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A data reduction program for the linac total-scattering amorphous materials spectrometer (LINDA)

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A DATA REDUCTION PROGRAM FOR THE LINAC TOTAL-SCATTERING AMORPHOUS MATERIALS SPECTROMETER (LINDA)

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ABSTRACT

A computer program has been written to reduce the data collected on the A.E.R.E., Harwell linac total-scattering spectrometer (TSS) to the differential scattering cross-section. This instrument, used for studying the structure of amorphous materials such as liquids and glasses, has been described in detail [1]. Time-of-flight spectra are recorded by several arrays of detectors at different angles using a pulsed incident neutron beam with a continuous distribution of wavelengths.

The program performs all necessary background and container subtractions and also absorption corrections using the method of Paalman and Pings [2]. The incident neutron energy distribution is obtained from the intensity recorded from a standard vanadium sample, enabling the observed differential scattering cross-section $\frac{d\sigma}{d\Omega}(\theta,\lambda)$ and the structure factor S(Q) to be obtained.

Various sample and vanadium geometries can be analysed by the program and facilities exist for the summation of data sets, smoothing of data, application of Placzek corrections [3] and the output of processed data onto magnetic tape or punched cards.

A set of example data is provided and some structure factors are shown with absorption corrections.

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ILLUSTRATIONS

1. Introduction

A schematic diagram of the spectrometer is shown in Fig. 1. A more detailed description of the apparatus is given by Sinclair et al [1].

Pulsed neutrons, at a repetition rate of 192 Hz, are incident on the sample from the moderator. The energy distribution of these neutrons is shown in Fig. 2. The time taken for each neutron after emission from the moderator to travel the 4.75m to the detector is called its time-of-flight. Between each burst it is possible to record the arrival of these neutrons and to sort them into 2048 channels of width 2 μs. An initial timing delay of a few hundred μseconds is used in the system to select neutrons with the shortest wavelength of interest.

After some hours a time-of-flight distribution will have been recorded for each detector. In general, each experiment would consist of several samples, e.g. sample, container, vanadium and background.

The samples may be changed automatically after a preset monitor count, usually taking some minutes, so that several time-of-flight distributions can be recorded for different samples and detectors. These distributions can be written onto magnetic tape for subsequent analysis using the computer program described in this report. The collection of the time-of-flight data and the transfer to magnetic tape is described in the program DATIN and TAPRIT, Johnson [2].

2. Calculations used in this program

(a) The Q-value

If it is assumed that the scattering process was elastic with no recoil of the scattering molecule the velocity of the neutron is given by:

$$V = \frac{L_o + L_s}{ID + (n - ½)\Delta t} \qquad \text{... (1)}$$

ID is the initial timing delay or the time period after the firing of the electron pulse at which the counting began, n is the number and Δt is the width of the time channel, L_o and L_s are the lengths of the initial and secondary flight paths. The Q-value for this event is given by:

$$Q = \frac{4\pi \sin(\theta/2)(L_o + L_s)252.7}{ID + (n - ½)\Delta t} \qquad \text{... (2)}$$

Where θ is the angle of the detector (scattering angle). If L_o and L_s are in metres, ID and Δt are in microseconds then Q will be in reciprocal Ångströms.

If in the model adopted for the data analysis the nucleus of effective mass number M is allowed to recoil then:

$$Q = \frac{2\pi(L_o + L_s)252.7}{[ID + (n - ½)\Delta t]\ x}\left(\frac{L_s}{L_o} + \left[1 - \frac{L_s}{L_o}\right] x\right)\sqrt{1 + x^2 - 2\,x\cos\theta} \qquad \ldots (3)$$

and

$$x = \sqrt{1 - \frac{2M}{(M+1)^2}\left\{1 - \cos\left[\theta + \sin^{-1}\frac{(\sin\theta)}{M}\right]\right\}} \qquad \ldots (4)$$

x is the ratio of the neutron velocity after being scattered to its initial velocity.

One of the three options can be requested for the form of the output data. These are Q-value, time-of-flight or wavelength. The recoil correction can be requested but the default option in the program will calculate the Q-scale from equation (2).

(b) The scattered intensity $I^s(Q)$

If time-of-flight distributions are recorded for a sample and container $I^{s+c}(Q)$ and for an empty container $I^c(Q)$, then the sample intensity $I^s(Q)$ is:

$$I^s(Q) = \frac{I^{s+c}(Q)}{M^{s+c}\ Ass} - \frac{I^c(Q)\ Acs}{M^c\ Ass\ Acc} \qquad \ldots (5)$$

M^{s+c} and M^c are the monitor counts for the two experiments. Ass, Acc and Acs are correction terms for absorption effects, calculated for cylindrical samples by the technique of Paalman and Pings [3].

For flat plates a similar calculation is performed. If A_1 is the attenuation factor for one window of the container of thickness t_w where;

$$t_w = (t_c - t_s)/2$$

with t_c and t_s the inner and outer widths of the can, and if A_2 is the attenuation factor for the sample then it can be shown that;

In transmission ($\theta \leqslant \pi/2$)

$$I^s(Q) = \frac{I^{s+c}(Q)}{A_1^2 A_2} - \frac{I^c(Q)}{A_1^2} \qquad \ldots (6)$$

Where $$A_1 = \frac{\cos\phi\cos(\theta-\phi)}{\rho_c t_w \sigma_c\,[\cos\phi - \cos(\theta-\phi)]}\left\{\exp\left[-\frac{\rho_c\sigma_c t_w}{\cos\phi}\right] - \exp\left[-\frac{\rho_c\sigma_c t_w}{\cos(\theta-\phi)}\right]\right\} \qquad \ldots (7)$$

and $$A_2 = \frac{\cos\phi\cos(\theta-\phi)}{\rho_s t_s \sigma_s\,[\cos\phi - \cos(\theta-\phi)]}\left\{\exp\left[-\frac{\rho_s\sigma_s t_s}{\cos\phi}\right] - \exp\left[-\frac{\rho_s\sigma_s t_s}{\cos(\theta-\phi)}\right]\right\} \qquad \ldots (8)$$

In reflection ($\theta \geqslant \pi/2$)

$$I^s(Q) = \frac{I^{s+c}(Q)}{A_1^2 A_2} - \frac{I^c(Q)(1 + A_1^2 A_2^2)}{(1 + A_1^2)\,A_1^2 A_2} \qquad \ldots (9)$$

Where $$A_1 = \frac{\cos\phi\cos(\theta+\phi)}{\rho_c t_w \sigma_c\,[\cos\phi - \cos(\theta+\phi)]}\left\{\exp\left[-t_w\rho_c\sigma_c\left(\frac{1}{\cos\phi} - \frac{1}{\cos[\theta+\phi]}\right)\right] - 1\right\} \qquad \ldots (10)$$

and $$A_2 = \frac{\cos\phi\cos(\theta+\phi)}{\rho_s t_s \sigma_s\,[\cos\phi - \cos(\theta+\phi)]}\left\{\exp\left[-t_s\rho_s\sigma_s\left(\frac{1}{\cos\phi} - \frac{1}{\cos[\theta+\phi]}\right)\right] - 1\right\} \qquad \ldots (11)$$

ϕ is the angle between the incident beam and a vector drawn normal to the can surface. θ is the scattering angle and σ_s and σ_c are the sample and can removal cross-sections (absorption + scattering).

Equations (7) and (8) above describing the attenuation of a plate in transmission geometry have a singularity when the scattering process is symmetric i.e. when $2\phi = \theta$. This is overcome in the program by setting the attenuation factor equal to the value obtained at $\theta = 0°$ as for symmetric scattering the neutron path lengths are identical. So that

$$A_1 = \exp\left[-\frac{\rho_c\sigma_c t_c}{\cos\phi}\right] \qquad (2\phi = \theta) \qquad \ldots (7a)$$

and $$A_2 = \exp\left[-\frac{\rho_s\sigma_s t_s}{\cos\phi}\right] \qquad (2\phi = \theta) \qquad \ldots (8a)$$

The calculated value of this attenuation factor should be compared with the experimentally observed transmission ratio on the downstream fission chamber which is evaluated in the program when $\theta = 0°$ as,

$$R_s(t) = \frac{I^{c+s}(t)\,M^c}{I^c(t)\,M^{c+s}} = 1 - \exp\left[-\frac{t_s\rho_s\sigma_s^{(abs+scatter)}}{\cos\phi}\right]$$

for both sample and vanadium. The calculated value of this ratio is also plotted as a continuous line.

The sub-routine ABSORP evaluates these terms. As the incident neutrons have an energy distribution, the absorption cross-section is computed for each time channel and the program requires the value of the absorption cross-sections at 1.88Å as provided in BNL-325 [4].

The total cross-section may also be used in the Paalman and Pings routine to give a correction for self-shielding i.e. the reduction of the intensity of the incident beam by the scattering of the sample. The effect of this correction on any subsequent multiple scattering correction must be considered. The scattering cross-section is read by the program through the sub-routine, READ1. It requires the cross-section as a two dimensional array of energy versus cross-section of up to 40 values.

The function BARN1 interpolates this array to produce a scattering cross-section for ABSORP if required and for the calculation of S(Q), the structure factor. The default state of the program does not apply a self-shielding correction.

If the energy variation of the scattering cross-section is not used in the program, then the provision of one cross-section value at any energy will cover the whole spectrum.

(c) The spectrum shape $I^v(Q)$

A standard sample of vanadium is studied together with the background. Because vanadium is an almost isotropic, incoherent neutron scatterer, the measured time-of-flight distribution, after background subtraction and absorption correction, represents the energy distribution of the incident neutron beam as shown in Fig. 2.

The measured sample intensity $I^s(Q)$ can then be divided by the appropriate component of the incident energy spectrum $I^v(Q)$. The vanadium standard, which may be a cylinder, an annular sleeve (to reduce absorption) or a flat plate, is corrected for self-absorption and the normalized counting ratio R(Q) is obtained if the parameter CRYOST=T is coded in the data list &CONTRL.

$$R(Q) = \frac{\dfrac{I^{s+c}(Q)}{M^{s+c}\,Ass} - \dfrac{I^c(Q)\,Acs}{M^c\,Ass\,Acc}}{\dfrac{I^{v+b}(Q)}{M^{v+b}\,A^vss} - \dfrac{I^b(Q)}{M^b\,A^vss}} \qquad \ldots (12)$$

The absorption corrections are simpler for the vanadium standard because there is negligible absorption of neutrons by the background. M^b and M^{v+b} are the background and vanadium monitor counts and $A^v ss$ is the self absorption of the vanadium sample.

An additional correction may be made for the absorption of the background intensity by the sample. In equation (5) Section 2(b) the Paalman and Pings absorption correction procedure reduces the intensity of the empty container $I^c(Q)$ by the factor Acs. This represents the absorption of neutrons which are scattered by the container and absorbed by the sample. However, a proportion of these neutrons $I^b(Q)$ are not from the container but are due to external background sources such as air scattering in the counter aperture and in the incident collimator.

If these neutrons are assumed to have passed through the sample en route to the detector, too large a background contribution will be subtracted, particularly in the case of strongly absorbing samples such as bromine or carbon tetrachloride. This is best corrected experimentally by evacuating the sample area as in a cryostat or furnace.

If a vacuum enclosure has been used the ratio R(Q) is calculated according to equation (12). However, if air scattering was present, an option exists in the program to calculate R(Q), i.e. if CRYOST=F in the list &CONTRL.

$$R(Q) = \frac{\left[\frac{I^{s+c}(Q)}{M^{s+c}} - \frac{I^b(Q)}{M^b}\right]\frac{1}{Ass} - \left[\frac{I^c(Q)}{M^c} - \frac{I^b(Q)}{M^b}\right]\frac{Acs}{AssAcc}}{\left[\frac{I^{v+b}(Q)}{M^{v+b}} - \frac{I^b(Q)}{M^b}\right]\frac{1}{A^v ss}} \quad \ldots (13)$$

(d) The observed differential scattering cross-section $\frac{d\sigma}{d\Omega}(\theta,\lambda)$ at each angle

The differential scattering cross-section $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$ can be calculated at each detector angle by using the known scattering cross-section of the vanadium standard so that if the parameter EXPO=T is coded in the input list &CONTRL,

$$\left.\frac{d\sigma}{d\Omega}\right|^{eff} = \frac{R(Q)\,A_v\,[1 - \exp(-\rho_v\sigma_v t_v)]\,\sigma_s^T}{A_s 4\pi\,[1 - \exp(-\rho_s\sigma_s t_s)]} \quad \ldots (14)$$

R(Q) is the ratio (12,13), ρ_v and ρ_s are the number of atoms and molecules per cubic Ångström in the vanadium and sample respectively, t_v and t_s are the effective plate thicknesses of the vanadium and sample in centimetres, A_V and A_S are the effective areas, σ_S^T is the total scattering cross-section of the sample and σ_V is the scattering cross-section of vanadium.

For a cylinder radius r, the effective plate thickness is

$$2rt = \pi r^2$$

$$t = \frac{\pi r}{2} \qquad \text{... (15)}$$

and A = 2r is the area/unit height presented to the beam.

This function is tabulated and plotted for each counter. If EXPO=F is coded in the input list &CONTRL, a simpler formalism is used.

$$\left.\frac{d\sigma}{d\Omega}\right|^{eff} = \frac{R(Q)\, r_V^2 \rho_V \sigma_V}{r_S^2 \rho_S} \qquad \text{if VROD=T \& SROD=T} \qquad \text{... (16)}$$

$$\left.\frac{d\sigma}{d\Omega}\right|^{eff} = \frac{R(Q)\,(r_V''^2 - r_V'^2)\, \rho_V \sigma_V}{r_S^2 \rho_S} \qquad \text{if VCOIL=T \& SROD=T} \qquad \text{... (17)}$$

and

$$\left.\frac{d\sigma}{d\Omega}\right|^{eff} = \frac{R(Q)\, t_V \rho_V \sigma_V \cos\theta_S}{t_S \rho_S \cos\theta_V} \qquad \text{if VPLATE=T \& SPLATE=T} \qquad \text{... (18)}$$

where r_S, r_V, r_V' and r_V'' are the radii of the sample and vanadium and θ_S, θ_V are the angles of the normals of the plates to the beam.

(e) The structure factor S(Q) at each angle

The structure factor S(Q) can be calculated at each angle by the expression

$$S(Q) = 1 + \frac{4\pi}{\sigma_S^{coh}} \left.\frac{d\sigma}{d\Omega}\right|^{eff} - \frac{\sigma_S^T}{\sigma_S^{coh}} \left\{1 + P1 + P2 + \frac{P3}{Q^2}\right\} \qquad \text{... (19)}$$

σ_S^{coh} is the sample coherent scattering cross-section, P1, P2 and P3 are Placzek correction terms [5-7]. These are

$$P1 + P2 = \frac{2}{M}\left[1 - f(1-2n)\right] \sin^2\frac{\theta}{2} + \frac{2}{M^2}\left[1 - f(1-2n)(1+2nf)\sin^2\frac{\theta}{2}\right] \sin^2\frac{\theta}{2} \qquad \text{... (20)}$$

and $$P3 = \frac{1.9366\bar{E}\sin^2\frac{\theta}{2}}{3MQ^2}\left[\cos\theta - 2f(1+2n)(1-2f[1+n]\sin^2\frac{\theta}{2})\right]$$

Where $\bar{E}$ is the mean kinetic energy of the molecule in meV and M is the effective molecular mass in amu. f is the fractional flight path;

$$f = \frac{L_s}{L_o + L_s} \qquad \ldots (21)$$

and n is the spectrum index ($\approx$ .83) [7].

S(Q) is listed and plotted for each counter. In addition if specified in the input options, S(Q) or $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$ will be punched to cards as Q,S(Q) or [Q, $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$].

Due to the complexity of Placzek corrections [6,7,10] for a linac experiment, it is suggested that a user wishing to apply his own form of corrections should use this program to evaluate the observed differential scattering cross-section $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$. These data may be then obtained on cards for subsequent Placzek correction.

(f) The deadtime correction

The mathematical formalism used to correct for the effect of a deadtime in the counting system has been described by Egelstaff [8]. If there are n_d dead channels after each recorded count and there are a total of N machine cycles, then the true count in channel n is given by

$$C_n^1 = \frac{C_n N}{\left[N - \sum_{m=n-n_d}^{m=n-1} C_m\right]} \qquad \ldots (22)$$

In the PDP-11 computer used to record data on the Linac total-scattering spectrometer, each detector has a separate input buffer store so that the deadtime corrections are not cross-linked between different counters.

(g) Equal Q-steps option

In the study of liquids and glasses most forms of data analysis, Fourier transforms in particular, require the data to be in equal Q-value increments.

As the data are collected as time-of-flight spectra the data increments as a function of Q-value are inversely proportional to the time-of-flight and are non-linear.

The option of equal Q-value steps is specified by

EQUALQ=T in &LINAC   Section 3(b)   (Default is T)

The routine QBIN first reads the stored S(Q) or $\frac{d\sigma}{d\Omega}\Big|^{eff}$ from a scratch disc. A set of data points are then produced at $.002Å^{-1}$ intervals by linear interpolation using a cubic spline. This distribution is then smoothed by a rectangular smoothing function, Section 2(h). The width of this function is the fractional Q-value resolution for each detector. Default values are used in the program but can be overwritten. Data points are then obtained from every $0.05Å^{-1}$ Q-value point in the spectrum. These values are listed, plotted and, if required, punched to cards. The namelist &QEQUAL is described in Section 3(j).

(h) Data smoothing options

Two options exist for smoothing data in the program and can both be specified in the &CONTRL list described in Section 3(f).

(i) SMOOTH=T, will smooth the vanadium and background patterns.

(ii) CAN=T, will smooth the container pattern.

The routine SMTH removes the peak due to the Linac Cell I neutron booster. This is observed in Cell II between 2550 and 2750 μsecs, after the firing of the electron pulse. The routine linearly interpolates the pattern between the two intensities at 2550 μsecs and 2750 μsecs.

A rectangular smoothing function is then convoluted with the data. The width of this function is equal to the incident neutron pulse width and is thus proportional to the time-of-flight channel number. The smoothed intensity $I_s(\bar{t})$ is given by

$$I_s(\bar{t}) = \frac{\sum_{t_1}^{t_2} I(t)\,\Delta t}{t_2 - t_1} \left[\begin{array}{l} t_1 = \bar{t} - w\bar{t} \\ t_2 = \bar{t} + w\bar{t} \end{array} \right] \qquad \ldots (23)$$

t_1 and t_2 are the lower and upper time limits and w is the fractional pulse width. The default value for w is 0.1, this can be overwritten in the name list, &CONTRL. SMTH plots graphs of each pattern after smoothing which are compared with the input data.

The use of the smoothing option is not advisable if there are Bragg peaks present in the data.

3. The format of the input data

(a) Use of the NAMELIST statement

The IBM function NAMELIST is used to input the majority of the program control data. This function is described in greater detail in [9]. Briefly, a list of variables is specified in the program and read into the program in a simple format, e.g. the list called LINAC is read as follows

&LINAC NRUN=1,ID=390,TFP=4.615,.....,&END

The first column of each card must be blank and the keywords LINAC and END must be preceded by Ampersands. The variables can be listed in any order. If a variable is not listed the program uses a default option. Logical variables such as ABSORB can be assigned values by the statements ABSORB=.TRUE. or ABSORB=T.

Multiple values may be input in two ways, e.g.

NC = 0,0,0,0,1,0,0,0,

or NC = 4*0,1,3*0,

All data relevant to the recorded data will be written onto the header block of the magnetic tape, e.g. monitors, counter angles etc. These data can also be overwritten by the input list described in this section. A minimum default input case is shown in section 4 together with a maximum input case.

All namelist parameters are printed on channel 13 immediately after they have been read.

(b) The calling routine &LINAC

&LINAC has the following variables of which the majority are default values written on the control block of the magnetic tape.

Variable	Description	Program-supplied value
VOLUME	'Name of magnetic tape' in apostrophes e.g. 'A3CMPH'	No default
NC(8)	Number of counters at each angle	(8*1)
TRANS(8)	If .TRUE. sample was studied in transmission If .FALSE. sample was studied in reflection (Applies to flat-plate experiments only)	.TRUE.

Unless there is a special reason, from this point the remaining variables need not be coded.

Variable	Description	Program-supplied value
NRUN	No. of sets of data to be analysed	1
ID	Initial timing delay in microseconds	Read from tape
TFP	Total flight path in metres	Read from tape
SFP	Second flight path in metres	Read from tape
CA(8)	Counter angles in degrees	Read from tape
ITAPE	7 or 9-track input tape	9
EQUALQ	If .TRUE. the routine QBIN is called and the data will be placed in equal Q-steps	.TRUE.
MON	If .TRUE. monitors will be read from tape If .FALSE. monitors will be read from cards	.TRUE.
DEAD	If .TRUE. deadtime corrections are applied	.TRUE.
NDEAD	No. of dead channels in TOF scaler	Read from tape
CHAN	Width of TOF channels in microseconds (integer)	Read from tape
NCTRS	No. of counters written on tape	Read from tape

The program then reads a list of runs required which must be on the magnetic tape. The list is in free format so that the last run number must be followed by a slash. These runs are read from the magnetic tape and then stored on a disk for random access. The magnetic tape input channel is 10 and the disk channel is 1. There are ITMAX ($\leqslant 80$) runs.

e.g.

```
&LINAC VOLUME='A3CMPH',NC=3*1,5*0,&END
2101 2102 2103 2104 2105 2109 2107 2108 2200
2250 2760/
```

or if the control record on the tape is incorrect;

```
&LINAC VOLUME='A3CMPH',NC=3*1,5*0,MON=F,CA=15.,25.,38.,
5*0., ID=236,&END
2101 2102 2103 2104/
```

(c) The title and run numbers

The program from this point onwards is called NRUN times with the following variables.

TITLE 72 characters describing the experiment (18A4)

Run Number, Run type (1 to 4), Monitors for each counter if MON=F (Free Format Input)

If the monitors are to be read from the magnetic tape then input;

Run Number, Run type

The last run must have a negative number on input, e.g.

2110	1
2111	2
2113	3
-2114	4

The program will use this as a sentinel and then reset it positively to its true value.

The run types are:

1. Sample + Can
2. Can
3. Vanadium + Background
4. Background

All runs of the same type will be added together including their monitors.

There are JMAX $\leqslant$ 80 runs acceptable

e.g.

24610	1	Three sample runs
24620	1	One can run
24630	1	One vanadium run
24611	2	Three background runs
24612	3	
24613	4	
24623	4	
-24633	4	

(d) The scattering cross-sections via the routine READ1

READ1 is called three times to input the scattering cross-section versus energy mesh for the sample, container and vanadium.

e.g. Energy, Cross-section, Sentinel (2F10.0,I1)

Sentinel = 1 for the final card, up to a maximum of 40 cards. The program sets the integers IMAX1, IMAX2 and IMAX3 as the sizes of the arrays. The energy is in eV and the Cross-section is in barns/molecule.

e.g. 0. 5.13 1 If only one card is provided for each type the program will execute more quickly.

