IDENTIFICATION

- a) ANGIR, a Computer Program System for the Semi-Quantitative and Quantitative Analysis of Trace Elements from Gamma Spectra of Neutron Activated Materials, obtained with Germanium Lithium Drifted Detectors.
- b) G. GUZZI - August 1966
- c) EURATOM C.C.R. Ispra: Nuclear Chemistry Laboratory

2. INSTRUMENTS COMPUTERS AND CODE

- a) Coaxial Ge(Li) detectors with active volume of 18 cc. 512 channels spectrometer (LABEN Milano) with the output of data on tapes punched by a High Speed Tape Punch (TELETYPE Corp.).
- b) IBM 7090
IBM 360/30
- c) Fortran IV

3. USE AND COMPOSITION OF THE PROGRAM

A) Use of the program:

INPUT consists of:

- i) IME: one card for the computation of decay times of the radioisotopes after the irradiation in the reactor.
FORMAT (12I6)
- ii) One card with a set of switches which allow the program to read the succeeding cards in a prefixed sequence. Three switches are used at present, i.e. SS, L5 and L6.
FORMAT (12X, 4F6.2, 6I1, 5A6).

- iii) NTAB3: the number of elements present in the succeeding cards.
FORMAT (I3).

- iv) TAB3: eight cards with the values of the resolution (full width at half maximum) of the Ge(Li) spectrometer in KeV vs. energy from 0 to 5 Mev, in intervals of 50 KeV.
FORMAT (12F6.3)

- v) One card with the number of the different libraries (KOMAX) used by the program, and the number of radioelements for each library (NUPIC).

- vi) One card for each radioelement in the library. This card contains:
 - ENE: Energy in KeV either of the analytical peaks or of the interfering peaks of the radioisotope. Values of energy are taken from (4).

 - ELE: Name of the radioelement.

 - AAS: Specific activity for a μg sample irradiated in a flux of 10^{13} neutron/sq cm.sec.

 - XIAM: Decay constant of the isotope in minutes.

 - KT: Number of control peaks for the interfering radioisotope.
FORMAT (F10.3,A6,2E12.6, I1)

- vii) One card for each interfering peak, containing:
 - ALEN: Energy of the control peak of the interfering isotopes

 - RAR: Ratio between the area of the control peak and that of the analytical peak.
FORMAT (10F7.3)

- viii) One card for each set of spectra with the lower (KLOW) and the higher (KHIGH) channels considered for the scanning of the spectra, the number of the spectra of each set (NSPCT), the number of peaks taken into consideration for the calibration of the spectrometer (KE) and the energies in KeV (E) of the peaks chosen.

FORMAT (2I3,2I6,9F6.2/(12F6.2)).

- ix) One card for completion of the preceding one, with the number of peaks (KM) and the number of the channel in which each peak falls (KLA, KLB).

FORMAT (35I2)

- x) One card for each measurement made with the spectrometer, with:

KOL: Type of library to be chosen

NIRR: Irradiation number

IRRORA: End of the irradiation stating its hour, minute, day and month

TIRR: Irradiation duration in minutes

NCAMP: Identification number of the sample

PESOC: Weight of the sample in grams

MISORA: hour, minute, day and month of the counting

TIME: Counting time in minutes

IPEC: Number of the spectrum

FLUSSO: Thermal neutron flux during the irradiation

FORMAT (2I4,4I2,F8.3,I4,F11.8,4I2,F8.3,I6,E11.3)

After each set of measurements there is a blank card which allows the program to start the calculations for the spectra belonging to that set.

- xi) A magnetic tape obtained by transformation of the punched paper tape by means of the 360/30 computer. This tape contains all the spectra produced by the gamma spectrometer.

OUTPUT consists of:

1) The following input data:

- i) DETECTOR RESOLUTION TABLE: A table of 96 values representing the f.w.h.m. in KeV vs. energy, from 0 to 5 MeV.
- ii) LIBRARIES: one sheet for each library composed by one line for each radioelement.
- iii) The calibration spectrum WHICH MUST BE ALWAYS THE FIRST OF EACH SET.
- iv) The peaks found for calibration with their energies, the boundaries of each peak, and the equation of the calibration line.
- v) One sheet for each spectrum to be analyzed with the data of the measurement.

2) After each spectrum there is:

- i) ELOW and EHIGH, low and high energy boundaries of the spectrum (according to the calibration line).
- ii) PHOTPEAK LIST: list of the photopeaks found with the energy of each peak (and the channel in which its maximum falls). For each peak the left side and the right side minima are given, the area in counts per minute, the associate statistical error (in counts) and finally the resolution (f.w.h.m.) in channels and in KeV.

iii) A sheet with the results of the analysis of each spectrum, with:

ELEMENT: The name of the radioelement found.

TH.ENERGY: the theoretical energy of the analytical peaks, of the interfering peaks and of the control peaks given in library.

EXP.ENERGY: Same energies, but found by the program on the basis of the calibration equation. If a control peak is not found, the minimum detectable activity is calculated and this value is printed out preceded by the word SENSIT.

P.P.M.: part per millions calculated on the bases of the area found and the values in library.

ERROR: Statistical error in part per million.

CONTRIBUTION: percent contribution of the interfering peaks over the analytical peaks.

iv) Three sheets with the drawing of the spectrum divided into three superposed parts (170 channels each part) each plotted with different marks. The channel content of the second and of the third parts are multiplied by factors chosen by the program, to make them comparable with the first part.

B) Composition of the program:

The program is composed of a deck of Fortran Cards and its listing is given in Appendix 2.

- MAIN PROGRAM: Reading and printing of the input data, coordination of the subroutines, printing of the photo-peaks list.
- SUBROUTINE RITE: reading of the magnetic tape and transformation of the data in a suitable format, by means of FUNCTION KONV. This subroutine numbers each spectrum and gives sign and corrects eventual invalid characters.

- SUBROUTINE PIKAR: Research of the gamma peaks, evaluation of the photopeak area, and of the associated statistical error. For each peak found, its symmetry axis, its corrected energy and its full width at half maximum is calculated.
- SUBROUTINE KALIP: control that the peaks found are those indicated for the calibration and fit, by means of SUBROUTINE FITN, a polynomial of order $N=1$ (in our case), to the points used for the calibration.
- FUNCTION TDEC : evaluation of the decay times.
- SUBROUTINE DETER: calculation of the concentration of the stable elements and of the associated errors. For the analytical peaks of the elements not completely free from interfering radioisotopes, this subroutine controls the presence and the amount of the interference. It checks for the presence of control peaks and measures their counting rates. If control peaks are not found, determines by means of the:
- SUBROUTINE IPOL the minimum counting rate, measures, on the bases of photopeak ratios, what is the highest fraction of the analytical peak which could be due to the interfering element, and prints the results.
- SUBROUTINE GRAPH: plotting of the spectra as stated above.

4. RESTRICTIONS

The maximum number of different libraries is 5, for each library 20 elements (analytical and interfering elements) are allowed and each element can have a maximum of 5 control peaks. Each set of spectra (calibration and unknown spectra) is composed by a maximum of 10.

The maximum number of channels of the spectrometer which can be used is 512.

If one wants to give to the program higher possibilities all the dimensions must be changed.

5. TYPICAL RUNNING TIME

For a typical analysis of 10 spectra produced by a Ge(Li) detector (calibration spectrum plus nine unknown) plotting included, the running time (COMP./LOAD AND EXECUTION) is about two minutes.

6. MATERIAL AVAILABLE

The list of the program is given. Upon request, the deck of cards in symbolic code and binary cards are available to scientists working in this field.

