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Institut für Neutronenphysik und Reaktortechnik
Projekt Schneller Brüter

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A Multi-Level Shape-Analysis Program for Resonance Parameter Determination by Least-Squares Fitting of Several Sets of Neutron Transmission Data Simultaneously

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Gesellschaft für Kernforschung mbH, Karlsruhe

ABSTRACT

The present report describes a least-squares shape analysis program which is used at the Karlsruhe Nuclear Research Center for the extraction of resonance parameters from neutron transmission data. The program allows simultaneous fitting of up to 5 different experimental data sets, uses the multi-level R-matrix formalism and includes resolution broadening. A listing of the program and examples for input and output are given.

FANAL - ein Multiniveau-Formanalysenprogramm zur Resonanzparameterbestimmung durch Anpassung an mehrere Neutronentransmissionsdatensätze gleichzeitig nach der Methode der kleinsten Quadrate.

ZUSAMMENFASSUNG

Der vorliegende Bericht beschreibt ein nach der Methode der kleinsten Quadrate arbeitendes Formanalysenprogramm, das am Kernforschungszentrum Karlsruhe zur Bestimmung von Resonanzparametern aus Neutronentransmissionsdaten benutzt wird. Das Programm gestattet das gleichzeitige Anpassen an bis zu 5 experimentelle Datensätze, basiert auf dem Multiniveau-R-Matrix-Formalismus und berücksichtigt die instrumentelle Auflösung. Eine Liste des Programms und Beispiele für Ein- und Ausgabe sind beigefügt.

1. INTRODUCTION

The present report, essentially an extended version of an internal report (Ref. 1), describes a FORTRAN IV program which has been in use at the Karlsruhe Nuclear Research Center since 1971. This program, FANAL 2, extracts resonance parameters and total cross sections from neutron transmission data obtained by the time-of-flight technique. It permits the determination of up to 50 parameters characterizing the total cross section by simultaneously fitting calculated transmission curves to experimental values from up to 5 different transmission measurements which may differ e.g. with respect to sample thickness or flight path. The measured and calculated transmission values and the resulting cross sections are plotted with a general-purpose plotting subroutine available at Karlsruhe (program PLOT, Ref. 2).

Total cross sections are normally derived from transmission data. One measures the probability

$$T(E) = e^{-n\sigma(E)} \qquad (1)$$

that a neutron with energy E passes a sample of thickness n (atoms per barn) without interaction. In practice the data are often affected by resolution effects and one observes actually the resolution-broadened transmission

$$\bar{T}(E) = \int R(E,E')\, T(E')\, dE' \qquad (2)$$

where $R(E,E')\,dE'$ is the probability that a neutron with an energy E' (in dE') is registered as if it had the energy E.

Another complication results from the thermal motion of the sample atoms. Strictly speaking the cross section appearing in Eq. (1) is the Doppler-broadened cross section. For light and medium-weight nuclei, however, Doppler broadening can usually be neglected.

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The program FANAL 2 treats instrumental resolution according to Eq. (2) but neglects Doppler broadening for broad (s-wave) levels. It is therefore applicable only to resonance data where the Doppler width $\Delta = \sqrt{4\ EkT/A}$ is much smaller than the width of the (resolution-broadened) s-wave resonances, e.g. to data for light and medium-weight nuclei or near-magic heavy nuclei such as lead. Narrow (p-wave) levels are Doppler broadened.

The total cross section is parametrized with an R-matrix multi-level formula (Ref. 3). The program starts by calculating cross sections and transmission values with guess values for the parameters. These guess values are then improved by application of the least-squares method (cf. e.g. Ref. 4). In order to make this method applicable the problem is linearized by Taylor expansion with respect to the parameters and truncation after the linear terms. The solution of the linearized problem is thus an approximation which can be improved by iteration. The program iterates until the relative variation of the summed squares, χ^2, from one step to the next remains below a given small threshold,

$$\left| \frac{\chi_i^2 - \chi_{i-1}^2}{\chi_i^2} \right| < \varepsilon \ , \qquad (3)$$

where

$$\chi_i^2 = \sum_{n=1}^{N} \left(\frac{T_n - \bar{T}\ (i, E_n)}{\delta T_n} \right)^2 \qquad (4)$$

(T_n : n-th transmission value measured at energy E_n; δT_n : uncertainty of T_n; $\bar{T}(i, E_n)$: transmission at E_n calculated from the parameters of the i-th iteration).

2. LIMITS OF THE PROGRAM

FANAL 2 is written in FORTRAN IV. Resonance cross sections are treated as pure s-wave cross sections with a potential-scattering contribution from the p-wave. Up to 45 resonances are accepted per nuclide and compound spin. For each of them one must specify E_λ (resonance energy), $\Gamma_{n\lambda}$ (neutron width),

$\Gamma_{n'\lambda}$ (partial width for inelastic scattering), and $\Gamma_{\gamma\lambda}$ (radiation width). Inelastic scattering is treated as a 1-channel reaction. The s-wave potential scattering cross section is characterized by 2 parameters, viz. by a_J (channel radius for compound spin J) and by S_J (a pseudo strength function summarily describing the influence of distant levels). The total number of resonance and potential-scattering parameters must not exceed 200, of which not more than 50 can be adjusted while the rest is held constant during the fit. The constant resonances can lie within or without the energy range of measured data points so that the influence of strong levels outside this range can be taken into account explicitly.

The maximum number of data points is 5,120; they may belong to 5 different time-of-flight runs. The sample material, however, must be the same for all runs, and must not contain more than 5 different nuclides.

3. FORMULAE

The total cross section for a single nuclide is taken as

$$\sigma = \sigma_0 + \sigma_1 \quad , \tag{5}$$

σ_0 representing the s-wave cross section,

$$\sigma_0 = 2\pi \lambda\!\!\!^{-2} \sum_{J=I-1/2}^{J=I+1/2} g_J(1-\mathrm{Re}\ U_J) \quad , \tag{6}$$

while σ_1 describes p-wave interactions; higher partial waves are neglected. The notation is as follows: $2\pi\lambda\!\!\!^{-}=2\pi/k_n$ is the neutron wave length in the center-of-mass system and

$$g_J = \frac{2J+1}{2(2I+1)} \tag{7}$$

the statistical spin factor, i.e. the probability that neutron spin (1/2) and target spin (I) combine in such a way as to yield compound spin J. According to R-matrix theory the relevant collision matrix element can be written as

$$U_J = e^{-ik_n R'_J} \left[(\underline{1} - iK_J)^{-1} (\underline{1} + iK_J) \right]_{nn} \qquad (8)$$

where $\underline{1}$ is the 2 x 2 unit matrix and K_J a 2 x 2 matrix with elements

$$K_{J,cc'} = \frac{1}{2} \sum_\lambda \frac{\Gamma_{\lambda c}^{1/2} \Gamma_{\lambda c'}^{1/2}}{E_\lambda - E - i\Gamma_{\gamma\lambda}/2} \qquad (9)$$

The sum runs over all levels with spin J. The channel subscripts c and c' can assume the values n (elastic channel) or n' (inelastic channel). For the inelastic channel one has

$$k_{n'} = \frac{\sqrt{2m(E-E_t)}}{\hbar} \qquad (10)$$

(E_t: inelastic threshold; m: reduced mass).

In this formulation all radiation channels are eliminated following the prescription given by Teichmann and Wigner (Ref. 3). They make themselves felt only by way of the imaginary term in each resonance denominator of k_J (Eq. 9).

The width amplitudes

$$\Gamma_{\lambda c}^{1/2} = (2\, k_c a_c)^{1/2}\, \gamma_{\lambda c} \qquad (11)$$

vary with energy as $E^{1/2}$ in contrast to the energy-independent reduced width amplitudes $\gamma_{\lambda c}$. They are to be understood as having the sign of $\gamma_{\lambda c}$.

The effective channel radius R'_J is calculated as

$$R'_J = a_J - \lambdabar \text{ arc tan } (S_J \sqrt{\frac{E}{1eV}} \text{ ar tanh } \frac{E-\bar{E}}{\Delta E/2}). \qquad (12)$$

This expression with two free parameters (a_J and S_J) is obtained if one approximates the levels outside the range of explicitly treated resonances by a picket fence model with strength function S_J (ratio of reduced neutron width to level spacing), replacing sums by integrals. $\bar{E}$ and ΔE are midpoint and length of the region of explicitly treated resonances, respectively.