(e) The absorption cross-sections &SIGMA

The three absorption cross-sections are read into the program via the namelist &SIGMA.

&SIGMA	SABS	= Sample Absorption Cross-section
	CABS	= Can Absorption Cross-section
	VABS	= Vanadium Absorption Cross-section
	SCOH	= Sample Coherent Scattering Cross-section

Absorption cross-sections are in barns/molecule at 2200 m/sec and are usually taken from BNL 325 [4].

e.g. &SIGMA SABS=3.9, CABS=4.98, VABS=4.98, SCOH=22.8, &END

(f) The control statement, &CONTRL

The namelist &CONTRL specifies all the options used by the program. Default values are specified for all variables.

Variable	Description	Default Value
PRINT	List all input data	F
PLOT	Plot graphs	T
PUNCH	Punch output data	F
SCATTR	Use scattering cross-section in ABSORP	F
ABSORB	Apply absorption corrections	T
Q	Compute Q-scale $Å^{-1}$	F
TOF	Compute Time-of-flight scale μsec	F
LAMBDA	Compute Wavelength scale Å	F
CRYOST	Is sample in vacuum enclosure?	F
SMOOTH	Smooths vanadium and background	F
CAN	Smooths container	F
W	Pulse width for smoothing option 0. < W < 1.0	.1
EXPO	Uses exponential scattering formalism	F
SMQ	Punches S_m(Q) to cards and puts S_m(Q) into equal Q.steps If .FALSE. does these operations for $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$	T

e.g. &CONTRL PRINT=T, Q=T, SMOOTH=T, &END.

(g) Control data for graphs &SCALE

The scale of the graphs of S(Q) can be specified at this stage if desired.

&SCALE SQMAX=8 Values, SQMIN=8 Values, XMAX=8 Values, XMIN=8 Values, &END

SQMAX(1)=YMAX for counter 1

SQMIN(2) =YMIN for counter 2

XMAX(3) =XMAX for counter 3 etc.

The graphs are scaled automatically if these values are zero.

e.g. &SCALE SQMIN=8*0., SQMAX=2.,2.5,6*3., &END

(h) The sizes and geometry of the sample and vanadium &SIZES, &DENSTY

The namelist &SIZES specifies all the shapes and dimensions of the sample, can and vanadium.

RADIUS defines the dimensions of either a cylinder or plate depending on the variables SROD, SPLATE, VROD, VCOIL and VPLATE

SROD	= Sample is a cylinder	(F)
SPLATE	= Sample is a plate	(F)
VROD	= Vanadium is a cylinder	(F)
VCOIL	= Vanadium is an annular coil	(F)
VPLATE	= Vanadium is a plate	(F)

If the sample is a cylinder, i.e. SROD=T, then;

RADIUS(1)=Sample radius in cm.

RADIUS(2)=Can radius (external) in cm.

RADIUS(3)=Increment in radius for absorption integral in cm.

$$\left[\frac{\text{RADIUS(1)}}{\text{RADIUS(3)}}\right] \text{ and } \left[\frac{\text{RADIUS(2)}}{\text{RADIUS(3)}}\right] \text{ must be integers} \leqslant 20$$

If the sample is a plate, i.e. SPLATE=T, then;

RADIUS(1)=Thickness of sample in cm.

RADIUS(2)=Outer thickness of can in cm. [RADIUS(2) > RADIUS(1)]

RADIUS(3)=Angle of normal to plate with the incident beam in degrees.

In transmission RADIUS(3)=0. and in general $0 \leqslant$ RADIUS(3) $\leqslant 90$.

If the Vanadium is a cylinder, i.e. VROD=T, then;

RADIUS(4)=Vanadium rod radius in cm.

RADIUS(5)=Not used.

RADIUS(6)=Increment in radius for absorption correction in cm.

$$\left[\frac{\text{RADIUS(4)}}{\text{RADIUS(6)}}\right] \text{ must be an integer} \leqslant 20$$

If the Vanadium is an annular coil, i.e. VCOIL=T, then;

RADIUS(4)=Inner radius of vanadium coil in cm.

RADIUS(5)=Outer radius of vanadium coil in cm.

RADIUS(6)=Increment in radius for absorption correction in cm.

$$\left[\frac{\text{RADIUS(4)}}{\text{RADIUS(6)}}\right] \text{ and } \left[\frac{\text{RADIUS(5)}}{\text{RADIUS(6)}}\right] \text{ must be integers} \leqslant 20.$$

If the Vanadium is a plate, i.e. VPLATE=T, then;

RADIUS(4)=Thickness of vanadium plate in cm.

RADIUS(5)=Not used.

RADIUS(6)=Angle of normal to plate with the incident beam in degrees.

$0 \leqslant$ RADIUS(6) $\leqslant 90$.

WIDTH=Beam width in cm.

HEIGHT=Beam height in cm.

A second namelist &DENSTY specifies the densities of the sample, can and vanadium.

SDENS = Sample density (gm.cm^{-3})

CDENS = Can density (gm.cm^{-3})

VDENS = Vanadium density (gm.cm^{-3})

SMW = Sample Molecular Weight

CMW = Can Molecular Weight

VMW = Vanadium Molecular Weight (50.942)

e.g. &SIZES RADIUS = .5,.55,.05,.6,.7,.05, WIDTH = 2.5, HEIGHT = 2.5, VROD=T, SROD = T, &END

or &SIZES RADIUS = .5,.55,30.,.1,.2,30., WIDTH = 2.5, HEIGHT = 2.5, SPLATE = T, VPLATE = T, &END

&DENSTY SDENS = 6.15., CDENS = 6.1, VDENS = 6.1, SMW = 69., CMW = 50.9, VMW = 50.9, &END

(i) Placzek corrections &PLZCK

The namelist &PLZCK provides input of the mean kinetic energy of the molecule and the effective mass. If these are both zero no corrections are applied.

&PLZCK

EBAR = Kinetic energy in meV (0.)

ANU = Effective mass in A.M.U. (1.0E + 3)

(j) Equal Q-step calculation &QEQUAL

Variable	Description	Default value
YMIN(8)	Minimum value of y-axis in graph)	0. provides automatic scaling
YMAX(8)	Maximum y-axis value)	
SCALE	Scale factor i.e. S(Q) = SCALE*S(Q)	1
PUNCH	Punches S_m (Q) or $\left.\frac{d\sigma}{d\Omega}\right\|^{eff}$ (depends on SMQ in &CONTRL)	F
QSTEP	Increment in Q-value	0.05Å^{-1}

In all the data input sections the program attempts to check the form of the data and will print messages if the data is unsuitable, e.g. if [RADIUS(1)/RADIUS(3)] is >20 or if a flat plate sample is parallel to the beam. At this stage the program may now recycle starting with Section 3(c) again.

4. How to run the program (including a sample set of input data as used for liquid nitrogen)

The first example shows the minimum default input data required for a 9-track tape data set with all the control information correctly typed onto the header block. Counter angles, flight paths, initial delay and all information for &LINAC is read from the header of the first run. The monitors are read from each header. The second example shows the maximum default with every parameter input via the NAMELIST statements.

Default case

```
//G.SYSIN DD *
 &LINAC NC=1,1,1,0, TRANS=4*T, &END
 24779 24699 25128 25127 /
 LIQUID NITROGEN 77K JHCLARKE UNIVERSITY OF KENT
 24779 1
 24699 2
 25128 3
 -25127 4
```

```
.001        22.8        1    SAMPLE SCATTERING X-SECTION
.001        5.13        1    CAN SCATTERING X-SECTION
.001        5.13        1    VANADIUM SCATTERING X-SECTION
&SIGMA SABS=3.7,CABS=4.98,VABS=4.98,SCOH=22.206,&END
&CONTRL Q=T,CRYOST=T,&END
&SCALE &END
&SIZES RADIUS=.55,.6,.05,.675,.72,.045,WIDTH=2.5,HEIGHT=2.5,
SROD=T,VCOIL=T,&END
&DENSTY SDENS=.81,CDENS=6.1,VDENS=6.81,SMW=28.,CMW=50.9,VMW=50.,
&END
&PLZCK ANU=17.,&END
&QEQUAL SCALE=.5,&END
/*
```

No default case

```
//G.SYSIN DD *
&LINAC NRUN=1,ID=390,TFP=4.615,SFP=0.4,ITAPE=9,CA=14.,28.,58.,
150., 150.,58.,28.,14.,NC=1,1,1,1,1,1,1,1,EQUALQ=T,CHAN=2,
NCTRS=8,VOLUME='BG7MPH',MON=F,TRANS=8*T,&END
24779 24699 25128 25127 /
LIQUID NITROGEN 77K JHCLARKE UNIVERSITY OF KENT
24779 1 32861 32861 32861 32861 32861 32861 32861 32861
24699 2 98290 98290 98290 98290 98290 98290 98290 98290
25128 3 70305 70305 70305 70305 70305 70305 70305 70305
-25127 4 68271 68271 68271 68271 68271 68271 68271 68271
.001        22.8
1.00        22.8        1
.001        5.13
1.00        5.13
2.00        5.13        1
0.001       5.13
1.000       5.13
2.000       5.13        1
&SIGMA SABS=3.7,CABS=4.98,VABS=4.98,SCOH=22.206,&END
&CONTRL PRINT=F,PLOT=T,PUNCH=F,SCATTR=F,ABSORB=T,Q=T,TOF=F,
LAMBDA=F,RECOIL=F,CRYOST=T,SMOOTH=T,CAN=T,W=.1,
EXPO=F,SMQ=T,&END
```

```
&SCALE SQMAX=2.,2.,2.,2.,2.,2.,2.,2.,SQMIN=0.,0.,0.,0.,0.,0.,0.,
0.,XMAX=5.,10.,20.,35.,0.,0.,0.,0.,XMIN=8*0.,&END
&SIZES RADIUS=.55,.6,.05,.675,.72,.045,WIDTH=2.5,HEIGHT=2.5,
SROD=T,VCOIL=T,SPLATE=F,VPLATE=F,VROD=F,&END
&DENSTY SDENS=.81,CDENS=6.1,VDENS=6.81,SMW=28.,CMW=50.9,
VMW=50.9,&END
&PLZCK ANU=14.,EBAR=0.,&END
&QEQUAL YMIN=0.,0.,0.,0.,0.,0.,0.,0.,YMAX=2.,2.,2.,2.,2.,2.,
2.,2.,PUNCH=F,SCALE=.5,&END
/*
```

On the Harwell computer the program can be executed as follows:

```
//UIDxxx JOB (,HMPH,2,360,,7,1,,2000,1,,0.5),NAME
/*SETUP        31UMPH
//**MAGTAPE A3CMPH FP/...READ ONLY../FP
// EXEC LINDA,TAPE=A3CMPH,SEQ=1,
// PARM='*P="5" *L="YES" *T="TITLE"'
//SYSIN DD *
(DATA)
/*
```

The procedure is an in-line catalogued procedure and is listed in Section 7. The parameters are as follows;

(1) UID = User identifier code on the Harwell computer.

(2) 31UMPH = Demountable Disk containing the program LINDA.

(3) A3CMPH = Archive magnetic tape.

(4) TAPE = A3CMPH, this expands into the full IBM tape control cards.

(5) SEQ = 1,2 etc., this expands into the file on the magnetic tape e.g. LABEL=(SEQ,SL).

(6) PARM = '*P="5"' etc is the input for the Harwell Ghost System [10].

5. An Explanation of the Form of the Output Data

An initial output page lists the information provided in &LINAC and also lists each run and its disposition on disk as it is found.

For each set of data the title is printed in a box at the top of the first page. The list of runs with their identifiers, monitors, etc. is printed, followed by the absorption cross-sections. The options specified in &CONTRL are then printed followed by the sample, can and vanadium dimensions. Number densities and Placzek correction constants follow with the scattering cross-section versus energy meshes.

As each run is read off disk, a log is written on channel 12 specifying its control numbers and locations. For each sample and counter, mean and total values of counts per monitor are listed. The Paalman and Pings correction terms are tabulated for every 10th channel followed by the size of the Placzek correction terms P_1, P_2 and P_3.

Q and S(Q) are printed in two columns followed by Q and $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$. This sequence is repeated for each counter. A running log of the computing time and the state of the graph plotter is also printed. Figures 3-5 show the input spectra for the program, the computed Paalman and Pings correction terms and $\left.\frac{d\sigma}{d\Omega}\right|^{eff}$ as plotted by the program for liquid nitrogen [11]. The form of the prepared data control block is given below.

LINAC Liquids Machine - Magnetic tape header block as prepared by DATIN

Position	Contents	Origin
1	No. of blocks for present sample	Calculated
2	No. of time channels per detector	Type in (default 2048)
3	Run number	Type in
4	Day)	From DOS (Disk operating system)
5	Month)	
6	Year)	
7	Sample No.	Calculated from interface
8	Total number of samples	Type in (default 1)
9	No. of counters	Type in (default 8)
10	Channel width in 1/10 μs	(default 20)
11	Initial delay in 1/10 μs	Type in
12	Total flight path in mm	(default 4750)
13	Second flight path in mm	(default 460)
14	Dead time in 1/10 μs	(default 30)
15		
16		

Position	Contents	Origin
17-24	Monitors etc. for Ctr 1	
25-32	" " " 2	
33-40	" " " 3	
41-48	" " " 4	
49-56	" " " 5	
57-64	" " " 6	
65-72	" " " 7	
73-80	" " " 8	
81-100	Users name Type in	
128 →	General text	

For Each Counter

Position	Contents	Origin
1	Angle (1/100 degree)	Type in (default values)
2	Time (1/50 sec)	Calculated
3	prf	Calculated
4	mon 1	Calculated
5	mon 2	Calculated
6	mon 3	Calculated
7	mon 4	
8	mon 5	

6. Glossary of variable names

A(2048)	Sample + Can run and finally $\frac{d\sigma}{d\Omega}$ array ≡ SA.
AB(60,20)	$\alpha_{nm} + \beta_{nm}$ in Paalman and Pings [3] ≡ IARR.
ABSORB	If true, applies absorption corrections.
ABSORP	Subroutine to calculate Paalman and Pings correction terms [3].
ACC1(54)	A_{cc} array in Paalman and Pings [3] for sample and can.
ACS1(54)	A_{cs} array in Paalman and Pings [3] for sample and can.
ACS2(54)	A_{cs} array in Paalman and Pings [3] for vanadium.
ADUM	Unity.
ANU,ANO,ANØ	Atomic Mass.
AS(60,20)	$\alpha_{nm} + \beta_{nm} - \sigma_{nm}$ in Paalman and Pings [3] ≡ IARR.
ASS1(54)	A_{ss} array in Paalman and Pings [3] for sample and can.
ASS2(54)	A_{ss} array in Paalman and Pings [3] for vanadium.
B(2048)	Can data array ≡ SB.
BARN1	Function to generate cross-section for time channel IT from E, SIGMA arrays.
B2CON	Absorption cross-section constant = .0022/TFP(μs.m^{-1}).
B2C1	Absorption constant for can.
B2S1	Absorption constant for sample.
B2V1	Absorption constant for vanadium.
C(2048)	Vanadium + background run ≡ SC.
CA(8)	Counter angle in degrees, then changed to half-angle in radians.
CABS	Can absorption cross-section at 2200 ms^{-1} (barns).
CAN	If true, smooths can scattering.
CDENS	Can density (g cm^{-3}).
CHAN	Channel width in microseconds.
CMW	Can molecular weight.
CONTRL	Control data input list.
CRYOST	If true, computes cryostat-configuration absorption corrections.
CSUM(4)	Counts per monitor, etc. (working array).

D(2048)	Background data array ≡ SD.
DASH	–
DATE1 * 1(12)	Date in control record (ASCII) DATE1(1-12) ≡ JAY1(13-24)
DATE2 * 1(12)	Date in control record (EBCDIC).
DAY	Day of month.
DEAD	If true, applies deadtime corrections.
DEADT	Subroutine to apply deadtime corrections to data.
DENSTY	Number-density input list.
DISC	Routine to retrieve run from archive disk and sum monitors and machine pulses.
DRAW	Graph plotting subroutine.
DUMR	Dummy radius for vanadium rod.
EBAR	Mean energy of molecule.
ENU(60,20)	$\eta_{nm} + \nu_{nm}$ in Paalman and Pings [3] ≡ IARR.
EQUALQ	If true, computes equal Q-value data for $S_m(Q)$ or $\frac{d\sigma}{d\Omega}$ depending on the value of SMQ.
EXPO	If true, uses exponential scattering formalism.
E0CON1	Energy constant.
E1(40)	Energy array for SIGMA1.
E2(40)	Energy array for SIGMA2.
E3(40)	Energy array for SIGMA3.
FORM(20)	Free format input array ON02A.
FPI	(4π) 4×3.14159.
FPIS	$(4\pi^2)$ 4×3.14159^2.
HCHAN	Half-channel width (μs).
HEIGHT	Height of neutron beam (cm).

IARR(16384)	Data record on magnetic tape.
	IARR(1-16384) ≡ JAY3 * 1(1-65536)
	IARR(1-1200) ≡ AB(1,1)
	IARR(1-6144) ≡ WK(1-6144)
	IARR(1201-2400) ≡ SI(1,1)
	IARR(2401-3600) ≡ AS(1,1)
	IARR(3601-4800) ≡ ENU(1,1)
	IARR(4801-6000) ≡ NU(1,1)
	IARR(6001-8192) ≡ R(1-2192)
ICHNL	No. of time-channels per counter.
ICON(256)	Control record of magnetic tape.
	ICON(1-128) ≡ JAY1 * 1(1-512)
	ICON(129-512) ≡ JAY2 * 1(1-512)
ID	Initial delay in microseconds.
IDUM	Dummy.
IMAX1	Size of E1 and SIGMA1.
IMAX2	Size of E2 and SIGMA2.
IMAX3	Size of E3 and SIGMA3.
INC	Counter number in DO loops.
ITAPE	Number of input tape 7, 8, 9.
ITIND	Working integer.
ITMAX	Number of runs archived to disk.
JAY1 * 1(512)	Control record ≡ ICON(256).
JAY2 * 1(512)	
JAY3 * 1(65536)	Data ≡ IARR(16384).
JCY, JJJ	Run counters.
JMAX	Number of runs to be processed in this cycle.
JOBNAM * 8	Alphanumeric text-name of computer job.
JSHIFT	Working array shift.

LAMBDA	If true, computes wavelength scale.
LINAC	Spectrometer data input list.
M(8,80)	Monitor count for counter (1-8) run (1-80).
MON	If true, monitors are read from magnetic tape control record. If false, from cards.
MONTH	Month of year.
MPRF(8,80)	Machine pulses for counter (1-8) run (1-80).
NBLKS	Number of blocks on tape.
NC(8)	On-off switch for (1-8) counters.
NCPK	Number of tof channels per array element of ASS1 etc.
NCTRS	Number of detectors on the magnetic tape file.
NDEAD	Number of dead channels.
NM(8,80)	Monitor count array as read from archive.
NMPRF(8,80)	Machine pulse array as read from archive.
NRMAX	Maximum number of archive runs.
NRUN	Number of cycles of data.
NTRN(80)	List of input run numbers for archive disk.
NU(60,20)	ν_{nm} in Paalman and Pings [3] ≡ IARR.
OJOHNA	Modified Harwell routine to give tabular lineprinter output.
PI	(π) 3.14159.
PLOT	If true, plot all graphs.
PLZCK	Placzek input list.
PRINT	If true, print raw summed data.
PUNCH	If true, punches $S_m(Q)$ or $\frac{d\sigma}{d\Omega}$ to cards depending on value of SMQ.
P1,P2,P3,P4	Placzek correction terms.
Q	If true, computes Q-scale.
QK(1200)	Q-scale in QBIN routine.
R(2192)	Radius array in ABSORP (working array) ≡ IARR.
RADIUS(6)	Dimensions of sample, can and vanadium.

RADIUS(1)	Radius of sample or thickness of sample.
RADIUS(2)	Outer radius of can or outer thickness of sample.
RADIUS(3)	Increment for integral or angle of normal to beam.
RADIUS(4)	Radius of vanadium rod or thickness of vanadium plate, or inner radius of coil.
RADIUS(5)	Outer radius of coil. Not used.
RADIUS(6)	Increment in integral or angle of normal to beam.
RATIO(2048)	Working array and finally, S(Q) array.
RD	Initial delay μs.
READ1	Reads E1,2,3 and SIGMA1, 2 and 3.
SA,SB,SC,SD	Single elements of arrays A,B,C,D.
SABS	Sample absorption cross-section at 2200 ms^{-1} (barns).
SCALE	Graph scale input list.
SCATTR	If true, uses scattering cross-sections (SIGMA1-3) in ABSORP.
SCOH	Sample coherent cross-section (barns).
SDENS	Sample density ($g.cm^{-3}$).
SFP	Second flight path in metres.
SI(60,20)	σ_{nm} in Paalman and Pings [3] $\equiv$ IARR.
SIGMA	Absorption cross-section input list.
SIGMA1(40)	Scattering cross-section of sample array.
SIGMA2(40)	Scattering cross-section of container array.
SIGMA3(40)	Scattering cross-section of vanadium array.
SIZES	Sample dimensions etc. data input list.
SMOOTH	If true, smooths vanadium and background.
SMTH	Subroutine to smooth an array of data.
SMW	Sample molecular weight.
SMQ	If true, punches $S_m(Q)$, if false, $\frac{d\sigma}{d\Omega}$.
SPLATE	If true, sample is a plate.
SQMAX(8)	Maximum value of S(Q) for counter (1-8) for graph.
SQMIN(8)	Minimum value of S(Q) for counter (1-8) for graph.

SROD	If true, sample is a cylinder.
SST	sin $(CA)^2$.
STAR	*
SUM(4,8,80)	No. of counts for sample type (1-4), counter (1-8) and run sequence (1-80).
T(2048)	Working array and Q, time-of-flight or wavelength array.
TAPE7	If true, data is input on PDP-4 magnetic tape.
TAPE8	If true, data is input from PDP-4 archive tape.
TAPE9	If true, data is input from PDP-11 archive tape.
TBEG,TEND,TDIFF	Elapsed time-constants.
TEXT * 1(192)	Alphanumeric text in control record (ASCII).
TEXT(1-192) ≡	JAY1(321-512).
TFP	Total flight path in metres.
TITLE(18)	72 character title.
TOF	If true, computes time-of-flight scale.
TXT * 1(80)	Alphanumeric text in control record (EBCDIC).
TYPE(80)	(1-4) run-type of run number RUN.
VABS	Vanadium absorption cross-section at 2200 ms^{-1} (barns).
VCOIL	If true, vanadium is an annulus.
VDENS	Vanadium density (g cm^{-3}).
VMW	Vanadium molecular weight.
VOLUME * 8	Alphanumeric text and name of magnetic tape volume.
VOLSP	Volume term for sample plate.
VOLSR	Volume term for sample cylinder.
VOLVC	Volume term for vanadium coil.
VOLVP	Volume term for vanadium plate.
VOLVR	Volume term for vanadium rod.
VPLATE	If true, vanadium is a plate.
VROD	If true, vanadium is a cylinder.
W	Smoothing width.