Appendix 2 : Listing of the program : ANGIR

		ANGIR			02/15/67				
		EXTERNAL FORMULA NUMBER	-	SOURCE STATEMENT	-	INTERNAL FORMULA NUMBER			
DIMENSION									
1	AA(5,12),	XLAM(5,20),	ALEN(5,20,5),	ENGH(80),	ARP(60),	10			
2	AB(127,15),	ELE(5,20),	RAR(5,20,5),	ENG(80),	SD(60),	11			
3	NEP(127),	ENE(5,20),	KEV(127,15),	ENGL(80),	NHI(60),	12			
4	ELEM(127),	AAS(5,20),	Y(200,3),	RES(60),	FE(60),	13			
5	TP(127),	KT(5,20),	TAB3(100),	KLAS(60),	X(200),	14			
6	A(5,12),	B(5,12),	NUPIC(5),	NLOW(60),	ALFA(5),	15			
7	T(127),	NE(127),				16			
DIMENSION									
1	PESOC(25),	IRRORA(4,25),	NIRR(25),	KLS(25),	KLA(60),	17			
2	NCAMP(25),	MISORA(4,25),	TIRR(25),	KOL(25),	KLB(60),	18			
3	M128(6),	E(25),	RE(60),	TIME(25),	IME(12)	19			
						20			
						21			
COMMON NP,Y,X,N,R,INDA,LOGA,LOGO,IS									
COMMON									
1	ENG,	ENGH,	ENGL,	TDEC,	TIR,	PESO,	FLUSS,	NUPIC,	22
2	ENE,	ELE,	AAS,	XLAM,	KT,	ALEN,	RAR,	KO,	23
3	EHIGH,	ELOW,	RES,	A,	B,	NLOW,	FE,	NHI,	24
4	L1,	L2,	L3,	L4,	L5,	L6,	ELEM,	TP,	25
5	T,	NE,	NEP,	KEV,	AB,	KLOW,	KHIGH,	JMAX,	26
6	IFIT,	KLAS,	ARP,	SD,	TAB3,	AKK,	BKK,	AA,	27
									28
									29
M128(1)=1									
M128(2)=128									
M128(3)=128*128									
M128(4)=128*128*128									
M128(5)=128*128*128*128									
READ (5,1001) IME									
1001	FORMAT (1216)								
100	READ (5,201) PP,QQ,RR,SS,L1,L2,L3,L4,L5,L6,ALFA								
ARMIN=20.0									
EKTW=1.2									
IF(PP)102,102,104									
102	PP=1.0								
104	IF(QQ)106,106,108								
106	QQ=1.1								
108	IF(RR)110,110,112								
110	RR=0.5								
112	IF(L1)666,666,115								
666	READ (5,600) NTAB3								
READ (5,601) (TAB3(I),I=1,NTAB3)									
600	FORMAT (13)								
601	FORMAT (12F6.3)								
WRITE (6,700) (I,I=1,5)									
WRITE (6,701) (TAB3(I),I=1,NTAB3)									
700	FORMAT (1H1,25HDETECTOR RESOLUTION TABLE/1H0,6X11,4(10X11)/1H0)								
701	FORMAT (11H0,1P5E11.3)								
READ (5,212) KOMAX,(NUPIC(I),I=1,KOMAX)									
212	FORMAT (3512)								
DO 1 I=1,KOMAX									
WRITE (6,702)									

ANGIR 02/15/67
 EXTERNAL FORMULA NUMBER - SOURCE STATEMENT - INTERNAL FORMULA NUMBER

```

    NU=NUPIC(I)
    DO 2 J=1,NU
    READ (5,214) ENE(I,J),ELE(I,J),AAS(I,J),XLAM(I,J),KT(I,J)
    WRITE (6,703) ELE(I,J),ENE(I,J),AAS(I,J),XLAM(I,J)
    702 FORMAT (1H1,7HLIBRARY//778H ISOTOPE,3X6HENERGY,5X9HSPEC. ACT.,5X,12
    1HDECAY CONST.,3X13HCONTROL PEAKS,5X6HRATIOS//)
    703 FORMAT (1HC,A6,F10.3,5X,1PE9.3,8X,E9.3)
    IF(KT(I,J)-1)2,4,5
    4 READ (5,215) ALEN(I,J,1),RAR(I,J,1)
    WRITE (6,704) ALEN(I,J,1),RAR(I,J,1)
    704 FORMAT (1H+,53X,F8.3,7X,F8.3)
    GO TO 2
    5 KTI=KT(I,J)
    READ (5,216) (ALEN(I,J,K),RAR(I,J,K),K=1,KTI)
    WRITE (6,704) ALEN(I,J,1),RAR(I,J,1)
    WRITE (6,710) (ALEN(I,J,K),RAR(I,J,K),K=2,KTI)
    710 FORMAT (1H,53X,F8.3,7X,F8.3)
    2 CONTINUE
    1 CONTINUE
    214 FORMAT (F10.3,A6,2E12.6,I2)
    215 FORMAT (2F10.3)
    216 FORMAT (10F7.3)
    115 READ (5,202) KLOW,KHIGH,NSPCT,KE,(E(I),I=1,KE)
    READ (5,240) KM,(KLA(I),KLB(I),I=1,KM)
    DO 116 I=1,KM
    116 KLS(I)=16*KLA(I)+KLB(I)
    I=0
    124 I=I+1
    READ (5,210) KOL(I),NIRR(I),(IRRORA(L,I),L=1,4),TIRR(I),NCAMP(I),P
    1ESOC(I),(MISORA(L,I),L=1,4),TIME(I),IPEC(I),FLUSSO(I)
    210 FORMAT (2I4,4I2,F8.3,I4,F11.8,4I2,F8.3,I6,E11.3)
    IF(IPEC(I))122,122,124
    122 MAPX=I-1
    C CALL RITE(KHIGH,NSPCT,AA)
    C DO 117 I=1,KHIGH
    117 A(I)=AA(I,1)
    WRITE (6,205) KLOW,EN,PP,KHIGH,KE,QQ,RR,SS
    WRITE (6,206) (I,I=1,10)
    IMX=KHIGH/10+1
    DO 118 I=1,IMX
    IP=I-1
    IL=IP*10+1
    IH=MIN0(I*10,KHIGH)
    118 WRITE (6,207) IP,(A(J),J=IL,IH)
    C
    WRITE (6,155)
    CALL PIKAR(PP,QQ,RR,1.0)
    CALL KALIP(EN,FE,E,KE,KLS,KM,RES)
    AKK=B(1)
    BKK=B(2)

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ANGIR 02/15/67
 EXTERNAL FORMULA NUMBER - SOURCE STATEMENT - INTERNAL FORMULA NUMBER