Doppler broadening is neglected for s-wave resonances as already mentioned. For narrow (p-wave) levels this may cause difficulties. The term σ_1 in eq. (5) is therefore taken as

$$\sigma_1 = 4\pi\lambda\!\!\!^{-2} \cdot 3 \sin^2 (k_n R_1' - \text{arc tan } k_n R_1') + \sum_\lambda (\sigma_0 \psi)_\lambda \ , \qquad (13)$$

with

$$\sigma_0 \psi = 4\pi\lambda\!\!\!^{-2} g_J \Gamma_n \frac{\sqrt{\pi}}{2\Delta'} \ \exp \left[-\left(\frac{E-E_0}{\Delta'} \right)^2 \right] \ , \qquad (14)$$

i.e. as the usual p-wave potential scattering term (R_1': effective radius for p-wave channels) plus a sum over Doppler-broadened resonances. Interference between resonance and potential scattering is neglected. Resonance profiles are approximated as Gaussians with 1/e widths Δ', where

$$\Delta'^2 = \Delta^2 + \Gamma^2/\ln 16 \ , \qquad (15)$$

$$\Delta^2 = 4kTE_0/A. \qquad (16)$$

The normalization is such that the peak areas have the correct value $\pi\sigma_0\Gamma/2$. The factor ln 16 in Eq. 15 ensures the correct half width (Γ) for negligibly small Doppler width ($\Delta \ll \Gamma$). The quantity kT is the effective (i.e. Lamb-corrected) sample temperature in energy units, E_0 the resonance energy, A the target nuclear mass divided by the neutron mass.

The resolution function is taken as Gaussian,

$$R(E,E')\ dE' = \frac{1}{w\sqrt{\pi}}\ e^{-(t-t')^2/w^2} \qquad (17)$$

with

$$w^2 = \frac{h^2}{\ln 16} + \frac{1}{6} \left(\frac{\Delta L}{L} t\right)^2 , \qquad (18)$$

where t and t' are the flight times corresponding to E and E', respectively, h is the half width (FWHM) of the γ peak in the time-of-flight spectrum, ΔL the effective thickness of the neutron detector (e.g. boron slab or lithium glass thickness) and L the flight path. This form of the resolution function accounts for four effects:

1) time shifts of the electronis (h)
2) finite burst width of the accelerator-pulsed neutron source (h)
3) finite channel width of the flight time analyzer (h)
4) flight path differences due to finite detector thickness (ΔL).

Note: The effective thickness of the detector may deviate from the geometrical thickness due to multiple scattering and self-shielding.

4. INPUT

All numeric input must be stated as FORTRAN-readable floating-point numbers. The present version of the program uses card input. A field of 10 columns is reserved for each number. Within this field the number can be arbitrarily placed in E or F format. Each potential-scattering or resonance parameter is accompanied by an uncertainty. If this uncertainty is set equal to 0. the associated parameter is treated as constant. If, on the other hand, it differs from zero the parameter is adjusted in each iterative step. All energies must be given in keV, all channel radii in fm, all flight times and flight-time increments in ns and all lengths (flight paths, sample thicknesses and sample radii) in m.

1st Card (Title Card)

Columns 1-60: Arbitrary alphameric text. This text appears on the listing and also below the plotted results.

2nd Card (Iteration Data)

Columns 1-10: Maximum number of iterations to be followed through;

Columns 11-20: Largest relative variation of χ^2 between successive iterations which is to be considered as sufficient to terminate the iterative process and to declare convergence achieved (values of the order 1 % were found to be reasonable).

Columns 21-30: Lower limit E_{min} (keV),

Columns 31-40: upper limit E_{max} (keV), of the range of explicitly treated resonances, i.e. of the range for which the extracted parameters are valid. (Note that this range may exceed the range of data points if additional constant resonances outside the latter are used).

3rd Card (Isotope Card)

Columns 1-10: Isotopic abundance of the first (main) sample nuclide (i.e. the number of nuclei of this nuclide divided by the total number of all sample atoms).

Columns 11-20: Atomic mass of main nuclide divided by neutron mass (for practical purposes it is usually sufficient to use simply the nucleon number A of the target nucleus);

Columns 21-30: Nuclear spin quantum number I of main nuclide;

Columns 31-40: Effective nuclear radius R_1' (cf. Eq. 6) for p-wave scattering of main nuclide;

4th Card (Potential-Scattering Card)

Columns 1-10:	Effective s-wave strenght function $S_{I+1/2}$ describing the influence of distant levels (cf. Eq. 11) for main isotope;
Columns 11-20:	uncertainty $^{+)}$ of $S_{I+1/2}$
Columns 21-30:	Channel radius $a_{I+1/2}$ (fm) for main isotope;
Columns 31-40:	Uncertainty $^{+)}$ of $a_{I+1/2}$ for main isotope;
Columns 41-50:	Threshold E_t(keV) for first inelastic channel, for main isotope, compound spin I+1/2;

5th Card (Resonance Card)

Columns 1-10:	Resonance energy E_1(keV)
Columns 11-20:	Uncertainty $^{+)}$ of E_1
Columns 21-30:	Neutron width Γ_{1n}(keV)
Columns 31-40:	Uncertainty $^{+)}$ of Γ_{1n}.
Columns 41-50:	Partial width for inelastic scattering $\Gamma_{1n'}$(keV) multiplied with the sign of $\gamma_{1n}\ \gamma_{1n'}$ (Eq. 11)
Columns 51-60:	Uncertainty $^{+)}$ of $\Gamma_{1n'}$.
Columns 61-70:	Radiation width $\Gamma_{1\gamma}$ (keV)
Columns 71-80:	Uncertainty $^{+)}$ of $\Gamma_{1\gamma}$.

A similar "resonance card" follows for each resonance of the main isotope with spin I + 1/2. If I > 0 a second compound spin, I - 1/2, can be formed by s-wave neutrons. For this second compound spin one must prepare another similar set of cards consisting of atleast a "potential-scattering card" and possibly a number of "resonance cards". If p-wave levels are to be analyzed they must be treated as levels of an additional isotope with vanishing potential scattering ($S_J = a_J = 0.$), see the example in Section 6. Note that spin or parity reassignment is effected simply by repositioning of the relevant resonance card(s) in the input deck.

+) Uncertainty = 0.: associated parameter is kept constant,
Uncertainty ≠ 0. (arbitrary): associated parameter is adjusted.

If sample impurities (e.g. other isotopes or oxygen in oxide samples) must be taken into account a completely analogous sequence of input cards must be prepared for each nuclide: "isotope card" followed by "potential scattering card" plus "resonance cards" for I + 1/2 (and then for I - 1/2 if I > 0). Resonance cards are optional. If they are missing only a potential scattering cross section is calculated for the relevant isotope and compound spin.

After the input cards specifying the cross section parameters other cards follow which contain information on the time-of-flight runs. For each run one needs a set of cards consisting of "sample card", "time-of-flight card", "transmission data cards" and one blank card.

Sample Card

Columns 1-10:	Sample thickness n(total number of nuclei, including impurities, per barn) (atoms/b).

Time-of-flight-Card

Columns 1-10:	Flight path L (m);
Columns 11-20:	Effective detector thickness ΔL(m), cf. Eq. 18;
Columns 21-30:	Channel width Δt(ns);
Columns 31-40:	Full width at half maximum of gamma peak h (ns) cf. Eq. 18;
Columns 41-50:	largest flight time t_{max} (ns).

Transmission Card

Columns 1-10:	Measured transmission T_1;
Columns 11-20:	Uncertainty δT_1(one standard deviation)
Columns 21-30:	Measured transmission T_2;
Columns 31-40:	Uncertainty δT_2 etc.

Thus four transmission values and associated uncertainties can be put on one 80-column card. The last transmission card of a given card may contain less than four. The first transmission, T_1, must correspond to the maximum flight time t_{max}, the second to $t_{max}-\Delta t$, the third to $t_{max}-2\Delta t$, etc. In other words the T-values should be entered in the order of ascending energy. Card sets for more time-of-flight runs may follow each consisting of "sample card", "time-of-flight card" and "transmission data cards". The maximum number of time-of-flight runs which can be treated simultaneously is 5.

A blank card signals the end of the input for one calculation. Input for more calculations may follow, i.e. problems can be stacked.

