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DOCHAP
A FORTRAN IV PROGRAM FOR THE CORRECTION AND CALIBRATION OF NEUTRON INELASTIC SCATTERING DATA

by

K. KREBS and D.J. WINFIELD

1971

Joint Nuclear Research Centre
Ispra Establishment - Italy

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ABSTRACT

This program is used to correct raw data obtained from the Ispra-1 Double Chopper Neutron Spectrometer Facility.

Corrections available are for background, air attenuation, detector efficiency and sample thickness. In addition, the data may be normalised with spectra obtained from a vanadium reference specimen. A smoothing routine may also be utilised if the data have low statistical accuracy. The corrected data output is available in either punched, printed or graphical format.

KEYWORDS

FORTRAN
PROGRAMMING
COMPUTERS
CORRECTIONS
CALIBRATION
INELASTIC SCATTERING
NEUTRONS
CHOPPERS
NEUTRON SPECTROMETERS
AIR
ATTENUATION
RADIATION DETECTORS
SAMPLING
THICKNESS
VANADIUM

CONTENTS

1. INTRODUCTION *)

The first stage in the analysis of the inelastic neutron scattering data produced by the ISPRA-I Double Chopper Spectrometer consists of the conversion of paper tape output, from an on line PDP8 computer [1] into punched cards and an optional CALCOMP plot.

In the second stage of the analysis the present program, DOCHAP, processes the neutron time of flight data on the punched cards and produces an output, which may be printed, punched or plotted as required, representing the final calibrated and corrected neutron data.

Section 2 of the report describes the available program subroutines and their various outputs.

Appendix 1 is a tabulation of the data input required for the program. Interpretations are also listed of all the input variables. Where these variables are controls for the initiation of subroutines or the selection of the various outputs from these subroutines, then the required values have been given in brackets.

Appendix 2 gives a listing of the program. All essential variables used which are not data input are labelled by comment statements.

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*) Manuscript received on 17 October 1970

2. PROGRAM DESCRIPTION

2.1 Main Routine

The function of the main routine is to read in the raw data and the respective mode cards. The mode cards determine the form of the data input and the selection of the subroutines required for the various corrections. All the subroutines and data input/output modes are initiated from this main routine. As many data as required, comprising time of flight spectra and corresponding background data from up to 20 detectors may be processed by the program. Each data set may have any of the available corrections applied according to the mode cards for that particular set.

To provide a check on the consistency of the data the routine also computes and prints out the mean positions, widths and integrated intensities of the elastic peaks of the raw data. The mean elastic peak positions are calculated, in terms of the average time of flight channel number i_o, between channel numbers NSSEP and NFSEP of the raw data, from the equation

$$i_o = \frac{\sum_{i=NSSEP}^{NFSEP} N_i \, i}{\sum_{i=NSSEP}^{NFSEP} N_i}$$

where N_i is the number of counts in channel number i. Assuming the elastic peak may be represented by a Gaussian then the full width at half height is given by

$$SWID = 2\sqrt{2 \ln 2} \; \frac{\sum_{i=NSSEP}^{NFSEP} N_i (i-i_o)^2}{\sum_{i=NSSEP}^{NFSEP} N_i}$$

and the total integrated peak intensity by

$$\text{TOTEL} = \sum_{i=\text{NSSEP}}^{\text{NFSEP}} N_i$$

The results of the calculations for the above three parameters are printed out for each counter in a given data set, at the end of the data processing of that particular set.

If required, this routine may also print and plot the raw data of each counter. The switches for these modes are the variables NWD and NGRD. The graphical output is plotted by the internal subroutine GRAPH [2]. This on-line representation is only convenient for a quick assessment of the data and is produced by the printer itself. All other subsequently mentioned graphs refer to this on-line printer mode unless it is specified that the CALCOMP graph plotter is being utilised. CALCOMP plots of the final corrected spectra are initiated by the variable NCALCD. The spectra are produced on a suitable scaled and labelled frame for each data set. Punched and printed output of the final data for each spectrum of the data sets being processed are called by the variables NPUND and NWRITD. A print out of the energy calibration (section 2.2.2) for each separate data set may also be called by the variable NWCAL. Channel numbers with corresponding neutron times of flight and energies are listed in this mode.

2.2 Subroutines

The program name of a subroutine is quoted after the respective sub-section heading, with the list of required arguments. Where these arguments are not specifically mentioned in the subsequent description, reference should be made to Appendix 1 for their interpretation. Initation of subroutine processing is performed by a calling variable and output options of the subroutines are called by output option variables. These variables are listed beneath the subroutine name in each sub-section. In general output may be in numerical or graphical form for each spectra; the output option variables being prefixed by NW and NGR respectively.

2.2.1 Vanadium Calibration

Subroutine : VAN (LA,LE,KKK, NVAN,NSIV,NFIV, NSEV, NFEV,
SVTOT,SVABS,VSTH,ALPHAD,BETAD,SUMCRR)

Calling Variable : NVAN

Output Option Variables: NWVAN,NGRVAN

This subroutine is described for each available option, determined by the switch variable NVAN in the main routine.

- OPTION : NVAN = 0

In this option the data input to the main program DOCHAP is the vanadium spectra only. The output is a number, KKK, of punched cards with vanadium correction factors SUMCCR for each counter.

The routines calculate the average number of counts/channel, denoted by AV, between the channel numbers NFIV and NSIV, for each spectrum. These channel numbers are taken to lie outside the channel numbers containing the vanadium inelastic peak and the elastic peak so that the average will give a good representation of the background level in each counter.

This average is given by:

$$AV = \sum_{i=NSIV}^{NFIV} N_i \Big/ \Big((NFIV - NSIV) + 1 \Big)$$

where N_i is the number of raw counts in channel number i. The resulting number of background corrected counts in the vanadium elastic peak is then given by

$$SUM = \sum_{i=NSEV}^{NFEV} (N_i - AV)$$

The value of SUM is then normalised to unity for the first spectra of each data set being processed.

A flat background subtraction is justified as any time dependent background will be eliminated by the subtraction of a sample holder background for a particular run. The correction factor by which the raw vanadium data is then multiplied to correct for sample absorption and scattering is given in the transmission mode (see fig.1(a)) by

$$VTHCRR = \frac{a \exp - \left(\frac{a\,\Sigma_a}{\sin(\alpha-\beta)}\right)\left(\frac{\Sigma_t}{\sin\beta} + \frac{\Sigma_a}{\sin(\alpha-\beta)}\right)}{1 - \exp - \left(\frac{a\,\Sigma_t}{\sin\beta} + \frac{a\,\Sigma_a}{\sin(\alpha-\beta)}\right)} \quad \ldots. (1)$$

Here Σ_a and Σ_t represent the vanadium absorption and total scattering cross section at the incident neutron energy in barns and are denoted in the program by SVABS and SVTOT respectively. The variables, together with the angles α and β and the sample thickness a are printed out for each spectrum. The correction factor is given relative to the vanadium thickness $a/\sin\alpha$ measured in the direction of the incident beam. Relative to the vanadium thickness a the correction will be VTHCRR x sin α. The final correction factor by which the sample data of each corresponding counter is normalised is then given by

$$SUMCRR = SUM \times VTHCRR$$

The correction factors are printed out for each counter together with the respective components SUM and VTHCRR.

Vanadium runs should be compared before and after a sample run, a comparison between the various SUMCRR values of each counter being made to check whether fluctuations in background, counter efficiency or electronic noise are apparent. Agreement to 3-4% in the two sets of vanadium correction factors should be obtained to guarantee satisfactory normalisation of the sample data.

No correction has been made for the Debye-Waller factor dependence of the vanadium scattering. This is given, at room temperature, by $\exp(-0.006\ Q^2)$ and is small enough to be neglected for small incident energies up to ~ 10meV.

Used in the present mode no other program subroutines are utilised.

- OPTION : NVAN = 1

In this mode the data input to the main routine is the raw sample data and the corresponding vanadium spectra. The output are again KKK correction cards for the subsequent use in option NVAN = 2 but the raw data fed in are corrected at the same time for vanadium normalisation. The print out is the same as for NVAN = 0 but any other program subroutines may be used in this mode.

- OPTION : NVAN = 2

In this mode data input are the raw sample data and the set of KKK punched cards. Data is then corrected for vanadium normalisation via the subroutine VAN.

- OPTION : NVAN = 3

No correction by the vanadium subroutine is performed in this mode.

2.2.2 Background Subtraction

Subroutine : BAGD (LA,LE,KKK)
Calling Variable : NBG
Output Option Variables : NWBG,NGRBG

This subroutine enables a background subtraction to be performed for each set of sample data which is read into the main routine. When NBG = 1 sample background data is initially read by the main routine and suitable normalised to the sample data by multiplication of the background data by the variable BAKNOR. This variable is given by the ratio : total number of monitor counts during sample run / total number of monitor counts during background run. The value of BAKNOR is read into the main routine. After the normalisation the background is subtracted from the raw sample data for each corresponding channel.