WIDTH	Width of neutron beam (cm).
WK(6144)	Working array in QBIN routine.
X	Ratio used in recoil correction $\frac{(\text{scattered neutron velocity})}{(\text{incident neutron velocity})}$.
XMAX(8) XMIN(8)	Maximum and minimum values for X-axes in graphs.
YEAR	Year.
Z	Zero.

7. LISTING OF CATALOGUED HARWELL PROCEDURE LINDA

```
//LINDA PROC TAPE=A3CMPH,TAPE7=7JBELA,POS1='DUMMY,',SEQ=1,POS2=
//    EXEC PGM=DISKPGM,COND=EVEN,REGION=390K
//*===== LINDA PROGRAM ON DISC MPHB =========================
//STEPLIB DD DSN=LOAD.MPH.JHCLINDA.VOL=REF=MPHB.DISP=SHR
//*===== CARD PUNCH ==========================================
//SYSPCH DD SYSOUT=B,DCB=BLKSIZE=80
//*===== SCRATCH DISC FILES FOR INPUT DATA ===================
//FT01F001 DD DISP=(NEW,DELETE),DSN=&&DATA,VOL=REF=SCRATCH,
//    SPACE=(CYL,(5,1),RLSE),DCB=(RECFM=VBS,LRECL=1028,BLKSIZE=12340)
//*===== CARD READER =========================================
//FT05F001 DD DDNAME=SYSIN
//*===== LINEPRINTER =========================================
//FT06F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//*===== CARD PUNCH ==========================================
//FT07F001 DD SYSOUT=B
//*===== FILE FOR SUMMED COUNTERS ============================
//FT08F001 DD VOL=REF=SCRATCH1,SPACE=((8192,32),RLSE,CONTIG),DSN=&&SUM
//*===== ARCHIVE TAPE A3CMPH =================================
//FT01F001 DD &POS2,DISP=(OLD,KEEP),VOL=SER=&TAPE,
//    LABEL=(&SEQ,SL),UNIT=(TAPE9,,DEFER),DSN=DATA.MPH.JHCARCH,
//    DCB=(RECFM=VS,LRECL=16388,BLKSIZE=16392,DEN=3)
//*===== OUTPUT PRINT CHANNELS FOR LINEPRINTER ===============
//FT11F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//FT12F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//FT13F001 DD SYSOUT=A,DCB=(RECFM=FA,BLKSIZE=133)
//*===== SCRATCH DISC FILE FOR EQUAL G-STEP =================
//FT14F001 DD VOL=REF=SCRATCH1,SPACE=((8194,8),RLSE,CONTIG),DSN=&&GBIN
//*===== INPUT CHANNEL FOR 7-TRACK PDP-4 TAPE ===============
//F1 DD &POS1,UNIT=(TAPE7,,DEFER),VOL=SER=&TAPE7,DISP=(OLD,KEEP),
        //    DCB=(RECFM=F,BLKSIZE=768,DEN=0,DSORG=PS),LABEL=(2,NL)
//*===== GHOST GRAPHPLOTTING JCL ============================
//GRIDINDX DD DISP=SHR,DSN=HAR.GRIDINDX

//GRID DD VOL=REF=GRID,SPACE=(768,(2000,20),RLSE)
//SYSIN DD *
//M EXEC PGM=PPLP,REGION=140K,ACCT=GHOSTLF
//STEPLIB DD DSN=HAR.GHOSTLIB,DISP=SHR
//FT06F001 DD SYSOUT=A
//SYSUDUMP DD SYSOUT=A
//FT49F001 DD SYSOUT=A
//GRIDINDX DD DSN=HAR.GRIDINDX,DISP=SHR
//PRINT DD SYSOUT=A
//DDSPOOL1 DD VOL=SER=SPOOL1,DISP=OLD,UNIT=3330
//DDSPOOL2 DD VOL=SER=SPOOL1,DISP=OLD,UNIT=3330
//DD318COM DD VOL=SER=318COM DISP=OLD,UNIT=3330
//DD319SYS DD VOL=SER=319SYS,DISP=OLD,UNIT=3330
//PROC PEND
```

```
C---- SPECTROMETER DATA ANALYSIS PROGRAM (LINDA) ----------------------
C==== MARK XLIV      5TH JANUARY 1976 --------------------------------
C
C      ***************************************************
C      * N1= NUMBER OF TIME-OF-FLIGHT CHANNELS PER COUNTER     *
C      * N2= NUMBER OF COUNTERS                                *
C      * N3= TOTAL NUMBER OF RUNS                              *
C      * N4= NUMBER OF TOTAL CROSS-SECTION VALUES              *
C      * N5= NUMBER OF INCREMENTS IN ABSORPTION INTEGRAL       *
C      * N6= NUMBER OF INTERPOLATION STEPS IN                  *
C      *       ABSORPTION CORRECTION TERMS                     *
C      * N7= NUMBER OF Q-STEPS IN EQUAL Q-VALUE ROUTINE        *
C      ***************************************************
C
C      ************************************************************
C      * RATIO(N1)  A(N1)   B(N1)  C(N1)  D(N1)  T(N1)                *
C      * SQMAX(N2)  SQMIN(N2)  XMAX(N2)  XMIN(N2)                     *
C      * RMC(N2,4)  CA(N2)  RPULSE(N2,4)                              *
C      * M(N2,N3)  MPRF(N2,N3)  NM(N2,N3)  NMPRF(N2,N3)  SUM(4,N2,N3) *
C      * NTRN(N3)  TYPE(N3)  RUN(N3)  NSEQ(N3)                        *
C      * SIGMA1(N4)  SIGMA2(N4)  SIGMA3(N4)  E1(N4)  E2(N4)  E3(N4)   *
C      * AB(3*N5,N5)  SI(3*N5,N5) AS(3*N5,N5) NU(3*N5,N5) ENU(3*N5,N5) *
C      * ASS1(N6)  ACC1(N6)  ACS1(N6)  ASS2(N6)  ACS2(N6)             *
C      * QK(N7)  RSK(N7)                                              *
C      ************************************************************
C
      REAL RTP*8(4)/'SAMPLE','CAN','VANADIUM','BACKGRND'/,
     *     RATIO(2048),A(2048),B(2048),C(2048),D(2048),T(2048),
     *     SUM(4,8,80)/2560*0./,RMC(8,4)/32*0./,RPULSE(8,4)/32*0./,
     *     SIGMA1(40),SIGMA2(40),SIGMA3(40),E1(40),E2(40),E3(40),
     *     SQMAX(8)/8*0./,SQMIN(8)/8*0./,XMAX(8)/8*0./,XMIN(8)/8*0./,
     *     AB(60,20),SI(60,20),AS(60,20),ENU(60,20),NU(60,20),
     *     ASS1(54)/54*1./,ACC1(54)/54*1./,ACS1(54)/54*1./,
     *     ASS2(54)/54*1./,ACS2(54)/54*1./,
     *     VOLUME*8/'UNKNOWN'/,JOBNAM*8/'        '/,
     *     CA(8)/8*0./,CSUM(4),RADIUS(6),TITLE(18),FORM(20),R(2192),
     *     WK(6144),QK(1200),RSK(1200),DSN*8(3)/3*'        '/
C
      INTEGER ICON(256),IARR(16384),DAY,YEAR,CHAN/0/,
     *     NTRN(80)/80*0/,RUN(80)/80*0/,TYPE(80)/80*0/,NSEQ(80)/80*0/,
     *     M(8,80)/640*0/,MPRF(8,80)/640*0/,NM(8,80)/640*0/,
     *     NMPRF(8,80)/640*0/,NC(8)/8*1/
C
      LOGICAL PRINT/F/,PLOT/T/,PUNCH/F/,SCATTR/F/,ABSORB/T/,ERRORS/F/,
     *        Q/F/,TOF/F/,LAMBDA/F/,RECOIL/F/,SMOOTH/F/,CAN/F/,
     *        CRYOST/F/,EXPO/F/,SMQ/T/,ENABLE/F/,EQUALQ/T/,DEAD/F/,
     *        SROD/F/,SPLATE/F/,VROD/F/,VPLATE/F/,VCOIL/F/,
     *        MON/T/,TAPE7/F/,TAPE8/F/,TAPE9/T/,TRANS(8)/8*T/,TRANSM/F/,
     *        JAY1*1(512),JAY2*1(512),JAY3*1(65536),
     *        TEXT*1(192),TXT*1(80),DATE1*1(12),DATE2*1(12)/12*' '/
C
      EQUIVALENCE (AB(1,1),WK(1),QK(1),IARR(1),JAY3(1)),
     *            (ICON(1),JAY1(1)),(ICON(129),JAY2(1)),
     *            (TEXT(1),JAY1(321)),(DATE1(1),JAY1(13)),
     *            (NCH,ICNL2),(CHAN,ICHNLW),(NBLKS,NBL),
     *            (RSK(1),SI(1,1),IARR(1201)),(AS(1,1),IARR(2401)),
     *            (ENU(1,1),IARR(3601)),(NU(1,1),IARR(4801)),
     *            (R(1),IARR(6001))
C
      DATA NRMAX,NRUN,NDEAD,JCY,JJJ,IDUM,ID,W,TFP,SFP/80,1,5*0,.1,2*0./,
     *     ECON1,Z,ADUM/2.609E6,0.,1./,
     *     PI,FPI,FPIS/3.14159,12.566,39.478/,
     *     EBAR,CBAR,RKBAR,ANU,ANO,AN[illegible]/3*0.,3*1.E3/,
     *     ITIND,ITAPE,NCTRS/1,9,0/,
     *     STAR,DASH/'*','_'/
C
      NAMELIST /LINAC/ NRUN,ID,TFP,SFP,ENABLE,ITAPE,CA,NC,EQUALQ,
     *                 NCTRS,CHAN,VOLUME,RPULSE,DEAD,NDEAD,MON,TRANS
     *         /SIGMA/ SABS,CABS,VABS,SCOH
     *         /SIZES/ RADIUS,WIDTH,HEIGHT,SROD,SPLATE,VROD,VCOIL,VPLATE
     *         /DENSTY/SDENS,SMW,CDENS,CMW,VDENS,VMW
     *         /PLZCK/ EBAR,CBAR,RKBAR,ANU,ANO,AN[illegible]
     *         /SCALE/ SQMAX,SQMIN,XMAX,XMIN
     *         /CONTRL/PRINT,PLOT,PUNCH,SCATTR,ABSORB,Q,TOF,LAMBDA,
     *                 ERRORS,RECOIL,CRYOST,SMOOTH,CAN,W,EXPO,SMQ
C
C---- READ IN LINAC CONTROL PARAMETERS /LINAC/ ------------------------
      READ (5,LINAC)
      WRITE(13,LINAC)
```

```
      IF(ITAPE.EQ.7)TAPE7=.TRUE.
      IF(ITAPE.EQ.9)TAPE9=.TRUE.
      IF(ITAPE.NE.9)TAPE9=.FALSE.
C
C----- FILE FOR SUMMED COUNTERS AND =Q -------------------------------
      DEFINE FILE 8(32,2048,U,IV8),14(8,2049,U,IV14)
C
C---- COMPUTE HEADER INFORMATION & GRAPH PLOTTER HEADER ---------------
      CALL ZA11AS(DAY,MONTH,YEAR)
      CALL ZA08AS(TIME)
      CALL ZA17AS(JOBNAM)
      CALL ZV01AD(10,VOLUME,DSN)
      CALL FILM  (1)
      CALL GHFROR(1)
      CALL CSPACE(0.,1.414,0.,1.)
      CALL PSPACE(.1,1.35,.1,.95)
      CALL PLACE (20,20)
      CALL TYPECS('LINAC LIQUIDS SPECTROMETER DATA',31)
      CALL PLACE (20,25)
      CALL TYPECS('PROGRAM RUN AT ',15)
      CALL TYPECS(TIME,8)
      CALL TYPECS(' ON ',4)
      CALL TYPENI(DAY)
      CALL TYPECS(' ',1)
      CALL TYPECS(MONTH,4)
      CALL TYPECS(' ',1)
      CALL TYPENI(YEAR)
      CALL CTRMAG(10)
C
      WRITE(6,10)DAY,MONTH,YEAR,TIME,JOBNAM,VOLUME,DSN
   10 FORMAT(/,T10,'TOTAL SCATTERING LIQUIDS SPECTROMETER,',
     *            'ALL SINGING,ALL DANCING DATA ANALYSIS PROGRAM,',
     *            ' RUN ON',I3,1X,A4,I5,' AT ',A8,//,
     *       T10,'JOBNAME IS ',A8,//,
     *       T10,'MAGTAPE VOLUME IS ',A8,//,
     *       T10,'DATA SET NAME IS ',5A8,//,
     *       T10,'PROGRAM MK XLIV    5TH JANUARY    1976 (J.H.CLARKE)')
C
C---- CHECK COUNTER OPTIONS -------------------------------------------
      IF(NC(1).EQ.0.AND.NC(2).EQ.0.AND.
     *   NC(3).EQ.0.AND.NC(4).EQ.0.AND.
     *   NC(5).EQ.0.AND.NC(6).EQ.0.AND.
     *   NC(7).EQ.0.AND.NC(8).EQ.0) GOTO1630
   20 IF(TAPE9)REWIND10
C
C---- READ LIST OF RUNS REQUIRED FOR PROCESSING -----------------------
      READ(5,*)NTRN
      DO 30 I=1,NRMAX
      IF(NTRN(I).EQ.0)GOTO40
   30 CONTINUE
C
C---- SET MAXIMUM NO. OF RUNS FOR SPOOLING (ITMAX) --------------------
   40 ITMAX=I-1
      WRITE(6,50)ITAPE,ITMAX
      WRITE(12,60)(NTRN(I),I=1,ITMAX)
      IF(MON)WRITE(6,70)
      IF(.NOT.MON)WRITE(6,80)
   50 FORMAT(/,T10,'NUMBER OF RUNS SPOOLED FROM',I2,'-TRACK TAPE ',
     *            'TO SCRATCH DISK IS',I3,//,
     *       T10,'SEE CHANNEL 12 FOR TAPE READING LOG')
   60 FORMAT(/,T10,'TAPE SPOOLING LOG OUTPUT CHANNEL 12',//,
     *       T10,'RUN NUMBERS (IN ORDER OF ASKING)',//,
     *       8(T10,10I10,/))
   70 FORMAT(/,T10,'MONITORS WILL BE READ FROM MAGTAPE CONTROL RECORD'/)
   80 FORMAT(/,T10,'MONITORS WILL BE READ FROM INPUT CARDS',/)
C
C---- READ FIRST CONTROL RECORD ---------------------------------------
C---- READ PDP4 7-TRACK MAGNETIC TAPE ---------------------------------
   90 IF(TAPE7)CALL RPDP47(1,1,ICON,0,0,0)
C---- READ PDP11 9-TRACK TAPE -----------------------------------------
      IF(TAPE9)READ(10,END=290)ICON
      NBLKS=ICON(1)
      IF(TAPE9)ICON(2)=NBLKS*128
C
C---- CHECK END OF TAPE -----------------------------------------------
      IF(ICON(3).EQ.9999.OR.JJJ.GT.ITMAX)GOTO300
C---- COMPUTE DATE ----------------------------------------------------
      IF(TAPE9)CALL ZA05AS(DATE1,DATE2,12,LDONE,1,IERR)
      WRITE(12,100)ICON(3),ICON(2),DATE2
  100 FORMAT(1X,'RUN NO.',I10,' OF',I6,' CHANNELS ON ',12A1)
```

```
C
C---- HUNT FOR RUN IN RUN LIST ------------------------------------------
      DO 110 K2=1,ITMAX
      IF(ICON(3).EQ.NTRN(K2))GO TO 120
  110 CONTINUE
C
C---- MOVE ON TO NEXT RECORD --------------------------------------------
      IF(TAPE7)CALL RPDP47(2,1,0,0,0,0)
      IF(TAPE9)READ(10,END=290)
      GOTO90
C
C---- RUN FOUND ---------------------------------------------------------
  120 WRITE(12,140)ICON(3)
C---- COMPUTE TEXT STRING FROM CONTROL RECORD ---------------------------
      IF(TAPE9)CALL ZA05AS(TEXT,TXT,80,LDONE,1,IERR)
      IF(TAPE9)WRITE(11,130)ICON(3),DATE2,TXT
  130 FORMAT(2X,'RUN NO. ',I10,2X,12A1,2X,80A1)
  140 FORMAT(1H+,T51,'*',I10,' FOUND')
C---- IF 7 TRACK  TAPE SKIP THIS SECTION --------------------------------
      IF(.NOT.TAPE9)GOTO170
      DO 160 K=1,8
C---- READ OFF ANY REMAINING RUN PARAMETERS FROM FIRST RUN ON TAPE -----
      IF(JJJ.GT.0)GOTO150
C
C---- COUNTER ANGLES FIRST ----------------------------------------------
      IF(CA(K).EQ.0.)CA(K)=FLOAT(ICON(9+8*K))*.01
C
C---- NOW THE MONITORS AND PRF PULSES IF MON HAS NOT BEEN SET TO FALSE -
  150 IF(MON)NM(K,K2)    =ICON(15+8*K)
      IF(MON)NMPRF(K,K2)=ICON(11+8*K)
  160 CONTINUE
      IF(JJJ.GT.0)GOTO230
C
C---- CHANNEL WIDTH,INITIAL DELAY,DEADTIME,NCTRS & FLIGHT PATHS --------
      IF(CHAN.EQ.0) CHAN =ICON(10)/10
      IF(ID.EQ.0)     ID   =ICON(11)/10
      IF(NDEAD.EQ.0)NDEAD=ICON(14)/ICON(10)
      IF(NCTRS.EQ.0)NCTRS=ICON(9)
      IF(TFP.EQ.0.) TFP   =FLOAT(ICON(12))*.001
      IF(SFP.EQ.0.) SFP   =FLOAT(ICON(13))*.001
C
C---- IF THIS IS THE FIRST RUN READ OFF THEN PRINT OUT THE CONTROL DATA-
C---- OTHERWISE GOTO 230 AND READ IN RUN -------------------------------
  170 IF(JJJ.GT.0)GOTO230
      F=SFP/TFP
      HCHAN=.5*FLOAT(CHAN)
      RD=ID
      RI=RD-HCHAN
      WRITE(6,190)NRUN,ID,TFP,SFP,NDEAD
      DO 180 K=1,NCTRS
      IF(      TRANS(K))WRITE(6,210)K,NC(K),CA(K)
      IF(.NOT.TRANS(K))WRITE(6,200)K,NC(K),CA(K)
  180 CONTINUE
  190 FORMAT(/,T10,'THERE ARE ',I3,' SETS OF DATA TO BE ANALYSED',//,
     *         T10,'THE INITIAL TIMING DELAY IS',I4,' MICROSECONDS',//,
     *         T10,'THE FLIGHT PATH LENGTH IS',F6.3,' METRES',//,
     *         T10,'THE SECOND FLIGHT PATH IS',F6.3,' METRES',//,
     *         T10,'THERE ARE ',I2,' DEAD CHANNELS',/)
  200 FORMAT(/,T10,'COUNTER POSITION NUMBER',I2,' HAS',I3,
     *              ' COUNTERS AT',F8.3,' DEGREES IN REFLECTION')
  210 FORMAT(/,T10,'COUNTER POSITION NUMBER',I2,' HAS',I3,
     *              ' COUNTERS AT',F8.3,' DEGREES IN TRANSMISSION')
C
C----- CONVERT TO RADIANS , HALF COUNTER ANGLE --------------------------
      DO 220 K=1,NCTRS
  220 CA(K)=CA(K)*.0087266
  230 JJJ=JJJ+1
C
C---- READ RUN INTO CORE ------------------------------------------------
      DO 240 K=1,16384
  240 IARR(K)=0
C---- 7-TRACK PDP-4 TAPE ------------------------------------------------
      IF(TAPE7)CALL RPDP47(2,1,IARR,ICON(2),2,NER)
      IF(.NOT.TAPE9)GOTO260
C---- 9-TRACK PDP-11 TAPE -----------------------------------------------
      NCHNL=ICON(1)*128
      READ(10,END=290)(IARR(K1),K1=1,NCHNL)
C
C---- FUDGE FUNNY CHARACTERS --------------------------------------------
      IARR(ICON(2))=IARR(ICON(2)-1)
```

```
C
C---- CORRECT FOR ODD HIGH ORDER PART OF WORD CREATED WITH OLD DATIN
      DO 250 J=1,NBLKS
      JSHIFT=(J-1)*512
      JAY3(1+JSHIFT)=JAY3(5+JSHIFT)
  250 JAY3(2+JSHIFT)=JAY3(6+JSHIFT)
  260 WRITE(12,270)
  270 FORMAT(1H+,T63,',READ FROM TAPE')
C
C---- WRITE RUN ONTO DISC 1 -------------------------------------------------
      WRITE(1)ICON,IARR
      WRITE(12,280)K2,ICON(3)
  280 FORMAT(1H+,T63,',WRITTEN TO DISC AS FILE',I3,' RUN',I10)
C
C---- INCREASE RUN NUMBER BY 1 ----------------------------------------------
      JCY=JCY+1
C---- SEQUENCE NUMBER OF RUN NTRN(K2) ON SCRATCH DISC
      NSEQ(K2)=JCY
C
C---- SET UP ARRAY DIMENSIONS FOR DUMMY ARGUMENTS OF SUBPROGRAMS -------
      IF(JCY.EQ.1.AND..NOT.TAPE9)ICNL2=ICON(2)
      IF(JCY.EQ.1.AND..NOT.TAPE9)ICHNL=ICON(2)/NCTRS
      IF(JCY.EQ.1.AND.TAPE9)ICNL2=ICON(1)*128
      IF(JCY.EQ.1.AND.TAPE9)ICHNL=ICNL2/NCTRS
      ICHNLW=CHAN
C
C---- CHECK ARRAY OVERFLOW OR END OF RUN LIST --------------------------------
      IF(JCY.GT.NRMAX.OR.JCY.GE.ITMAX)GOTO310
C---- READ IN NEXT RUN -------------------------------------------------------
      GO TO 90
C
C---- END OF TAPE OR DATA SET -----------------------------------------------
  290 WRITE(6,340)
  300 WRITE(12,320)
  310 WRITE(6,330)
  320 FORMAT(T10,'9999 FOUND')
  330 FORMAT(T45,'**********')
  340 FORMAT(T10,'EOF MARK FOUND ON MAGNETIC TAPE')
      ENDFILE 1
C
C---- CYCLE OVER SETS OF INPUT DATA ------------------------------------------
      IF(NRUN.EQ.0)STOP
      DO 1620 KRUN=1,NRUN
      READ(5,350)TITLE
      WRITE(6,360)(STAR,I=1,83),TITLE,(STAR,I=1,83)
      WRITE(6,370)(DASH,I=1,49)
  350 FORMAT(18A4)
  360 FORMAT(1H1,T30,80A1,/,T30,A1,T109,A1,/,T30,A1,T34,18A4,T109,A1,/,
     *T30,A1,T109,A1,/,T30,80A1,/,/,T5,'IDENTIFIER',T20,'RUN-NO.',T33,
     *'MON1',T43,'MON2',T53,'MON3',T63,'MON4',T73,'MON5',T83,'MON6',T93,
     *'MON7',T103,'MON8')
  370 FORMAT(1H+,T5,10A1,T20,7A1,T33,8(4A1,6X))
C
C---- INITIALIZE VARIABLES --------------------------------------------------
      DO 400 K1=1,NRMAX
      RUN(K1)=0
      TYPE(K1)=0
      DO 390 K2=1,3
      M(K2,K1)=0
      MPRF(K2,K1)=0
      DO 380 K3=1,4
  380 SUM(K3,K2,K1)=0.
  390 CONTINUE
  400 CONTINUE
      DO 420 K=1,4
      CSUM(K)=0.
      DO 410 L=1,8
      RMC(L,K)=0.
      RPULSE(L,K)=0.
  410 CONTINUE
  420 CONTINUE
C
C---  INPUT RUN NO. MONITOR COUNT -------------------------------------------
      DO 490 K=1,NRMAX
      CALL ONE2A(FORM)
      IF(.NOT.MON)READ(5,FORM)RUN(K),TYPE(K),(M(L,K),L=1,NCTRS)
      IF(.NOT.MON)GOTO460
      IF(MON)READ(5,FORM)RUN(K),TYPE(K)
C
C---- FIND POSITION OF RUN(K) IN ARCHIVE LIST NTRN --------------------
```