5. OUTPUT

The output consists of listing and plots.

The listing shows first the contents of the "title", "isotope", "potential-scattering", "resonance", "sample" and "time-of-flight" cards. Next it contains tables of measured and calculated transmission values for all utilized experimental runs. Subsequently the values of the squared-error sum χ^2 and the usual error adjustment factor $(\chi^2/(N-P))^{1/2}$ are printed (N: number of measured transmission values, P: number of adjusted parameters). For a good fit the error adjustment factor should be close to 1.

After that one gets a table with the adjusted (and constant) parameters and their uncertainties. The uncertainties are the square roots of the corresponding diagonal elements of the covariance matrix of the least-squares problem. They result from the experimental transmission uncertainties by normal error propegation. If the maximum number of iterative steps specified on the second input card exceeds 1 a similar printout (transmission table plus improved parameters) is obtained for each iterative step.

The subroutine PLOT yields for each iterative step a plot with all experimental data points including error bars. The calculated values are plotted in the same plot in curve form. The text of the "title card" appears under each plot after a figure number. The curve in Abb. 1 corresponds to the input (guess) parameters, that in Abb. 2 to the improved parameters after the first iteration, etc.

For the last set of parameters neither transmission nor χ^2 values are calculated, printed or plotted. If the convergence criterion (Eq. 3) with reasonably chosen ε is satisfied there should not be any essential change in the last step anyway.

6. EXAMPLE

Fig. 1 shows the input cards for a realistic fitting problem which illustrates most features of FANAL 2:

Two transmission measurements taken with Fe_2O_3 samples enriched to 90.7 % ^{57}Fe are to be analyzed between 20 and 80 keV (for experimental details see Refs. 5,6). ^{57}Fe has a $1/2^-$ ground state and a first excited state with $3/2^-$ at 14.4 keV. Thus there are two s-wave level sequences ($J^\pi = 0^-, 1^-$), one inelastic channel being open for the 1^- sequence. The signs of the inelastic widths indicate the relative signs of $\Gamma_n^{1/2}\Gamma_{n'}^{1/2}$ (cf. Eq. 9).

The p-wave levels of ^{57}Fe+n are represented as levels of a fictitious, spinless target isotope with zero potential scattering ($a_J = S_J = 0.$). Thus the neutron widths in the input and output are actually $g_J\Gamma_n$ values (cf. Eq. 14).

The main impurity was ^{56}Fe. It is represented by another s-wave level sequence. The smooth oxygen cross section is specified by a potential scattering card without resonance cards following.

Sample and transmission cards contain the experimental data of the two utilized time-of-flight runs.

Figs. 2 - 4 show the cross section parameter input and the tables with measured and calculated data as printed by the computer. Fig. 5 shows the measured data (points with error bars) together with the calculated transmission curves.

The CPU time needed for the whole job (3 iterations) was 18 min 44 sec on an IBM 370/168. The required memory capacity was 252 kbytes.

7. REFERENCES

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Ref. 4 J. MATTHEWS and R.L. WALKER, Mathematical Methods of Physics, New York-Amsterdam, 1965, p. 365.

Ref. 5 G. ROHR and K.-N. MÜLLER, Z. Physik 227 (1969) 1

Ref. 6 H. BEER and R.R. SPENCER, KFK 2063 (1974)

Figure Captions

Fig. 1 - Representative example: input cards.

Fig. 2 - Representative example: printout of cross section parameter input.

Fig. 3 - Representative example: printout of transmission data input and calculated values.

Fig. 4 - Representative example: printout of cross section parameter after 1 iteration. Note that uncertainties are now the results of error propagation of transmission uncertainties rather than indicators for parameter adjustment as in Fig. 2.

Fig. 5 - Representative example: plots of measured point data and calculated curves. The calculated curves of Abb. 1, 2, 3 correspond to the cross section parameters before 1, 2, 3 iterations, respectively.

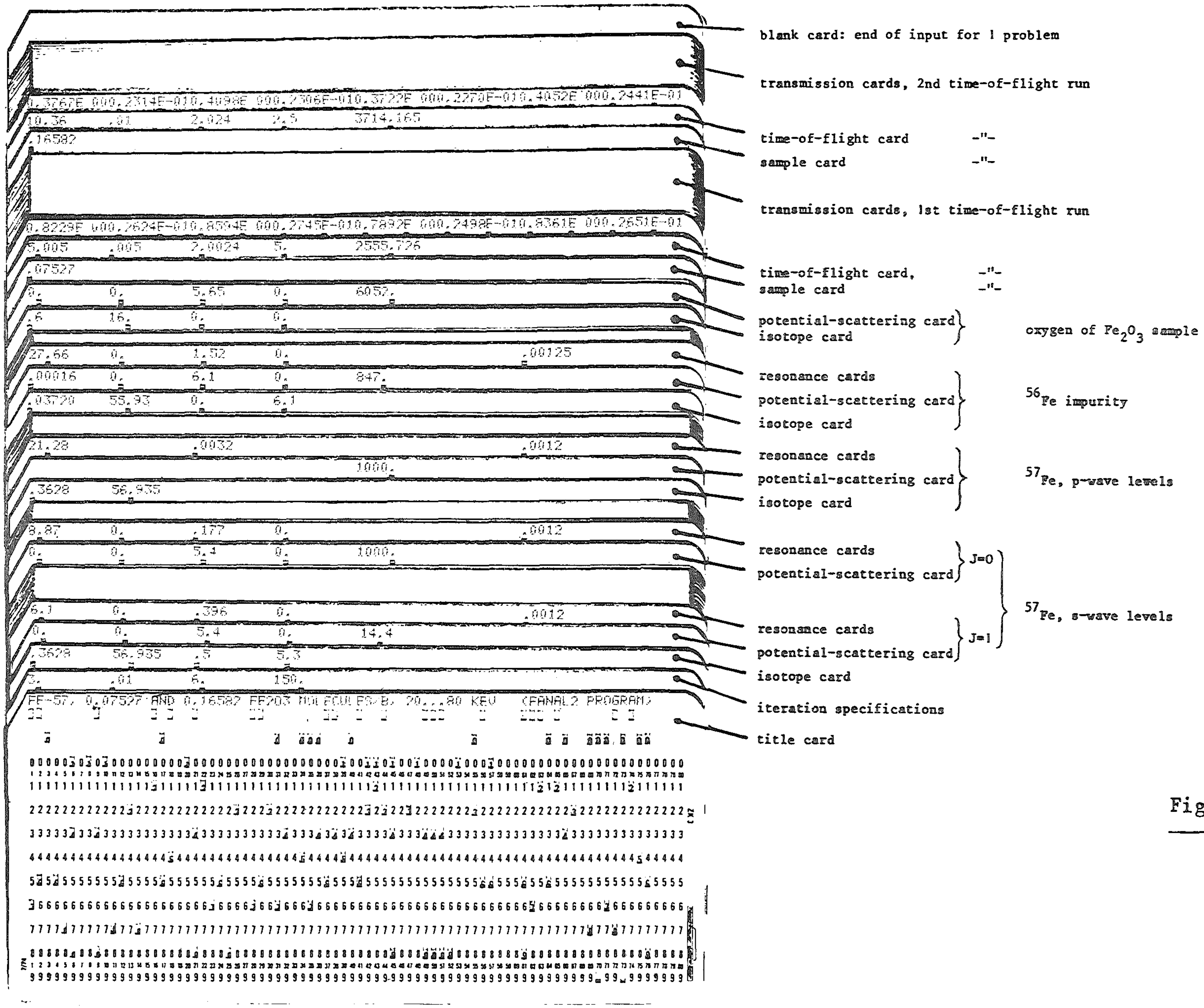
blank card: end of input for 1 problem
transmission cards, 2nd time-of-flight run
time-of-flight card -"-
sample card -"-
transmission cards, 1st time-of-flight run
time-of-flight card, -"-
sample card -"-
potential-scattering card
isotope card
oxygen of Fe_2O_3 sample
resonance cards
potential-scattering card
isotope card
^{56}Fe impurity
resonance cards
potential-scattering card
isotope card
^{57}Fe, p-wave levels
resonance cards
potential-scattering card
J=0
resonance cards
potential-scattering card
J=1
^{57}Fe, s-wave levels
isotope card
iteration specifications
title card