2.2.3 Time of Flight Calibration

The time of flight calibration is performed by calling two independent subroutines discussed below. The first of these, subroutine CHANA, corrects the spectra for frame overlap and the second, subroutine CAL, then calculates the correct time of flight values of the data in their new channel number assignments.

i) Subroutine : CHANA (NFR,NEND)
Calling Variable : NCHA
Output Option Variables : NWCHA, NGRCHA

With this subroutine frame overlap is corrected for by transferring the whole block of channels which precede channel number NFR, representing infinite energy, to the right hand side of the spectra such that they form a continuation from the last channel NEND of the observed spectra.

ii) Subroutine : CAL (NFR,NEND,NW,ND,N1,N2,NEL,SM,SZ,TT)
Calling Variable : NCAL
Output Option Variable: NWCAL

This subroutine produces a time of flight calibration for the spectra as a function of channel number. Two monitors placed at a fixed distance (SM meters) apart in the straight-through beam enable the incident neutron energy to be determined. The average channel number, to the nearest integer of the peak from each monitor is fed into the main routine as integers N1 and N2. ND is the delay, in units of 16 μsec, which is applied by the time of flight interface after the rotor start pulse is received. SZ represents the sample-detector flight path in meters and NEL is the average channel number of the elastic peak at the detector. For reference the total sample running time in hours TT, is included in the subroutine.

With all the above data input the subroutine calculates and prints the energy, wavelength, and velocity of the incident neutrons. Time of flight correction required to produce the correct time of flight values for each channel with the time origin taken when the incident pulse hits the center of the sample is also printed out.

2.2.4 Smoothing Routine

Subroutine : SMOOTH (N,NSMA,LA,LE)
Calling Variable : NSM
Output Option Variables : Graphical and numerical output is automatically produced via the subroutine in this case.

This subroutine may be utilised if the data has low statistical accuracy and is called by use of the switch variable NSM in the main routine. A full description of the smoothing technique, known as an n point moving polynominal fit is given in reference [3].

The smoothing routine described there has been modified and 7 different options incorporated into this program. Values of n between 5 and 11, and degreees of polynomials from 2 to 5 are utilised (see comment labels in the subroutine listing).

The options are called from the main routine using values of NSMA from 1 to 7. With NSMA = 1 the data has minimum smoothing applied to it by using a 5 point moving polynomial fit of order 2. When NSMA = 7 maximum smoothing is available, with an 11 point moving polynominal fit of order 5. After processing by the routine the number of data points is reduced by (n-1) relative to the initial number N as a result of the smoothing procedure.

2.2.5 Air Attenuation Correction

Subroutine	:	AIR (LA,LE)
Calling Variable	:	NAIR
Output Option Variable	:	NWAIR

This routine calculates the attenuation resulting from air scattering and absorption in the neutron flight path, of length L, from sample to the detector.

Wavelength dependent scattering occurs primarily from oxygen and nitrogen molecules, the presence of water vapour in the atmosphere can be neglected. The cross sections of oxygen and nitrogen were taken from BNL-325 and are represented in the subroutine as a data set over the energy range from 4 meV to 100 meV. The correction factor by which the data is multiplied is given by

$$AN = \exp(\Sigma_N L + \Sigma_O L)$$

where Σ_N and Σ_O are the total macroscopic cross sections of nitrogen and oxygen atoms in the atmosphere as a function of energy, at a temperature of 22°C and a pressure of 745 torr.

2.2.6 Counter Efficiency Correction

Subroutine : CTR (LA,LE)
Calling Variable : NCTR
Output Option Variables : NWCTR,NGRCTR

The counter efficiency CN is calculated for 4 atmosphere He^3 detectors of radius R = 1.25 cm. placed with their axes perpendicular to the scattered beam, with reference to fig.2, by

$$CN = 1 - \int_0^{\pi/2} \exp(-2\Sigma_a R \cos\Theta)\cos\Theta \, d\Theta$$

where Σ_a is the macroscopic absorption cross section of He^3 at room temperature and 4 atmospherespressure.

Assuming Σ_a follows the 1/v law the efficiency CN is calculated as a function of energy and the sample data is multiplied by the 1/CN value at the corresponding energy of the time of flight calibrated data.

2.2.7 Sample Thickness Correction

Subroutine : THICK(LA,LE,NCC,ATW,DENS,STOT,SABS,STH, ALPHAD,BETA)
Calling Variable : NTC
Output Option Variables : NWTC,NGRTC

This routine calculates and corrects for the attenuation of the scattered neutrons resulting from transmission through parallel side samples as a function of the angle of scatter. The average atomic weight ATW, density DENS and the sample thickness STH are read into the main routine together with the absorption cross section SABS of the sample at 25.3 meV and the total cross section STOT at the incident energy. The sample absorption cross section is assumed to follow the 1/v law, in all cases.

The expressions by which the experimental data at a given energy and scattering angle must be multiplied to correct for sample transmission are calculated for 2 different sample arrangements, determined by the value of NCC, and are listed below:

a) NCC = 1. Sample in transmission mode.
In this case the expression for the correction factor, labelled SN in the subroutine is identical to that given in equation 1, Σ_a and Σ_t now referring to the sample specimen.

b) NCC = 2. Sample in reflection mode.
Reference to fig.1(b) shows that in the reflection mode the correction factor is given by

$$SN = \frac{\left(\frac{\Sigma_t}{\sin\beta} + \frac{\Sigma_a}{\sin(\alpha - \beta)} \right) a}{1 - \exp-\left(\frac{a\Sigma_t}{\sin\beta} + \frac{a\,\Sigma_a}{\sin(\alpha - \beta)} \right)}$$

REFERENCES

[1] METZDORF, H.J. Euratom Report EUR 3933.e (1968)

[2] MONGINI-TAMAGNINI,C., PIRE,J.
Euratom Report EUR 2238.e (1965)

[13] SAVITZKY,A., GOLAY,M.J.E.,
Analytical Chemistry 36, 1627 (1964)

APPENDIX 1

DATA INPUT LIST WITH INTERPRETATION

A list of the data input variables and their required format specification is given in the order of occurence of the variables together with an interpretation. All variables are either integer or floating point according to the standard FORTRAN IV convention. The number of each data card required is specified. Where different values of the same data variable are required on a set of consecutive cards, then the set is counted as one card. Where a control variable is specified the number required for different modes to be initiated is given in brackets in the interpretation. It should be noted however that in certain options some data cards are not required.

Number of card	Variable Name	Format	Interpretation
1	NSPL	12I5	Number of sets of sample data.
	NREP		Number of spectra comprising one data set.
2ff	SCANG(I), I=1, NREP	F 10.4	Detector scattering angle (degrees) for NREP detectors.
3	TEXT(1)... TEXT(18)..	18A4	Title card.
4	NSSEP, NFSEP	12I5	Channel numbers defining start and finish respectively of sample elastic peak of raw data,
	NSIV, NFIV		Channel numbers defining start and finish respectively of region outside the inelastic and elastic peaks of raw vanadium data.
	NSEV, NFEV		Channel numbers defining start and finish respectively of vanadium elastic peak of raw data.

Number of card	Variable Name	Format	Interpretation
5	NFR	12I5	Channel number corresponding to frame overlap position
	NEND		Last channel + 1 containing observed data points
	NCHASS		Number of counter inputs to PDP8 (either 12,6,3, or 1). This determines the number of channels, 3072/NCHASS allocated to one spectrum.
6	NWD,NGRD	24I3	Controls for printing (1) and online plotting (1) of raw sample data.
	NWRITD,NPUND, NCALCD		Controls for printing (1) punching (1) and CALCOMP plotting (1) of final corrected sample data.
7	NVAN,NWAN, NGRWAN	24I3	Controls for initiation (0,1,2), printing (1) and plotting of the vanadium subroutine calibration.
	NCHA,NWCHA, NGRCHA		Controls for initiation (1), printing (1) and plotting of the channel shift subroutine data.
	NCAL,NWCAL		Controls for initiation (1) and printing (1) of time of flight calibration routine.
	NBG,NWBG, NGRBG		Controls for initiation (1), printing (1) and plotting (1) of the background subtraction routine.
	NSM,NSMA		Controls for initiation (1) and the smoothing option (1 to 7) of the smoothing routine.
	NAIR,NWAIR, NGRAIR		Controls for initiation (1), printing (1) and plotting (1) of the air attenuation correction.
	NCTR,NWCTR, NGRCTR		Controls for initiation (1), printing (1) and plotting (1) of the counter efficiency correction.
	NTC,NWTC, NGRTC,NCC		Controls for initiation (1), printing (1), plotting (1), and mode (1 or 2) of the sample thickness correction

Number of card	Variable Name	Format	Interpretation
8	NW	5I6,3F6.3	Channel width (μsec)
	DN		Analyser trigger delay (16 μsec)
	N1, N2		Positions of 1st and 2nd monitor peaks, in channel numbers.
	NEL		Position of elastic peak in the detectors, in channel numbers.
	SM		Flight path between monitors (meters).
	SZ		Flight path between sample and detectors (meters).
	TT		Total sample measurement time (hrs).
9	SVTOT,SVABS	4F10.4	Vanadium total and absorption cross sections at the incident energy (barns).
	VSTH		Vanadium sample thickness (cm).
	BETAD		Vanadium sample inclination to the direct beam (degrees).