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C---- DON'T FORGET THAT LAST RUN IN LIST RUN(ITMAX) IS NEGATIVE --------
      DO 450 K1=1,ITMAX
      IF(IABS(RUN(K)).NE.NTRN(K1))GOTO440
C
C---- SET MONITOR OF RUN(K) TO VALUE NM IN ARCHIVE LIST --------------
      DO 430 L=1,NCTRS
      M(L,K)=NM(L,K1)
      MPRF(L,K)=NMPRF(L,K1)
  430 CONTINUE
  440 IF(IABS(RUN(K)).EQ.NTRN(K1))GOTO460
  450 CONTINUE
C---- LIST RUN NUMBERS AND MONITORS ------------------------------------
  460 WRITE(6,470)RTP(TYPE(K)),RUN(K),(M(L,K),L=1,NCTRS)
      IF(TYPE(K).LT.0.OR.TYPE(K).GT.4)WRITE(6,480)RUN(K)
      IF(TYPE(K).LT.0.OR.TYPE(K).GT.4)GOTO1620
  470 FORMAT(T5,A8,T16,I10,T27,8I10)
  480 FORMAT(T10,'RUN NUMBER',I10,' HAS AN INVALID RUN TYPE INDICATOR')
      IF(RUN(K).LT.0)JMAX=K
C---- CHECK FOR LAST RUN IN LIST AND RESET  TO POSITIVE VALUE ----------
      IF(RUN(K).LT.0)GOTO500
  490 CONTINUE
  500 RUN(JMAX)=-RUN(JMAX)
C
C---- INITIALIZE T -----------------------------------------------------
      DO 510 K2=1,2048
  510 T(K2)=0.
C
C---- READ IN SCATTERING CROSS SECTION ARRAYS 1<IMAX<40 --------------
      CALL READ1(SIGMA1,E1,IMAX1)
      CALL READ1(SIGMA2,E2,IMAX2)
      CALL READ1(SIGMA3,E3,IMAX3)
C
C---- READ ABSORPTION CROSS SECTIONS AND COHERENT CROSS SECTION /SIGMA/
      READ(5,SIGMA)
      WRITE(13,SIGMA)
      WRITE(6,520)SABS,CABS,VABS,SCOH
  520 FORMAT(   /,T10,'ABSORPTION CROSS SECTION OF SAMPLE IS ',T65,F8.3,
     *' BARNS',/,T10,'ABSORPTION CROSS SECTION OF CAN IS     ',T65,F8.3,
     *' BARNS',/,T10,'ABSORPTION CROSS SECTION OF VANADIUM IS',T65,F8.3,
     *' BARNS',/,T10,'COHERENT SCATTERING CROSS SECTION OF MOLECULE IS'
     * ,T65,F8.3,' BARNS',/)
C
C---- INPUT CONTROL CARD -----------------------------------------------
      READ ( 5,CONTRL )
      WRITE(13,CONTRL)
      IF(.NOT.PLOT)CALL GHPEN(0)
      WRITE(6,530)
      IF(PRINT)          WRITE(6,540)
      IF(PLOT)           WRITE(6,550)
      IF(.NOT.PLOT)      WRITE(6,560)
      IF(PUNCH)          WRITE(6,570)
      IF(SCATTR)         WRITE(6,580)
      IF(ABSORB)         WRITE(6,590)
      IF(CRYOST)         WRITE(6,600)
      IF(RECOIL)         WRITE(6,610)
      IF(ERRORS)         WRITE(6,620)
      IF(SMOOTH)         WRITE(6,630)
      IF(CAN)            WRITE(6,640)
      IF(EXPO)           WRITE(6,670)
      IF(SMOOTH.OR.CAN)WRITE(6,650)W
      IF(W.LE.0.OR.W.GE.1.)W=.1
      IF(W.LE.0.OR.W.GE.1.)WRITE(6,660)
C
  530 FORMAT(T10,'PROGRAM WILL COMPUTE D(SIGMA)/D(OMEGA) AND S(Q) WITH P
     *LAZCEK CORRECTIONS')
  540 FORMAT(T10,'RAW COUNTS WILL BE LISTED')
  550 FORMAT(T10,'RATIOES ETC. WILL BE PLOTTED')
  560 FORMAT(T10,'GRAPHS WILL NOT BE PLOTTED')
  570 FORMAT(T10,'RATIOES WILL BE PUNCHED TO CARDS')
  580 FORMAT(T10,'SCATTERING CROSS SECTION USED IN ABSORPTION STEP')
  590 FORMAT(T10,'ABSORPTION CORRECTIONS WILL BE APPLIED')
  600 FORMAT(T10,'AIR BACKGROUND NOT SUBTRACTED FROM SAMPLE AND CAN')
  610 FORMAT(T10,'RECOIL CORRECTIONS APPLIED')
  620 FORMAT(T10,'STANDARD ERRORS WILL BE COMPUTED')
  630 FORMAT(T10,'SMOOTHING WILL BE PERFORMED ON VANADIUM & BACKGROUND')
  640 FORMAT(T10,'SMOOTHING WILL BE PERFORMED ON CAN')
  650 FORMAT(T10,'SMOOTHING WIDTH W IS ',F6.3)
  660 FORMAT(T10,'W RESET TO  .05')
  670 FORMAT(T10,'EXPONENTIAL SCATTERING FORMALISM USED')
C
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C-----READ MAXIMUM AND MINIMUM SCALE VALUES FOR GRAPH PLOTTING /SCALE/
      READ(5,SCALE)
      WRITE(13,SCALE)
      DO 680 I=1,NCTRS
      IF(SQMAX(I).NE.0.0)WRITE(6,690)SQMAX(I),SQMIN(I),I
      IF(XMAX(I).NE.0.0)WRITE(6,700)XMAX(I),XMIN(I),I
  680 CONTINUE
      WRITE(6,710)CHAN
  690 FORMAT(T10,'YMAX = ',F8.3,' YMIN = ',F8.3,' FOR COUNTER',I2)
  700 FORMAT(T10,'XMAX = ',F8.3,' XMIN = ',F8.3,' FOR COUNTER',I2)
  710 FORMAT(T10,'CHANNEL WIDTH IS ',I6,' MICROSECONDS')
C
C-----READ SAMPLE AND VANADIUM GEOMETRIES /SIZES/ ---------------------
      READ(5,SIZES)
      WRITE(13,SIZES)
      IF(.NOT.SPLATE)R3=20.5*RADIUS(3)
      IF(.NOT.VPLATE)R4=20.5*RADIUS(4)
      IF(((RADIUS(4).GT.R4.OR.RADIUS(5).GT.R4).AND.(VROD.OR.VCOIL)).OR.
     *  ((RADIUS(1).GT.R3.OR.RADIUS(2).GT.R3).AND.SROD))GOTO830
      IF(SPLATE.AND.(RADIUS(2).LT.RADIUS(1)))GOTO870
      IF(SROD)  WRITE(6,720)(RADIUS(K),K=1,3)
      IF(SPLATE)WRITE(6,730)(RADIUS(K),K=1,3)
      IF(VROD)  WRITE(6,740)RADIUS(4),RADIUS(6)
      IF(VCOIL) WRITE(6,750)(RADIUS(K),K=4,6)
      IF(VPLATE)WRITE(6,760)RADIUS(4),RADIUS(6)
      WRITE(6,770)HEIGHT,WIDTH
      IF(RADIUS(3).EQ.90..OR.RADIUS(6).EQ.90.)GOTO850
C
C---- COMPUTE PLATE ANGLES IN RADIANS ---------------------------------
      IF(SPLATE)RADIUS(3)=RADIUS(3)*PI/180.
      IF(VPLATE)RADIUS(6)=RADIUS(6)*PI/180.
C
  720 FORMAT(T10,'RADIUS OF SAMPLE IS      ',T50,F7.4,' CM.',/,
     *        T10,'RADIUS OF CAN (OUTER) IS',T50,F7.4,' CM.',/,
     *        T10,'INCREMENT IN ABSORPTION INTEGRAL IS',T50,F7.4,
     *        T10,'CYLINDRICAL SAMPLE GEOMETRY')
  730 FORMAT(T10,'THICKNESS OF SAMPLE PLATE IS',T50,F7.4,' CM.',/,
     *        T10,'THICKNESS OF SAMPLE +CAN IS ',T50,F7.4,' CM.',/,
     *        T10,'ANGLE OF SAMPLE NORMAL TO BEAM IS',T50,F7.4,' DEGS.',/
     *      ,T10,'FLAT PLATE SAMPLE GEOMETRY')
  740 FORMAT(T10,'RADIUS OF VANADIUM ROD IS   ',T50,F7.4,' CM.',
     *     /,T10,'INCREMENT IN ABSORPTION INTEGRAL IS',T50,F7.4,' CM.',
     *     /,T10,'VANADIUM STANDARD HAS CYLINDRICAL GEOMETRY')
  750 FORMAT(T10,'RADIUS OF VANADIUM COIL (INNER) IS',T50,F7.4,' CM.',/,
     *        T10,'RADIUS OF VANADIUM COIL (OUTER) IS',T50,F7.4,' CM.',/,
     *        T10,'INCREMENT IN ABSORPTION INTEGRAL IS',T50,F7.4,' CM.',
     *     /,T10,'VANADIUM STANDARD IS IN FORM OF COIL')
  760 FORMAT(T10,'THICKNESS OF VANADIUM PLATE IS',T50,F6.3,' CM.',/,
     *        T10,'ANGLE OF VANADIUM NORMAL TO BEAM IS',T50,F6.3,' DEGS.'
     *    ,/,T10,'VANADIUM STANDARD IS IN FORM OF A FLAT PLATE')
  770 FORMAT(T10,'HEIGHT OF BEAM IS',F6.3,' CM.',/,
     *        T10,'WIDTH  OF BEAM IS',F6.3,' CM.')
C
C---- INPUT NUMBER DENSITIES OF SAMPLE,CAN AND VANADIUM ---------------
      READ(5,DENSTY)
      WRITE(13,DENSTY)
      RHOS=.6023*SDENS/SMW
      RHOC=.6023*CDENS/CMW
      RHOV=.6023*VDENS/VMW
      WRITE(6,780)SDENS,SMW,RHOS,CDENS,CMW,RHOC,VDENS,VMW,RHOV
  780 FORMAT(T10,'SAMPLE DENSITY IS  ',T30,F8.3,' GM./C.C.',
     *             'MOLECULAR WEIGHT IS',T68,F9.3,
     *        T80,'NUMBER DENSITY IS  ',T98,F8.5,/,
     *        T10,'CAN DENSITY IS     ',T30,F8.3,' GM./C.C.',
     *             'MOLECULAR WEIGHT IS',T68,F9.3,
     *        T80,'NUMBER DENSITY IS  ',T98,F8.5,/,
     *        T10,'VANADIUM DENSITY IS',T30,F8.3,' GM./C.C.',
     *             'MOLECULAR WEIGHT IS',T68,F9.3,
     *        T80,'NUMBER DENSITY IS  ',T98,F8.5,/)
C
C---- READ PARAMETERS FOR PLACZEK CORRECTIONS -------------------------
      READ(5,PLZCK)
      WRITE(13,PLZCK)
      IF(ANO.NE.1.0E+3 )ANU=ANO
      IF(ANO.NE.1.0E+3 )ANU=ANO
      WRITE(6,790)EBAR,CBAR,RKBAR,ANU
  790 FORMAT(T10,'MEAN KINETIC ENERGY OF MOLECULE IS',F10.5,' MILLI EV '
     *    ,/,T10,'MEAN VALUE OF CBAR IS',F10.5,'          ',/,
     *        T10,'MEAN VALUE OF KBAR IS',F10.5,' EV    ',/,
     *        T10,'EFFECTIVE MOLECULAR MASS IS',E12.3,' A.M.U.')
```

```
C
C---- PRINT SCATTERING CROSS SECTION/ENERGY MESHES -------------------
      WRITE(6,800)
      CALL OJOHNA(E1,SIGMA1,IMAX1,10,6,6,'EF',' SIGMA S',0)
      WRITE(6,810)
      CALL OJOHNA(E2,SIGMA2,IMAX2,10,6,6,'EF',' SIGMA C',0)
      WRITE(6,820)
      CALL OJOHNA(E3,SIGMA3,IMAX3,10,6,6,'EF',' SIGMA V',0)
  800 FORMAT(//,T10,'SAMPLE SCATTERING CROSS SECTION/ENERGY MESH')
  810 FORMAT(//,T10,'CAN SCATTERING CROSS SECTION/ENERGY MESH ')
  820 FORMAT(//,T10,'VANADIUM SCATTERING CROSS SECTION/ENERGY MESH')
      GOTO890
C
C---- CYLINDRICAL SAMPLE ERROR -----------------------------------------
  830 WRITE(6,840)
  840 FORMAT(' **',' RADII OF SAMPLES/DELTAR IS GREATER THAN 20 ')
      WRITE(6,SIZES)
      GOTO1620
C
C---- PLATE SAMPLE ERROR -----------------------------------------------
  850 WRITE(6,860)RADIUS(3),RADIUS(6)
  860 FORMAT(T10,'**** SAMPLE IS PARALLEL TO BEAM, THETA(SAMPLE)=',F6.3,
     *           ' THETA(VANADIUM)=',F6.3)
      WRITE(6,SIZES)
      GOTO1620
  870 WRITE(6,880)RADIUS(2),RADIUS(1)
  880 FORMAT(T10,'**** (SAMPLE+CAN) WIDTH IS GREATER THAN SAMPLE WIDTH')
      WRITE(6,SIZES)
      GOTO1620
C
C----- COMPUTE SECANTS OF PLATE ANGLES COSS AND COSV ------------------
  890 IF(SPLATE)COSS=1./COS(RADIUS(3))
      IF(VPLATE)COSV=1./COS(RADIUS(6))
C
C----- CHECK FOR FORM OF DATA OUTPUT ----------------------------------
      IF(Q)      WRITE(6,900)
      IF(TOF)    WRITE(6,910)
      IF(LAMBDA)WRITE(6,920)
  900 FORMAT(/,T10,'DATA IS PRESENTED IN FORM OF Q-VALUES',/)
  910 FORMAT(/,T10,'DATA IS PRESENTED IN TIME OF FLIGHT VALUES',/)
  920 FORMAT(/,T10,'DATA IS PRESENTED IN WAVELENGTH VALUES',/)
C
C---- SET UP ODD VARIABLES -------------------------------------------
      R1=RADIUS(1)
      R2=RADIUS(2)
      R3=RADIUS(3)
      R4=RADIUS(4)
      R5=RADIUS(5)
      R6=RADIUS(6)
      IF(VROD)         DUMR=R4+R6
      IF(VPLATE)       DUMR=R4*1.1
      IF(.NOT.ABSORB)GOTO930
C---- B2CON=TIME IN MICRO SECONDS FOR ABSORPTION X-SECTION ------------
      B2CON=.0022/TFP
      B2S1=SABS*B2CON
      B2C1=CABS*B2CON
      B2V1=VABS*B2CON
C
C---- LOOP OVER ALL COUNTERS WRITING THEM TO DISC 8 ------------------
  930 DO 1010 INC=1,NCTRS
      IF(NC(INC).EQ.0)GOTO1010
      DO 940 K=1,2048
      A(K)=0.
      B(K)=0.
      C(K)=0.
  940 D(K)=0.
C
C---- READ OFF RUNS FROM SCRATCH DISC AND SUM TOGETHER ----------------
C---- ACCORDING TO TYPE K=1,2,3 OR 4 ----------------------------------
      J=1
  950 K=TYPE(J)
      NR=RUN(J)
      GOTO(960,970,980,990),K
C
C---- READ OFF SAMPLE AND CAN RUN,RETURNS WITH RUN ADDED IN TO ARRAY A -
C---- ,MONITORS FROM M INTO RMC AND PRF PULSES FROM MPRF INTO RPULSE ---
  960 CALL DISC(A,IARR,NR,ICHNL,INC,ICON,SUM,K,J,RMC,&950,&1000,NTRN,M,
     *          MPRF,RPULSE,JMAX,NSEQ)
  970 CALL DISC(B,IARR,NR,ICHNL,INC,ICON,SUM,K,J,RMC,&950,&1000,NTRN,M,
     *          MPRF,RPULSE,JMAX,NSEQ)
```