Fig. 1

FE-57, 0.07527 AND 0.16582 FE2C3 MCLECULES/B, 20...80 KEV

MAXIMAL NUMBER OF ITERATIVE STEPS: 3.
STOP IF RELATIVE CHANGE OF CHI-SQUARE IS LESS THAN 0.010
PARAMETERS VALID BETWEEN 6.000 AND 150.000 KEV

ABUN-DANCE	ATOMIC WEIGHT	TARGET SPIN	P-WAVE RADIUS (FM)	COMP. SPIN	S-WAVE STRNTH.F. /UNCERT.	S-WAVE RADIUS (FM) /UNCERT.	INEL. THRESH. (KEV)	RESONANCE ENERGY (KEV) /UNCERT.	PARTIAL WIDTHS FOR EL. SCATT. (KEV) /UNCERT.	INEL. SCATT. (KEV) /UNCERT.	CAPTURE (KEV) /UNCERT.
0.3628	56.9	0.5	5.300	1.0	0.0	5.400	14.400	6.100	3.960E-01	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								26.980	2.940E+00	7.680E-01	2.300E-03
								1.000	0.100E+01	0.100E+01	C.0
								39.380	3.000E-02	0.0	1.200E-03
								1.000	0.100E+01	0.100E+01	C.0
								41.410	7.200E-01	2.100E+00	5.000E-04
								1.000	0.100E+01	0.100E+01	0.0
								47.000	3.820E-01	1.230E-01	5.500E-04
								1.000	0.100E+01	0.100E+01	0.0
								61.257	3.370E+00	4.650E-01	1.200E-03
								1.000	0.100E+01	0.100E+01	C.0
								65.750	3.000E-01	-1.500E+00	1.200E-03
								1.000	0.100E+01	0.100E+01	C.0
								77.250	1.600E+00	8.500E-01	5.000E-04
								1.000	0.100E+01	0.100E+01	C.0
								93.700	2.000E-01	2.000E-01	1.200E-03
								0.0	0.0	0.0	C.0
								109.600	2.300E+00	2.000E-01	1.900E-03
								0.0	0.0	0.0	0.0
								110.150	1.200E+00	1.550E+00	2.000E-03
								0.0	0.0	0.0	0.0
								125.000	1.500E+00	1.000E+00	1.200E-03
								0.0	0.0	0.0	C.0
								129.500	4.200E+00	8.000E+00	1.200E-03
								0.0	0.0	0.0	C.0
				0.0	0.0	5.400	1000.000	8.870	1.770E-01	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								56.290	9.000E+00	0.0	1.200E-03
								1.000	0.100E+01	0.0	0.0
								126.000	2.500E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								134.500	3.300E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								141.000	1.500E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
0.3628	56.9	0.0	0.0	0.5	0.0	0.0	1000.000	21.280	3.200E-03	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	C.0
								37.010	4.000E-03	0.0	1.200E-03
								0.0	0.0	0.0	C.0
								41.930	1.000E-02	0.0	1.200E-03
								1.000	0.100E+01	0.0	0.0
								52.660	1.600E-02	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								56.195	2.900E-03	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								72.600	1.500E-02	0.0	1.200E-03
								1.000	0.100E+01	0.0	C.0
0.0372	55.9	0.0	6.100	0.5	1.600E-04	6.100	847.000	27.660	1.520E+00	0.0	1.250E-03
					0.0	0.0		0.0	0.0	0.0	C.0
								74.360	5.390E-01	0.0	1.250E-03
								0.0	0.0	0.0	0.0
								83.500	9.120E-01	0.0	4.400E-04
								0.0	0.0	0.0	C.0
								90.200	5.000E-02	0.0	1.300E-03
								0.0	0.0	0.0	0.0
0.6000	16.0	0.0	0.0	0.5	0.0	5.650	6052.000				
					0.0	C.0					

UTILIZED TIME-OF-FLIGHT RUNS:

RUN NO.	SAMPLE THICKNESS (ATOMS/B)	FLIGHT PATH (M)	EFF. DETECTOR THICKNESS (M)	CHANNEL WIDTH (NS)	FWHM OF GAMMA PEAK (NS)	MAXIMAL FLIGHT-TIME (NS)
1	7.527E-02	5.005	0.005	2.00240	5.000	2555.726
2	1.658E-01	10.360	0.010	2.02400	2.500	3714.165

Fig. 2

```
COMPLETED ITERATIONS  :  1
TIME-OF-FLIGHT RUN NO.:  1
SAMPLE THICKNESS      :  7.527E-02 ATOMS/B
FLIGHT PATH           :  5.005E+00 M
```

FLIGHT TIME (NS)	NEUTRON ENERGY (KEV)	MEASURED TRANSMISSION	CALCULATED TRANSMISSION	TOTAL X-SECTION (B)
2555.726	20.045	0.8225+-0.0262	0.8033	2.911
2553.723	20.077	0.8594+-0.0274	0.8032	2.913
2551.721	20.108	0.7892+-0.0250	0.8031	2.915
2549.719	20.140	0.8361+-0.0265	0.8030	2.917
2547.716	20.171	0.8652+-0.0278	0.8028	2.920
2545.714	20.203	0.8267+-0.0259	0.8027	2.922
2543.711	20.235	0.8376+-0.0265	0.8026	2.924
2541.709	20.267	0.8115+-0.0255	0.8025	2.927
2539.706	20.299	0.8541+-0.0268	0.8023	2.929
2537.704	20.331	0.8260+-0.0261	0.8022	2.932
2535.701	20.363	0.8052+-0.0252	0.8020	2.934
2533.699	20.395	0.8571+-0.0263	0.8019	2.937
2531.697	20.427	0.8328+-0.0258	0.8017	2.940
2529.694	20.460	0.8566+-0.0261	0.8015	2.94[illegible]
2527.692	20.492	0.8385+-0.0261	0.8014	[illegible]
2525.689	[illegible]	0.8070+-0.0250	0.8012	
2523.687		[illegible]8408+-0.026[illegible]		
		[illegible]94+-0.[illegible]		
⋮	⋮	⋮	⋮	⋮
	[illegible]4.718			[illegible]
	64.901	0.[illegible]	0.491[illegible]	9.398
1418.339	65.084	0.51[illegible]12	0.4945	9.308
1416.337	65.268	0.5040+-0.0111	0.4950	9.303
1414.334	65.453	0.4575+-0.0112	0.4933	9.373
1412.332	65.639	0.5092+-0.0115	0.4910	9.473
1410.329	65.826	0.5005+-0.0116	0.4903	9.524
1408.327	66.013	0.5193+-0.0119	0.4926	9.464
1406.324	66.201	0.5363+-0.0127	0.4986	9.287
1404.322	66.390	0.5388+-0.0128	0.5073	9.032
1402.320	66.580	0.5359+-0.0131	0.5177	8.746
1400.317	66.770	0.5430+-0.0132	0.5286	8.460
1398.315	66.962	0.5570+-0.0141	0.5394	8.188
1396.312	67.154	0.5470+-0.0143	0.5497	7.937
1394.310	67.347	0.6013+-0.0157	0.5593	7.706
1392.307	67.541	0.5786+-0.0156	0.5684	7.494
1390.305	67.735	0.5817+-0.0160	0.5768	7.300
1388.302	67.931	0.5717+-0.0161	0.5847	7.119
1386.300	68.127	0.5979+-0.0173	0.5922	6.952
1384.298	68.325	0.6057+-0.0179	0.5992	6.796
1382.295	68.523	0.5892+-0.0194	0.6059	6.649
1380.293	68.722	0.5586+-0.0189	0.6123	6.510
1378.290	68.921	0.6607+-0.0219	0.6184	6.379

```
COMPLETED ITERATIONS  :  1
TIME-OF-FLIGHT RUN NO.:  2
SAMPLE THICKNESS      :  1.658E-01 ATOMS/B
FLIGHT PATH           :  1.036E+01 M
```