IF NVAN ≠ 2 THE NEXT SET OF DATA CARDS [10 ff] ARE NOT READ IN :

Number of card	Variable Name	Format	Interpretation
10 ff	SUM(I),I=1, NREP	F10.4	Vanadium correction factors for NREP detectors, produced by vanadium subroutine options: NVAN = 0 or 1 .
11	ATW	6F10.4	Average atomic weight of sample.
	DENS		Density of sample (gm/cc).
	STOT		Total neutron cross section of sample for incident energy (barns).
	SABS		Total neutron absorption cross section of sample at 25.3 meV (barns).
	STH		Sample thickness (cm).
	BETA		Sample inclination to incident beam (degrees).

Number of card	Variable Name	Format	Interpretation
IF NBG ≠ 1 DATA CARD [12] AND THE FOLLOWING DATA SET [13ff] ARE NOT BEAD IN :			
12	BAKNOR	F10.4	Ratio of sample /background motion counts
13ff	NADR1,(NBK (KKK, I),I = NIADR, NEADR)	11(I6,1X)	Background data from channel number 1 to NCHNN, on format produced from the paper tape conversion routine, for NREP sets of spectra (KKK = 1, NREP)
IF NVAN ≥ 2 THE FOLLOWING DATA SET [14ff] ARE NOT READ IN:			
14ff	NADR1,(NVDAT(KKK, I), I = NIADR, NEADR)	11(I6,1X)	Vanadium data read in as above for NREP sets
IF NVAN = 0 THE FOLLOWING DATA SET [15ff] ARE NOT READ IN:			
15ff	NADR1,(NDAT(I), I = NIADR, NEADR)	11(I6,1X)	Sample data read in as above for NREP sets
IF NCALCD ≠ 1 THE FOLLOWING DATA SET [16ff] ARE NOT READ IN:			
16ff	NC(K),(A(K,I), I = 1,66)(K=1,6)	3X,I3,66 A1	Title cards for a given data set. The NC(K) set specify the title card numbers and the (A(K,I) set contain any alphanumeric information required. The A(K,I) matrix is printed out on the CALCOMP output.
THE DATA READ IN NOW RETURNS TO THE THIRD CARD OF THE LIST, [3] AND REPEATS FOR THE SECOND DATA SET UNTIL ALL THE NSPL SETS HAVE BEEN READ IN.			

FIG1(a). GEOMETRY OF VANADIUM SAMPLE IN TRANSMISSION MODE.

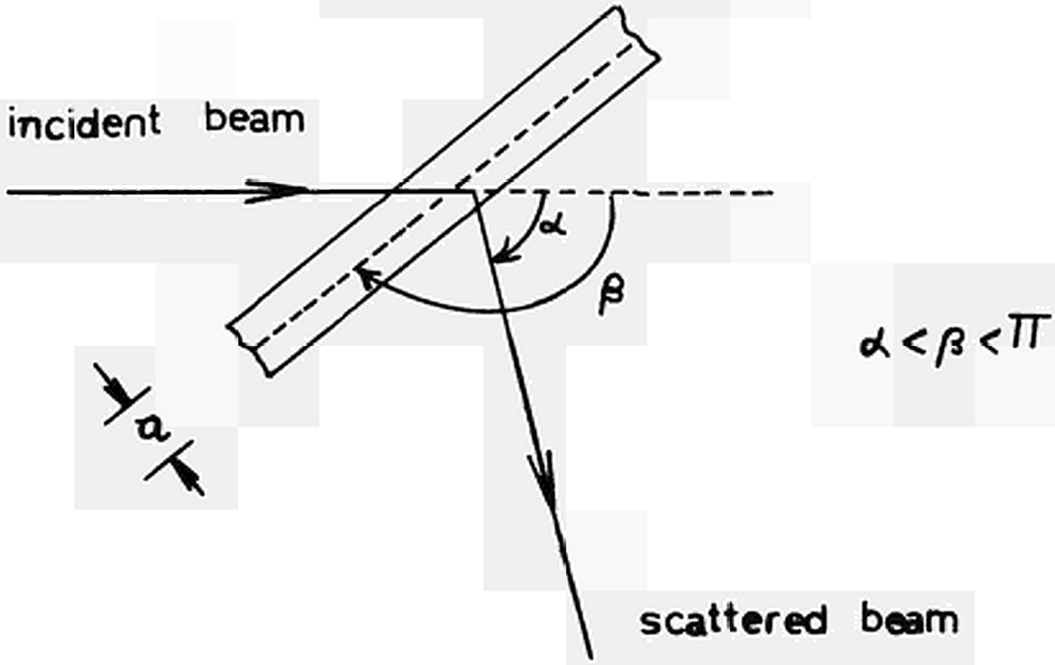
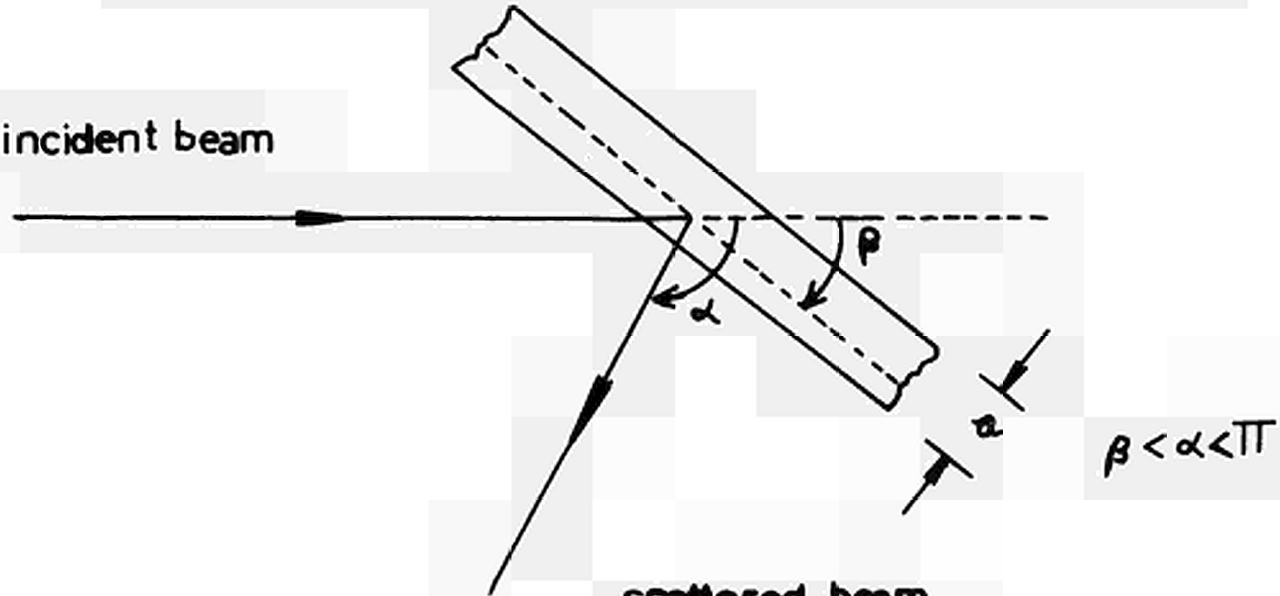
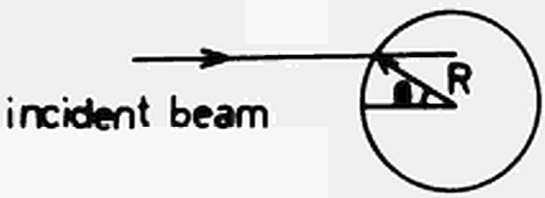


FIG1(b). SAMPLE GEOMETRY IN REFLECTION MODE.



Both α and β are positive for clockwise rotation.