```
  980 CALL DISC(C,IARR,NR,ICHNL,INC,ICON,SUM,K,J,RMC,&950,&1000,NTRN,M,
     *              MPRF,RPULSE,JMAX,NSEQ)
  990 CALL DISC(D,IARR,NR,ICHNL,INC,ICON,SUM,K,J,RMC,&950,&1000,NTRN,M,
     *              MPRF,RPULSE,JMAX,NSEQ)
C
C---- PUT A,B,C,D TO DISC 8 -------------------------------------------
 1000 WRITE(8'4*INC-3)A
      WRITE(8'4*INC-2)B
      WRITE(8'4*INC-1)C
      WRITE(8'4*INC)D
 1010 CONTINUE
      ENDFILE 8
C
      DO 1600 INC=1,NCTRS
      TBEG=ZA02AS(DUMMY)
      IF(NC(INC).EQ.0)GOTO1600
      FIND(8'4*INC-3)
      IF(Q)      GOTO1060
      IF(TOF)    GOTO1020
      IF(LAMBDA)GOTO1040
C
C---- PRODUCE TIME CHANNELS -------------------------------------------
 1020 DO 1030 I=1,ICHNL
 1030 T(I)=RI+FLOAT(ICHNLW*I)
      GOTO1100
C
C---- PRODUCE WAVELENGTH VALUES ---------------------------------------
 1040 CON2=TFP*252.7
      DO 1050 I=1,ICHNL
 1050 T(I)=(RI+FLOAT(ICHNLW*I))/CON2
      GOTO1100
C---- PRODUCE Q VALUES ------------------------------------------------
C
 1060 IF(.NOT.RECOIL)GOTO1070
C---- RECOIL CORRECTION -----------------------------------------------
      X=1.-COS(CA(INC)*2.+ARSIN(SIN(CA(INC)*2.)/ANU))
      X=SQRT(1.-2.*ANU*X/(ANU+1.)**2)
C---- APPLY CENTRE OF MASS TRANSFORMATION -----------------------------
      C3=1587.761*TFP*((1.-F)*X+F)*SQRT(X*X+1.-2.*X*COS(CA(INC)*2.))/X
      DCA=CA(INC)*114.5915
 1070 IF(.NOT.RECOIL)C3=3175.5218*SIN(CA(INC))*TFP
C---- Q-SCALE ---------------------------------------------------------
      DO 1090 K=1,ICHNL
      IF(K.EQ.1.AND.RECOIL)WRITE(6,1080)X,DCA
 1080 FORMAT(T10,'RATIO OF V2 TO V1 IS',F6.3,' AT',F6.3,' DEGREES')
 1090 T(K)=C3/(RI+FLOAT(CHAN*K))
C
C----- SET UP AN ARRAY OF 54 PAALMAN AND PINGS TERMS ------------------
C---- CHECK TO SEE IF WE HAVE DOWNSTREAM MONITOR ----------------------
 1100 IF(CA(INC).EQ.0.)TRANSM=.TRUE.
      IF(CA(INC).NE.0.)TRANSM=.FALSE.
      IF(TRANSM)GOTO1150
      IF(.NOT.ABSORB)GOTO1130
      TCON=RI
      DO 1110 I=1,20
      R(I)=0.
      DO 1110 J=1,6
      AB(J,I)=0.
      SI(J,I)=0.
      AS(J,I)=0.
      NU(J,I)=0.
      ENU(J,I)=0.
 1110 CONTINUE
C
C----- # OF CHANNELS PER ARRAY ELEMENT (NCPK)    ----------------------
      NCPK=10*ICHNL/512
      CHAN2=FLOAT(CHAN*NCPK)
      IF(IMAX1.EQ.1)B1S=SIGMA1(1)
      IF(IMAX2.EQ.1)B1C=SIGMA2(1)
      IF(IMAX3.EQ.1)B1V=SIGMA3(1)
      DO 1120 K=1,54
      TCON=TCON+CHAN2
C
C----- ABSORPTION X-SECTIONS FOR ARRAY ELEMENT (B2S,B2C & B2V) ---------
      B2S  =TCON*B2S1
      B2C  =TCON*B2C1
      B2V  =TCON*B2V1
C
C---- CHECK FOR SCATTERING CROSS SECTION SHORT CUT  -------------------
      IF(IMAX1.GT.1)B1S=BARN1(K,SIGMA1,E1,RI,TFP,CHAN,1)
```

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      IF(IMAX2.GT.1)B1C=BARN1(K,SIGMA2,E2,R1,TFP,CHAN,2)
      IF(IMAX3.GT.1)B1V=BARN1(K,SIGMA3,E3,R1,TFP,CHAN,3)
C
C---- SAMPLE ABSORPTION CORRECTION TERMS -----------------------------------
      CALL ABSORP(B1S,B2S,B1C,B2C,RHOS,RHOC,R1,R2,R3,ASS1(K),ACC1(K),
     *              ACS1(K),CA(INC),1,AB,SI,AS,ENU,NU,R,ABSORB,SCATTR,
     *              SPLATE,VPLATE,TRANS(INC))
C
C---- VANADIUM ROD CORRECTION TERMS ----------------------------------------
      IF(VROD)CALL ABSORP(B1V,B2V,Z,Z,RHOV,Z,R4,DUMR,R6,ASS2(K),ADUM,
     *                        ACS2(K),CA(INC),2,AB,SI,AS,ENU,NU,R,ABSORB,
     *                        SCATTR,SPLATE,VPLATE,TRANS(INC))
C
C---- VANADIUM COIL CORRECTION TERMS ---------------------------------------
      IF(VCOIL)CALL ABSORP(Z,Z,B1V,B2V,Z,RHOV,R4,R5,R6,ADUM,ASS2(K),
     *                        ADUM,CA(INC),2,AB,SI,AS,ENU,NU,R,ABSORB,
     *                        SCATTR,SPLATE,VPLATE,TRANS(INC))
C
C---- VANADIUM PLATE CORRECTION TERMS --------------------------------------
      IF(VPLATE)CALL ABSORP(B1V,B2V,Z,Z,RHOV,Z,R4,DUMR,R6,ASS2(K),ADUM,
     *                         ADUM,CA(INC),2,AB,SI,AS,ENU,NU,R,ABSORB,
     *                         SCATTR,SPLATE,VPLATE,TRANS(INC))
 1120 CONTINUE
C
C---- WRITE ABSORPTION CORRECTION TERMS ------------------------------------
 1130 FIND(8'4*INC-3)
      WRITE(6,1140)
      WRITE(6,1150)(ASS1(K),ACC1(K),ACS1(K),ASS2(K),ACS2(K),
     *    ASS1(K+1),ACC1(K+1),ACS1(K+1),ASS2(K+1),ACS2(K+1),K=1,54,2)
 1140 FORMAT(/,T10,'PAALMAN AND PINGS ABSORPTION CORRECTION TERMS ',
     * 'ARE:',//,T11,'ASS1',T18,'ACC1',T25,'ACS1',T32,'ASS2',T39,
     * 'ACS2',T46,'ASS1',T53,'ACC1',T60,'ACS1',T67,'ASS2',T74,'ACS2')
 1150 FORMAT(T8,10F7.4)
C
C----- RECOVER A,B,C,D   ---------------------------------------------------
 1160 READ(8'4*INC-3)A
      READ(8'4*INC-2)B
      READ(8'4*INC-1)C
      READ(8'4*INC)D
C
C---- LIST COUNTS,MONITORS AND COUNTS PER MONITOR  --------------------------
      WRITE(6,1170)
 1170 FORMAT(/,T10,'COUNTS,MONITORS,PULSES & COUNTS PER MONITOR',//)
C
C---- LOOP OVER RUN TYPE K=1,2,3,4 -----------------------------------------
      DO 1180 K=1,4
      CSUM(K)=0.
C
C---- LOOP OVER RUN SEQUENCE ON DISC J=1,2,...JMAX -------------------------
      DO 1180 J=1,JMAX
      SK=SUM(K,INC,J)
      MPRFK=MPRF(INC,J)
      MK=M(INC,J)
      IF(SK.GT..1.AND.MK.GT.0)CPM=SK/FLOAT(MK)
      IF(SK.GT..1)WRITE(6,1210)SK,MK,MPRFK,CPM,RTP(K),INC,RUN(J),J
 1180 CSUM(K)=CSUM(K)+SK
C
C---- PRINT MONITORS AND SUMMED COUNTS FOR EACH COUNTER --------------------
      WRITE(6,1220)INC,(RMC(INC,K),K=1,4),INC,CSUM,INC,
     *           (RPULSE(INC,L),L=1,4)
C
C---- PRINT COUNTS PER MONITOR ---------------------------------------------
      DO 1190 K=1,4
 1190 CSUM(K)=CSUM(K)*.01/RMC(INC,K)
      WRITE(6,1230)INC,CSUM
C
C---- PRINT COUNTS PER PULSE -----------------------------------------------
      DO 1200 K=1,4
      IF(RPULSE(INC,K).EQ.0.)CSUM(K)=0.
      IF(RPULSE(INC,K).EQ.0.)GOTO1200
      CSUM(K)=CSUM(K)*RMC(INC,K)/RPULSE(INC,K)*100.
 1200 CONTINUE
      WRITE(6,1240)INC,CSUM
C
 1210 FORMAT(T10,'SUM=',F12.0,' MONITOR=',I10,' PRF=',I10,
     *              ' SUM/MON=',F12.5,' TYPE=',A8,' COUNTER=',I2,
     *              ' RUN=',I10,' NO.=',I2)
 1220 FORMAT(/,T10,'MONITOR COUNTS FOR CTR:',I2,
     *               ' S+C',F10.0,' C',F10.0,' V+B',F10.0,' B',F10.0,/,
     *          T10,'SUMMED COUNTS FOR CTR:',I2,
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     *               ' S+C',F10.0,' C',F10.0,' V+B',F10.0,' B',F10.0,/,
     *         T10,'PRF PULSES     FOR CTR:',I2,
     *               ' S+C',F10.0,' C',F10.0,' V+B',F10.0,' B',F10.0,/)
 1230 FORMAT(T10,'COUNTS/MONITOR FOR CTR:',I2,
     *               ' S+C',F10.3,' C',F10.3,' V+B',F10.3,' B',F10.3,/)
 1240 FORMAT(T10,'COUNTS/PULSE   FOR CTR:',I2,
     *               ' S+C',F10.3,' C',F10.3,' V+B',F10.3,' B',F10.3,/)
C
C---- LIST RAW DATA ----------------------------------------------------------
      ICHNL1=(ICHNL/6)+1
      IF(.NOT.PRINT)GOTO1290
      WRITE(13,1250)INC
      CALL OJOHNA(T,A,ICHNL,ICHNL1,4,6,'FF','S+C      ',13)
      WRITE(13,1260)INC
      CALL OJOHNA(T,B,ICHNL,ICHNL1,4,6,'FF','CAN      ',13)
      WRITE(13,1270)INC
      CALL OJOHNA(T,C,ICHNL,ICHNL1,4,6,'FF','V+B      ',13)
      WRITE(13,1280)INC
      CALL OJOHNA(T,D,ICHNL,ICHNL1,4,6,'FF','BACK     ',13)
 1250 FORMAT(1H1,'SAMPLE+CAN RUN:COUNTER',I3)
 1260 FORMAT(1H1,'CAN RUN:COUNTER',I3)
 1270 FORMAT(1H1,'VANADIUM+BACKGROUND RUN:COUNTER',I3)
 1280 FORMAT(1H1,'BACKGROUND RUN:COUNTER',I3)
 1290 SIG1=SIGMA1(1)
C
C----- APPLY DEAD TIME CORRECTIONS --------------------------------------------
      CALL DEADT(RATIO,A,ICHNL,NDEAD,RPULSE,NCTRS,INC,DEAD,RMC,1)
      CALL DEADT(RATIO,B,ICHNL,NDEAD,RPULSE,NCTRS,INC,DEAD,RMC,2)
      CALL DEADT(RATIO,C,ICHNL,NDEAD,RPULSE,NCTRS,INC,DEAD,RMC,3)
      CALL DEADT(RATIO,D,ICHNL,NDEAD,RPULSE,NCTRS,INC,DEAD,RMC,4)
      DO 1300 K=1,ICHNL
 1300 RATIO(K)=0.
      A(1)=1.
      B(1)=1.
      C(1)=1.
      D(1)=1.
C
C---- PLOT RAW DATA ----------------------------------------------------------
      IF(.NOT.PLOT)GOTO1310
      CALL DRAW(0,T,A,11,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *             ABSORB,XMAX,XMIN)
      CALL DRAW(0,T,B,12,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *             ABSORB,XMAX,XMIN)
      CALL DRAW(0,T,C,12,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *             ABSORB,XMAX,XMIN)
      CALL DRAW(0,T,D,12,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *             ABSORB,XMAX,XMIN)
 1310 IF(TRANSM)GOTO1320
      IF(CAN)CALL FRAME
      IF(CAN)CALL SCALES
      IF(CAN)CALL BORDER
C
C
C---- SMOOTH CONTAINER -------------------------------------------------------
      IF(CAN)CALL SMTH(B,RATIO,T,ICHNL,CHAN,RD,W)
      IF(SMOOTH.AND..NOT.CAN)CALL FRAME
      IF(SMOOTH.AND..NOT.CAN)CALL SCALES
      IF(SMOOTH.AND..NOT.CAN)CALL BORDER
C
C---- SMOOTH VANADIUM AND BACKGROUND ------------------------------------------
      IF(SMOOTH)CALL SMTH(C,RATIO,T,ICHNL,CHAN,RD,W)
      IF(SMOOTH)CALL SMTH(D,RATIO,T,ICHNL,CHAN,RD,W)
      IF(.NOT.CAN.AND..NOT.SMOOTH)GOTO1320
      CALL CTRMAG(10)
      CALL PLACE(20,10)
      CALL TYPECS('SMOOTHED ',9)
      CALL TYPECS('COUNTER',8)
      CALL TYPENI(INC)
      CALL PLACE(20,2)
      CALL TYPECS(TITLE,72)
C
C---- DUMMY NO. TO SCRATCH DISC    -------------------------------------------
 1320 IF(EQUALQ)WRITE(14'INC)NC(INC)
      IF(EQUALQ)WRITE(12,1330)INC,NC(INC)
 1330 FORMAT(1X,'NC(INC) WRITTEN TO DISC #14 FOR COUNTER',I3,' AS',I3)
C
C---- PLACZEK CONSTANTS   ----------------------------------------------------
      IF(TRANSM)GOTO1480
      ECCON2=TFP*SIN(CA(INC))
      ECCON2=1./(ECCON2*ECCON2*ECCON1)
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      TEND=ZA02AS(DUMMY)
      TDIFF=TEND-TBEG
      WRITE(6,1340)INC,TDIFF
 1340 FORMAT(/,T10,'COUNTER',I3,' ABSORPTION + DISC SPOOLING',
     *              ' TAKES',F10.5,' SECS')
C
C----- COMPUTE PLACZEK TERMS -------------------------------------------
C----- RATIO OF PATH LENGTHS (F) AND SIN**2(THETA) (SST) ---------------
      SST=SIN(CA(INC))
      SST=SST*SST
      RANO=1./ANU
      RN=.83
      P1=-2.*SST*RANO*(1.-F*(1.-2.*RN))
      P2=2.*SST*RANO**2*(1.-F*(1.-2.*RN)*(1.+2.*F*RN)*SST)
      P3=EBAR*(COS(CA(INC)*2.)-2.*F*(1.+2.*RN)*(1.-2.*F*(1.+RN))*SST)*
     *    1.9366
      P4=1.+P1+P2
      WRITE(6,1350)P1,P2,P3
 1350 FORMAT(/,T10,'PLAZCEK TERMS ARE:',3F10.5)
C
C----- COMPUTE RHO*SIGMA TERMS  -----------------------------------------
      IF(.NOT.EXPO)GOTO1360
      IF(VROD  )VOLVR=RHOV*R4*1.570796
      IF(VCOIL )VOLVC=RHOV*(R5-R4*R4/R5)*1.570796
      IF(SROD  )VOLSR=RHOS*R1*1.570796
 1360 IF(VPLATE)VOLVP=RHOV*R4*COSV
      IF(SPLATE)VOLSP=RHOS*R1*COSS
      IF(EXPO  )GOTO1370
      IF(SROD  )VOLSR=RHOS*R1*R1*3.141592654
      IF(VROD  )VOLVR=RHOV*R4*R4*3.141592654
      IF(VCOIL )VOLVC=RHOV*(R5*R5-R4*R4)*3.141592654
C
C----- PLOT ABSORPTION CORRECTION TERMS ---------------------------------
 1370 CALL FRAME
      CALL MAP    (AMIN1(T(1),T(ICHNL)),AMAX1(T(1),T(ICHNL)),.5,1.05)
      CALL WINDOW(AMIN1(T(1),T(ICHNL)),AMAX1(T(1),T(ICHNL)),.5,1.05)
      CALL SCALES
      CALL BORDER
      CALL CTRMAG(1 )
      CALL PLACE(20,2)
      CALL TYPECS(TITLE,72)
      CALL CTRMAG(15)
      CALL PLACE(40,45)
      CALL TYPECS('PAALMAN AND PINGS CORRECTION TERMS:COUNTER',42)
      CALL TYPENI(INC)
      CALL CTRMAG(1)
      RIRT =1./FLOAT(NCPK)
C
C----- SET UP PAALMAN AND PINGS TERMS FOR EACH CHANNEL  ----------------
      RTIME=R1
      DO 1450 K=1,ICHNL
C---- CHOOSE ELEMENT OF ARRAY  -----------------------------------------
      J    =(K-1)/NCPK+1
      RK   =FLOAT(K-(J-1)*NCPK-1)*RIRT
      JP1  =J+1
      ASS  =ASS1(J)+RK*(ASS1(JP1)-ASS1(J))
      ACC  =ACC1(J)+RK*(ACC1(JP1)-ACC1(J))
      ACS  =ACS1(J)+RK*(ACS1(JP1)-ACS1(J))
      ASV  =ASS2(J)+RK*(ASS2(JP1)-ASS2(J))
      ASV2=1.
      CALL PLOTNC(T(K),ASS,43)
      CALL PLOTNC(T(K),ACC,43)
      CALL PLOTNC(T(K),ACS,43)
      CALL PLOTNC(T(K),ASV,43)
      CALL PLOTNC(T(K),ASV2,43)
C
C---- CHECK TO SEE IF BACKGROUND IS TO BE SUBTRACTED FROM -------------
C---- (SAMPLE AND CAN)  AND CAN SEPARATELY -----------------------------
      SC=C(K)
      SD=D(K)
      IF(CRYOST)GOTO1380
      SA=A(K)-SD
      SB=B(K)-SD
      GOTO1390
 1380 SA=A(K)
      SB=B(K)
C
C---- FINISHED WITH A,B,C & D  -----------------------------------------
 1390 IF(.NOT.ABSORB)GOTO1400
      TOP=(SA-SB*ACS/ACC)/ASS
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      BOTTOM=(SC-SD)/ASV
      GOTO1410
 1400 TOP=SA-SB
      BOTTOM=SC-SD
C
C---- ZERO DIVIDE CHECK FOR VANADIUM ------------------------------------
 1410 IF(BOTTOM.LE..000001)WRITE(6,1420)INC,K,BOTTOM,SC,SD
      IF(BOTTOM.LE..000001)GOTO1450
 1420 FORMAT(T10,'VANADIUM < .000001 FOR COUNTER',I3,' CHANNEL',I5,
     A ' BOTTOM =',F12.5,' SC=',F12.5,' SD=',F12.5)
      RATIO(K)=TOP/BOTTOM
      B1S=SIGMA1(1)
      B1V=SIGMA3(1)
C
C---- CORRECT FOR AREA OF SAMPLE AND VANADIUM STANDARD -----------------
      IF(.NOT.EXPO)GOTO1430
      IF(SROD  )RATIO(K)=RATIO(K)/(2.*R1)
      IF(SPLATE)RATIO(K)=RATIO(K)/WIDTH
      IF(VROD  )RATIO(K)=RATIO(K)*R4
      IF(VCOIL )RATIO(K)=RATIO(K)*R5
      IF(VPLATE)RATIO(K)=RATIO(K)*WIDTH
      IF(SROD  )RATIO(K)=RATIO(K)/(1.-EXP(-B1S*VOLSR))
      IF(SPLATE)RATIO(K)=RATIO(K)/(1.-EXP(-B1S*VOLSP))
      IF(VROD  )RATIO(K)=RATIO(K)*(1.-EXP(-B1V*VOLVR))
      IF(VCOIL )RATIO(K)=RATIO(K)*(1.-EXP(-B1V*VOLVC))
      IF(VPLATE)RATIO(K)=RATIO(K)*(1.-EXP(-B1V*VOLVP))
 1430 IF(EXPO)GOTO1440
      IF(VROD  )RATIO(K)=RATIO(K)*B1V*VOLVR
      IF(VCOIL )RATIO(K)=RATIO(K)*B1V*VOLVC
      IF(VPLATE)RATIO(K)=RATIO(K)*B1V*VOLVP
C
C---- COMPUTE D(SIGMA)/D(OMEGA) -----------------------------------------
 1440 IF(EXPO.AND.(SROD.OR.SPLATE))A(K)=RATIO(K)*.0795774715*B1S
      IF(.NOT.EXPO.AND.SROD     )   A(K)=RATIO(K)*.0795774715/VOLSR
      IF(.NOT.EXPO.AND.SPLATE   )   A(K)=RATIO(K)*.0795774715/VOLSP
C
C---- COMPUTE S(Q) ------------------------------------------------------
      RTIME=RTIME+CHAN
      QS=ECCON2*RTIME**2
      RATIO(K)=1.+(A(K)*FP1-B1S*(P4+P3*QS))/SCOH
 1450 CONTINUE
C
C---- PRINT OUT S(Q) AND D(SIGMA)/D(OMEGA) ------------------------------
      WRITE(6,1460)INC
      CALL OJOHNA(T,RATIO,ICHNL,ICHNL1,4,5,'FF','S(Q)     ',6)
      WRITE(6,1470)INC
      CALL OJOHNA(T,A,ICHNL,ICHNL1,4,5,'FF','DS/DW    ',6)
 1460 FORMAT(1H1,T10,'S(Q) FOR COUNTER',I3)
 1470 FORMAT(1H1,T10,'DS/DW FOR COUNTER',I3)
C
C---- COMPUTE,LIST AND PLOT TRANSMISSION RATIOS FOR SAMPLE AND VANADIUM
 1480 IF(.NOT.TRANSM)GOTO1540
      CON4=1./(TFP*252.7)
      DO 1490 K=1,ICHNL
C==== WAVELENGTH SCALE ==================================================
      T(K)=(R1+FLOAT(CHAN*K))*CON4
C---- SAMPLE/CONTAINER --------------------------------------------------
      RATIO(K)=A(K)/B(K)
C---- VANADIUM/BACKGROUND -----------------------------------------------
 1490 A(K)=C(K)/D(K)
C
C---- LIST --------------------------------------------------------------
      WRITE(6,1500)INC
      CALL OJOHNA(T,RATIO,ICHNL,ICHNL1,4,5,'FF','SAMPLE  ',6)
      WRITE(6,1510)INC
      CALL OJOHNA(T,A,ICHNL,ICHNL1,4,5,'FF','VANADIUM',6)
 1500 FORMAT(1H1,T10,'TRANSMISSION RATIO FOR SAMPLE COUNTER',I3)
 1510 FORMAT(1H1,T10,'TRANSMISSION RATIO FOR VANADIUM',I3)
C
C---- PLOT RATIOS -------------------------------------------------------
      CALL DRAW(3,T,RATIO,INC,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *          ABSORB,XMAX,XMIN)
C==== COMPUTE TRANSMISSION RATIO FROM CROSS SECTIONS IN READ1 AND ASIGMA
C==== ABSORPTION CROSS SECTION CONSTANT =================================
      B2S2=B2S1/CON4
C==== SCATTERING CROSS SECTION IN SHORT CUT CASE OF ONE VALUE IN READ1 =
      IF(IMAX1.EQ.1)B1S2=SIGMA1(1)
      VOLSP=-RHOS*R1*COSS
      VOLSR=-RHOS*R1*1.570796
      DO 1520 K=1,ICHNL
```

```
C==== SCATTERING CROSS SECTION FROM READ1 ARRAYS SIGMA AND E ===========
      IF(IMAX1.GT.1)B1S2=BARN1(K,SIGMA1,E1,RI,TFP,CHAN,1)
C==== FIRST FLAT PLATE CASE ============================================
      IF(SPLATE)RATIO(K)=EXP(VOLSP*(B2S2*T(K)+B1S2))
C==== SECONDLY ROD WITH EFFECTIVE THICKNESS PI*RADIUS/2 ================
      IF(SROD  )RATIO(K)=EXP(VOLSR*(B2S2*T(K)+B1S2))
 1520 CONTINUE
C==== NOW PLOT AS A LINE ON MEASURED RATIO =============================
      CALL PTPLOT(T,RATIO,1,ICHNL,-43)
C
C==== REPEAT SEQUENCE FOR VANADIUM STANDARD ============================
      CALL DRAW(4,T,A,INC,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,LAMBDA,
     *          ABSORB,XMAX,XMIN)
      B2V2=B2V1/CON4
      VOLVP=-RHOV*R4*COSV
      VOLVR=-RHOV*R4*1.570796
      VOLVC=-RHOV*(R5-R4*R4/R5)*1.570796
      IF(IMAX3.EQ.1)B1V2=SIGMA3(1)
      DO 1530 K=1,ICHNL
      IF(IMAX3.GT.1)B1V2=BARN1(K,SIGMA3,E3,RI,TFP,CHAN,3)
      IF(VPLATE)RATIO(K)=EXP(VOLVP*(B2V2*T(K)+B1V2))
      IF(VROD  )RATIO(K)=EXP(VOLVR*(B2V2*T(K)+B1V2))
      IF(VCOIL )RATIO(K)=EXP(VOLVC*(B2V2*T(K)+B1V2))
 1530 CONTINUE
      CALL PTPLOT(T,RATIO,1,ICHNL,-43)
      GOTO1550
C
C
C---- PLOT -------------------------------------------------------------
 1540 IF(.NOT.PLOT)GOTO1550
      CALL DRAW(1,T,RATIO,INC,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,
     *          LAMBDA,ABSORB,XMAX,XMIN)
      CALL DRAW(2,T,A    ,INC,ICHNL,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,
     *          LAMBDA,ABSORB,XMAX,XMIN)
C
C---- PUNCH  -----------------------------------------------------------
 1550 IF(.NOT.PUNCH)GOTO1580
      DO 1560 I=1,ICHNL,12
      II=(I/12)+1
      IF(.NOT.SMQ)WRITE(7,1570)(A(I+K-1),K=1,12),II
 1560 IF(SMQ)WRITE(7,1570)(RATIO(I+K-1),K=1,12),II
 1570 FORMAT(12F6.3,I8)
C
C---- WRITE S(Q) OR DS/DW TO SCRATCH DISC ------------------------------
 1580 IF(EQUALQ.AND.SMQ)WRITE(14'INC)NC(INC),RATIO
      IF(EQUALQ.AND..NOT.SMQ)WRITE(14'INC)NC(INC),A
      WRITE(6,1590)
 1590 FORMAT(T10,'DATA FILE WRITTEN TO DISC #14')
C
C---- END TIMING SEQUENCE ----------------------------------------------
      TEND =ZA02AS(DUMMY)
      TDIFF=TEND-TBEG
      WRITE(6,1610)INC,TDIFF
 1600 CONTINUE
 1610 FORMAT(T10,'COMPLEAT COUNTER',I3,' TAKES ',F10.5,' SECONDS')
C
C---- EQUAL QBIN SUBROUTINE --------------------------------------------
      IF(.NOT.TRANSM)CALL QBIN(TITLE,ICHNL,RI,CHAN,CA,TFP,NCTRS,RATIO,
     *                         T,D,WK,QK,RSK,NC,EQUALQ)
 1620 CONTINUE
      CALL GREND
      STOP
C
C---- ERROR MESSAGE WHEN ALL COUNTERS HAVE BEEN SWITCHED OFF -----------
 1630 WRITE(6,1640)
 1640 FORMAT(T10,'*****************************************************
     ***************',/,T10,'DO YOU REALLY WANT TO SWITCH OFF ALL YOUR CO
     *UNTERS ???',/,T10,'PROGRAM HAS RESET COUNTER 1 NC(1) TO 1 AND WILL
     & CONTINUE',/)
     NC(1)=1
     GOTO20
     END
      FUNCTION BARN1(IT,S,E,RI,TFP,ICHNLW,N)
C
C---- FUNCTION (BARN1) TO FIND SCATTERING CROSS-SECTION AS A FUNCTION
C---- OF TIME CHANNEL (IT) FROM THE CROSS-SECTION ARRAY (SIGMA) VERSUS
C---- ENERGY (E) ------------------------------------------ ----------
C---- INITIAL DELAY (RI) MICROSECONDS ---------------------------------
C---- TOTAL FLIGHT PATH (TFP) METRES ----------------------------------
C---- CHANNEL WIDTH (ICHNLW) MICROSECONDS ------------------------------
```

```
C---- SAMPLE TYPE (N) 1 TO 3 (SAMPLE,CAN,VANADIUM) --------------------
C
      REAL CON5/5225.8/,S(1),E(1)
C---- CONVERT TIME OF FLIGHT TO ENERGY IN EV ---------------------------
      CHANL=FLOAT(ICHNLW*IT)
      SPEED=TFP/(R1+CHANL)
      DE=CON5*SPEED*SPEED
C---- CHECK LOWER ENERGY END OF MESH ----------------------------------
      J=1
      IF(DE.LT.E(1))WRITE(6,40)DE,N
   10 J=J+1
C---- CHECK UPPER ENERGY END OF MESH ----------------------------------
      IF(J.GT.40)WRITE(6,50)DE,N
      IF(DE-E(J))30,20,10
   20 BARN1=S(J)
      RETURN
C---- LINEARLY INTERPOLATE FOR FUNCTION -------------------------------
   30 JM1=J-1
      BARN1=S(JM1)+(S(J)-S(JM1))*(DE-E(JM1))/(E(J)-E(JM1))
   40 FORMAT(' ***** ENERGY MESH DOES NOT GO LOW ENOUGH IN ENERGY RANGE
     1 AT ',E12.3,' EV FOR SAMPLE TYPE ',I3)
   50 FORMAT(' ENERGY MESH DOES NOT GO HIGH ENOUGH IN ENERGY RANGE AT',
     1 E12.3,' EV   FOR SAMPLE TYPE ',I3)
      RETURN
      END
      SUBROUTINE OJOHNA (X,Y,M,NC,NSX,NSY,NF,H,IOUTP)
C
C---- MODIFIED HARWELL LIBRARY ROUTINE (OA03A) --------------------------
C---- WILL PRINT X AND Y ARRAYS OF M ELEMENTS IN NC COLUMNS--------------
C---- NSX FIGURES IN X, NSY FIGURES IN Y --------------------------------
C---- 'FF' 'EF ''FE' 'EE' FORMATS (NF) ----------------------------------
C---- HEADER CAPTION (H) OF 8 CHARACTERS --------------------------------
C---- OUTPUT CHANNEL (IOUTP) --------------------------------------------
C
      REAL*4 X(1),Y(1),H*8
      INTEGER*2 F1(16)/'(1X,00( 4X,0PF00. 00,2X ,1PE00. 00))'/,
     A F2(11)/'( 00X,A8, 00( 00X,A8))'/,NFL,NF,C0/'0'/,C1/'1'/,
     B PF/'PF'/,PE/'PE'/,FF/'FF'/,FE/'FE'/,EF/'EF'/
      INTEGER*4 MXFW/60/,LLL/128/
      LOGICAL*1 LF(2)
      EQUIVALENCE (NFL,LF(1))
      NFL=NF
      IF(NF.EQ.FF.OR.NF.EQ.FE) GO TO 20
   10 NXDEC=MAX0(NSX-1,0)
      NXW=NXDEC+7
      F1(6)=C1
      F1(7)=PE
      GO TO 30
   20 CALL OA03B (X,M,NXW,NXDEC,NSX)
      IF(NXW.GT.MXFW) GO TO 10
      F1(6)=C0
      F1(7)=PF
   30 CALL OA03C (F1,6,NXW)
      CALL OA03C (F1,10,NXDEC)
      IF(NF.EQ.FF.OR.NF.EQ.EF) GO TO 50
   40 NYDEC=MAX0(NSY-1,0)
      NYW=NYDEC+7
      F1(13)=C1
      F1(14)=PE
      GO TO 60
   50 CALL OA03B (Y,M,NYW,NYDEC,NSY)
      IF(NYW.GT.MXFW) GO TO 40
      F1(13)=C0
      F1(14)=PF
   60 CALL OA03C (F1,15,NYW)
      CALL OA03C (F1,17,NYDEC)
      NCOL=LLL/(NXW+NYW+6)
      IF(NCOL.EQ.0) GO TO 140
      CALL OA03C (F1,3,NCOL)
      K=NYW+NXW-2
      J=NXW+NYW/2+4
      CALL OA03C (F2,2,J)
      CALL OA03C (F2,8,K)
      CALL OA03C (F2,6,NCOL-1)
      K=NCOL
      IM=(M-1)/NC+1
      IK=(IM-1)/K+1
      IT=M-(IM-1)*NC
      ITAB=0
      I1=NC
```

```
      I3=NC*(K-1)
      NC3=NCOL
   70 IF(IK.LE.0)RETURN
      IF(IK.GT.1) GO TO 90
   80 I1=IT
      I3=(IM-1)*NC
      NC3=IM
   90 WRITE(IOUTP,F2) (H,J=1,NC3)
      DO 100 I=1,I1
      I2=ITAB+I
      I4=I2+I3
  100 WRITE(IOUTP,F1) (X(J),Y(J),J=I2,I4,NC)
      IF(IM.EQ.1.OR.I1.EQ.NC) GO TO 120
      I31=I3-NC
      I11=I1+1
      DO 110 I=I11,NC
      I2=ITAB+I
      I4=I2+I31
  110 WRITE(IOUTP,F1) (X(J),Y(J),J=I2,I4,NC)
  120 ITAB=ITAB+NC*K
      IK=IK-1
      IM=IM-K
      WRITE(IOUTP,130)
  130 FORMAT(' ')
      GO TO 70
  140 WRITE(IOUTP,150)
  150 FORMAT('0 ***** OJOHNA ERROR: FIELD WIDTHS OF COLUMNS TOO WIDE FOR
     *PAGE')
      WRITE(IOUTP,160) LF(1),NXW,NXDEC,LF(2),NYW,NYDEC
  160 FORMAT('            FORMATS  X: ',A1,I2,'.',I2,'  Y: ',A1,I2,'.',I2)
      RETURN
      END
      SUBROUTINE DRAW(IW,X,Y,J,IMAX,SQMAX,SQMIN,TITLE,SIG1,Q,TOF,
     * LAMBDA,ABSORB,XMAX1,XMIN1)
C
C---- ROUTINE PLOTS ARRAY (Y) AGAINST ARRAY (X) OF (IMAX) POINTS-----------
C---- BETWEEN (XMIN1) AND (XMAX1)  AND SQMIN AND SQMAX --------------------
C---- IW IS THE FUNCTION TYPE INDICATOR (1-4) S(Q),DS/DW,RATIOS -----------
C---- TITLE IS ON EVERY GRAPH ---------------------------------------------
C---- SIG1 IS THE MEAN VALUE FOR DS/DW GRAPHS -----------------------------
C---- Q,TOF AND LAMBDA INDICATE TYPE OF X-SCALE ---------------------------
C---- ABSORB INDICATES ABSORPTION CORRECTION FOR MESSAGE BOX ON GRAPH   ---
C
      REAL X(2048),Y(2048),TITLE(18),SQMAX(8),SQMIN(8),XMAX1(8),XMIN1(8)
      INTEGER DAY,YEAR
      LOGICAL Q,TOF,LAMBDA,ABSORB
C
C---- J=11,12,13,14 ARE SAMPLE+CAN,CAN,VANADIUM+BACKGROUND & BACKGROUND-
      IF(J.GT.11)GOTO40
      YMIN=Y(MN01A(Y(1),Y(2),IMAX))
      YMAX=Y(MX01A(Y(1),Y(2),IMAX))*1.1
      XMIN=X(MN01A(X(1),X(2),IMAX))
      XMAX=X(MX01A(X(1),X(2),IMAX))
C
C---- SAMPLE ETC RUNS RAW DATA GOTO 4  ----------------------------------
      IF(J.GT.8)GOTO30
      IF(SQMAX(J).LT..0001)GOTO20
      YMAX=SQMAX(J)
      YMIN=SQMIN(J)
      WRITE(12,10)J,SQMAX(J),SQMIN(J)
   10 FORMAT(1X,'COUNTER',I3,' YMAX SET TO',F7.3,' YMIN SET TO',F7.3)
C
C---- PLOT DS/DW ---------------------------------------------------------
   20 IF(IW.EQ.2)YMIN=0.
      IF(IW.EQ.2)YMAX=SIG1*.5/3.14159
      IF(XMAX1(J).LT..0001)GOTO30
      XMAX=XMAX1(J)
      XMIN=XMIN1(J)
   30 IF(XMAX.LE.XMIN.OR.YMAX.LE.YMIN)RETURN
C
C---- OVERPLOT SAMPLE+CAN,CAN,VANADIUM+BACKGROUND AND BACKGROUND -------
   40 IF(J.LT.12)CALL FRAME
      CALL MAP   (XMIN,XMAX,YMIN,YMAX)
      CALL WINDOW(XMIN,XMAX,YMIN,YMAX)
      IF(J.GT.11)GOTO50
      CALL SCALES
      CALL BORDER
   50 CALL CTRMAG(10)
      IF(J.GT.8)GOTO60
C
```

```
C---- PLOT PATTERN ---------------------------------------------------
      CALL PTPLOT(X,Y,1,IMAX,43)
   60 IF(J.LE.8)GOTO70
      CALL CTRMAG(1)
      CALL PTPLOT(X,Y,1,IMAX,37)
      CALL CTRMAG(10)
   70 IF(J.GT.11)RETURN
C
C---- POSITION TITLE --------------------------------------------------
      CALL PLACE (20,2)
      CALL TYPECS(TITLE,72)
      CALL PLACE (2,50)
      CALL CTRORI(1.)
      CALL CTRMAG(15)
C
C---- CHOOSE AND PRINT THE APPROPIATE Y-AXIS CAPTION ------------------
      IF(J.EQ.11)CALL TYPECS('SAMPLE,CAN,VANADIUM + BACKGROUND',32)
      CALL CTRORI(0.)
      IF(J.GT.8)GOTO90
      CALL CTRORI(1.)
      IF(IW.NE.2)GO TO 80
      CALL CTRSET(2)
      CALL TYPENC(14)
      CALL CTRSET(4)
      CALL TYPENC(29)
      CALL TYPENC(46)
      CALL CTRSET(2)
      CALL TYPENC(14)
      CALL CTRSET(3)
      CALL TYPENC(33)
      CALL CTRSET(1)
   80 IF(IW.EQ.1)CALL TYPECS('S(Q)',4)
      IF(IW.EQ.3)CALL TYPECS('SAMPLE TRANSMISSION RATIO',25)
      IF(IW.EQ.4)CALL TYPECS('VANADIUM TRANSMISSION RATIO',27)
      CALL TYPECS(' FOR COUNTER ',13)
      CALL TYPENI(J)
      CALL CTRORI(0.)
C
C---- CHOOSE AND PRINT THE APPROPIATE X-AXIS CAPTION ------------------
   90 CALL PLACE(40,45)
      IF(IW.LT.3)GOTO100
      CALL TYPECS('LAMBDA ANGSTROMS ',17)
      IF(IW.GE.3)GOTO110
  100 IF(Q)      CALL TYPECS(' Q RECIPROCAL ANGSTROMS',23)
      IF(TOF)    CALL TYPECS(' T.O.F. MICROSECONDS    ',23)
      IF(LAMBDA)CALL TYPECS(' LAMBDA ANGSTROMS       ',23)
  110 IF(J.GT.8)RETURN
C
C---- DRAW BOX IN TOP RIGHT HAND CORNER AXIS CAPTION ------------------
      YTOP=.8*YMAX+.2*YMIN
      XTOP=.8*XMAX+.2*XMIN
      CALL BOX(XTOP,XMAX,YTOP,YMAX)
      CALL CTRMAG(10)