FLIGHT TIME (NS)	NEUTRON ENERGY (KEV)	MEASURED TRANSMISSION	CALCULATED TRANSMISSION	TOTAL X-SECTION (B)
3714.165	40.665	0.3767+-0.0231	0.3795	5.842
3712.141	40.710	0.4098+-0.0251	0.3725	5.954
3710.116	40.754	0.3722+-0.0227	0.3656	6.068
3708.092	40.799	0.4052+-0.0244	0.3586	6.183
3706.068	40.843	0.3552+-0.0224	0.3518	6.300
3704.044	40.888	0.3613+-0.0238	0.3450	6.418
3702.020	40.933	0.3235+-0.0217	0.3383	6.535
3699.996	40.978	0.4046+-0.0254	0.3319	6.652
3697.971	41.022	0.3445+-0.0226	0.3256	6.768
3695.947	41.067	0.2951+-0.0210	0.3195	6.881
3693.923	41.112	0.3227+-0.0221	0.3137	6.992
3691.899	41.157	0.3170+-0.0223	0.3083	7.098
3689.875	41.203	0.2925+-0.0223	0.3031	7.200
3687.851	41.248	0.2866+-0.0210	0.2983	7.297
3685.826	41.293	0.2752+-0.0211	0.2939	7.387
3683.802	41.339	0.3020+-0.0215	0.2899	7.470
3681.778	41.384	0.2422+-0.0202	0.2863	7.546
3679.754	41.430	0.2973+-0.0216	0.2831	7.613
3677.730	41.475	0.2655+-0.0217	0.2804	7.672
3675.706	41.521	0.2884+-0.0217	0.2781	7.72[illegible]
3673.6[illegible]	41.567	0.2740+-0.0213	0[illegible]763	7.[illegible]
	[illegible]1.612	[illegible]0.0219		
	[illegible]58	[illegible]		
⋮	⋮	⋮	⋮	⋮
[illegible]			[illegible]20[illegible]	[illegible]072
2677.790	[illegible]	0.2430+-[illegible]	0.2078	9.475
2675.766	78.3[illegible]	0.2430+-0.00[illegible]	0.2151	9.266
2673.741	78.471	0.2578+-0.0079	0.2228	9.052
2671.717	78.590	0.2635+-0.0080	0.2308	8.839
2669.693	78.709	0.2570+-0.0078	0.2389	8.631
2667.669	78.829	0.2828+-0.0082	0.2470	8.429
2665.645	78.948	0.2791+-0.0081	0.2550	8.236
2663.621	79.068	0.2954+-0.0084	0.2629	8.053
2661.596	79.189	0.2942+-0.0083	0.2706	7.879
2659.572	79.309	0.3108+-0.0085	0.2781	7.715
2657.548	79.430	0.3090+-0.0085	0.2849	7.560
2655.524	79.551	0.3245+-0.0087	0.2919	7.414
2653.500	79.673	0.3219+-0.0087	0.2986	7.276
2651.476	79.794	0.3196+-0.0086	0.3051	7.146
2649.451	79.916	0.3256+-0.0086	0.3114	7.024
2647.427	80.039	0.3507+-0.0090	0.3175	6.908

```
CHI**2:                    9.638E+03
ERROR ADJUSTMENT FACTOR:   2.974E+00
```

Fig. 3

ABUNDANCE	ATOMIC WEIGHT	TARGET SPIN	P-WAVE RADIUS (FM)	COMP. SPIN	S-WAVE STRNTH.F. /UNCERT.	S-WAVE RADIUS (FM) /UNCERT.	INEL. THRESH. (KEV)	RESONANCE ENERGY (KEV) /UNCERT.	PARTIAL WIDTHS FOR EL. SCATT. (KEV) /UNCERT.	INEL. SCATT. (KEV) /UNCERT.	CAPTURE (KEV) /UNCERT.
0.3628	56.9	0.5	5.300	1.0	0.0	5.400	14.400	6.100	3.960E-01	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								29.326	3.188E+00	7.209E-01	2.300E-03
								0.008	0.105E-01	0.172E-01	C.0
								39.380	1.805E-02	7.436E-03	1.200E-03
								0.017	0.234E-02	0.698E-02	0.0
								41.463	7.177E-01	1.973E+00	9.000E-04
								0.019	0.102E-01	0.482E-01	0.0
								47.014	3.715E-01	1.412E-01	5.500E-04
								0.004	0.461E-02	0.101E-01	0.0
								61.101	2.596E+00	7.855E-01	1.200E-03
								0.013	0.318E-01	0.415E-01	0.0
								65.865	1.355E-01	-1.286E+00	1.200E-03
								0.052	0.127E-01	0.113E+00	0.0
								77.110	1.390E+00	8.062E-01	5.000E-04
								0.014	0.202E-01	0.277E-01	0.0
								93.700	2.000E-01	2.000E-01	1.200E-03
								0.0	0.0	0.0	0.0
								109.600	2.300E+00	2.000E-01	1.900E-03
								0.0	0.0	0.0	0.0
								110.150	1.200E+00	1.550E+00	2.000E-03
								0.0	0.0	0.0	0.0
								125.000	1.500E+00	1.000E+00	1.200E-03
								0.0	0.0	0.0	C.0
								129.500	4.200E+00	8.000E+00	1.200E-03
								0.0	0.0	0.0	C.0
				0.0	0.0	5.400	1000.000	8.870	1.770E-01	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								56.677	9.533E+00	0.0	1.200E-03
								0.053	0.145E+00	0.0	0.0
								126.000	2.500E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								134.500	3.300E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								141.000	1.500E+00	0.0	1.200E-03
								0.0	0.0	0.0	0.0
0.3628	56.9	0.0	0.0	0.5	0.0	0.0	1000.000	21.280	3.200E-03	0.0	1.200E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								37.010	4.000E-03	0.0	1.200E-03
								0.0	0.0	0.0	C.0
								41.921	~~7.528E-03~~	~~0.0~~	~~1.200E-03~~
								0.010	0.193E-02	0.0	0.0
								52.660	1.600E-02	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								56.195	2.900E-03	0.0	1.200E-03
								0.0	0.0	0.0	0.0
								72.619	4.419E-04	0.0	1.200E-03
								0.013	0.502E-03	0.0	0.0
0.0372	55.9	0.0	6.100	0.5	1.600E-04	6.100	847.000	27.660	1.520E+00	0.0	1.250E-03
					0.0	0.0		0.0	0.0	0.0	0.0
								74.360	5.390E-01	0.0	1.250E-03
								0.0	0.0	0.0	0.0
								83.500	9.120E-01	0.0	4.400E-04
								0.0	0.0	0.0	0.0
								90.200	5.000E-02	0.0	1.300E-03
								0.0	0.0	0.0	0.0
0.6000	16.0	0.0	0.0	0.5	0.0	5.650	6051.956				
					0.0	0.0					