FIG 2. DETECTOR GEOMETRY.



```
                C       PROGRAM DOCHAP
                C
                C       DOCHAP EVALUATES AND CORRECTS DATA FROM THE ISPRA 1 DOUBLE CHOPPER
                C       NEUTRON SPECTROMETER FACILITY
                C
 0001                   DIMENSION NC(20),A(20,66),CHNNL(3080),CALSPC(3080),XECK(6),YECK(6)
 0002                   DIMENSION AVSP(20),SWID(20),NDAT(260),FDAT(20,260),TOTEL(20),NBK(2
                      10,260),SUMC(20),SCANG(20),X(260),NVDAT(20,260)
                C
 0003                   COMMON/MACAL/TEXT(18),TF(260),T1,T2,T3,E0,WLAM0,E01,V0,E02,E03,TCO
                      1RR
 0004                   COMMON /MAVAN/VDAT(20,260)
 0005                   COMMON /MABAG/BG(20,260)
 0006                   COMMON DATA(260),E(260)
                C
 0007                   LOGICAL BLOOP,VLOOP
                C
 0008                   CALL INTCTR(180)
 0009                   READ  (5,1000) NSPL,NREP
                C
                C       NSPL...NO OF SETS OF SAMPLE DATA
                C       NREP...NO OF SPECTRA IN ONE DATA SET
                C
 0010                   READ (5,1001) (SCANG(I),I=1,NREP)
                C
                C       SCANG(I)...SCATTERING ANGLES FOR NREP DETECTORS (DEGREES)
                C
 0011                   DO 6 KKS=1,NSPL
 0012                   READ (5,1002) (TEXT(I),I=1,18)
                C
                C       TEXT(I)...TITLE CARD
                C
 0013                   READ (5,1000) NSSEP,NSFEP,NSIV,NFIV,NSEV,NFEV
                C
                C       NSSEP...CH NO OF START OF SAMPLE ELASTIC PEAK (RAW DATA)
                C       NSFEP...CH NO OF FINISH OF SAMPLE ELASTIC PEAK (RAW DATA)
                C       NSIV,NFIV...START AND FINISH CHANNELS FOR BACKGROUND AVERAGING
                C       NSEV,NFEV...START AND FINISH CHANNELS FOR VANADIUM ELASTIC PEAK
                C
 0014                   READ (5,1000) NFR,NEND,NCHASS
                C
                C       NFR   ...CHANNEL NO AT FRAME EVERLAP POSITION
                C       NEND ...LAST CHANNEL NO OF OBSERVED SPECTRA
                C       NCHASS...NO OF COUNTER INPUTS TO TOF INTERFACE
                C
 0015                   READ (5,1003) NWD,NGRD,NWRITD,NPUND,NCALCD
                C
                C       NWD    ...CONTROL FOR INITIATION OF RAW DATA PRINT
```

```
             C      NGRD  ...CONTROL FOR INITIATION OF RAW DATA PLOT
             C      NWRITD...CONTROL FOR INITIATION OF FINAL DATA PRINT
             C      NPUND ...CONTROL FOR INITIATION OF FINAL DATA PUNCH
             C      NCALCD...CONTROL FOR INITIATION OF FINAL DATA CALCOMP PLOT
             C
0016                READ (5,1003) NVAN,NWVAN,NGRVAN,NCHA,NWCHA,NGRCHA,NCAL,NWCAL,NBG,N
                   1WBG,NGRBG,NSM,NSMA,NAIR,NWAIR,NGRAIR,NCTR,NWCTR,NGRCTR,NTC,NWTC,NG
                   2RTC,NCC
             C
             C      VAN...CONTROLS FOR CALIBRATION OF DATA WITH VANADIUM SCATTERING
             C      CHA...CONTROLS FOR CHANNEL SHIFTING ROUTINE
             C      CAL...CONTROLS FOR TIME OF FLIGHT CALIBRATION ROUTINE
             C      BG ...CONTROLS FOR BACKGROUND CORRECTION ROUTINE
             C      SM ...CONTROLS FOR SMOOTHING ROUTINE
             C      AIR...CONTROLS FOR AIR ATTENUATION CORRECTION
             C      CTR...CONTROLS FOR COUNTER SENSITIVITY CORRECTION
             C      NTC...CONTROLS FOR SAMPLE THICKNESS CORRECTION
             C      NCC...CONTROLS FOR SAMPLE THICKNESS CORRECTION MODE
             C
0017                READ (5,1004) NW,ND,N1,N2,NEL,SM,SZ,TT
             C
             C      NW   ...CHANNEL WIDTH(IN MICROSEC)
             C      ND   ...ANALYSER TRIGGER DELAY (16 MICROSEC)
             C      N1   ...FIRST MONITOR PEAK (CHANNEL NUMBER)
             C      N2   ...SECOND MONITOR PEAK (CHANNEL NUMBER)
             C      NEL  ...ELASTIC PEAK (ORIGINAL CHANNEL NUMBER)
             C      SM   ...FLIGHT PATH BETWEEN MONITORS(IN M)
             C      SZ   ...FLIGHT PATH SAMPLE-COUNTER(IN M)
             C      TT   ...TOTAL MEASURING TIME (IN HOURS)
             C
0018                READ (5,1005) SVTOT,SVABS,VSTH,BETAD
             C
             C      SVTOT...TOTAL CROSS SECTION OF VANADIUM FOR E0 IN BARNS
             C      SVABS...ABSORPTION CROSS SECTION OF VANADIUM FOR E0 IN BARNS
             C      VSTH ...VANADIUM SAMPLE THICKNESS IN CM.
             C      BETAD...ANGLE FROM KI TO VANADIUM INCLINATION IN DEGREES
             C
0019                IF (NVAN.NE.2) GO TO 10
             C
0020                READ (5,1001) (SUMC(I),I=1,NREP)
             C
             C      SUMC(I)...VANADIUM CALIBRATION CORRECTION FACTORS
             C
0021             10 CONTINUE
             C
0022                READ (5,1006) ATW,DENS,STOT,SABS,STH,BETA
             C
             C      ATW ..ATOMIC RESP.MOLECULAR WEIGHT
```

```
                C      DENS..DENSITY
                C      STOT..TOTAL NEUTRON CROSS SECTION OF SAMPLE FOR EO IN BARN
                C      SABS..ABSORPTION CROSS SECTION OF SAMPLE AT 25.3 MEV IN BARN
                C      STH ..SAMPLE THICKNESS IN CM
                C      BETA..ANGLE FROM KI TO SAMPLE INCLINATION IN GRAD
                C
 0023                  NCHNN=3072/NCHASS
 0024                  IF (NBG.NE.1) GO TO 8
                C
 0025                  READ (5,1001) BAKNOR
                C
                C      BAKNOR ...RATIO OF MONITOR COUNTS FOR SAMPLE TO BACKGROUND RUNS
                C
                C      READ IN BACKGROUND DATA
                C
 0026                  DO 5 KKK=1,NREP
 0027                  BLOOP=.FALSE.
 0028                  DO 98 L=1,308
 0029                  IF (BLOOP)  GO TO 99
 0030                  NADR=(L-1)*10
 0031                  NIADR=NADR+1
 0032                  NEADR=NADR+10
 0033                  IF (NCHNN.LE.NEADR) NEADR=NCHNN
                C
 0034                  READ (5,1007) NADR1,(NBK(KKK,I),I=NIADR,NEADR)
                C
 0035                  IF (NADR1.NE.NADR) GO TO 199
 0036                  IF (NCHNN.LE.(NADR+10))  BLOOP=.TRUE.
 0037               98 CONTINUE
 0038              199 WRITE (6,4000)
 0039               99 CONTINUE
 0040                5 CONTINUE
                C
 0041                  DO 9 KKK=1,NREP
 0042                  DO 7 I=1,NEADR
 0043                  BG(KKK,I)=NBK(KKK,I)
 0044                  BG(KKK,I)=BG(KKK,I)*BAKNOR