      CALL POSITN(.9*XTOP+.1*XMAX,.9*YMAX+.1*YTOP)
      IF(.NOT.ABSORB)CALL TYPECS(' NO ABSORPTION CORRECTIONS          ',33)
      IF(ABSORB)     CALL TYPECS(' ABSORPTION CORRECTIONS             ',33)
      CALL POSITN(.9*XTOP+.1*XMAX,.9*YMAX+.1*YTOP)
      CALL LINEFD(2)
      CALL TYPECS('          APPLIED',15)
      CALL POSITN(.9*XTOP+.1*XMAX,.9*YMAX+.1*YTOP)
      CALL LINEFD(4)
      CALL ZAIBAS(DAY,MONTH,YEAR)
      CALL TYPENI(DAY)
      CALL TYPECS(' ',1)
      CALL TYPECS(MONTH,4)
      CALL TYPECS(' ',1)
      CALL TYPENI(YEAR)
      WRITE(12,120)
  120 FORMAT(1X,'GRAPH PLOTTED')
      RETURN
      END
      SUBROUTINE SMTH(A,B,C,ICHNL,CHAN,RD1,WIDTH)
C
C
C---- SMOOTHS ARRAY (A) AS A FUNCTION OF ARRAY (C).-------------------------
C---- ELIMINATES BOOSTER PEAK AT 2600 MICROSECONDS ----------------------
C---- ICHNL POINTS IN ARRAY------------------------------------------
C---- CHANNEL WIDTH IS (CHAN) MICROSECONDS ---------------------------
C---- INITIAL DELAY (RD1) MICROSECONDS ------------------------------
C---- WRITES INTO ARRAY (B) THEN WRITES BACK TO (A) THEN ZEROES (B)---------
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C---- USES RECTANGULAR SMOOTHING FUNCTION PERCENTAGE WIDTH IS (WIDTH) -----
C
      REAL A(ICHNL),B(ICHNL),C(ICHNL)
      INTEGER CHAN
C---- DEFINE I FOR 255. AND 275. MICROSECS. ------------------------
      I2550=(2500.-RD1)/CHAN+.5
      I2750=(2700.-RD1)/CHAN+.5
      RIMI=FLOAT(I2750-I2550)
      OMW=1.-WIDTH
      OPW=1.+WIDTH
      RI=0.
C
C---- CORRECT FOR BOOSTER ------------------------------------------
      DO 10 I=1,ICHNL
      IF(I.GE.I2550.AND.I.LE.I2750)A(I)=A(I2550)+(A(I2750)-A(I2550))
     A *FLOAT(I-I2550)/RIMI
   10 CONTINUE
      DO 30 I=1,ICHNL
      SUM=0.
C---- COMPUTE I1 AND I2 --------------------------------------------
      RI=RI+1.
      I1=INT(RI*OMW+.5)
      I2=INT(RI*OPW+.5)
      IF(I1.LE.1)I1=2
      IF(I2.LE.1)I2=2
      IF(I2.GT.ICHNL)I2=ICHNL
C---- INTEGRATE A FROM I1 TO I2 AND STORE IN SUM -------------------
      DO 20 J=I1,I2
   20 SUM=SUM+A(J)
   30 B(I)=SUM/FLOAT(I2-I1+1)
C---- PLOT SMOOTHED AND UNSMOOTHED ARRAYS A AND B ------------------
      CALL CTRMAG(3)
      CALL PTPLOT(C,B,1,ICHNL,-43)
      CALL PTPLOT(C,A,1,ICHNL,43)
C
C---- RESET ARRAY B TO A  AND SET B TO ZERO ------------------------
      DO 40 I=1,ICHNL
      A(I)=B(I)
   40 B(I)=0.
      RETURN
      END
      SUBROUTINE DISC(A,IARR,NRUN,ICHNL,INC,ICON,SUM,K,J,RMC,*,*,
     A NTRN,M,MPRF,RPULSE,JMAX,NSEQ)
C
C----- FINDS A RUN OF NAME:NRUN ------------------------------------
C----- THERE ARE :ICHNL CHANNELS PER COUNTER,THE COUNTER NO. IS:INC ----
C----- READS RUN OFF THE DISC ADDS IT INTO ARRAY :A(ICHNL) ------------
C----- RETURNS THE CONTROL RECORD:ICON(256) --------------------------
C----- ADDS IN THE MONITOR COUNT TO ARRAY:RMC(INC,4) -----------------
C----- ADDS IN THE PRF PULSE TO ARRAY : RPULSE -----------------------
C----- RUN TYPE :K 1,2,3 OR 4 ----------------------------------------
C----- ADDS IN A TO TOTAL COUNT :SUM(K,INC,JJ) -----------------------
C----- INCREMENTS J AND RETURNS TO NEXT RUN OR TO REST OF PROGRAM ------
C
      REAL A(2048),RMC*4(8,4),SUM*4(4,8,80),RPULSE(8,4)
      INTEGER ICON(256),M(8,80),NTRN(80),NRMAX/80/,IARR(16384),
     *        MPRF(8,80),NSEQ(80)
C---- REWIND ALL DATA SETS ----------------------------------------
      REWIND 1
C---- DUMMY COUNT SUM ----------------------------------------------
      SK=SUM(K,INC,J)
C---- LABEL SHIFT -------------------------------------------------
      KSHIFT=(INC-1)*ICHNL
      IF(J.EQ.1)WRITE(12,10)
      WRITE(12,20)NRUN,ICHNL,INC,J
   10 FORMAT(//,1X,'LOG OF SCRATCH DISC OPERATIONS OUTPUT CHANNEL 12',/)
   20 FORMAT(1X,'LOOKING FOR RUN',I10,' OF',I6,' CHANNELS COUNTER',
     A I2,' RUN COUNTER',I3)
      DO 30 K1=1,NRMAX
C---- RUN IS THE K1 TH IN THE LIST AND IS IN POSITION NSEQ(K1) ON DISC
      IF(NRUN.EQ.NTRN(K1))GOTO90
   30 CONTINUE
      WRITE(12,40)NRUN
   40 FORMAT(1H+,T72,'RUN NUMBER',I10,' NOT FOUND IN INPUT RUN LIST')
      GOTO140
   50 WRITE(12,60)K2,NRMAX
   60 FORMAT(1X,'END-OF-FILE FOUND RUN COUNTER K2=',I4,' NRMAX =',I3)
      GOTO140
   70 WRITE(12,80)K2,NRMAX
   80 FORMAT(1X,'RUN NOT FOUND ON DISC K2=',I4,' NRMAX=',I3)
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      GOTO140
C---- READ CONTROL RECORD -----------------------------------------------
   90 NSEQ1=NSEQ(K1)-1
      IF(NSEQ1.EQ.0)GOTO110
      DO 100 K2=1,NSEQ1
  100 READ(1,END=50)
  110 READ(1,END=50)ICON,IARR
      WRITE(12,120)NRUN
  120 FORMAT(1H+,T72,'RUN NUMBER',I10,'     FOUND IN INPUT RUN LIST')
      DO 130 K3=1,ICHNL
      COUNT=FLOAT(IARR(K3+KSHIFT))
C---- TRANSFER COUNTS TO ARRAY A AND ADD IN TO SUM (SK) ----------------
      SK=SK+COUNT
  130 A(K3)=A(K3)+COUNT
C---- SUM IN MONITOR COUNTS AND PRF PULSES ------------------------------
      RPULSE(INC,K)=RPULSE(INC,K)+FLOAT(MPRF(INC,J))
      RMC(INC,K)=RMC(INC,K)+FLOAT(M(INC,J))
      SUM(K,INC,J)=SK
  140 IF(J.GE.JMAX)RETURN2
      J=J+1
      RETURN1
      END
      SUBROUTINE ABSORP(SSCAT,SABS,CSCAT,CABS,RHOS,RHOC,R1,R2,DELTAR,
     * ASS,ACC,ACS,THET,IROUTE,AB,SI,AS,ENU,NU,R,ABSORB,SCATTR,SPLATE,
     * VPLATE,TRANS)
C
C---- COMPUTES PAALMAN AND PINGS TERMS FOR A CYLINDRICAL SAMPLE----------------
C---- COMPUTES SIMILAR TERMS FOR A FLAT PLATE CONTAINER-----------------------
C---- SSCAT : SAMPLE SCATTERING CROSS-SECTION -------------------------------
C---- SABS  : SAMPLE ABSORPTION CROSS-SECTION -------------------------------
C---- CSCAT : CAN SCATTERING CROSS-SECTION ----------------------------------
C---- CABS  : CAN ABSORPTION CROSS-SECTION ----------------------------------
C---- RHOS : SAMPLE NUMBER DENSITY ------------------------------------------
C---- RHOC : CAN NUMBER DENSITY ---------------------------------------------
C---- R1 : SAMPLE RADIUS ----------------------------------------------------
C---- R2 : CAN RADIUS (OUTER) -----------------------------------------------
C---- DELTAR : INCREMENT IN RADIUS ------------------------------------------
C---- R1 : SAMPLE THICKNESS -------------------------------------------------
C---- R2 : (SAMPLE + CAN THICKNESS) -----------------------------------------
C---- DELTAR : ANGLE OF PLATE NORMAL TO BEAM --------------------------------
C---- IF CYLINDRICAL GEOMETRY (SROD,VROD, OR VCOIL)--------------------------
C---- IF PLATE GEOMETRY (VPLATE OR SPLATE) ----------------------------------
C---- ASS: PAALMAN AND PINGS SAMPLE ABSORPTION TERM -------------------------
C---- ACC AND ACS : PAALMAN AND PINGS CAN AND CROSS ABSORPTION TERMS --------
C---- THET: ANGLE OF DETECTOR IN RADIANS ------------------------------------
C---- IROUTE (1,2) SAMPLE OR VANADIUM (SAVES TIME NOT CALCULATING ACS)-------
C---- AB,SI,AS,ENU,NU: INTEGRAL TERMS IN ROUTINE --EQUIVALENCED IN MAIN------
C---- R : RADII OF SHELLS IN CYLINDRICAL SAMPLE INTEGRATION ----------------
C---- ABSORB: LOGICAL VARIABLE SWITCHING ON ABSORPTION ----------------------
C---- SCATTR: LOGICAL VARIABLE SWITCHING ON SCATTERING CROSS-SECTION -------
C---- SPLATE, VPLATE: SAMPLE AND VANADIUM PLATE SWITCHES --------------------
C---- TRANS: LOGICAL VARIABLE SPECIFYING TRANSMISSION OR REFLECTION --------
C
      REAL R(20),AB(60,20),SI(60,20),AS(60,20),ENU(60,20),NU(60,20),
     * PI/3.14159/,PIBY2/1.57073/,DRM/-.5/
      LOGICAL ABSORB,SCATTR,SPLATE,VPLATE,YESACC,NOACC,
     *L1,L2,L3,L4,L5,L6,L7,L8,L9,L10,L11,L12,L13,L14,L15,L16,L17,L18,L19
     *,L20,L21,TRANS
C----- IF THERE IS NO ABSORPTION CORRECTION REQUIRED PROGRAM
C----- LOOPS OUT AFTER SETTING ALL PAALMAN AND PINGS TERMS
C----- TO UNITY
      IF(.NOT.ABSORB)GOTO90
      IF(.NOT.SCATTR)SSCAT=0.
      IF(.NOT.SCATTR)CSCAT=0.
C----- 20 ZONES, SAMPLE RADIUS:R1,CAN OUTER RADIUS:R2,
C----- INCREMENT:DELTAR,ANGLE:THET(RADIANS)
C-----CONSTANTS
      TTHET=2.*THET
      TMPB2=THET-PIBY2
      TPPB2=THET+PIBY2
C-----N*SIGMA (SAMPLE) OR MU(SAMPLE)
      STS=(SSCAT+SABS)*RHOS
C-----N*SIGMA (CAN) OR MU(CAN)
      STC=(CSCAT+CABS)*RHOC
C-----IF THE SAMPLE SPECIFIED IS A PLATE PROGRAM CALCULATES
C----- DIFFERENT SET OF TERMS
      IF(SPLATE.OR.VPLATE)GOTO100
C----- NO OF RINGS IN SAMPLE
      MR=R1/DELTAR+.1
      R1DMR=R1/FLOAT(MR)
```

```
C-----NO OF RINGS IN SAMPLE AND CAN
      MMAX=R2/DELTAR+.1
      R1SQ=R1*R1
      R2SQ=R2*R2
C-----COMMON FACTOR
      FAK=.66666/FLOAT(MR*MR)
      SINT=SIN(THET)
      COST=COS(THET)
      R1OCST=R1/COST
C-----COMPUTE ALL TERMS ALPHA,BETA ETC.
      DRM=-.5
      DO 10 M=1,MMAX
C:::::R(M)=(FLOAT(M)-.5)*R1OMR
      DRM=DRM+1.
      R(M)=DRM*R1OMR
      ROM=R(M)
      RHO=R1/ROM
      RSQ=ROM*ROM
      NMAX=3*M
      PONMAX=PI/FLOAT(NMAX)
      DRN=-.5
      DO 10 N=1,NMAX
C_____________________________________________________________
C----- OMEGA(N,M)
      DRN=DRN+1.
C:::::ONM=TMPB2+(FLOAT(N)-.5)*PONMAX
      ONM=TMPB2+DRN*PONMAX
      SINOMT=SIN(ONM-THET)
      SONM=SIN(ONM)
      SSONM=SONM*SONM
      RSQSS=RSQ*SSONM
      SOM2T=SIN(ONM-TTHET)
      SSOM2T=SOM2T*SOM2T
      RSQSSM=RSQ*SSOM2T
C_____________________________________________________________
C       ALPHA(N,M)+BETA(N,M)
      AB(N,M)=SQRT(R2SQ-RSQSS)+SQRT(R2SQ-RSQSSM)
C_____________________________________________________________
C       SIGMA(N,M)
      SI(N,M)=2.*ROM*SINOMT*SINT
C_____________________________________________________________
C       ALPHA+BETA-SIGMA
      AS(N,M)=AB(N,M)-SI(N,M)
C_____________________________________________________________
C       CHECK VALIDITY OF NU
      IF(ABS(SONM).LT.RHO)NU(N,M)=SQRT(R1SQ-RSQSS)
      IF(ABS(SONM).GE.RHO)NU(N,M)=0.
C_____________________________________________________________
C       CHECK ETA LIMITS AND GET ETA +NU
      IF(ABS(SOM2T).LT.RHO)ENU(N,M)=SQRT(R1SQ-RSQSSM)+NU(N,M)
      IF(ABS(SOM2T).GE.RHO)ENU(N,M)=NU(N,M)
C_____________________________________________________________
   10 CONTINUE
C----- OMEGA LIMITS IN ZONE D,RLIMITS ARE 0<R(M)<R1
      DHIGH=TPPB2
      DLOW =TMPB2
      ASS=0.
      IF(RHOS.EQ.0.)GOTO30
      DO 20 M=1,MR
      NMAX=3*M
      PONMAX=PI/FLOAT(NMAX)
      FU=1.-1./FLOAT(2*M)
      DRN=-.5
      DO 20 N=1,NMAX
      DRN=DRN+1.
C:::::ONM=TMPB2+(FLOAT(N)-.5)*PONMAX
      ONM=TMPB2+DRN*PONMAX
C----- COMPUTE ASS IN ZONE D
      IF(ONM.LE.DHIGH.AND.ONM.GE.DLOW)ASS=ASS
     A +FU*EXP(-STS*(ENU(N,M)-SI(N,M))-STC*(AB(N,M)-ENU(N,M)))
   20 CONTINUE
      ASS=ASS*FAK
C_____________________________________________________________
   30 IF(RHOS.EQ.0.)ASS=1.
      ACC=0.
      ACS=0.
C----- CONSTANT
      FAK=FAK/(R2SQ/R1SQ-1.)
C     **************************************************************
C     * SET UP LIMITS FOR OMEGA AND R(M) IN EACH ZONE A1,A0,B0,B1, & C  *
```

```
C     * ALL ZONES HAVE TOPMOST LIMIT OF R2                                  *
C     * ZONES B0 AND C HAVE UPPER LIMIT OF R10CST <R1/COS(THET)>            *
C     * ZONES A1,B0 AND C HAVE LOWER LIMIT OF R1                            *
C     * ZONES A0 AND B1 HAVE LOWER LIMIT OF R10CST                          *
C     * COMPUTE NON M-DEPENDENT TERMS FIRST                                 *
C     ***********************************************************************
      A1HIGH=DHIGH
      A0LOW =DLOW
      CLOW  =DLOW
      YESACC=RHOC.NE.0.
      NOACC=RHOC.EQ.0.
C----- SUM OVER MR
      MMIN=MR+1
      DO 80 M=MMIN,MMAX
C----  COMPUTE M-DEPENDENT TERMS
      ROM=R(M)
      A1LOW =ARSIN(R1/ROM)
      A0HIGH=-A1LOW
      B0HIGH=A1LOW
      B0LOW =TTHET-PI+A1LOW
      B1HIGH=A1LOW
      B1LOW =-A1LOW
      CHIGH =B0LOW
      FU=1.-1./FLOAT(2*M)
      NMAX=3*M
      PONMAX=PI/FLOAT(NMAX)
C----- SUM OVER N
      DRN=-.5
      DO 80 N=1,NMAX
      DRN=DRN+1.
C----- COMPUTE OMEGA
C:::::ONM=TMPB2+(FLOAT(N)-.5)*PONMAX
      ONM=TMPB2+DRN*PONMAX
C----- COMPUTE ACC AND ACS
C----- CHECK FOR EACH ZONE IN TURN
C----- CALCULATE DUMMY ARRAY VALUES
      ASN    =AS(N,M)
      STCASN=FU*EXP(-STC*ASN)
      TNU    =2.*NU(N,M)
      STSTNU=EXP(-STS*TNU)
      SCASTN=FU*EXP(-STC*(ASN-TNU))
      TENU   =2.*ENU(N,M)
      SCASTE=FU*EXP(-STC*(ASN-TENU))
      L1=ONM.LE.A1HIGH
      L2=ONM.GE.A1LOW
      L3=ONM.LE.A0HIGH
      L4=ONM.GE.A0LOW
      L5=ROM.GE.R10CST
      L6=ONM.LE.B0HIGH
      L7=ONM.GE.B0LOW
      L8=ROM.LE.R10CST
      L9=ROM.LT.R2
      L10=ONM.LE.B1HIGH
      L11=ONM.GE.B1LOW
      L12=ONM.LE.CHIGH
      L13=ONM.GE.CLOW
      L14=ROM.LE.R2
C______________________________________________________________________
C       ZONE A1
      IF(.NOT.(L1.AND.L2))GOTO40
          IF(YESACC)ACC=ACC+STCASN
                    ACS=ACS+STCASN
C______________________________________________________________________
C       ZONE A0
   40 IF(.NOT.(L3.AND.L4.AND.L5))GOTO50
          IF(YESACC)ACC=ACC+STCASN
                    ACS=ACS+STCASN
C______________________________________________________________________
C       ZONE B0
   50 IF(.NOT.(L6.AND.L7.AND.L8.AND.L9))GOTO60
          IF(YESACC)ACC=ACC+SCASTN
                    ACS=ACS+SCASTN*STSTNU
C______________________________________________________________________
C       ZONE B1
   60 IF(.NOT.(L10.AND.L11.AND.L5))GOTO70
          IF(YESACC)ACC=ACC+SCASTN
                    ACS=ACS+SCASTN*STSTNU
C______________________________________________________________________
C       ZONE C
   70 IF(.NOT.(L12.AND.L13.AND.L14.AND.L8))GOTO80
```

```
          IF(YESACC)ACC=ACC+SCASTE
                    ACS=ACS+SCASTE*EXP(-STS*TENU)
   80 CONTINUE
      ACS=ACS*FAK
      ACC=ACC*FAK
      IF(NOACC)ACC=1.
      GOTO110
C---- RETURN STATE FOR NO ABSORPTION
   90 ASS=1.
      ACC=1.
      ACS=1.
      GOTO110
C
C     ******************************************
C     * FLAT PLATE ABSORPTION TERMS            *
C     *  CTHMPH =  COS(2THETA-PHI)             *
C     *  CTHPPH =  COS(2THETA+PHI)             *
C     *  CPTTMP=   COS(PHI)*COS(2THETA-PHI)    *
C     *  CPTTPP=   COS(PHI)*COS(2THETA+PHI)    *
C     *  CPMTMP=   COS(PHI)-COS(2THETA-PHI)    *
C     *  CPMTPP=   COS(PHI)-COS(2THETA+PHI)    *
C     ******************************************
C
  100 CTH=COS(TTHET)
      CPHI=COS(DELTAR)
C==== CHECK FOR SYMMETRIC  SCATTERING CASE IN TRANSMISSION ============
      TPHI=2.*PHI
      IF(((TPHI.LE.TTHET+.01).OR.(TPHI.GE.TTHET-.01)).AND.TRANS)GOTO140
      CTHMPH=COS(TTHET-DELTAR)
      CTHPPH=COS(TTHET+DELTAR)
      CPTTMP=CPHI*CTHMPH
      CPTTPP=CPHI*CTHPPH
      CPMTMP=CPHI-CTHMPH
      CPMTPP=CPHI-CTHPPH
C
C---- SAMPLE TERMS FOR AS  --------------------------------------------
      R1STS=R1*STS
      TM1=-R1STS/CPHI
      TM2=-R1STS/CTHMPH
      TM3=-R1STS*((1./CPHI)-(1./CTHPPH))
C
C---- CAN TERMS FOR AC  -----------------------------------------------
C---- THICKNESS OF CAN WALL *STC --------------------------------------
      R2MR1C=(R2-R1)*STC*.5
      TN1=-R2MR1C/CPHI
      TN2=-R2MR1C/CTHMPH
      TN3=-R2MR1C*((1./CPHI)-(1./CTHPPH))
C
C---- A1 AND A2 TERMS IN TRANSMISSION ---------------------------------
C---- DIVIDE BY ZERO CHECK --------------------------------------------
C     L15=THET.LE..785398
C     L16=THET.GT..785398
      L15=TRANS
      L16=.NOT.TRANS
      L17=R1STS.NE.0.
      L19=R2MR1C.NE.0.
      L20=IROUTE.EQ.1
      L21=IROUTE.EQ.2
      IF(L15.AND.L17)A2=CPTTMP*(EXP(TM1)-EXP(TM2))/(R1STS*CPMTMP)
      IF(L15.AND.L19.AND.L20)
     *                  A1=CPTTMP*(EXP(TN1)-EXP(TN2))/(R2MR1C*CPMTMP)
C---- A1 AND A2 TERMS IN REFLECTION -----------------------------------
      IF(L16.AND.L17)A2=CPTTPP*(EXP(TM3)-1.)/(R1STS*CPMTPP)
      IF(L16.AND.L19.AND.L20)
     *                  A1=CPTTPP*(EXP(TN3)-1.)/(R2MR1C*CPMTPP)
C
C     ************************************************
C     * SET UP ASS,ACS & ACC TERMS FROM A1 AND A2    *
C     * IN TRANSMISSION                              *
C     * ASS=A1**2*A2                                 *
C     * ACC=1.                                       *
C     * ACS=A2                                       *
C     * IN REFLECTION                                *
C     * ASS=A1**2*A2                                 *
C     * ACC=(1.+A1**2)*.5                            *
C     * ACS=(1.+(A1*A2)**2)*.5                       *
C     ************************************************
C
      IF(.NOT.L19)A1=1.
      IF(.NOT.L17)A2=1.
```

```
      IF(L21)A1=1.
      IF(L15)ASS=A1*A1*A2
      IF(L15)ACC=1.
      IF(L15)ACS=A2
      IF(L16)ASS=A1*A1*A2
      IF(L16)ACC=(1.+A1*A1)*.5
      IF(L16)ACS=(1.+A1*A1*A2*A2)*.5
C---- DIVIDE BY ZERO PATCH ------------------------------------------------
      IF(.NOT.L17)ASS=1.
      IF(.NOT.L19)ACC=1.
      IF(L21)ACC=1.
      IF(L21)ACS=1.
C---- RESET EVERYTHING ---------------------------------------------------
  110 DO 130 K=1,20
      R(K)=0.
      DO 120 J=1,60
      AB(J,K)=0.
      SI(J,K)=0.
      AS(J,K)=0.
      NU(J,K)=0.
      ENU(J,K)=0.
  120 CONTINUE
  130 CONTINUE
      RETURN
C==== SYMMETRIC SCATTERING CASE ==========================================
  140 A2=EXP(-R1*STS/CPHI)
      A1=EXP(-(R2-R1)*STC*.5/CPHI)
      IF(STC.EQ.0.)A1=1.
      IF(STS.EQ.0.)A2=1.
      ASS=A1*A1*A2
      ACC=1.
      ACS=A2
      GOTO110
      END
      SUBROUTINE DEADT(R,A,ICHNL,NDEAD,RPULSE,NCTRS,INC,DEAD,RMC,KI)
C
C---- APPLIES DEADTIME CORRECTIONS AND CORRECTS FOR MONITOR COUNTS ------------
C---- R : CORRECTION FACTOR ARRAY ---------------------------------------------
C---- A : DATA ARRAY ----------------------------------------------------------
C---- ICHNL : NUMBER OF CHANNELS IN ARRAY -------------------------------------
C---- NDEAD : NUMBER OF DEAD CHANNELS -----------------------------------------
C---- RPULSE : NUMBER OF MACHINE PULSES FIRED ---------------------------------
C---- NCTRS : NUMBER OF DETECTORS USED (UNNECCESSARY WHEN USING MK2
C----          SPECTROMETER ,AS ALL DETECTORS HAVE INDIVIDUAL BUFFERS) ----------
C---- INC : CURRENT COUNTER NUMBER --------------------------------------------
C---- DEAD : LOGICAL VARIABLE DESCRIBING DEAD TIME SWITCH ---------------------
C---- RMC : MONITOR COUNT ARRAY -----------------------------------------------
C---- KI : SAMPLE TYPE (1,2,3,4) SAMPLE,CAN,VANADIUM OR BACKGROUND ------------
C
      REAL A(ICHNL),R(ICHNL),RPULSE(8,4),RMC(8,4)
      LOGICAL DEAD
      DO 10 I=1,ICHNL
   10 R(I)=1.
C---- DIVIDE BY MONITORS ONLY IF NO DEADTIME CORRECTION -------------------
      IF(.NOT.DEAD.OR.NDEAD.EQ.0.OR.RPULSE(INC,KI).EQ.0.)GOTO40
      CALL FRAME
      CALL MAP(0.,FLOAT(ICHNL),0.95,1.1)
      CALL WINDOW(0.,FLOAT(ICHNL),0.95,1.1)
      CALL SCALES
      CALL BORDER
      CALL POSITN(FLOAT(ICHNL/3),1.07)
      CALL TYPECS('DEAD TIME CORRECTION FACTOR',28)
      CALL POSITN(0.,1.)
      DO 30 I=1,ICHNL
      SUM=0.
      N1=I-NDEAD
      N2=I-1
      IF(N1.LE.0)N1=1
      DO 20 J=N1,N2
   20 SUM=SUM+A(J)
      R(I)=1./(1.-SUM/RPULSE(INC,KI))
   30 CALL JOIN(FLOAT(I),R(I))
C---- CORRECT FOR MONITOR COUNTS ----------------------------------------------
   40 DO 50 K=1,ICHNL
   50 A(K)=A(K)*R(K)*100000./RMC(INC,KI)
      RETURN
      END
      SUBROUTINE READ1(S,E,IMAX)
C-----READ IN SCATTERING CROSS SECTION V ENERGY ARRAYS
C-----ROUTINE RETURNS VALUES OF CROSS SECTION,ENERGY & # OF POINTS
```

```
      REAL S(1),E(1)
      DO 20 I=1,40
      READ(5,10)E(I),S(I),K
   10 FORMAT(2F10.0,I1,59X)
C-----K IS SENTINEL FOR END OF DATA
      IF(K.EQ.1)GO TO 40
   20 CONTINUE
      WRITE(6,30)
   30 FORMAT('*** > THAN 40 SCATTERING CROSS SECTION VALUES IN MESH ***')
      STOP
   40 IMAX=I
      RETURN
      END
      SUBROUTINE QBIN(TITLE,ICHNL,RID,CHAN,CA,TFP,NCTRS,T,SQ,D,W,Q,RSQ,
     *                NC,EQUALQ)
C
C---- PUTS DATA INTO EQUAL WIDTH Q-BINS ------------------------------------
C---- TITLE : TITLE FOR GRAPHS ETC. ----------------------------------------
C---- ICHNL : NUMBER OF CHANNELS IN ARRAY ----------------------------------
C---- RID : INITIAL DELAY -------------------------------------------------
C---- CHAN: CHANNEL WIDTH IN MICROSECONDS ----------------------------------
C---- CA : COUNTER ANGLE --------------------------------------------------
C---- TFP : TOTAL FLIGHT PATH IN METRES ------------------------------------
C---- NCTRS : NUMBER OF DETECTORS -----------------------------------------
C---- T: TIME OF FLIGHT ARRAY ---------------------------------------------
C---- SQ :  S(Q) ARRAY READ FROM SCRATCH DISC AS WRITTEN IN MAIN PROGRAM -------
C---- D : ARRAY FOR SPLINE FITTING ROUTINE ---------------------------------
C---- W : ARRAY FOR SPLINE FITTING ROUTINE ---------------------------------
C---- Q : Q-SCALE ARRAY ---------------------------------------------------
C---- RSQ : EQUAL Q-BIN DATA ----------------------------------------------
C---- NC : COUNTER ON/OFF SWITCH FOR EACH DETECTOR POSITION ----------------
C---- EQUALQ: LOGICAL VARIABLE TO SWITCH ROUTINE ON/OFF ---------------------
C
      REAL    T(2048),SQ(2048),Q(1200),RSQ(1200),D(2048),W(6144),CA(8),
     *        TITLE(18),YMAX(8)/8*0./,QSTEP/.05/,SCALE/1./,XMIN(8)/8*0./
     *        ,XMAX(8)/8*0./,WIDTH(8)/8*.015/
      INTEGER NC(8),IQMAX(8),CHAN
      LOGICAL PUNCH/F/,PLOT/T/,EQUALQ
      NAMELIST/QEQUAL/ YMIN,YMAX,XMIN,XMAX,QSTEP,SCALE,PUNCH,PLOT,WIDTH
C
      IF(.NOT.EQUALQ)GOTO170
      N=ICHNL-1
C---- GRAPHS -----------------------------------------------------------
      CALL GHPEN(1)
      CALL FRAME
      CALL CTRMAG(15)
      CALL PLACE(20,20)
      CALL TYPECS('EQUAL-Q STEP OPTION',19)
      CALL PLACE(20,25)
      CALL TYPECS('MARK VI 16TH JUNE 1975',22)
C
C---- TIMING SEQUENCE ---------------------------------------------------
      TBEG=ZA02AS(DUMMY)
C
C---- Q-SCALE CONSTANT  -------------------------------------------------
      CONQ=TFP*3175.5216
      WRITE(6,10)
   10 FORMAT(1H1,T10,'EQUAL Q-STEP PROGRAM MARK VII  4TH DECEMBER 1975')
      READ(5,QEQUAL)
      WRITE(13,QEQUAL)
      CSCALE=.01*SCALE
      HQSTEP=.5*QSTEP
      CQSTEP=.01*QSTEP
C
C---- TOF SCALE  --------------------------------------------------------
      DO 20 KI=1,ICHNL
   20 T(KI)=RID+FLOAT((KI-1)*CHAN)
C
C---- LOOP OVER ALL COUNTERS --------------------------------------------
      DO 130 INC=1,NCTRS
      IF(NC(INC).EQ.0)GOTO130
      CON1=CONQ*SIN(CA(INC))
C
C---- READ S(Q) OR DS/DW FROM SCRATCH DISC -------------------------------
      READ(14'INC,ERR=150)NC(INC),(SQ(KI),KI=1,ICHNL)
C
C---- COMPUTE YMAX AND PRINT OUT HEADINGS  ------------------------------
      IF(YMAX(INC).EQ.0.)YMAX(INC)=SCALE*3.
      WRITE(6,30)QSTEP,SCALE,YMAX(INC),INC,NC(INC),WIDTH(INC),XMAX(INC)
   30 FORMAT(/,T10,'Q-STEP IS ',F5.2,' RECIPROCAL ANGSTROMS',
```

```
     *        /,T10,'SCALE FACTOR IS ',F5.3,
     *        /,T10,'YMAX IS ',F5.3,
     *        /,T10,'COUNTER NUMBER ',I2,' NC=',I3,
     *        /,T10,'SMOOTHING WIDTH IS ',F5.4,
     *        /,T10,'MAXIMUM Q-VALUE IS ',F6.3)
C
C==== FIT TO SPLINE=====================================================
      CALL TB04A(N,T,SQ,D,W)
C==== COMPUTE EQUAL Q AND PLOT =========================================
      QMX=CON1/T(1)
      QMN=CON1/T(ICHNL)
      IF(XMAX(INC).NE.0.)QMX=XMAX(INC)
      IF(XMIN(INC).NE.0.)QMN=XMIN(INC)
      IJ=-2
C==== LOOP OVER ALL Q-BINS =============================================
      DO 50 J=1,1200
      Q(J)=FLOAT(J)*QSTEP
      RSQ(J)=0.
      IF(Q(J).LT.QMN)GOTO50
      IF(Q(J).GT.QMX)GOTO60
      QJM=Q(J)-HQSTEP
C==== SUM OVER WIDTH OF Q-BIN ==========================================
      DO 40 K=1,100
      QJM=QJM+CQSTEP
   40 RSQ(J)=RSQ(J)+TG01B(IJ,N,T,SQ,D,CON1/QJM)
C==== APPLY SCALING FACTOR =============================================
      RSQ(J)=RSQ(J)*CSCALE
   50 CONTINUE
   60 IQMAX(INC)=J
C=
C==== SMOOTH WITH WIDTH FUNCTION PROPORTIONAL TO Q-RESOLUTION ==========
      RI=0.
      MAX=IQMAX(INC)
C==== CYCLE OVER EACH Q-VALUE ==========================================
      DO 80 K=1,MAX
      OMW=1.-WIDTH(INC)*Q(K)
      OPW=1.+WIDTH(INC)*Q(K)
      RI=RI+1.
C==== UPPER AND LOWER ELEMENTS OF INTEGRATION ==========================
      I1=INT(RI*OMW+.5)
      I2=INT(RI*OPW+.5)
      IF(I1.LE.1)I1=2
      IF(I2.LE.1)I2=2
      IF(I2.GT.MAX)I2=MAX
C==== INTEGRATE ========================================================
      DO 70 J=I1,I2
   70 SUM=SUM+RSQ(J)
C==== NORMALISE ========================================================
   80 D(K)=SUM/FLOAT(I2-I1+1)
      DO 90 K=1,MAX
C==== REST RSQ ARRAY TO REQUIRED VALUE =================================
   90 RSQ(K)=D(K)
      DO 100 K=1,2048
C==== CLEAR D ARRAY ====================================================
  100 D(K)=0.
C
C==== PLOT GRAPHS ======================================================
      CALL FRAME
      CALL MAP(0.,QMX,0.,YMAX(INC))
      CALL WINDOW(0.,QMX,0.,YMAX(INC))
      CALL SCALES
      CALL BORDER
C---- CAPTION ----------------------------------------------------------
      CALL CTRMAG(10)
      CALL PLACE(2,40)
      CALL CTRORI(1.)
      CALL TYPECS('SM(Q)',5)
      CALL CTRORI(0.)
      CALL PLACE(20,2)
      CALL TYPECS(TITLE,72)
      CALL TYPECS(' COUNTER ',9)
      CALL TYPENI(INC)
      CALL CTRMAG(15)
      CALL PLACE(40,45)
      CALL TYPECS('Q RECIPROCAL ANGSTROMS',23)
      CALL CTRMAG(5)
C
C---- LIST,PLOT,PUNCH AND WRITE EQUAL Q-STEP DATA TO DISC --------------
      CALL OJOHNA(Q,RSQ,IQMAX(INC),IQMAX(INC)/6+1,4,6,'FF','SM(Q)    ',6)
      CALL PTPLOT(Q,RSQ,1,IQMAX(INC),43)
```

```
      NQMAX=IQMAX(INC)
      IF(PUNCH)WRITE(7,110)((RSQ(K2-K1-1),K1=1,8),K2,K2=1,NQMAX,8)
      WRITE(14'INC)RSQ
      TEND=ZA02AS(DUMMY)-TBEG
      WRITE(6,120)TEND
  110 FORMAT(8F9.3,I8)
  120 FORMAT(T10,'TIME SO FAR IS ',F10.5,' SECONDS')
  130 CONTINUE
C
C---- PLOT ALL COUNTERS ON ONE GRAPH  ----------------------------------
      FIND(14'1)
      CALL FRAME
      CALL SCALES
      CALL BORDER
      CALL CTRMAG(6)
      DO 140 INC=1,NCTRS
      IF(NC(INC).EQ.0)GOTO140
      READ(14'INC)RSQ
      IF(INC.LT.NCTRS)FIND(14'INC+1)
      CALL PTPLOT(Q,RSQ,1,IQMAX(INC),INC)
  140 CONTINUE
      RETURN
  150 WRITE(6,160)
  160 FORMAT(T10,'DISC READ ERROR')
      RETURN
  170 READ(5,QEQUAL)
      WRITE(13,QEQUAL)
      RETURN
      END
```