AFTER 1 ITERATIONS NO CONVERGENCE YET

WARNING: INTERNAL GRID WAS TOO FINE IN ITERATION 2, KR REDUCED FROM 107 TO 100

Fig. 4

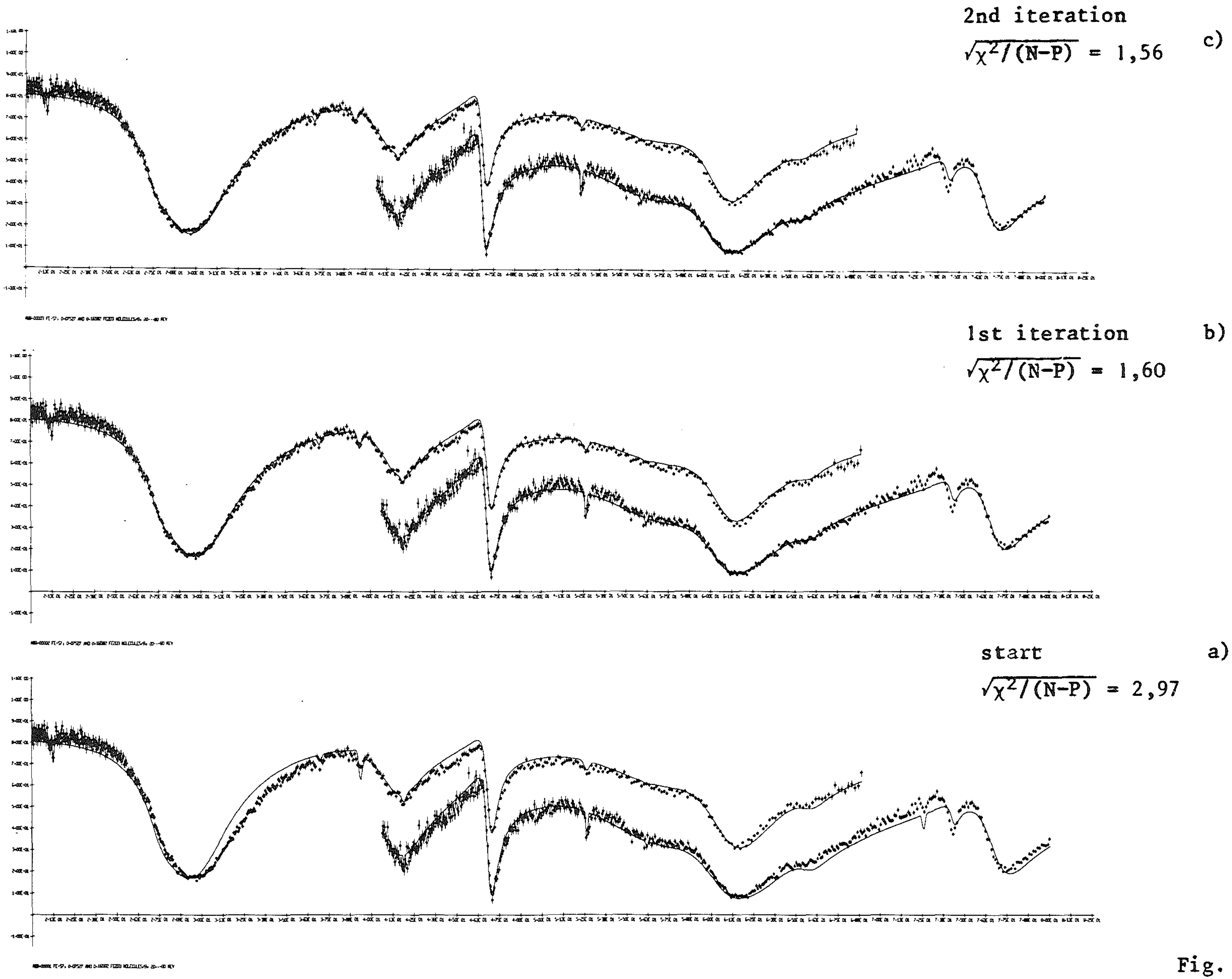
2nd iteration
$\sqrt{\chi^2/(N-P)}$ = 1,56
c)
1st iteration
b)
$\sqrt{\chi^2/(N-P)}$ = 1,60
start
a)
$\sqrt{\chi^2/(N-P)}$ = 2,97