 0045                7 CONTINUE
 0046                9 CONTINUE
                C
                C      END OF BACKGROUND DATA READ IN FOR ONE SAMPLE SET
                C
 0047                8 CONTINUE
 0048                  IF (NVAN.GE.2) GO TO 15
                C
                C      READ IN VANADIUM DATA
                C
 0049                  DO 11 KKK=1,NREP
```

```
                  VLOOP=.FALSE.
                  DO 97 L=1,308
                  IF (VLOOP) GO TO 91
                  NADR=(L-1)*10
                  NIADR=NADR+1
                  NEADR=NADR+10
                  IF (NCHNN.LE.NEADR) NEADR=NCHNN
            C
                  READ (5,1007) NADR1,(NVDAT(KKK,I),I=NIADR,NEADR)
            C
                  IF (NADR1.NE.NADR) GO TO 90
                  IF (NCHNN.LE.(NADR+10))  VLOOP=.TRUE.
               97 CONTINUE
               90 WRITE (6,4021)
               91 CONTINUE
               11 CONTINUE
            C
                  DO 16 KKK=1,NREP
                  DO 14 I=1,NEADR
                  VDAT(KKK,I)=NVDAT(KKK,I)
               14 CONTINUE
               16 CONTINUE
            C
               15 CONTINUE
            C
                  DO 1 KKK= 1,NREP
                  WRITE (6,9000)
                  WRITE (6,4001) (TEXT(I),I=1,18)
                  WRITE (6,9001)
            C
                  N=NEND-1
                  LA=1
                  LE=N
                  IF (NVAN.EQ.0) GO TO 300
            C
            C     READ IN SAMPLE DATA
            C
                  DO 100 L=1,308
                  NADR=(L-1)*10
                  NIADR=NADR+1
                  NEADR=NADR+10
                  IF (NCHNN.LE.NEADR) NEADR=NCHNN
            C
                  READ (5,1007) NADR1,( IDAT(I),I=NIADR,NEADR)
            C
                  IF (NWD.EQ.1) WRITE (6,1007) NADR1,(IDAT(I),I=NIADR,NEADR)
                  IF (NADR1.NE.NADR) GO TO  200
                  IF (NCHNN.LE.(NADR+10)) GO TO  300
```

```
0087              100 CONTINUE
            C
            C         END OF SAMPLE DATA READ IN FOR ONE SAMPLE SET
            C
0088              200 WRITE (6,4002)
0089              300 CONTINUE
0090                  WRITE (6,9001)
            C
0091                  DO 222 I=1,NEND
0092                  X(I)=I
0093                  IF (NVAN.EQ.0)  GO TO 222
0094                  DATA(I)=NDAT(I)
0095              222 CONTINUE
            C
0096                  IF (NVAN.EQ.0) GO TO 223
            C
            C         CALCULATION OF AVERAGE CHANNEL,WIDTH AND INTENSITY OF ELASTIC PEAK
            C
0097                  AVSCH=0.0
0098                  SUMSEL=0.0
0099                  DO 22 I=NSSEP,NSFEP
0100                  SI=I
0101                  SUMSEL=DATA(I)+SUMSEL
0102                  AVSCH=AVSCH+DATA(I)*SI
0103               22 CONTINUE
0104                  TOTEL(KKK)=SUMSEL
0105                  AVSCH=AVSCH/SUMSEL
0106                  AVSP(KKK)=AVSCH
0107                  SIGMAS=0.0
0108                  DO 27 I=NSSEP,NSFEP
0109                  SI=I
0110                  SIGMAS=SIGMAS+DATA(I)*(SI-AVSCH)**2
0111               27 CONTINUE
0112                  SIGMAS=SIGMAS/SUMSEL
0113                  IF (SIGMAS.GT.0.) GO TO 40
0114                  IF (SIGMAS.LE.0.) WRITE (6,4003)
0115                  GO TO 9999
0116               40 SWID (KKK)=2.3548*SQRT(SIGMAS)
0117              223 IF (NGRD.EQ.1.AND.NVAN.GE.1) CALL GRAPH(1,N,0.,0,-1,-1,X(2),DATA(2
                     1),Y2,Y3)
            C
            C         CALLING OF SUBROUTINES NOW BEGINS
            C
            C
            C         VANADIUM CALIBRATION CORRECTION
            C
0118                  ALPHAD=SCANG(KKK)
0119                  SUMCRR=SUMC(KKK)
```

```
0120          IF (NVAN.LE.2)   WRITE (6,4004)
0121          IF (NVAN.LE.2)   CALL VAN(LA,LE,KKK,NVAN,NSIV,NFIV,NSEV,NFEV,SVTOT
             1,SVABS,VSTH,ALPHAD,BETAD,SUMCRR)
0122          IF (NWVAN.EQ.1)  WRITE (6,4005)
0123          IF (NWVAN.EQ.1)  WRITE (6,4006) (DATA(I),I=LA,LE)
0124          WRITE (6,9001)
0125          NVPP=NFEV-NSEV
0126          IF (NGRVAN.EQ.1) CALL GRAPH (1,NVPP,0.,0,-1,-1,X(NSEV),VDAT(KKK,NS
             1EV),Y2,Y3)
        C
        C     BACKGROUND CORRECTION
        C
0127          IF (NBG.EQ.1)   WRITE (6,4007)
0128          IF (NBG.EQ.1)   CALL BAGD(LA,LE,KKK)
0129          IF (NWBG.EQ.1)  WRITE(6,4006) (DATA(I),I=LA,LE)
0130          WRITE (6,9001)
0131          IF (NGRBG.EQ.1) CALL GRAPH(1,N,0.,0,-1,-1,X(LA),DATA(LA),Y2,Y3)
        C
        C     CHANNEL SHIFT AND RE-NUMBERING (CHANNEL ASSIGNMENT)
        C
0132          IF (NCHA.EQ.1)   WRITE (6,4008)
0133          IF (NCHA.EQ.1)   CALL CHANA(NFR,NEND)
0134          IF (NWCHA.EQ.1)  WRITE (6,4006) (DATA(I),I=LA,LE)
0135          WRITE (6,9001)
0136          IF (NGRCHA.EQ.1) CALL GRAPH(1,LE,0.,0,-1,-1,X(1),DATA(1),Y2,Y3)
        C
        C     CALIBRATION
        C
0137          IF (NCAL.EQ.1)   CALL CAL(NFR,NEND,NW,ND,N1,N2,NEL,SM,SZ,TT)
        C
        C     SMOOTHING
        C
0138          IF (NSM.EQ.1) WRITE (6,4009)
0139          IF (NSM.EQ.1) CALL SMOOTH (N,NSMA,LA,LE)
        C
        C     AIR ATTENUATION CORRECTION
        C
0140          IF (NAIR.EQ.1)   WRITE (6,4010)
0141          IF (NAIR.EQ.1)   CALL AIR(LA,LE)
0142          IF (NWAIR.EQ.1)  WRITE (6,4006) (DATA(I),I=LA,LE)
0143          WRITE (6,9001)
0144          IF (NGRAIR.EQ.1) CALL GRAPH(1,N,0.,0,-1,-1,X(LA),DATA(LA),Y2,Y3)
        C
        C     COUNTER SENSITIVITY CORRECTION
        C
0145          IF (NCTR.EQ.1)   WRITE (6,4011)
0146          IF (NCTR.EQ.1)   CALL CTR(LA,LE)
0147          IF (NWCTR.EQ.1)  WRITE (6,4006) (DATA(I),I=LA,LE)
```

```
0148                WRITE (6,9001)
0149                IF (NGRCTR.EQ.1) CALL GRAPH(1,N,0.,0,-1,-1,X(LA),DATA(LA),Y2,Y3)
              C
              C     SAMPLE THICKNESS CORRECTION
              C
0150                IF (NTC.EQ.1)   WRITE (6,4012)
0151                IF (NTC.EQ.1)   CALL THICK (LA,LE,NCC,ATW,DENS,STOT,SABS,STH,ALPHA
                   1D,BETA)
0152                IF (NWTC.EQ.1)  WRITE (6,4006) (DATA(I),I=LA,LE)
0153                WRITE (6,9001)
0154                IF (NGRTC.EQ.1) CALL GRAPH(1,N,0.,0,-1,-1,X(LA),DATA(LA),Y2,Y3)
              C
              C
0155                DO 3 I=LA,LE
0156                FDAT(KKK,I)=DATA(I)
0157              3 CONTINUE
0158              1 CONTINUE
              C