```

WRITE (6,245) AKK,BKK
C
120 NSPMU=NSPCT-1
DO 127 IPC=1,NSPMU
DO 121 I=1,KHIGH
121 A(I)=AA(I,IPC+1)
ITST=IPC+1
KO=KOL(IPC)
DO 502 I=1,MAPX
IF(ITST-IPEC(I))502,503,502
502 CONTINUE
WRITE (6,220) ITST
TCON=1.0
GO TO 137
503 TCON=TIME(I)
TIR=TIRR(I)
PESO=PESOC(I)
FLUSS=FLUSSO(I)
TDEC=TDEC1(MISORA(1,I),IRRORA(1,I),IME)
137 WRITE (6,705)
WRITE (6,706) KO,ITST,NIRR(I),(IRRORA(L,I),L=1,4),TIR,FLUSS,(MISOR
1A(L,I),L=1,4),TDEC,TCON,NCAMP(I),PESO
705 FORMAT (1H1,31X,6HIRRORA,35X6HMISORA,34X6HSAMPLE/1H 123HPROBLEM S
1PEC.No. IRR.No. HOUR MIN DAY MONTH IRR.TIME FLUX HOUR MIN D
2AY MCNTH DECAY TIME TCON NUMBER WEIGHT)
706 FORMAT (15,2I9,4I5,F10.3,1PE12.4,15,2I4,15,6PF14.3,F9.3,15,3XF11.7
1/1H0)
WRITE (6,206) (I,I=1,10)
DO 138 I=1,IMX
IP=I-1
IL=IP*10+1
IH=MINO(I*10,KHIGH)
138 WRITE (6,207) IP,(A(J),J=IL,IH)
CALL PIKAR(PP,CQ,RR,TCON)
ELOW=FLOAT(KLOW+3)*AKK+BKK
EHIGH=FLOAT(KHIGH-3)*AKK+BKK
WRITE (6,151) ELOW,EHIGH
DO 150 J=1,JMAX
ENGL(J)=FLOAT(NLOW(J))*AKK+BKK
ENGH(J)=FLOAT(NHI(J))*AKK+BKK
RE(J)=RES(J)*AKK
150 ENGL(J)=FE(J)*AKK+BKK
DO 152 J=1,JMAX
152 WRITE (6,153) J,ENGL(J),NLOW(J),ENG(J),FE(J),ENGH(J),NHI(J),ARP(J)
1,SD(J),RE(J),RES(J)
C
151 FORMAT (1H1,6H ELOW=F9.4/1H0,6HEHIGH=F9.4/
1 1H0/1H0,10X12HLEFT-MINIMUM ,14X4HPEAK,12X13HRIGHT-MINIMUM
2,14X4HAREA/1H0)
155 FORMAT (1H1)
153 FORMAT (1H0,12,6XF9.4,2X1H(I3,1H),6XF9.4,2X1H(F6.2,1H),3XF9.4,2X1H
1(I3,1H),2F10.3,F10.3,2X1H(F6.2,1H))
201 FORMAT (12X,4F6.2,6I1,5A6)
202 FORMAT (2I3,2I6,9F6.2/(12F6.2))

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 EXTERNAL FORMULA NUMBER - SOURCE STATEMENT - INTERNAL FORMULA NUMBER

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203 FORMAT ((10F6.0,20X))
205 FORMAT (1H1,5HKLOW=14,10X3HEN=F6.1,10X2HP=F6.2/1H ,6HKHIGH=13,10X3
1HKE=13,13X2HQ=F6.2,10X2HR=F6.2,10X2HS=F6.2)
206 FORMAT (1HC,10(9X11)/)
207 FORMAT (1H ;12,10F10.0)
211 FORMAT (10F6.0,16)
220 FORMAT (1H0,28HWARNING..... SPECTRUM NUMBER 17,7HUNKNOWN/1H0)
240 FORMAT (35I2)
245 FORMAT (1H0,22HCALIBRATION LINE      Y=F7.5,3H*X+F9.5)

C
500 IF(K0)127,127,500
CALL DETER(TCON)
NP=3
X(1)=1.
DX=1.

C
2000 DO 2000 I=2,170
X(I)=X(I-1)+DX
DO 2001 I=1,170
2001 Y(I,1)=A(I)+2.0
B1=A(I)
DO 2004 J=2,170
IF(A(J)-B1)2004,2004,2005
2005 B1=A(J)
2004 CONTINUE
B2=A(171)
DO 2006 J=172,340
IF(A(J)-B2)2006,2006,2007
2007 B2=A(J)
2006 CONTINUE
B3=A(341)
DO 2008 J=342,510
IF(A(J)-B3)2008,2008,2009
2009 B3=A(J)
2008 CONTINUE
DO 2002 I=171,340
J=I-170
2002 Y(J,2)=A(I)*B1/B2
DO 2003 I=341,510
J=I-340
2003 Y(J,3)=A(I)*B1/B3
B12=B1/B2
B13=B1/B3
WRITE (6,2010) B12
WRITE (6,2011) B13
2010 FORMAT (41H THE SECOND CURVE HAS BEEN MULTIPLIED BY,E12.4)
2011 FORMAT (40H THE THIRD CURVE HAS BEEN MULTIPLIED BY,E12.4)
N=170
RINDA=0.
IS=0
LOGA=-1
LOGO=-1
CALL GRAPH
127 CONTINUE
GO TO 115
END

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SUBROUTINE RITE(JSX,MIX,A)
THIS RIET ONLY FOR PURE SPECTRA (L=5)
C
DIMENSION
1  A(512,10), XLAM(5,20), ALEN(5,20,5), ENGH(80), ARP(60), 10
2  AB(127,15), ELE(5,20), RAR(5,20,5), ENG(80), SD(60), 11 MODIF
3  NEP(127), ENE(5,20), KEV(127,15), ENGL(80), NHI(60), 12
4  ELEM(127), AAS(5,20), Y(200,3), RES(60), FE(60), 13
5  TP(127), KT(5,20), TAB3(100), KLAS(60), X(200), 14
6 MODIFA(512), B(512), NUPIC(5), NLOW(60), ALFA(5), 15
7  T(127), NE(127), IN(76) 16 MODIF
COMMON NP,Y,X,N,RINDA,LOGA,LOGO,IS 17 MODIF
COMMON
1  ENG, ENGH, ENGL, TDEC, TIR, PESO, FLUSS, NUPIC, 22
2  ENE, ELE, AAS, XLAM, KT, ALEN, RAR, KO, 23
3  EHICH, ELOW, RES, MODIFA, B, NLOW, FE, NHI, 24 MODIF
4  L1, L2, L3, L4, L5, L6, ELEM, TP, 25
5  T, NE, NEP, KEV, AB, KLOW, KHIGH, JMAX, 26
6  IFIT, KLAS, ARP, SD, TAB3, AKK, BKK, A 27 MODIF
701 DATA INC/0776060606060/
JSXME=JSX-1
IS=0
J=0
702 J=J+1
IF(J-MIX) 7021,7021,7022
7022 RETURN
7021 JS=0
703 JS=JS+1
READ (11,730) L,(IN(I),I=1,5)

DO 704 I=1,5
IF(IN(I).EQ. INC) GO TO 720
704 CONTINUE
IF(L.NE.5) GO TO 710
KAN=KONV(IN,1,5)
A(JS,J)=KAN
IF(IS.EQ.0) GO TO 705
A(JS-1,J)=(A(JS-2,J)+A(JS,J))*0.5
IS=0
705 IF(JS.EQ.1) GO TO 706
IF(JS-JSX)703,702,702
706 IF(MOD(KAN,16))708,703,708
708 WRITE (6,731) J,KAN
GO TO 703
710 IF(L-76)712,712,714
712 WRITE (6,732) J,JS,L,(IN(I),I=1,5)

JS=JS-1
GO TO 703
714 WRITE(6,736)
736 FORMAT(1H0,24HEND OF TAPE WITH SPECTRA)
IF(JS.NE.1) GO TO 715
RETURN
715 WRITE (6,733) J,JS
RETURN

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		02/15/67	
RITE			
EXTERNAL	FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER
720		IF (L.NE.5) GO TO 712	,59
		A(JS,J)=0.0	,62
		IF (IS.EQ.1.OR. JS.EQ.1.OR. JS.EQ.JSX) GO TO 724	,63
		IS=1	,66
		WRITE (6,734) J,JS	,67
		GO TO 703	,70
724		WRITE (6,735) J,JS	,71
		GO TO 703	,74
C			
730		FORMAT (16,5A1)	
731		FORMAT (1H0,32HWARNING FIRST CHANNEL NOT =MOD16,8X2HJ=I3,5X4HKAN=I15)	
732		FORMAT (1H0,30HWARNING INVALID RECORD SKIPPED ,10X2HJ=I3,15X4HKAN=I5,5X2HL=I2,5X5A1)	
733		FORMAT (1H0,34HWARNING LAST SPECTRUM NOT COMPLETE,6X2HJ=I3,6X3HJS=I5)	
734		FORMAT (1H0,37HWARNING INV. REC. SUBSTITUTED BY MEAN,3X2HJ=I3,6X3H1JS=I5)	
735		FORMAT (1H0,37HWARNING INV. REC. SUBSTITUTED BY ZERO,3X2HJ=I3,6X3H1JS=I5)	
		END	,75