Fig. 5

APPENDIX

Listing of FANAL 2

```
FORTRAN IV G1  RELEASE 2.0            MAIN              DATE = 75336          20/33/10              PAGE 0001

      C  FANAL2 MAIN PROGRAM
      C
      C
      C        NOTICE TO NON-KFK USERS:
      C
      C        PLOT(X,Y,N,NT,NP,NH,I,NS,NR,XMAX,XMIN,SX,YMAX,YMIN,SY,TEXT,ID)
      C        IS A STANDARD PLOTTER SUBROUTINE IN USE AT KFK (KARLSRUHE)
      C        WHICH MUST BE REPLACED BY AN EQUIVALENT  PLOTTER PACKAGE
      C        ELSEWHERE
      C
      C         1. X       ARRAY OF ABSCISSAE
      C         2. Y       ARRAY OF ORDINATES
      C         3. N       NUMBER OF CO-ORDINATE PAIRS
      C         4. NT=1    PLOT POINT SYMBOLS
      C              =2    DRAW LINE
      C              =3    DRAW LINE WITH POINT SYMBOLS
      C         5. NP      CHOOSE NP-TH POINT SYMBOL (FROM A LIST) IF NT=1 OR 3
      C         6. NH=1    HEIGHT OF POINT SYMBOL 0.12 IN.
      C              =2    HEIGHT OF POINT SYMBOL 0.16 IN.
      C              =3    HEIGHT OF POINT SYMBOL 0.24 IN.
      C         7. I=1     LINEAR INTERPOLATION  (FOR NT=2 OR 3)
      C             =2     QUADRATIC     ''        (FOR NT=2 OR 3)
      C             =3     CUBIC         ''        (FOR NT=2 OR 3)
      C         8. NS      SPACING: EVERY NS-TH POINT IS TO BE MARKED
      C                    (FOR NT=3)
      C         9. NR=0    DRAW ONTO EXISTING PLOT
      C              =1    BEGIN NEW PLOT, (XMAX-XMIN)/(YMAX-YMIN) = 1
      C              =2                     -''-                 = 2
      C              =3                     -''-                 = 3
      C              =4                     -''-                 = 4
      C             >=5                     -''-                 = 1.5
      C                    (NH,XMAX,XMIN,SX,YMAX,YMIN,SY,TEXT NEED NOT BE
      C                    SPECIFIED FOR NR=0)
      C        10. XMAX    MAXIMAL ABSCISSA
      C        11. XMIN    MINIMAL ABSCISSA
      C        12. SX      X-INCREMENT CORRESPONDING TO 0.01 IN.
      C        13. YMAX    MAXIMAL ORDINATE
      C        14. YMIN    MINIMAL ORDINATE
      C        15. SY      Y-INCREMENT CORRESPONDING TO 0.01 IN.
      C        16. TEXT    FIGURE CAPTION, 60 ALPHAMERIC CHARACTERS
      C        17. ID      FIGURE NUMBER
      C
      C  FANAL2 SUMMARY:
      C
      C  PROGRAMMING LANGUAGE: FORTRAN IV
      C  PURPOSE             : SHAPE ANALYSIS OF NEUTRON TRANSMISSION DATA,
      C                        EXTRACTION OF RESONANCE PARAMETERS,
      C                        CALCULATION OF TRUE CROSS SECTION.
      C  METHOD              : SIMULTANEOUS LEAST-SQUARES FIT TO SEVERAL
      C                        SETS OF TIME-OF-FLIGHT DATA (E. G. TAKEN
      C                        WITH DIFFERENT SAMPLES OR RESOLUTIONS).
      C  FORMALISM           : MULTI-LEVEL R-MATRIX FORMULA WITH 1 ELASTIC
      C                        AND 1 INELASTIC NEUTRON CHANNEL PER COMPOUND
      C                        SPIN AND PARITY. CAPTURE CHANNELS ARE ELIMI-
      C                        NATED FOLLOWING REICH AND MOORE BY TEICHMANN-
      C                        WIGNER REDUCTION METHOD.
      C  CORRECTIONS         : DOPPLER BROADENING IS APPLIED ONLY TO LEVEL
      C                        SEQUENCES WITH VANISHING POTENTIAL SCATTERING
```

```
              C                          (P-WAVE RESONANCES) AS FANAL2 WAS DEVELOPPED
              C                          FOR STRUCTURAL MATERIALS (CR, FE, NI ... )
              C                          WHERE DOPPLER BROADENING FOR TYPICAL S-WAVE
              C                          LEVELS IS NEGLIGIBLE.
              C                          RESOLUTION BROADENING IS APPLIED TO CALCULATED
              C                          TRANSMISSION (GAUSSIAN RESOLUTION FUNCTION).
              C
0001                COMMON Z11,Z21,Z22,HI,GI
0002                COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
                   1      XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                   2      TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
                   3      CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                   4      YY(201),DYY(50,201),
                   5      F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
                   6      CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
                   7      ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0003                COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
0004              1 IZ=0
0005                CHISQ=0.
0006                CALL EIN
0007                IZX=ZIT
0008                CALL PARAUS
0009                CALL INDEX
0010              2 CHISQO=CHISQ
0011                CHISQ=0.
0012                CALL HBN
0013                CALL MEV
0014                IZ=IZ+1
0015                CALL NGK
0016                CALL YTAB
0017                CALL ORTH(MA,A,B)
0018                CALL ADJ(MX,MA,X,DLX,B,C)
0019                CALL KEV
0020                CALL PARAUS
0021                VCHISQ=((CHISQ-CHISQO)/CHISQ)**2
0022                DLCHSQ=SQRT(VCHISQ)
0023                IF(DLCHSQ.LT.EPS)GO TO 3
0024                WRITE(6,100)IZ
0025            100 FORMAT(//' AFTER',I3,' ITERATIONS NO CONVERGENCE YET'//)        FA
0026                IF(IZ.LT.IZX)GO TO 2
0027                STOP
0028              3 WRITE(6,101)IZ
0029            101 FORMAT(//' CONVERGENCE CRITERION SATISFIED AFTER',I3,'ITERATIONS'
                   1//)
0030                STOP
0031                END
```

```
FORTRAN IV G1  RELEASE 2.0            MAIN              CATE = 75336          20/33/10                PAGE 0001

                C
0001                  SUBRCUTINE EIN
                C
                C  EIN READS INPUT CARDS
                C
0002                  COMMCN Z11,Z21,Z22,HI,GI
0003                  COMMCN TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
                    1        XN(5),XR(5),FP(5),DLFP(5),TC(5),TE(5),TJ(5),
                    2        TMX(5),ZH(5),Y(5120),CLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
                    3        CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                    4        YY(201),DYY(50,201),
                    5        F(201),A(50,5C),B(5C,5C),C(50),EZ(2C48),Z(5120),DZ(50),
                    6        CHISQ,CHISQO,MP(6,2),MR(6,2),CST(50),AL(6),RF(201),CC,KN,KH
                    7        ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004                  COMPLEX Z11,Z21,Z22,CZ11,CZ21,DZ22,HI,GI
0005                  I=0
0006                  N=0
0007                  MX=0
0008                  HI=(C.,.5)
0009                  GI=(C.,1.)
                C  I LABELS ISOTOPES
                C  J LABELS COMPOUND SPINS
                C  K LABELS MEASURED DATA POINTS
                C  L LABELS RESCNANCES
                C  M LABELS (ADJUSTED AND FIXED) CRCSS SECTICN PARAMETERS
                C  N LABELS MEASURED DATA SETS (TIME-CF-FLIGHT RUNS)
0010                1 READ(5,100)TITLE
0011              100 FORMAT(15A4)
0012                  WRITE(6,101)TITLE
0013              101 FORMAT(1H1//30X,15A4///)
0014                  READ(5,102)ZIT,EPS,E1(1),E2(1)
0015              102 FORMAT(4E10.5)
0016                  WRITE(6,103)ZIT,EPS,E1(1),E2(1)
0017              103 FORMAT(' MAXIMAL NUMBER OF ITERATIVE STEPS:  ',
                     1F4.0/  ' STOP IF RELATIVE CHANGE OF CHI-SQUARE IS LESS THAN',
                     2F6.3/  ' PARAMETERS VALID BETWEEN',F8.3,' ANC',F8.3,' KEV')
0018                2 I=I+1
                C  READ ISCTOPE CARD (I-TH ISOTOPE)
                C  H(I)    : ABUNDANCE
                C  AG(I)   : RATIO OF NUCLEAR MASS TC NEUTRON MASS
                C  SPIN(I): TARGET SPIN
                C  RP(I)   : EFFECTIVE RADIUS FCR P-WAVE SCATTERING (FM)
0019                  READ(5,104)H(I),AG(I),SPIN(I),RP(I)
0020              104 FORMAT(4E10.5)
0021                3 G(I,1)=.5*(1.+1./(2.*SPIN(I)+1.))
0022                  G(I,2)=1.-G(I,1)
0023                  IF(SPIN(I).EQ.0.)JX(I)=1
0024                  IF(SPIN(I).GT.0.)JX(I)=2
0025                  CS(I,1)=SPIN(I)+.5
0026                  CS(I,2)=SPIN(I)-.5
0027                  L=0
0028                  J=1
0029                  MN=MX+1
0030                  MX=MN+1
                C  READ POTENTIAL-SCATTERING CARC (I-TH ISCTOPE, J-TH SPIN)
                C  X(MN)   : S-WAVE STRENGTH FUNCTICN FROM CISTANT LEVELS
                C  DLX(MN): UNCERTAINTY (0. IF X(MN) IS TO BE TREATED AS FIXED)
                C  X(MX)   : EFFECTIVE RADIUS FOR S-WAVE SCATTERING (FM)
```

```
           C  DLX(MX): UNCERTAINTY (0. IF X(MX) IS TO BE TREATED AS FIXED)
           C  ES(I,J): INELASTIC THRESHOLD (ONLY NECESSARY WHERE RELEVANT)
0031             READ(5,105)(X(M),DLX(M),M=MN,MX),ES(I,J)
0032         105 FORMAT(5E10.5)
0033           4 L=L+1
0034             MN=MX+1
0035             MX=MN+3
           C  READ RESONANCE CARD
           C  X(MN)   : RESONANCE ENERGY (KEV)
           C  X(MN+1): NEUTRON WIDTH    (KEV)
           C  X(MN+2): INELASTIC WIDTH  (KEV)
           C  X(MX)   : RADIATION WIDTH  (KEV)
           C  DLX(M) : UNCERTAINTIES (0. IF ASSOCIATED PARAMETER X(M) IS FIXED)
0036             READ(5,106)(X(M),DLX(M),M=MN,MX)
0037         106 FORMAT(8E10.5)
           C  CHECK CARD TYPE
0038             IF(X(MX).NE.0.)   GO TO 4
0039             IF(J.LT.JX(I))    GO TO 5
0040             IF(DLX(MN).GE.1.) GO TO 6
0041                               GO TO 7
           C  LAST CARD WAS POTENTIAL-SCATTERING CARD
0042           5 LX(I,J)=L-1
0043             MX=MX-2
0044             J=2
0045             ES(I,J)=X(MN+2)
0046             L=0
0047             GO TO 4
           C  LAST CARD WAS ISOTOPE CARD
0048           6 LX(I,J)=L-1
0049             MX=MX-4
0050             I=I+1
0051             H(I)    =X(MN)
0052             AG(I)=  DLX(MN)
0053             SPIN(I)=X(MN+1)
0054             RP(I)   =DLX(MN+1)
0055             GO TO 3
           C  LAST CARD WAS SAMPLE CARD
           C  XN(N): SAMPLE THICKNESS (ATOMS/B)
0056           7 LX(I,J)=L-1
0057             N=N+1
0058             XN(N)=X(MN)
0059             MX=MX-4
0060             IX=I
0061             KH=0
           C  READ TIME-OF-FLIGHT CARD FOR N-TH RUN
           C  FP(N)   : FLIGHT PATH (M)
           C  DLFP(N): EFFECTIVE DETECTOR THICKNESS (M)
           C  TC(N)   : TIME CHANNEL WIDTH (NS)
           C  TB(N)   : FWHM OF GAMMA PEAK (NS)
           C  TMX(N)  : MAXIMAL FLIGHT TIME (NS)
0062           8 READ(5,107)FP(N),DLFP(N),TC(N),TB(N),TMX(N)
0063         107 FORMAT(5E10.5)
           C  READ DATA CARD
           C  Y(K)   : MEASURED TRANSMISSION
           C  DLY(K): UNCERTAINTY
0064           9 KN=KH+1
0065             KH=KN+3
0066             READ(5,108) (Y(K),DLY(K),K=KN,KH)
```

```
FORTRAN IV G1  RELEASE 2.0            EIN                DATE = 75336          20/33/10              PAGE 0003
 0067            108 FORMAT(8E10.5)                                                         002210
               C  WAS THIS LAST DATA CARD?                                                FA002220
 0068                IF(DLY(KH  ).NE.0.)GO TO 9                                             002230
 0069                IF(DLY(KH  ).EQ.0.)KX(N)=KH-1                                          002240
 0070                IF(DLY(KH-1).EQ.0.)KX(N)=KH-2                                          002250
 0071                IF(DLY(KH-2).EQ.0.)KX(N)=KH-3                                          002260
 0072                IF(DLY(KH-3).EQ.0.)KX(N)=KH-4                                          002270
 0073                KH=KX(N)                                                               002280
 0074                N=N+1                                                                  002290
 0075                IF(DLY(KN).EQ.0.)XN(N)=Y(KN)                                           002300
 0076                IF(DLY(KN).NE.0.)READ(5,109)XN(N)                                      002310
 0077            109 FORMAT(E10.5)                                                          002320
               C  END OF INPUT?                                                           FA002330
 0078                IF(XN(N).NE.0.)GO TO 8                                                 002340
 0079                NX=N-1                                                                 002350
 0080                RETURN                                                                 002360
 0081                END                                                                    002370
```

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FORTRAN IV G1  RELEASE 2.0          MAIN          DATE = 75336          20/33/10          PAGE 0001