0159                IF (NVAN.EQ.0)  GO TO 66
0160                WRITE (6,4013) NSSEP,NSFEP
0161                WRITE (6,4014)
0162                DO 2 KKK=1,NREP
0163                NCTR=KKK+2
              C
              C     PRINT OUT AVERAGE CHANNEL ,WIDTH AND INTENSITY OF ELASTIC PEAKS
              C
0164                WRITE (6,4015) NCTR,AVSP(KKK),SWID(KKK),TOTEL(KKK)
0165              2 CONTINUE
0166                IF (NWCAL.NE.1) GO TO 13
              C
0167                WRITE (6,4022) (TEXT(I), I=1,18)
0168                WRITE (6,4023) NW,ND,N1,N2,NEL,SM,SZ,TT
0169                WRITE (6,4024) T1,T2,T3,E0,WLAM0,E01,V0,E02,E03,TCORR
0170                WRITE (6,4016)
0171                WRITE (6,4017) (I,TF(I),E(I),I=LA,LE)
              C
0172             13 CONTINUE
0173                WRITE (6,4018)
0174                DO 4 KKK=1,NREP
0175                KNK=KKK+2
0176                IF (NWRITD.EQ.1) WRITE (6,4019) KNK
0177                IF (NWRITD.EQ.1) WRITE (6,4020) (FDAT(KKK,I),I=LA,LE)
0178                IF (NPUND.EQ.1)  PUNCH 2000, (FDAT(KKK,I),I=LA,LE)
0179              4 CONTINUE
0180             66 CONTINUE
              C
0181                IF (NCALCD.NE.1) GO TO 6
              C
```

```
C         START CALCOMP PLOTTING OF ALL DATA SETS
C
          DO 12 K=1,6
          READ (5,1008) NC(K),(A(K,I),I=1,66)
      12  CONTINUE
          CALL FINIM (2.,2.)
          DO 130 K=1,6
          YTEXT=28.-.5*K
          NCK=NC(K)
          DO 130 I=1,66
          XTEXT=2.+.25*I
     130  CALL SYMBL4(XTEXT,YTEXT,.3,0.,A(K,I),1)
     140  DO 135 I=LA,LE
     135  CHNNL(I)=I
          XDIAGR=2.
          YDIAGR=3.
          XDIA=0.
          YDIA=0.
C
          DO 160 KKK=1,NREP
          DO 145 I=LA,LE
          CALSPC(I)=FDAT(KKK,I)
     145  CALSPC(I)=CALSPC(I)+.00001
          CALL FINIM (XDIAGR,YDIAGR)
          XDIA=XDIA+XDIAGR
          YDIA=YDIA+YDIAGR
          NLELA=LE-LA
          CALL DESSIN (CHNNL(LA),CALSPC(LA),NLELA,1,1,1,1,1,15.,10.,0,0,7HCH
         1ANNEL,7,6HCOUNYS,6,-1)
          CALL SYMBL4(11.,9.,.3,0.,8HSPECTRUM,8)
          FNSPEC=KKK
          CALL NUMBER (13.4,9.,.3,0.,FNSPEC,-1)
          IF (KKK/2*2.EQ.KKK) GO TO 150
          XDIAGR=18.
          YDIAGR=14.
          GO TO 160
     150  YDIAGR=-14.
          XDIAGR=0.
     160  CONTINUE
C
          CALL FINIM(-XDIA-2.,-YDIA)
          KMM=(NREP+2)/2
C
          XECK(1)=18*KMM+4
          YECK(1)=30.
          YECK(2)=0.
          XECK(2)=XECK(1)
          XECK(3)=0.
```

```
0224            YECK(3)=0.0
0225            XECK(4)=0.
0226            YECK(4)=30.0
0227            XECK(5)=XECK(1)
0228            YECK(5)=YECK(1)
0229            XECK(6)=XECK(2)
0230            YECK(6)=YECK(2)
          C
0231            CALL LINE(XECK,YECK,5,1,1)
0232            CALL FINTRA
0233          6 CONTINUE
          C
0234       1000 FORMAT (12I5)
0235       1001 FORMAT (F10.4)
0236       1002 FORMAT (18A4)
0237       1003 FORMAT (24I3)
0238       1004 FORMAT (5I6,3F6.3)
0239       1005 FORMAT (4F10.4)
0240       1006 FORMAT (6F10.4)
0241       1007 FORMAT (11(I6,1X))
0242       1008 FORMAT (3X,I3,66A1)
          C
0243       2000 FORMAT (8(E10.4))
          C
0244       4000 FORMAT (///,'  CHECK BACKGROUND DATA SEQUENCE  ',///)
0245       4002 FORMAT (///,'  CHECK SAMPLE DATA SEQUENCE  ',///)
0246       4003 FORMAT (///,'  STANDARD DEVIATION IS NEGATIVE CHECK DATA  ',///)
0247       4004 FORMAT (///,'  VANADIUM CALIBRATION DATA  ',///)
0248       4005 FORMAT (///,'  DATA AFTER VANADIUM CALIBRATION  ',///)
0249       4007 FORMAT (///,'  DATA AFTER BACKGROUND SUBTRACTION  ',///)
0250       4008 FORMAT (///,'  DATA AFTER NEW CHANNEL ASSIGNMENT  ',///)
0251       4009 FORMAT (///,'  DATA AFTER SMOOTHING AFTER CAL  ',///)
0252       4010 FORMAT (///,'  DATA AFTER CORR. FOR AIR ATTENUATION  ',///)
0253       4011 FORMAT (///,'  DATA AFTER CORR. FOR COUNTER SENSITIVITY  ',///)
0254       4012 FORMAT (///,'  DATA AFTER SAMPLE THICKNESS CORRECTION  ',///)
0255       4018 FORMAT (///,'  DATA AT THE END OF DOCHAP IN PUNCH FORMAT  ',///)
0256       4021 FORMAT (///,'  CHECK VANADIUM DATA SEQUENCE  ',///)
0257       4001 FORMAT (///,18A4)
0258       4006 FORMAT (10(F10.2,2X))
0259       4013 FORMAT (1H1,2X,35HAVERAGE ELASTIC PEAK BETWEEN CH NOS,I6,3X,3HAND,
               1I6,3X,11HOF RAW DATA,//)
0260       4014 FORMAT (///,10X,14HCOUNTER NUMBER,33H    AVERAGE ELASTIC PEAK (CH
               1NOS),30H   WIDTH ELASTIC PEAK (CH NOS),4X,22HINTENSITY ELASTIC PEA
               1K,//)
0261       4015 FORMAT (15X,I6,13X,F10.6,21X,F10.6,20X,1PE12.4,/)
0262       4016 FORMAT (6X,7H CH.NO.,8X,5HTF(I),8X,4HE(I),//)
0263       4017 FORMAT (8X,I4,4X,1PE12.4,1PE12.4)
0264       4019 FORMAT (//,3X,11HCOUNTER NO=,I5,//)
```

```
0265        4020 FORMAT (10(1PE11.3,1X))
0266        4022 FORMAT (1H1,///1X,18A4,///)
0267        4023 FORMAT (6X,5HNW  =,I4,3X,5HND  =,I4,3X,5HN1  =,I4,3X,5HN2  =,I4,3X
               1,5HVEL =,I4,//,6X,6HSMON =,E12.5,3X,8HSSCOUN =,E12.5,3X,6HTOTT =,E
               212.5,//)
0268        4024 FORMAT (        6X,21HFIRST   MONITOR PEAK= ,E12.5,1X,8HMICROSEC,//
               16X,21HSECOND MONITOR PEAK =,E12.5,1X,8HMICROSEC,//6X,21HOBSERVATIO
               2N INTERVAL=,E12.5,1X,8HMICROSEC,////6X,10HINPUT BEAM,///8X,5HEO  =
               3,E12.5,1X,3HMEV,11X,8HLAMBDA =,E12.5,1X,8HANGSTROM,//8X,5HEO1 =,E1
               42.5,1X,4H1/CM,10X,8HVO      = ,E12.5,1X,5HM/SEC,//8X,5HEO2 =,E12.5,
               51X,8HE-15 ERG,//8X,5HEO3 =,E12.5,1X,7HE+12 HZ, 7X,9HTCORR   =,E12.
               65,1X,8HMICROSEC,////)
           C
0269        9000 FORMAT (1H1)
0270        9001 FORMAT (1H0)
           C
0271        9999 CONTINUE
           C
0272             STOP
0273             END
```

```
0001            SUBROUTINE VAN (LA,LE,KKK,NVAN,NSIV,NFIV,NSEV,NFEV,SVTOT,SVABS,VST
               1H,ALPHAD,BETAD,SUMCRR)
          C
          C
0002            COMMON /MAVAN/VDAT(20,260)
0003            COMMON DATA(260),E(260)
0004            DIMENSION SUMEL(20)
          C
          C     IF (NVAN.EQ.0)  VANADIUM  DATA  ONLY  READ  IN
          C     IF (NVAN.EQ.1)  VANADIUM  DATA  AND  SAMPLE  DATA  READ  IN
          C     IF (NVAN.EQ.2)  DATA  +  VANADIUM  CORRECTION FACTORS  ONLY  USED
0005            IF (NVAN.EQ.2)  GO TO 52
          C
0006            ALPHAV=ALPHAD/57.29578
0007            BETAV=BETAD/57.29578
0008            VATC=1.597
          C     VATC NUMBER OF VANADIUM ATOMS PER CCM (UNITS OF 10**23)