		02/15/67	
KONV			
EXTERNAL	FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER
		FUNCTION KONV(IN,KL,KH)	
		DIMENSION IN(80),N(10)	
		DATA (N(I),I=1,10)/1H0,1H1,1H2,1H3,1H4,1H5,1H6,1H7,1H8,1H9/	
		KONV=0	,1
		DO 20 K=KL,KH	,2
		DO 10 I=1,10	,3
10		IF (IN(K).EQ.N(I)) GO TO 20	,4
		WRITE (6,30) K	,8
		I=1	,11
20		KONV=KONV*10+I-1	,12
		RETURN	,14
30		FORMAT (1H0,29HWARNING CONVERSION ERROR I=I2)	
		END	,15

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SUBROUTINE DETER(TCON)
C
DIMENSION
1 AA(512,10), XLAM(5,20), ALEN(5,20,5), ENGH(80), ARP(60), 10
2 AB(127,15), ELE(5,20), RAR(5,20,5), ENG(80), SD(60), 11
3 NEP(127), ENE(5,20), KEV(127,15), ENGL(80), NHI(60), 12
4 ELEM(127), AAS(5,20), Y(200,3), RES(60), FE(60), 13
5 TP(127), KT(5,20), TAB3(100), KLAS(60), X(200), 14
6 A(512), B(512), NUPIC(5), NLOW(60), ALFA(5), 15
7 T(127), NE(127) 16
C
COMMON NP,Y,X,N,RINDA,LOGA,LOGO,IS 22
COMMON 23
1 ENG, ENGH, ENGL, TDEC, TIR, PESO, FLUSS, NUPIC, KO, 24
2 ENE, ELE, AAS, XLAM, KT, ALEN, RAR, KO, 25
3 EHIGH, ELOW, RES, A, B, NLOW, FE, NHI, 26
4 L1, L2, L3, L4, L5, L6, ELEM, TP, 27
5 T, NE, NEP, KEV, AB, KLOW, KHIGH, JMAX, 28
6 IFIT, KLAS, ARP, SD, TAB3, AKK, BKK, AA 29
C
NU=NUPIC(KO)
WRITE (6,201)
DO 1 J=1,NU
DO 4 NPEAK=1,JMAX
CFF=4.0
KEN=ENE(KO,J)
KEL=ENG(NPEAK)-(ENGH(NPEAK)-ENGL(NPEAK))/CFF-0.5
KEH=ENG(NPEAK)+(ENGH(NPEAK)-ENGL(NPEAK))/CFF-0.5
IF(KEL-KEN)3,3,4
IF(KEH-KEN)4,5,5
3 AREA1=ARP(NPEAK)/EXP(-XLAM(KO,J)*TDEC)
5 AROS=1.E13*AREAI/(1.-EXP(-XLAM(KO,J)*TIR))
PPM=AROS/(AAS(KO,J)*PESO*FLUSS)
ERR=SD(NPEAK)*PPM/ARP(NPEAK)
ELES=ELE(KO,J)
ENT=ENE(KO,J)
ENS=ENG(NPEAK)
KI=KT(KO,J)
WRITE (6,202) ELES,ENT,ENS,ARP(NPEAK),PPM,ERR
M=0
CON=100.
IF(KI-1)30,31,32
30 CONP=100.
50 WRITE (6,101) CONP
GO TO 61
31 IF(ALEN(KO,J,1)-EHIGH)112,444,444
112 IF(ALEN(KO,J,1)-ELOW)444,444,113
444 CONP=100.
WRITE (6,203) ALEN(KO,J,1),CONP
GO TO 61
113 M=M+1
N=0
DO 134 JIF=1,JMAX
IF(ALEN(KO,J,1)-ENGL(JIF))134,134,137
137 IF(ALEN(KO,J,1)-ENGH(JIF))138,134,134
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	DETER		02/15/67
	EXTERNAL FORMULA NUMBER	- SOURCE STATEMENT	- INTERNAL FORMULA NUMBER(S)
138	CON=100.*ARP(JIF)/(RAR(KO,J,1)*ARP(NPEAK))		,43
	WRITE (6,204) ALEN(KO,J,1),ARP(JIF),CON		,44
	N=N+1		,47
134	CONTINUE		,48
	IF(N)400,400,61		,50
400	AL=ALEN(KO,J,1)		,51
	CALL IPOL(DET,AL,TCON)		,52
	CON=100.*DET/(RAR(KO,J,1)*ARP(NPEAK))		,53
	WRITE (6,205) ALEN(KO,J,1),DET,CON		,54
	GO TO 61		,55
32	DO 33 K=1,KI		,56
	IF(ALEN(KO,J,K)-EHIGH)12,35,35		,59
12	IF(ALEN(KO,J,K)-ELOW)35,35,13		,60
35	WRITE (6,203) ALEN(KO,J,K),CON		,61
	GO TO 33		,64
13	M=M+1		,65
	N=0		,66
	DO 34 JIF=1,JMAX		,67
	IF(ALEN(KO,J,K)-ENGL(JIF))34,34,37		,68
37	IF(ALEN(KO,J,K)-ENGH(JIF))38,34,34		,69
38	CON=100.*ARP(JIF)/(RAR(KO,J,K)*ARP(NPEAK))		,70
	N=N+1		,71
	WRITE (6,204) ALEN(KO,J,K),ARP(JIF),CON		,72
34	CONTINUE		,75
	IF(N)40,40,41		,77
40	AL1=ALEN(KO,J,K)		,78
	CALL IPOL(DET,AL1,TCON)		,79
	CON=100.*DET/(RAR(KO,J,K)*ARP(NPEAK))		,80
	WRITE (6,205) ALEN(KO,J,K),DET,CON		,81
41	CONTINUE		,84
33	CONTINUE		,85
61	CONTINUE		,87
4	CONTINUE		,88
1	CONTINUE		,90
C			
101	FORMAT (1H+,82X,F7.3)		
201	FORMAT (1H1,92HELEMENT TH.ENERGY EXP.ENERGY	AREA CPM	
	1 P.P.M. ERROR CONTRIBUTION//)		
202	FORMAT (1H0,A7,F11.3,F12.3,6X,F12.3,F16.5,F14.5)		
203	FORMAT (1H0,7X,F11.3,64X,F7.3)		
204	FORMAT (1H0,7X,F11.3,18X,F12.3,34X,F7.3)		
205	FORMAT (1H0,7X,F11.3,12X,6HSENSIT,F12.3,34X,F7.3)		
	RETURN		,92
	END		,93

SUBROUTINE FITN(X,Y,B,N,IX)

THIS SUBPROGRAM FITS A POLYNOMIAL OF ORDER N TO A SET OF POINTS
 X(I),Y(I) OUTPUT ARE THE COEFFICIENTS B OF THE POLYNOMIAL (POWERS I
 N DECREASING ORDER

C
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DIMENSION
1  UT(20,20), U(20,20), SY(21), SX(40), B(1), Y(1), X(1)
    IF(N-2) 12,12,10
10  ITER=3
    GO TO 14
12  ITER=2
14  NE=N+1
    NT=N+2
    NKE=2*N+1
    DO 16 L=1,NKE
16  SX(L)=0.0
    DO 18 L=1,NE
18  SY(L)=0.0
    DO 22 I=1,IX
    P=1.0
    DO 22 L=1,NKE
    SX(L)=SX(L)+P
    IF(L-NE) 20,20,22
20  SY(L)=SY(L)+P*Y(I)
22  P=P*X(I)
    DO 26 K=1,NE
    DO 24 J=1,NE
    IND=K+J-1
24  U(K,J)=SX(IND)
26  U(K,NT)=SY(K)
    U(NT,NT)=-1.0
    DO 28 J=1,NE
28  U(NT,J)=0.0
    DO 30 I=1,NT
    DO 30 J=1,NT
30  UT(I,J)=U(J,I)
    DET=1.0
    DO 90 IL=1,ITER
    DO 80 I=1,NT
    C=0.0
    DO 1 K=1,NT
    1  C=C+U(I,K)*UT(K,I)
    IF(C) 2,99,2
    2  DET=DET*C
    DO 3 J=1,NT
    3  UT(J,I)=UT(J,I)/C
    DO 80 J=1,NT
    IF(J-I) 4,80,4
    4  H=0.0
    DO 5 K=1,NT
    5  H=H+U(I,K)*UT(K,J)
    DO 6 K=1,NT
    6  UT(K,J)=UT(K,J)-H*UT(K,I)
    