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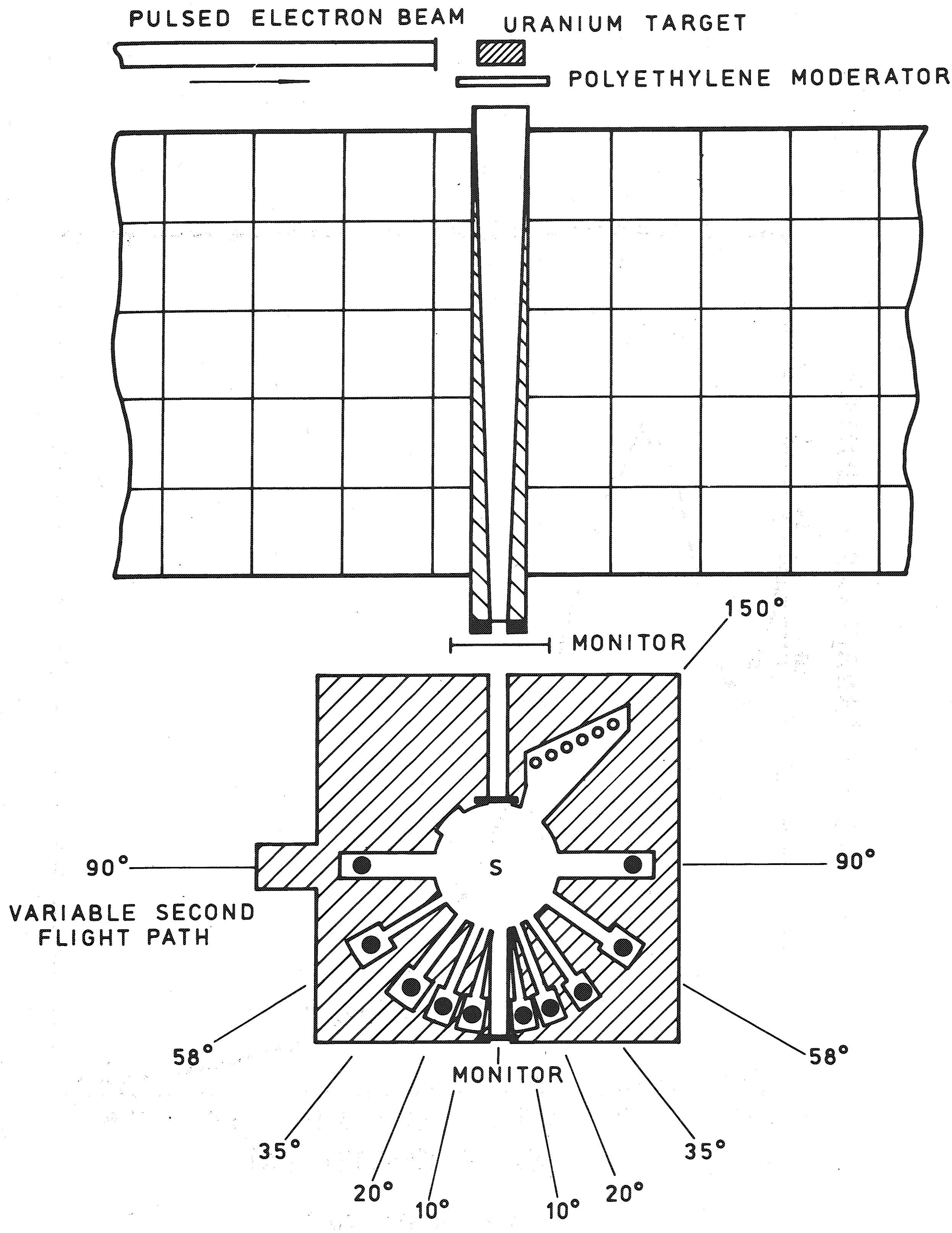
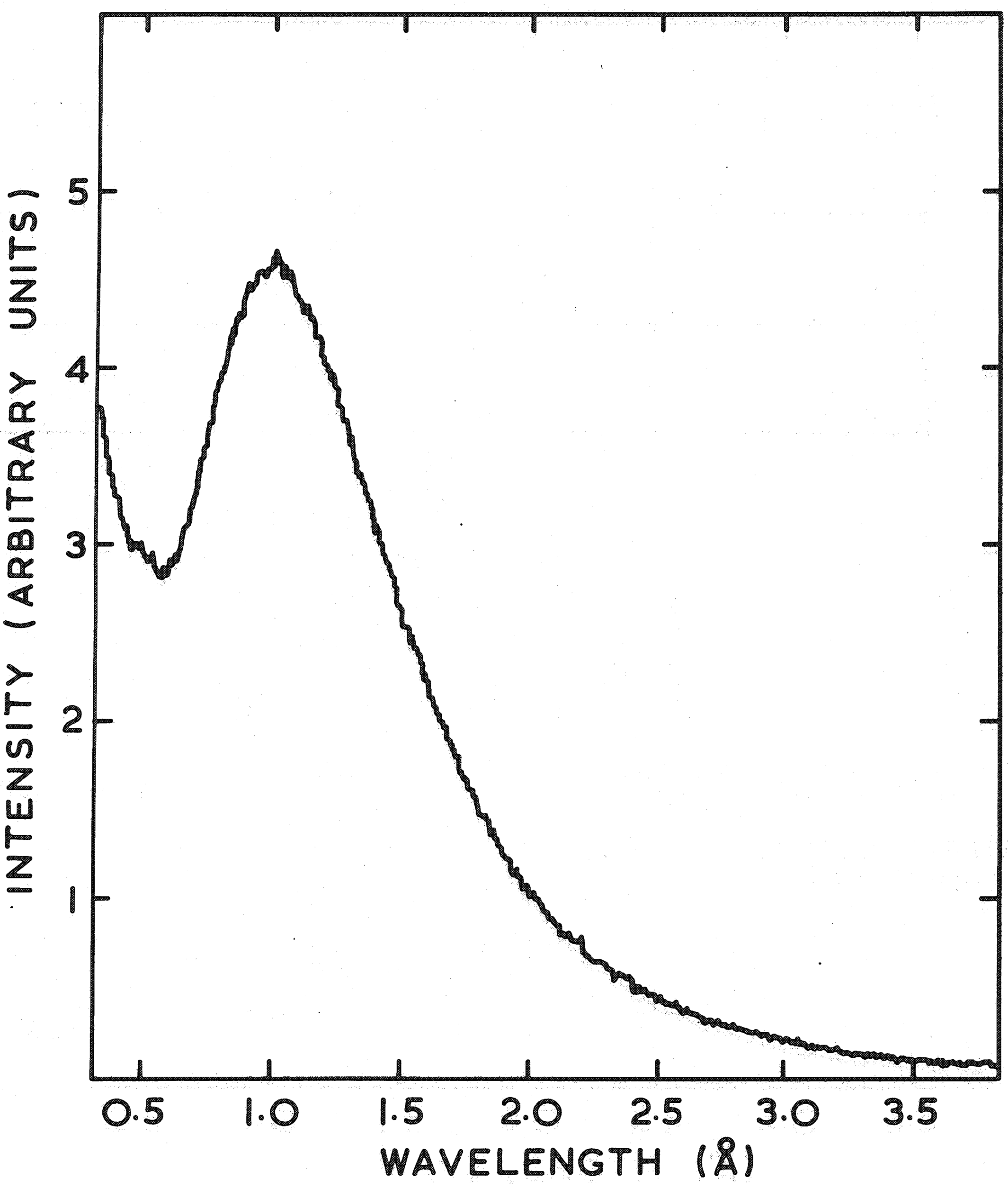
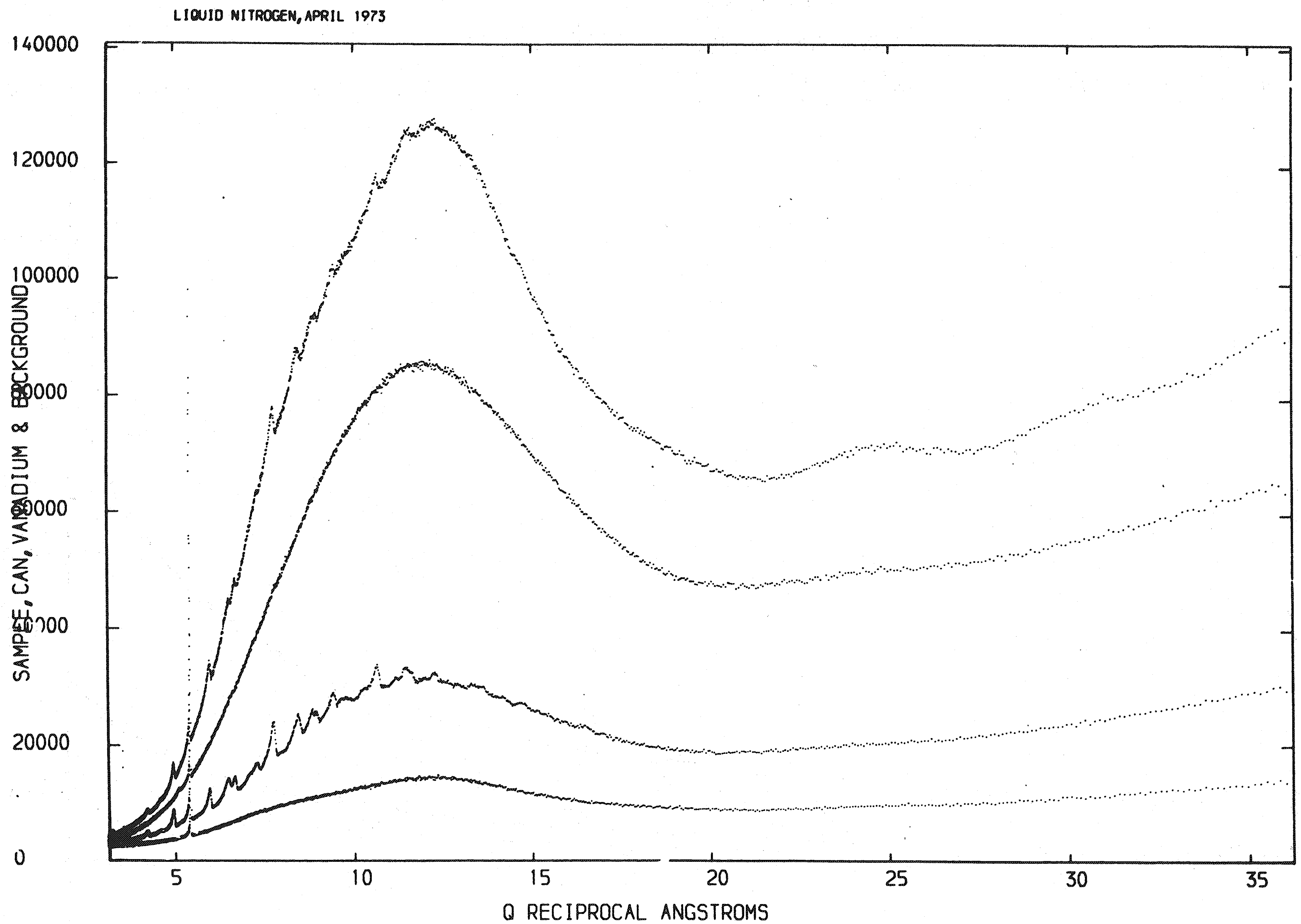
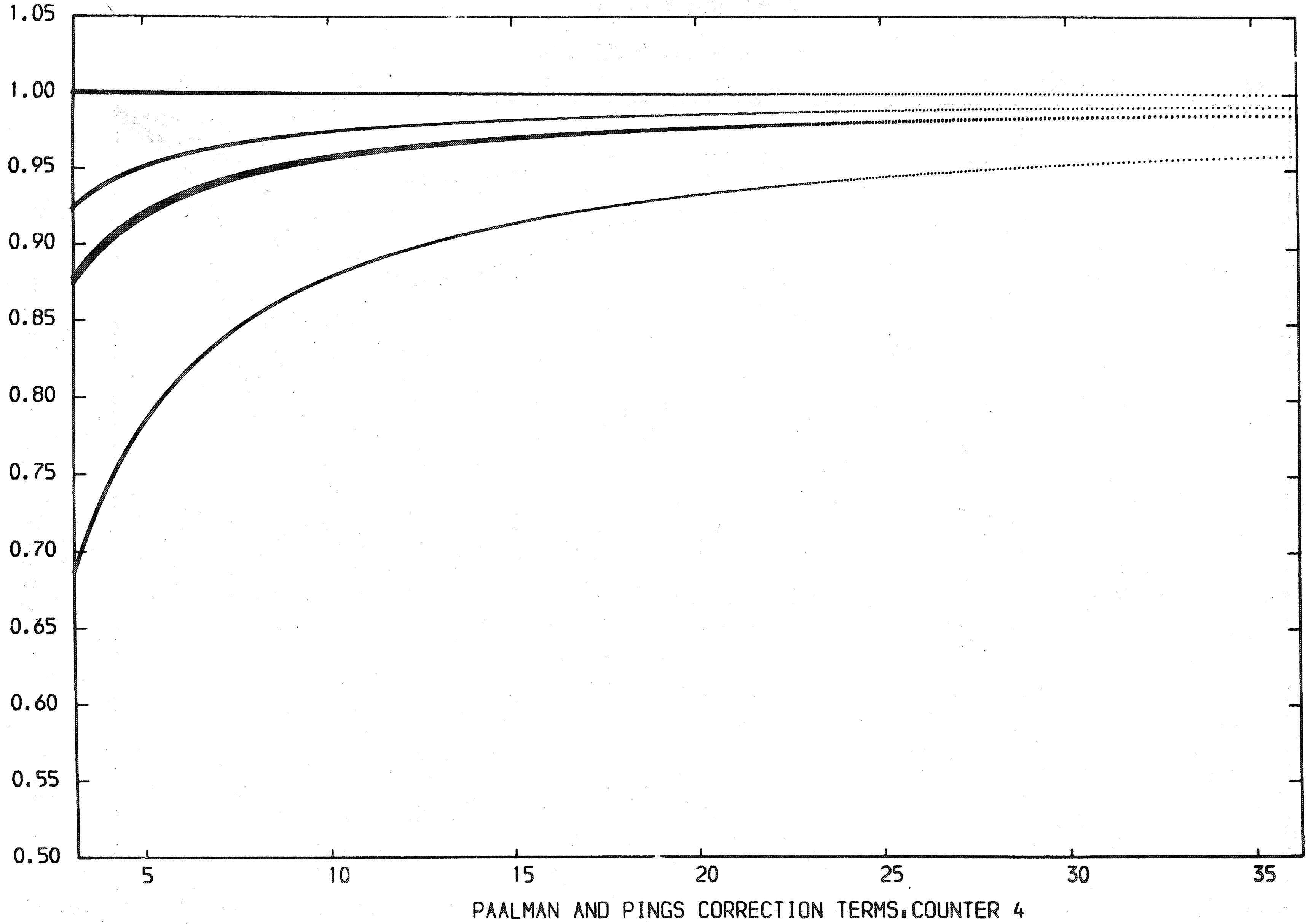