          C     FLAT SAMPLE IN TRANSMISSION MODE
0009            VVK=1./SIN(BETAV)
0010            VVL=1./SIN(ALPHAV-BETAV)
0011            VNUM=(VVK*SVTOT+VVL*SVABS)*0.1*VATC*VSTH
0012            VNAM=VVL*SVABS*0.1*VATC*VSTH
0013            VTHCRR=EXP(-VNAM)*VNUM
0014            VTHCRR=VTHCRR/(1.-EXP(-VNUM))
0015            AV=0.0
          C
0016            DO 22 I=NSIV,NFIV
0017            SUMIN=VDAT(KKK,I)
0018            AV=AV+SUMIN
0019         22 CONTINUE
          C
0020            INCH=NFIV-NSIV
0021            CH=FLOAT(INCH)+1.0
0022            AV=AV/CH
          C
0023            DO 23 J=LA,LE
0024            VDAT(KKK,J)=VDAT(KKK,J)-AV
0025            IF (NVAN.EQ.0) DATA(J)=VDAT(KKK,J)
0026         23 CONTINUE
          C
0027            SUMEL(KKK)=0.0
0028            AVCH=0.0
          C
0029            DO 24 K=NSEV,NFEV
0030            AK=K
0031            SUMEL(KKK)=VDAT(KKK,K)+SUMEL(KKK)
0032            AVCH=AVCH+VDAT(KKK,K)*AK
0033         24 CONTINUE
```

```
                C
 0034                 AVCH=AVCH/SUMEL(KKK)
 0035                 SUM=SUMEL(KKK)/SUMEL(1)
                C
                C     SUM..INTEGRATED ELASTIC PEAK INTENSITY RELATIVE TO COUNTER ONE
                C
 0036                 SUMCRR=SUM*VTHCRR
 0037                 PUNCH 2000,SUMCRR
 0038                 SIGMA=0.0
                C
 0039                 DO  27 I=NSEV,NFEV
 0040                 BI=I
 0041                 SIGMA=SIGMA+VDAT(KKK,I)*(BI-AVCH)**2
 0042              27 CONTINUE
                C
 0043                 SIGMA=SIGMA/SUMEL(KKK)
 0044                 IF (SIGMA.GT.0.) GO TO 40
 0045                 IF (SIGMA.LE.0.) WRITE (6,4000)
 0046                 SIGMA=0.000001
 0047              40 SIGMA=SQRT(SIGMA)
 0048                 WIDTH=2.3548*SIGMA
                C
 0049                 WRITE (6,4001) NSIV,NFIV,NSEV,NFEV
 0050                 WRITE (6,4002) SVTOT,SVABS
 0051                 WRITE (6,4003) VSTH,ALPHAD,BETAD,VTHCRR
 0052                 WRITE (6,4004) SUM,WIDTH,AVCH
 0053                 WRITE (6,4005) (VDAT(KKK,I),I=LA,LE)
                C
 0054                 DO 70 L=LA,LE
 0055                 DATA(L)=DATA(L)*SUMCRR
 0056              70 CONTINUE
                C
 0057                 IF (NVAN.LE.1) GO TO 101
 0058              52 CONTINUE
 0059                 WRITE (6,4006) SUMCRR,ALPHAD,BETAD
                C
 0060                 DO 25 L=LA,LE
 0061                 DATA(L)=DATA(L)*SUMCRR
 0062              25 CONTINUE
                C
 0063                 GO TO 9999
 0064             101 WRITE (6,4006) SUMCRR,ALPHAD,BETAD
                C
                C
 0065            2000 FORMAT (F10.4)
                C
 0066            4000 FORMAT (//,42H STANDARD DEVIATION IS NEGATIVE CHECK DATA,//)
 0067            4001 FORMAT (29H BACKGROUND TAKEN BETWEEN CHS,I5,1X,3HAND,I5,1X,24HAND
```

```
                1ELASTIC PEAK BETWEEN,I5,1X,3HAND,I5,//)
 0068      4002 FORMAT (21H VANADIUM TOTAL XSEC=,F8.3,3X,20HAND ABSORPTION XSEC=,F
                18.3,3X,5HBARNS//)
 0069      4003 FORMAT (1X,F6.3,46HCM  VANADIUM THICKNESS CORRECTION WITH ALPHA =,
                1F8.4,3X,9HAND BETA=,F8.4,3X,2HIS,F8.5,//)
 0070      4004 FORMAT (56H VANADIUM ELASTIC PEAK INTENSITY RELATIVE TO COUNTER 1
                1=,F8.4,3X,6HWIDTH=,F8.4,3X,18HAVERAGE CHANNEL = ,F8.2,//)
 0071      4005 FORMAT (10(F10.2,2X))
 0072      4006 FORMAT (//,32H VANADIUM NORMALISING FACTOR IS=,F8.4,3X,6HALPHA=,F8
                1.4,3X,5HBETA=,F8.4,//)
          C
 0073      9999 RETURN
          C
 0074           END
```



```
 0001           SUBROUTINE BAGD(LA,LE,KKK)
          C
          C
 0002           COMMON DATA(260),E(260)
 0003           COMMON /MABAG/BG(20,260)
          C
 0004           DO 1 I=LA,LE
 0005           DATA(I)=DATA(I)-BG(KKK,I)
 0006           IF (DATA (I).LT.0.0) DATA(I)=0.
 0007         1 CONTINUE
          C
 0008           RETURN
 0009           END
```

```
0001              SUBROUTINE CHANA(NFR,NEND)
            C
            C
            C     SHIFT AND RE-NUMBERING OF CHANNELS
            C
0002              COMMON D(260),E(260)
0003              DIMENSION DS(520)
0004              ND=NEND-NFR
0005              NA=ND+1
0006              NE=ND+NFR-1
            C
0007              DO 11 I=1,NFR
0008              DS(I+NEND)=D(I+1)
0009           11 D(I)=0.0
            C
0010              DO 22 I=1,ND
0011              D(I)=D(I+NFR)
0012           22 D(I+NFR)=0.0
            C
0013              DO 33 I=NA,NE
0014           33 D(I)=DS(I+NFR)
            C
0015              RETURN
0016              END
```

```
      SUBROUTINE CAL(NFR,NEND,NW,ND,N1,N2,NEL,SM,SZ,TT)
C
C
C     CAL CALIBRATES CHANNELS INTO UNITS OF TIME-OF-FLIGHT AND ENERGY
C
      COMMON/MACAL/TEXT(18),TF(260),T1,T2,T3,E0,WLAM0,E01,V0,E02,E03,TCO
     1RR
      COMMON D(260),E(260)
C
C
      NP=NEND
      T1=N1*NW+16*ND
      T2=N2*NW+16*ND
      T3=NP*NW+16*ND
      DELT=T3+T1-T2
      NSEL=NEL+NEND-NFR
C
      E0=5226.94*1000.*((SM/DELT)**2)
      E01=8.066973*E0
      E02=1.60209*E0
      E03=E02/6.62517
      WLAM0=9.04427/SQRT(E0)
      V0=3956.03/WLAM0
      TWEL=72.3*SZ/SQRT(E0/1000.)
      TMEL=NSEL*NW+16*ND
      TCORR=TWEL-TMEL
C
      NEND1=NEND-1
      DO 44 I=1,NEND1
      TF(I)=I*NW+16*ND
      TF(I)=(TF(I)+TCORR)/SZ
   44 E(I)=5226.94*1000./TF(I)**2
C
      RETURN
      END
```

```
      SUBROUTINE SMOOTH(N,NSMA,LA,LE)
C
C
      COMMON DATA(260),E(260)
      DIMENSION DATAS(260),PP(11)
      DIMENSION X(260)
C
      GO TO (71,72,73,74,75,76,77),NSMA
C
   71 WRITE (6,1071)
      M=N-4
      GO TO 99
   72 WRITE (6,1072)
      M=N-6
      GO TO 99
   73 WRITE (6,1073)
      M=N-6
      GO TO 99
   74 WRITE (6,1074)
      M=N-8
      GO TO 99
   75 WRITE (6,1075)
      M=N-8
      GO TO 99
   76 WRITE (6,1076)
      M=N-10
      GO TO 99
   77 WRITE (6,1077)
      M=N-10
C
   99 DO 200 I=LA,M
      PP(1)=DATA(I)
      PP(2)=DATA(I+1)
      PP(3)=DATA(I+2)
      PP(4)=DATA(I+3)
      PP(5)=DATA(I+4)
      PP(6)=DATA(I+5)
      PP(7)=DATA(I+6)
      PP(8)=DATA(I+7)
      PP(9)=DATA(I+8)
      PP(10)=DATA(I+9)
      PP(11)=DATA(I+10)
      GO TO (61,62,63,64,65,66,67),  NSMA
C
   61 SUM=17.*PP(3)+12.*(PP(2)+PP(4))-3.*(PP(1)+PP(5))
      DATAS(I+2)=SUM/35.
      GO TO 200
   62 SUM=7.*PP(4)+6.*(PP(3)+PP(5))+3.*(PP(2)+PP(6))-2.*(PP(1)+PP(7))
```

```
            DATAS(I+3)=SUM/21.
            GO TO 200