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FITN				02/15/67
EXTERNAL FORMULA NUMBER	-	SOURCE STATEMENT	-	INTERNAL FORMULA NUMBER(S)
80		CONTINUE		,60
90		CONTINUE		,63
		DO 7 I=1,NE		,65
		IND=NE+1-I		,66
7		B(IND)=UT(I,NT)		,67
		RETURN		,69
99		WRITE(6,98)N,IX,IL		,70
98		FORMAT (1H0,34HWARNING.....FITTING CANNOT PROCEED,3I4/1H0)		
		RETURN		,73
		END		,74

TDEC1				02/15/67
EXTERNAL FORMULA NUMBER	-	SOURCE STATEMENT	-	INTERNAL FORMULA NUMBER(S)
FUNCTION TDEC1(MO,IO,IME)				
DIMENSION MO(4),IO(4),IME(12)				
		I1=MO(4)		,1
		I2=IO(4)		,2
		TDEC1=((IME(I1)-IME(I2)+MO(3)-IO(3))*24+MO(1)-IO(1))*60+MO(2)-IO(2)		,3
		1)		,4
		RETURN		,5
		END		

IPOL
EXTERNAL FORMULA NUMBER - SOURCE STATEMENT - INTERNAL FORMULA NUMBER(S) 02/15/67

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SUBROUTINE IPOL(DT,EN,TE)
C
DIMENSION
1 AA(512,10), XLAM(5,20), ALEN(5,20,5), ENGH(80), ARP(60), 10
2 AB(127,15), ELE(5,20), RAR(5,20,5), ENG(80), SD(60), 11
3 NEP(127), ENE(5,20), KEV(127,15), ENGL(80), NHI(60), 12
4 ELEM(127), AAS(5,20), Y(200,3), RES(60), FE(60), 13
5 TP(127), KT(5,20), TAB3(100), KLAS(60), X(200), 14
6 A(512), B(512), NUPIC(5), NLOW(60), ALFA(5), 15
7 T(127), NE(127) 16
C
COMMON NP,Y,X,N,RINDA,LOGA,LOGO,IS 22
COMMON 23
1 ENG, ENGH, ENGL, TDEC, TIR, PESO, FLUSS, NUPIC, 24
2 ENE, ELE, AAS, XLAM, KT, ALEN, RAR, KO, 25
3 EHIGH, ELOW, RES, A, B, NLOW, FE, NHI, 26
4 L1, L2, L3, L4, L5, L6, ELEM, TP, 27
5 T, NE, NEP, KEV, AB, KLOW, KHIGH, JMAX, 28
6 IFIT, KLAS, ARP, SD, TAB3, AKK, BKK, AA 29
C
FK=3.0
P=1.3
VYFT=50.0
KN=(EN-BKK)/AKK+0.5
IND=EN/VYFT+1.0
ED=AMOD(EN,VYFT)
KD=P*0.5*(TAB3(IND+1)-TAB3(IND))*ED/VYFT+TAB3(IND)/AKK+0.5
IL=KN-KD
IH=KN+KD
SUM=0.0
DO 2 I=IL,IH
2 SUM=SUM+A(I)
DET=FK*FK/(1.66*TE)*(1.0+SQRT(1.0+8.0*SUM/(FK*FK)))
RETURN
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SUBROUTINE KALIP(EN,FR,E,KE,KLS,KM,RE)
C
DIMENSION
1 AA(512,10), XLAM(5,20), ALEN(5,20,5), ENGH(80), ARP(60), 10
2 AB(127,15), ELE(5,20), RAR(5,20,5), ENG(80), SD(60), 11
3 NEP(127), ENE(5,20), KEV(127,15), ENGL(80), NHI(60), 12
4 ELEM(127), AAS(5,20), Y(200,3), RES(60), FE(60), 13
5 TP(127), KT(5,20), TAB3(100), KLAS(60), X(200), 14
6 A(512), R(512), NUPIC(5), NLOW(60), ALFA(5), 15
7 T(127), NE(127), LLOW(10), LHI(10) 16
DIMENSION 17 MOD
1 KLS(25), FR(25), FN(25), REI(25), RE(25), EG(25), E(25) 18
COMMON NP,Y,X,N,RINDA,LOGA,LOGO,IS 22
COMMON 23
1 ENG, ENGH, ENGL, TDEC, TIR, PESO, FLUSS, NUPIC, 24
2 ENE, ELE, AAS, XLAM, KT, ALEN, RAR, KO, 25
3 EHIGH, ELOW, RES, A, B, NLOW, FE, NHI, 26
4 L1, L2, L3, L4, L5, L6, ELEM, TP, 27
5 T, NE, NEP, KEV, AB, KLOW, KHIGH, JMAX, 28
6 IFIT, KLAS, ARP, SD, TAB3, AKK, BKK, AA 29
C
80 DO 82 I=1,KM
LLOW(I)=KLS(I)-5
82 LHI(I)=KLS(I)+5
88 N=1
J=1
M=1
DO 39 I=1,KHIGH
KR=FR(J)+0.5
IF(I-KR)31,33,31
31 IF(I-LHI(M))30,30,32
32 M=M+1
GO TO 30
33 IF(I-LHI(M))34,34,36
34 IF(I-LLOW(M))36,35,35
35 FI=I
FN(N)=FR(J)
REI(N)=RE(J)
B(N)=A(I)
EG(N)=E(M)
N=N+1
M=M+1
36 J=J+1
30 IF(J-JMAX)37,37,40
37 IF(M-KE)39,39,40
39 CONTINUE
C
40 N=N-1
WRITE(6,91)N
DO 41 I=1,N
41 WRITE(6,92) I,E(I),LLOW(I),LHI(I),FN(I),B(I),REI(I)
NPE=N+1
IF(NPE-KE)42,42,45
42 DO 43 I=NPE,KE

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	KALIP		02/15/67
	EXTERNAL FORMULA NUMBER	- SOURCE STATEMENT -	INTERNAL FORMULA NUMBER(S)
	43	WRITE(6,92)I,E(I),LLOW(I),LHI(I)	,40
	45	CALL FITN (FN,EG,B,I,N)	,44
		RETURN	,45
C	92	FORMAT (1H0,I2,F10.3,2I10,3F10.3)	
	91	FORMAT (1HC/1HC,6X23HDATA OF ESTIMATED PEAKS,5X21HPEAKS FOR CALIBR 1ATION/1HC,5X6HENERGY,7X3HLOW,6X4HHIGH,4X7HCHANNEL,4X6HCOUNTS,6X4HF 2WHM,10X12)	
		END	,46