PULSED ELECTRON BEAM
URANIUM TARGET
POLYETHYLENE MODERATOR
150°
MONITOR
90°
S
90°
VARIABLE SECOND FLIGHT PATH
58°
58°
MONITOR
35°
35°
20°
10°
10°
20°



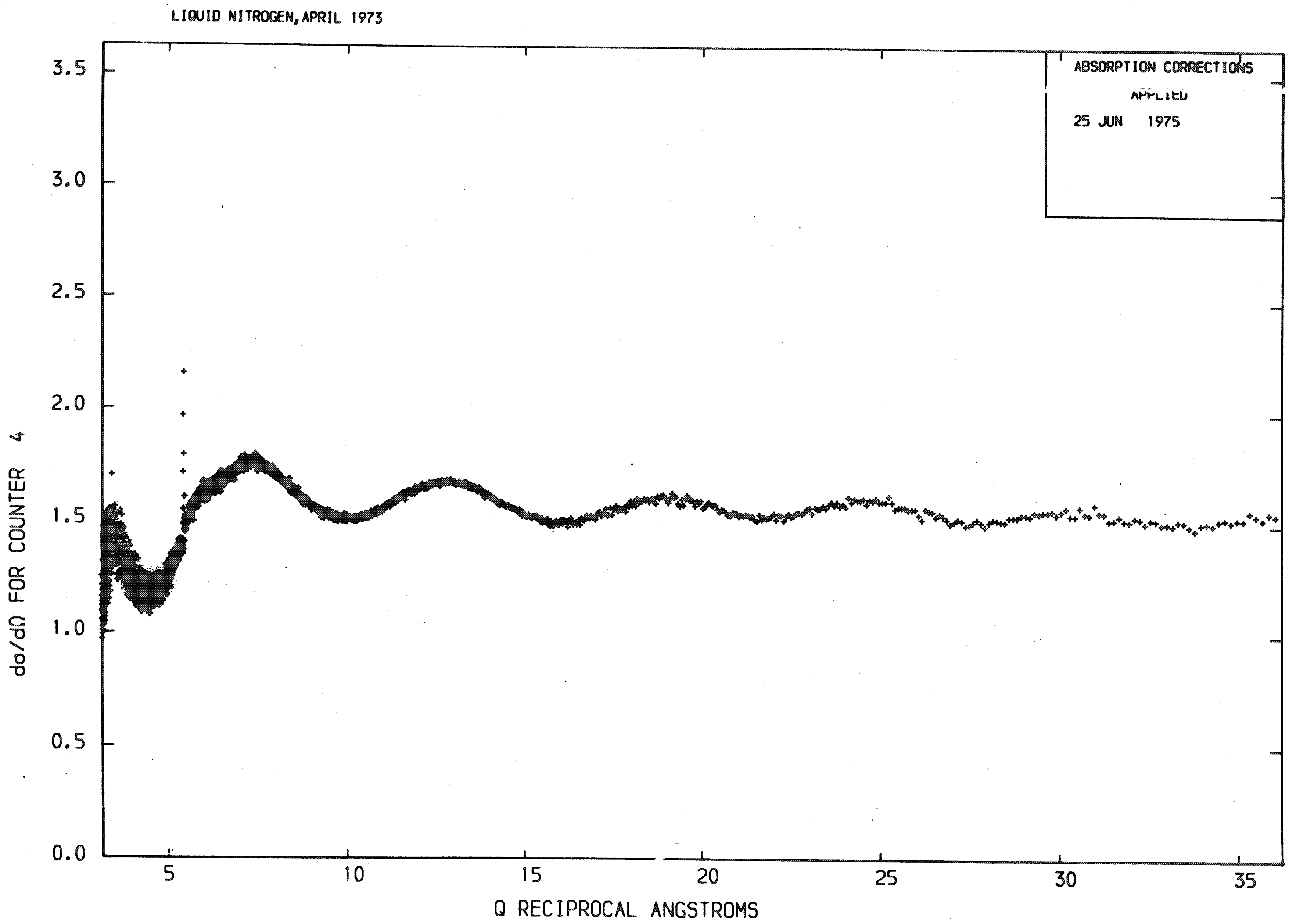
AERE - R 8121 Fig. 2
The energy distribution of the incident beam.



AERE - R 8121 Fig. 3
The input spectra for the program normalised for monitor counts.



AERE - R 8121 Fig. 4
The computed Paalman and Pings correction terms.



AERE - R 8121 Fig. 5

$d\sigma/d\Omega|^{eff}$ for liquid nitrogen as computed by the program (ϕ = 150°).