         63 SUM=131.*PP(4)+75.*(PP(3)+PP(5))-30.*(PP(2)+PP(6))+5.*(PP(1)+PP(7)
           1)
            DATAS(I+3)=SUM/231.
            GO TO 200
         64 SUM=59.*PP(5)+54.*(PP(4)+PP(6))+39.*(PP(3)+PP(7))+14.*(PP(2)+PP(8)
           1)-21.*(PP(1)+PP(9))
            DATAS(I+4)=SUM/231.
            GO TO 200
         65 SUM=179.*PP(5)+135.*(PP(4)+PP(6))+30.*(PP(3)+PP(7))-55.*(PP(2)+PP(
           18))+15.*(PP(1)+PP(9))
            DATAS(I+4)=SUM/429.
            GO TO 200
         66 SUM=89.*PP(6)+84.*(PP(5)+PP(7))+69.*(PP(4)+PP(8))+44.*(PP(3)+PP(9)
           1)+9.*(PP(2)+PP(10))-36.*(PP(1)+PP(11))
            DATAS(I+5)=SUM/429.
            GO TO 200
         67 SUM=143.*PP(6)+120.*(PP(5)+PP(7))+60.*(PP(4)+PP(8))-10.*(PP(3)+PP(
           19))-45.*(PP(2)+PP(10))+18.*(PP(1)+PP(11))
            DATAS(I+5)=SUM/429.
        200 CONTINUE
      C
            DO 201 I=LA,LE
            DATA(I)=DATAS(I)
        201 CONTINUE
      C
            GO TO (51,52,53,54,55,56,57 ),  NSMA
         51 LA=LA+2
            LE=LE-2
            GO TO 100
         52 LA=LA+3
            LE=LE-3
            GO TO 100
         53 LA=LA+3
            LE=LE-3
            GO TO 100
         54 LA=LA+4
            LE=LE-4
            GO TO 100
         55 LA=LA+4
            LE=LE-4
            GO TO 100
         56 LA=LA+5
            LE=LE-5
            GO TO 100
         57 LA=LA+5
            LE=LE-5
```

```
              GO TO 100
          100 N=M
      C
              WRITE (6,1078) (DATA(I),I=LA,LE)
              WRITE (6,1079)
              DO 220 I=LA,LE
          220 X(I)=I
              CALL GRAPH (1,M,0.,0,-1,-1,X(LA),DATA(LA),Y2,Y3)
      C
      C       NSMA=1  POL=2,3    5 POINTS
      C       NSMA=2  POL=2,3    7 POINTS
      C       NSMA=3  POL=4,5    7 POINTS
      C       NSMA=4  POL=2,3    9 POINTS
      C       NSMA=5  POL=4,5    9 POINTS
      C       NSMA=6  POL=2,3   11 POINTS
      C       NSMA=7  POL=4,5   11 POINTS
      C
         1071 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.2/3, 5 PNTS,//)
         1072 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.2/3, 7 PNTS,//)
         1073 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.4/5, 7 PNTS,//)
         1074 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.2/3, 9 PNTS,//)
         1075 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.4/5, 9 PNTS,//)
         1076 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.2/3,11 PNTS,//)
         1077 FORMAT (      //,7X,41HSMOOTHING WITH POLYNOM OF DEG.4/5,11 PNTS,//)
         1078 FORMAT (10(F10.2,2X))
         1079 FORMAT (1H0)
      C
      C
              RETURN
              END
```

```
      SUBROUTINE AIR(K1,K2)
C
C
      COMMON D(260),E(260)
      DIMENSION A1(15),B1(15),A2(18),B2(18),AN(260)
C
      DATA A1/2.,4.,7.,7.4,10.,11.5,14.5,20.,30.,37.,40.,70.,100.,185.,7
     100./
      DATA B1/8.6,6.6,5.3,5.2,4.75,4.6,4.45,4.3,4.15,4.1,4.05,3.9,3.85,3
     1.75,3.71/
      DATA A2/2.,4.,5.5,5.6,7.4,7.5,9.2,10.,13.,15.,20.,24.,40.,62.,100.
     1,120.,330.,700./
      DATA B2/24.,20.8,18.7,18.6,16.6,16.5,15.5,15.1,14.2,13.8,13.2,12.9
     1,12.3,11.8,11.4,11.2,10.65,10.5/
C
      G=0.007379
C     G ...NUMBER OF AIR MOLECULES PER CCM*FLIGHT PATH LENGTH*2
C           AT T=298 K AND P=745 TORR FOR L=153 CM
C           IN UNITS OF 10**24 CM**3*CM
C           G=(6.0248*10**23*L/V)*2.
C           V=P0*T*V0/(P*T0)
C
      K9=K1
      DO 1 N=K1,K2
      IF((E(N)-2.0)*(E(N)-700.0))3,2,2
    2 K9=N+1
      GO TO 1
    3 DO 6 I=1,14
      IF((E(N)-A1(I))*(E(N)-A1(I+1)))7,7,6
    7 STO=(B1(I)*A1(I+1)-A1(I)*B1(I+1)+E(N)*(B1(I+1)-B1(I)))/(A1(I+1)-A1
     1(I))
C
C     STO...TOTAL CROSS SECTION OF OXYGEN IN BARN
C
      GO TO 8
    6 CONTINUE
    8 DO 9 I=1,17
      IF((E(N)-A2(I))*(E(N)-A2(I+1)))10,10,9
C
   10 STN=(B2(I)*A2(I+1)-A2(I)*B2(I+1)+E(N)*(B2(I+1)-B2(I)))/(A2(I+1)-A2
     1(I))
C
C     STN...TOTAL CROSS SECTION OF NITROGEN IN BARN
C
      GO TO 11
    9 CONTINUE
   11 AN(N)=EXP(-G*(0.2*STO+0.8*STN))
      D(N)=D(N)/AN(N)
```

```
FORTRAN IV G LEVEL 1, MOD 2                AIR                DATE = 70321           09/21/19

0026              1 CONTINUE
           C
0027                RETURN
0028                END
```

```
FORTRAN IV G LEVEL 1, MOD 2                CTR                DATE = 70321           09/21/19

0001                SUBROUTINE CTR(K1,K2)
           C
           C
0002                COMMON DATA(260),E(260)
0003                DIMENSION CN(260)
           C
0004                FINTF(X)=EXP(PSR*SQRT(1.-X**2))
           C
0005                F=0.58034
0006                R=1.25
           C
           C        F   ...MACROSCOPIC CROSS SECTION OF HE3 AT 25,3 MEV IN 1/CM FOR 4AT
           C        R   ...DETECTOR RADIUS IN CM
           C
0007                DO 1 I=K1,K2
0008                PSR=-2.0*R*F*SQRT(25.3/E(I))
0009                H=0.01
0010                FPAIR=0.0
0011                FIMP=0.0
           C
0012                DO 4 K=1,99,2
0013              4 FIMP=FIMP+FINTF(H*FLOAT(K))
           C
0014                DO 5 K=2,100,2
0015              5 FPAIR=FPAIR+FINTF(H*FLOAT(K))
           C
0016                CN(I)=1.0-H*(1.0+FINTF(1.0)+2.*FPAIR+4.*FIMP)/3.
0017                DATA(I)=DATA(I)/CN(I)
           C
0018              1 CONTINUE
           C
0019                RETURN
0020                END
```

```
      SUBROUTINE THICK (LA,LE,NCC,ATW,DENS,STOT,SABS,STH,ALPHAD,BETA)
C
C
      COMMON DATA(260),E(260)
      DIMENSION SN(260)
C
      ALPHAS=ALPHAD/57.29578
      BETAS=BETA/57.29578
      VK=1./SIN(BETAS)
      VL=1./SIN(ALPHAS-BETAS)
      ATC=6.02252*DENS/ATW
C
      GO TO  (1,2),NCC
C
C     FLAT SAMPLE IN TRANSMISSION POSITION
    1 DO 30 N=LA,LE
      SA=SABS*SQRT(25.3/E(N))
      SNUM=(VK*STOT+VL*SA)*0.1*ATC*STH
      SNAM=VL*SA*0.1*ATC*STH
   30 SN(N)=EXP(-SNAM)*SNUM/(1.-EXP(-SNUM))
      GO TO 4
C
C     FLAT SAMPLE IN REFLEXION POSITION
    2 DO 5 N=LA,LE
      SA=SABS*SQRT(25.3/E(N))
      SNUM=(VK*STOT+VL*SA)*0.1*ATC*STH
    5 SN(N)=SNUM/(1.-EXP(-SNUM))
      GO TO 4
C
    4 DO 7 N=LA,LE
      DATA(N)=DATA(N)*SN(N)
    7 CONTINUE
C
      RETURN
      END
```

To disseminate knowledge is to disseminate prosperity — I mean general prosperity and not individual riches — and with prosperity disappears the greater part of the evil which is our heritage from darker times.

Alfred Nobel

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