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SUBROUTINE PIKAR(P,Q,R,TCON)
DIMENSION
1 AA(512,10), XLAM(5,20), ALEN(5,20,5), ENGH(80), ARP(60), 10
2 AB(127,15), ELE(5,20), RAR(5,20,5), ENG(80), SD(60), 11
3 NEP(127), ENE(5,20), KEV(127,15), ENGL(80), NHI(60), 12
4 ELEM(127), AAS(5,20), Y(200,3), RES(60), FE(60), 13
5 TP(127), KT(5,20), TAB3(100), KLAS(60), X(200), 14
6 A(512), B(512), NUPIC(5), NLOW(60), ALFA(5), 15
7 T(127), NE(127) 16
DIMENSION 17
1 C(512), REST(512) 18
C COMMON NP,Y,X,N,RINDA,LOGA,LOGO,IS 22
COMMON 23
1 ENG, ENGH, ENGL, TDEC, TIR, PESO, FLUSS, NUPIC, 24
2 ENE, ELE, AAS, XLAM, KT, ALEN, RAR, KO, 25
3 EHIGH, ELOW, RES, A, B, NLOW, FE, NHI, 26
4 L1, L2, L3, L4, L5, L6, ELEM, TP, 27
5 T, NE, NEP, KEV, AB, KLOW, KHIGH, JMAX, 28
6 IFIT, KLAS, ARP, SD, TAB3, AKK, BKK, AA 29
C
RL=1.00
RR=1.05
DO 10 I=KLOW,KHIGH
10 C(I)=A(I)+P*SQRT(A(I))
I=KLOW+2
J=0
12 I=I+1
IF(I-KHIGH+3)16,84,84
16 IF(A(I)-A(I-1))12,18,18
18 IF(A(I)-A(I+1))12,12,20
20 IL=I
KLS=100
IF(A(I)-C(I-1))24,24,26
24 IL=IL-1
KLS=200
IH=I
26 IF(A(I)-C(I+1))28,28,30
28 IH=IH+1
KLS=KLS+100
C
30 IF(A(IL-1)-C(IL-2))38,38,36
36 IF(A(IH+1)-C(IH+2))38,38,42
38 IF(A(IL)-0.333*Q*RL*(A(IL-1)+A(IL-2)+A(IL-3)))12,12,39
39 IF(A(IH)-0.333*Q*RR*(A(IH+1)+A(IH+2)+A(IH+3)))12,12,40
40 KLS=KLS+500
C
42 IL=IL-1
IF(IL-KLOW-3)54,54,44
44 IF(A(IL)-A(IL-1))46,42,42
46 IF(A(IL)-0.333*RL*(A(IL-3)+A(IL-2)+A(IL-1)))54,54,48
48 IF(J-1)52,52,50
50 IF(IL-NHI(J-1))54,54,52
52 KLS=KLS+10

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PIKA
EXTERNAL FORMULA NUMBER - SOURCE STATEMENT - INTERNAL FORMULA NUMBER(S) 02/15/67

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C      GO TO 42
54  IH=IH+1
    IF(IH-KHIGH+3)56,62,62
56  IF(A(IH)-A(IH+1))58,54,54
58  IF(A(IH)-0.333*RR*(A(IH+3)+A(IH+2)+A(IH+1)))62,62,60
60  KLS=KLS+1
    GO TO 54
C      62  ART=0.0
    DO 64 L=IL,IH
64  ART=ART+A(L)
    FLT=IH-IL+1
    AP=ART-0.5*FLT*(A(IL)+A(IH))
    SDEV=SQRT(ART+FLT*FLT*(A(IL)+A(IH))*0.25)
    IF(AP*R-SDEV)12,12,66
66  IF(J-60)68,67,67
67  WRITE (6,201)
    GO TO 84
201  FORMAT (1H0,26HWARNING JMAX LIMITED TO 60/1H0)
C      68  J=J+1
    IMEM=IH
    DO 90 KLEBS=IL,IH
    FLEBS=KLEBS
    FIL=IL
    FIH=IH
    FLH=(A(IH)-A(IL))/(FIH-FIL)
    FOND=FLH*(FLEBS-FIL)+A(IL)
90  REST(KLEBS)=A(KLEBS)-FOND
93  IF(REST(I)-REST(I-1))91,92,92
91  I=I-1
    GO TO 93
92  IF(REST(I)-REST(I+1))94,95,95
94  I=I+1
    GO TO 92
95  SUM1=0.
    SUM2=0.
    DO 96 KLEB=IL,IH
    IF(2.*REST(KLEB)-REST(I))96,97,97
97  FLEB=KLEB
    SUM1=SUM1+FLEB*REST(KLEB)
    SUM2=SUM2+REST(KLEB)
96  CONTINUE
    FE(J)=SUM1/SUM2
    IFE=FE(J)+0.5
    DIFE=IFE
    DELTA=FE(J)-DIFE
    IF(DELTA)70,70,71
70  XMAS=(1.-DELTA)*REST(IFE)+DELTA*REST(IFE-1)
    GO TO 72
71  XMAS=(1.-DELTA)*REST(IFE)+DELTA*REST(IFE+1)
72  RES(J)=2.*AP/XMAS*SQRT(0.693/3.14)
103  NHI(J)=IH
    NLOW(J)=IL
    KLAS(J)=KLS

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		PIKA			02/15/67
	EXTERNAL FORMULA NUMBER	-	SOURCE STATEMENT	-	INTERNAL FORMULA NUMBER(S)
			ARP(J)=AP/TCON		,89
			SD(J)=SDEV/TCON		,90
			I=IMEM		,91
			GO TO 12		
C					
	84		JMAX=J		,92
			RETURN		,93
			END		,94
					,95

	SUBROUTINE GRAPH	0010	
	DIMENSION Y(200,3), X(200), V(18), E1(6), E2(6), E3(6), Y2(200,3), X2(200	0020	
	1), M1(200,3), M2(200), IMIN(3), IMAX(3)	0030	
	DIMENSION MM(4,1), G(4,1)	0040	
C	THE FOLLOWING STATEMENT(S) HAVE BEEN MANUFACTURED BY THE TRANSLATOR TO	0050	
C	COMPENSATE FOR THE FACT THAT EQUIVALENCE DOES NOT REORDER COMMON---	0060	
	COMMON NP , Y , X , N , RINDA , LOGA	0070	
	COMMON LOGO , IS	0080	
C	DIMENSION MM(4,1), G(4,1)	0110	
C	COMMON NP, Y, X, N, RINDA, LOGA, LOGO, IS	0120	
	DO 10 I=1, 18	0130	,1
	DATA Q000HL/6H /	0140	
10	V(I)=Q000HL	0150	,2
	DATA Q001HL/6H. /	0160	
	E1(1)=Q001HL	0170	,4
	DATA Q002HL/6H. /	0180	
	E1(2)=Q002HL	0190	,5
	DATA Q003HL/6H. /	0200	
	E1(3)=Q003HL	0210	,6
	DATA Q004HL/6H. /	0220	
	E1(4)=Q004HL	0230	,7
	DATA Q005HL/6H. /	0240	
	E1(5)=Q005HL	0250	,8
	DATA Q006HL/6H. /	0260	
	E1(6)=Q006HL	0270	,9
	DATA Q007HL/6H* /	0280	
	E2(1)=Q007HL	0290	,10
	DATA Q008HL/6H* /	0300	
	E2(2)=Q008HL	0310	,11
	DATA Q009HL/6H* /	0320	
	E2(3)=Q009HL	0330	,12
	DATA Q010HL/6H* /	0340	
	E2(4)=Q010HL	0350	,13
	DATA Q011HL/6H* /	0360	
	E2(5)=Q011HL	0370	,14
	DATA Q012HL/6H* /	0380	
	E2(6)=Q012HL	0390	,15
	DATA Q013HL/6H+ /	0400	
	E3(1)=Q013HL	0410	,16
	DATA Q014HL/6H+ /	0420	
	E3(2)=Q014HL	0430	,17
	DATA Q015HL/6H+ /	0440	
	E3(3)=Q015HL	0450	,18
	DATA Q016HL/6H+ /	0460	
	E3(4)=Q016HL	0470	,19
	DATA Q017HL/6H+ /	0480	
	E3(5)=Q017HL	0490	,20
	DATA Q018HL/6H+ /	0500	
	E3(6)=Q018HL	0510	,21
	DO 60 J=1, NP	0520	,22
	IMIN(J)=1	0530	,23
	IMAX(J)=1	0540	,24
	LLL=IMIN(J)	0550	,25
	MMM=IMAX(J)	0560	,26
	DO 24 K=2, N	0570	,27

	B	EXTERNAL FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER	02/15/67	NUMBER(S)
23			IF(Y(K,J)-Y(LLL,J))23,23,24	0580		,28
			IMIN(J)=K	0590		,29
			LLL=IMIN(J)	0600		,30
24			CONTINUE	0610		,31
			DO 34 K=2,N	0620		,32
			IF(Y(K,J)-Y(MMM,J))34,34,33	0630		,34
33			IMAX(J)=K	0640		,35
			MMM=IMAX(J)	0650		,36
34			CONTINUE	0660		,37
60			CONTINUE	0670		,39
			IF(NP-1)81,81,80	0680		,41
80			LMIN=1	0690		,42
			KMIN=IMIN(1)	0700		,43
			DO 64 J=2,NP	0710		,44
			K=IMIN(J)	0720		,45
			IF(Y(K,J)-Y(KMIN,LMIN))63,63,64	0730		,46
63			LMIN=J	0740		,47
			KMIN=K	0750		,48
64			CONTINUE	0760		,49
			LMAX=1	0770		,51
			KMAX=IMAX(1)	0780		,52
			DO 65 J=2,NP	0790		,53
			K=IMAX(J)	0800		,54
			IF(Y(K,J)-Y(KMAX,LMAX))65,66,66	0810		,55
66			LMAX=J	0820		,56
			KMAX=K	0830		,57
65			CONTINUE	0840		,58
			GO TO 149	0850		,60
81			LMIN=1	0860		,61
			KMIN=IMIN(1)	0870		,62
			LMAX=1	0880		,63
			KMAX=IMAX(1)	0890		,64
149			IF(15)150,150,151	0900		,65
151			IF(Y(KMAX,LMAX))8002,152,8001	0910		,66
8002			D1=Y(KMIN,LMIN)/Y(KMAX,LMAX)	0920		,67
			GO TO 8015	0930		,68
8001			D1=Y(KMAX,LMAX)/Y(KMIN,LMIN)	0940		,69
8015			IF(D1-10.E+02)152,152,153	0950		,70
152			LOGO=-1	0960		,71
			GO TO 8003	0970		,72
153			LOGO=+1	0980		,73
8003			IF(X(N))8012,155,8011	0990		,74
8012			D2=X(1)/X(N)	1000		,75
			GO TO 8016	1010		,76
8011			D2=X(N)/X(1)	1020		,77
8016			IF(D2-10.E+02)155,155,156	1030		,78
155			LOGA=-1	1040		,79
			GO TO 150	1050		,80
156			LOGA=+1	1060		,81
150			IF(LOGA)43,43,44	1070		,82
44			DO 45 K=1,N	1080		,83
45			X2(K)=ALOG(ABS(X(K)))*0.43429*X(K)/ABS(X(K))	1090		,84
			WRITE(6,1012)	1100		,86
1012			FORMAT(23H LOG SCALE IN ABSCISSA/)	1110		
			GO TO 47	1120		,88
43			DO 46 K=1,N	1130		,89

	B	EXTERNAL FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER(S)	02/15/67
46			X2(K)=X(K)	1140	,90
			WRITE (6,1008)	1150	,92
1008			FORMAT (26H NORMAL SCALE IN ABSCISSA/)	1160	
47			IF(LOGO)48,48,49	1170	,94
49			DO 50 K=1,N	1180	,95
			DO 50 J=1,NP	1190	,96
50			Y2(K,J)=ALOG(ABS(Y(K,J)))*0.43429*Y(K,J)/ABS(Y(K,J))	1200	,97
			WRITE (6,1011)	1210	,100
1011			FORMAT (23H LOG SCALE IN ORDINATE/)	1220	
			GO TO 51	1230	,102
48			DO 52 K=1,N	1240	,103
			DO 52 J=1,NP	1250	,104
52			Y2(K,J)=Y(K,J)	1260	,105
			WRITE (6,1009)	1270	,108
1009			FORMAT(26H NORMAL SCALE IN ORDINATE/)	1280	
51			XINTM=X2(2)-X2(1)	1290	,110
			DO 700 J=3,N	1300	,111
			XINT=X2(J)-X2(J-1)	1310	,112
			IF(XINT-XINTM)701,700,700	1320	,113
701			XINTM=XINT	1330	,114
700			CONTINUE	1340	,115
			DO 53 K=1,N	1350	,117
			M2(K)=2.5+((X2(K)-X2(1))/XINTM)	1360	,118
			DO 53 J=1,NP	1370	,119
53			M1(K,J)=((Y2(K,J)-Y2(KMIN,LMIN))/(Y2(KMAX,LMAX)-Y2(KMIN,LMIN)))*	1380	
			1(96.0-(10.0*(FLOAT(NP)-1.0)))+1.5	1390	,120
			IF (RINDA)702,702,703	1400	,123
703			DO 704 K=1,N	1410	,124
704			M2(K)=2.0+(78.0-(10.0*(FLOAT(NP)-1.0)))*RINDA*(X2(K)-X2(1))/(X2(N)	1420	
			1-X2(1))+0.5	1430	,125
702			AA=Y2(KMAX,LMAX)	1440	,127
			BB=Y2(KMIN,LMIN)	1450	,128
			DIF=AA-BB	1460	,129
			TAC=10.E-35	1470	,130
			IF(DIF-TAC)73,73,7	1480	,131
73			CALL EXIT	1490	,132
6			TAC=TAC*10.0	1500	,133
7			TEC=TAC*10.0	1510	,134
			IF(DIF-4.0*TEC)4,4,6	1520	,135
4			IF(LOGO)8700,8700,8701	1530	,136
8701			IF(TAC-1.0)8702,8700,8700	1540	,137
8702			TAC=1.0	1550	,138
8700			BBB= AINT((BB/TAC)*1.00001)*TAC	1560	,139
			AAA= AINT((AA/TAC)*1.00001)*TAC	1570	,140
			IF(ABS((BBB-BB)/BB)-1.E-05)8500,8500,8800	1580	,141
8800			IF(BB-BBB)8500,8500,8501	1590	,142
8501			BBB=BBB+TAC	1600	,143
8500			IF(ABS((AAA-AA)/AA)-1.E-05)8600,8600,8801	1610	,144
8801			IF(AA-AAA)8601,8600,8600	1620	,145
8601			AAA=AAA-TAC	1630	,146
8600			DIFV=AAA-BBB	1640	,147
			NQP= AINT((DIFV/TAC)*1.00001)+1.0	1650	,148
			DO 18 I=1,NQP	1660	,149
			P=FLOAT(I)-1.0	1670	,150
18			G(I)=BBB+TAC*P	1680	,151
			IF(ABS(G(I)-BB)-1.E-05)8900,8900,8901	1690	,153

		B			02/15/67		
EXTERNAL FORMULA NUMBER	SOURCE STATEMENT				INTERNAL FORMULA NUMBER(S)		
8900	G(1)=BB				1700		,154
8901	DO 19 J=1,NQP				1710		,155
19	MM(J)=((G(J)-BB)/(AA-BB))*(96.0-(10.0*(FLOAT(NP)-1.0)))+1.5				1720		,156
	IF(LOGO)9001,9001,9002				1790		,158
9002	EBBB=10.0**BBB						,159
	ETAC=10.0**TAC				1740		,160
	IF(Y(KMIN,LMIN))8705,8706,8706				1750		,161
8705	ETAC=1.0/ETAC				1760		,162
	EBBB=-1.0/EBBB				1770		,163
8706	CONTINUE				1780		,164
	WRITE (6,999)EBBB,ETAC						,165
999	FORMAT (55H INFORMATIONS ON ORDINATE SCALE - LEFT SCALING POINT =				1810		
	1PE12.3,31H-FACTOR BETWEEN SCALING POINTS=1PE12.3)				1820		
	GO TO 8000				1830		,168
9001	WRITE (6,99)BBB,TAC				1840		,169
99	FORMAT (55H INFORMATIONS ON ORDINATE SCALE - LEFT SCALING POINT =				1850		
	1PE12.3,33H-INTERVAL BETWEEN SCALING POINTS=1PE12.3)				1860		
8000	DO 28 J=1,NQP				1870		,172
	IF(J-1)20,20,21				1880		,173
20	KKK=1				1890		,174
	GO TO 22				1900		,175
21	KKK=4				1910		,176
22	MIAO=NP*KKK				1920		,177
	N2=MM(J)/6				1930		,178
	IF(N2)83,83,84				1940		,179
83	N3=MM(J)				1950		,180
103	GO TO(6001,6002,6003,6009,6009,6009,6009,6005,6005,6005,6006)				1960		
	1,MIAO				1970		,181
6001	WRITE (6,1015)E1(N3)				1980		,182
	GO TO 28				1990		,185
6002	WRITE (6,1025)E1(N3)				2000		,186
	GO TO 28				2010		,189
6003	WRITE (6,1035)E1(N3)				2020		,190
	GO TO 28				2030		,193
6005	WRITE (6,1205)E1(N3)				2040		,194
	GO TO 28				2050		,197
6006	WRITE (6,1305)E1(N3)				2060		,198
	GO TO 28				2070		,201
6009	WRITE (6,1105)E1(N3)				2080		,202
	GO TO 28				2090		,205
84	N3=MM(J)-N2*6				2100		,206
	IF(N3)86,86,87				2110		,207
86	N2=N2-1				2120		,208
	IF(N2)7003,7003,7002				2130		,209
7003	N3=6				2140		,210
	GO TO 103				2150		,211
7002	N3=6				2160		,212
87	GO TO(6011,6012,6013,6019,6019,6019,6019,6015,6015,6015,6016)				2170		
	1,MIAO				2180		,213
6011	WRITE (6,1015)(V(L),L=1,N2),E1(N3)				2190		,214
	GO TO 28				2200		,220
6012	WRITE (6,1025)(V(L),L=1,N2),E1(N3)				2210		,221
	GO TO 28				2220		,227
6013	WRITE (6,1035)(V(L),L=1,N2),E1(N3)				2230		,228

EXTERNAL FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER(S)
		02/15/67
6015	GO TO 28 WRITE (6,1205)(V(L),L=1,N2),E1(N3)	2240 ,234 2250 ,235
6016	GO TO 28 WRITE (6,1305)(V(L),L=1,N2),E1(N3)	2260 ,241 2270 ,242
6019	GO TO 28 WRITE (6,1105)(V(L),L=1,N2),E1(N3)	2280 ,248 2290 ,249
28	CONTINUE	2300 ,255
1015	FORMAT (1H0,21X,17A6)	2310
1025	FORMAT (1H0,31X,15A6)	2320
1035	FORMAT (1H0,41X,14A6)	2330
1205	FORMAT (1H+,31X,15A6)	2340
1305	FORMAT (1H+,41X,14A6)	2350
1105	FORMAT (1H+,21X,17A6)	2360
	IF(NP-1)1001,1001,1002	2370
1001	WRITE (6,1005)	2380 ,257
	WRITE (6,3005)	2390 ,258
	GO TO 1010	2400 ,260
1002	IF(NP-2)1006,1006,1007	2410 ,262
1006	WRITE (6,1004)	2420 ,263
	WRITE (6,3004)	2430 ,264
	GO TO 1010	2440 ,266
1007	WRITE (6,1003)	2450 ,268
	WRITE (6,3003)	2460 ,269
1005	FORMAT(20H X	2470 ,271
1004	FORMAT(30H X	2480
1003	FORMAT(41H X	2490
3003	FORMAT(38H	2500
3004	FORMAT(27H	2510
3005	FORMAT(17H	2520
1010	M=0	2530
	DO 500 K=1,N	2540 ,273
12	M=M+1	2550 ,274
	IF(M-M2(K))9,40,2000	2560 ,275
2000	M=M-1	2570 ,276
	GO TO 500	2580 ,277
9	WRITE (6,11)	2590 ,278
	GO TO 12	2600 ,279
40	D08J=1,NP	2610 ,281
	MIAO=J*NP	2620 ,282
	N2=M1(K,J)/6	2630 ,283
	IF(N2)13,13,14	2640 ,284
13	N3=M1(K,J)	2650 ,285
110	GO TO(2001,2002,2003,2005,2005,2006,2006,2006,2009),MIAO	2660 ,286
2001	WRITE (6,15)X(K),(Y(K,L),L=1,NP),E1(N3)	2670 ,287
		2680 ,288
		2690 ,294
2002	GO TO 8 WRITE (6,25)X(K),(Y(K,L),L=1,NP),E1(N3)	2680 ,295
		2690 ,296
		2700 ,302
2003	GO TO 8 WRITE (6,35)X(K),(Y(K,L),L=1,NP),E1(N3)	2710 ,303
		2720 ,304
		2730 ,310
	GO TO 8	2740 ,311

EXTERNAL FORMULA NUMBER	SOURCE STATEMENT	INTERNAL FORMULA NUMBER(S)
2005	WRITE (6,205)X(K),(Y(K,L),L=1,NP),E2(N3)	2730
	GO TO 8	2740
2006	WRITE (6,305)X(K),(Y(K,L),L=1,NP),E2(N3)	2750
	GO TO 8	2760
2009	WRITE (6,305)X(K),(Y(K,L),L=1,NP),E3(N3)	2770
	GO TO 8	2780
14	N3=M1(K,J)-N2=6	2790
	IF(N3)16,16,17	2800
16	N2=N2-1	2810
	IF(N2)3,3,2	2820
3	N3=6	2830
	GO TO 110	2840
2	N3=6	2850
17	GO TO (2011,2012,2013,2015,2015,2016,2016,2016,2019),MIAO	2860
2011	WRITE (6,15)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E1(N3)	2870
	GO TO 8	2880
2012	WRITE (6,25)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E1(N3)	2890
	GO TO 8	2900
2013	WRITE (6,35)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E1(N3)	2910
	GO TO 8	2920
2015	WRITE (6,205)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E2(N3)	2930
	GO TO 8	2940
2016	WRITE (6,305)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E2(N3)	2950
	GO TO 8	2960
2019	WRITE (6,305)X(K),(Y(K,L),L=1,NP),(V(L),L=1,N2),E3(N3)	2970
8	CONTINUE	2980
500	CONTINUE	2990
11	FORMAT (2H)	3000
15	FORMAT (1H ,1P2E10.2,1X,17A6)	3010
25	FORMAT (1H ,1P3E10.2,1X,15A6)	3020
35	FORMAT (1H ,1P4E10.2,1X,14A6)	3030
205	FORMAT (1H+,1P3E10.2,1X,15A6)	3040
305	FORMAT (1H+,1P4E10.2,1X,14A6)	3050
	RETURN	3060
	END	3070

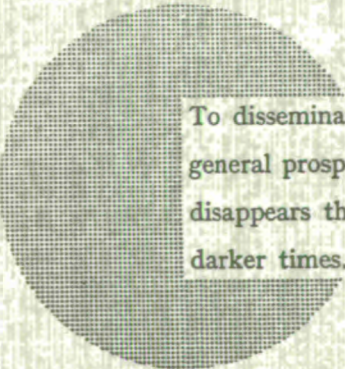
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Alfred Nobel

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