               C
0001                 SUBROUTINE PARAUS
               C
               C          PARAUS PRINTS CROSS SECTION PARAMETERS
               C
0002                 COMMON Z11,Z21,Z22,HI,GI
0003                 COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
                    1        XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                    2        TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
                    3        CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                    4        YY(201),DYY(50,201),
                    5        F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),LZ(50),
                    6        CHISQ,CHISQ0,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
                    7        ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004                 COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
0005                 MH=MX
0006                 WRITE(6,100)
0007             100 FORMAT(1H0//'  ABUN-    ATOMIC  TARGET P-WAVE    COMP.  S-WAVE
                    1S-WAVE     INEL.      RESONANCE        PARTIAL WIDTHS FOR'/
                    2           '  DANCE    WEIGHT   SPIN  RADIUS     SPIN  STRNTH.F.
                    3RADIUS     THRESH.    ENERGY     EL. SCATT.   INEL. SCATT. CAPTURE'/
                    4           '                                 (FM)
                    5(FM)       (KEV)      (KEV)      (KEV)        (KEV)        (KEV)'/
                    6           '                                                  /UNCERT.
                    7/UNCERT.              /UNCERT.   /UNCERT.     /UNCERT.     /UNCERT.'/)
0008                 MX=0
0009                 DO 1 I=1,IX
0010                 J=1
0011                 IF(LX(I,1).EQ.0)GO TO 2
0012                 MN=MX+1
0013                 MX=MN+5
0014                 WRITE(6,101)H(I),AG(I),SPIN(I),RP(I),CS(I,J),X(MN),X(MN+1),ES(I,J)
                    1,X(MN+2),X(MN+3),X(MN+4),X(MX),(DLX(M),M=MN,MX)
0015             101 FORMAT(F7.4,F8.1,F7.1,F9.3,F8.1,1PE12.3,0PF8.3,F9.3,F12.3,1P3E12.3
                    1,     /39X,0PE12.3,F8.3,9X,F12.3,3E12.3/)
0016                 GO TO 3
0017               2 MN=MX+1
0018                 MX=MN+1
0019                 WRITE(6,102)H(I),AG(I),SPIN(I),RP(I),CS(I,1),X(MN),X(MX  ),ES(I,1)
                    1,DLX(MN),DLX(MX)
0020             102 FORMAT(F7.4,F8.1,F7.1,F9.3,F8.1,1PE12.3,0PF8.3,F9.3/39X,E12.3,F8.3
                    1/)
0021                 GO TO 4
0022               3 IF(LX(I,J).LE.1)GO TO 4
0023                 LMX=LX(I,J)
0024                 DO 5 L=2,LMX
0025                 MN=MX+1
0026                 MX=MN+3
0027                 WRITE(6,103)(X(M),M=MN,MX),(DLX(M),M=MN,MX)
0028             103 FORMAT(68X,F12.3,1P3E12.3/68X,0PF12.3,3E12.3/)
0029               5 CONTINUE
0030               4 IF(J.EQ.JX(I))GO TO 1
0031                 J=2
0032                 IF(LX(I,2).EQ.0)GO TO 6
0033                 MN=MX+1
0034                 MX=MN+5
0035                 WRITE(6,104)CS(I,2),X(MN),X(MN+1),ES(I,2),X(MN+2),X(MN+3),X(MN+4),
                    1X(MX),(DLX(M),M=MN,MX)
```

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FORTRAN IV G1  RELEASE 2.0              PARAUS              DATE = 75336          20/33/10              PAGE 0002

 0036              104 FORMAT(31X,F8.1,1PE12.3,0PF8.3,F9.3,F12.3,1P3E12.3       /39X,0PE12.   002960
                      13,F8.3,9X,F12.3,3E12.3/)                                              002970
 0037                  GO TO 3                                                               002980
 0038                6 MN=MX+1                                                               002990
 0039                  MX=MN+1                                                               003000
 0040                  WRITE(6,105)CS(I,2),X(MN),X(MX),ES(I,2),DLX(MN),DLX(MX)               003010
 0041              105 FORMAT(31X,F8.1,1PE12.3,0PF8.3,F9.3/39X,E12.3,F8.3/)                  003020
 0042                1 CONTINUE                                                              003030
 0043                  MX=MF                                                                 003040
 0044                  IF(IZ.GT.0)RETURN                                                     003050
 0045                  WRITE(6,106)                                                          003060
 0046              106 FORMAT(1H0///' UTILIZED TIME-OF-FLIGHT RUNS:'//                     FA003070
                      1' RUN     SAMPLE        ',           'FLIGHT     EFF. DETECTOR CHANNEL  003080
                      2      FWHM OF       MAXIMAL'/                                       FA003090
                      3' NO.      THICKNESS    ',           'PATH          THICKNESS    WIDTH  F 003100
                      4      GAMMA PEAK  FLIGHT-TIME'/                                     FA003110
                      5'          (ATOMS/B)    ',           '(M)           (M)          (NS)   003120
                      6      (NS)          (NS)'/)                                         FA003130
 0047                  DO 51 N=1,NX                                                          003140
 0048                  WRITE(6,107)N,XN(N),        FP(N),DLFP(N),TC(N),TB(N),TMX(N)          003150
 0049              107 FORMAT(I3,1PE16.3,          0PF10.3,F12.3,F12.5, F12.3,F16.3)         003160
 0050               51 CONTINUE                                                              003170
 0051                  RETURN                                                                003180
 0052                  END                                                                   003190
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```
      C
0001        SUBRCUTINE INDEX
      C
      C        INDEX GENERATES INITIAL SUBSCRIPTS FOR THE PARAMETER GROUPS:
      C
      C        MP(I,J): FIRST SUBSCRIPT OF POTENTIAL-SCATTERING PARAMETERS,
      C        MR(I,J): FIRST SUBSCRIPT OF RESONANCE PARAMETERS,
      C        MX: TOTAL NUMBER OF CROSS SECTION PARAMETERS,
      C        MA: NUMBER OF ADJUSTED CROSS SECTION PARAMETERS.
      C
0002        COMMCN Z11,Z21,Z22,HI,GI
0003        COMMCN TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
           1      XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
           2      TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
           3      CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
           4      YY(201),DYY(50,201),
           5      F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
           6      CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
           7      ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004        COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
0005        MSUM=1
0006        DO 1 I=1,IX
0007        JH=JX(I)
0008        DO 1 J=1,JH
0009        MP(I,J)=MSUM
0010        MR(I,J)=MSUM+2
0011      1 MSUM=MR(I,J)+4*LX(I,J)
      C        ZAHL DER PARAMETER:
0012        MX=MSUM-1
0013        MA=0
0014        DO 2 M=1,MX
0015        IF(DLX(M).GT.0.)MA=MA+1
0016      2 CONTINUE
0017        RETURN
0018        END
```

```
FORTRAN IV G1  RELEASE 2.0            MAIN              DATE = 75336          20/33/10              PAGE 0001
                 C
 0001                  SUBROUTINE HBN
                 C
                 C          HBN PRODUCES QTL, THE RATIO OF SMALLEST HALF-WIDTH
                 C          (ON A TIME-OF-FLIGHT SCALE) TO FLIGHT PATH.
                 C
 0002                  COMMON Z11,Z21,Z22,HI,GI
 0003                  COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
                      1         XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                      2         TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MO,E,FT,ST,SC,SG,
                      3         CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                      4         YY(201),DYY(50,201),
                      5         F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
                      6         CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
                      7        ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
 0004                  COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
 0005                  QTL=1000.
 0006                  DO 1 I=1,IX
 0007                  JH=JX(I)
 0008                  DO 1 J=1,JH
 0009                  IF(LX(I,J).EQ.0)GO TO 1
 0010                  M1=MR(I,J)
 0011                  M2=MR(I,J)+4*LX(I,J)-4
 0012                  DO 1 MM=M1,M2,4
 0013                  GT=ABS(X(MM+1))+ABS(X(MM+2))+X(MM+3)
 0014                  IF(X(M1-1).EQ.0..AND.DLX(M1-2).EQ.0..AND.DLX(M1-1).EQ.0.)
                      1GT=SQRT(GT**2+2.81E-4*X(MM)/AG(I))
 0015                  Q=GT/X(MM)*36.148/SQRT(.001*X(MM))
 0016                  IF(Q.LT.QTL)QTL=Q
 0017                1 CONTINUE
 0018                  RETURN
 0019                  END
```

```
           C
0001             SUBROUTINE MEV
           C
           C          MEV CALCULATES RESONANCE PARAMETERS IN MEV AND WIDTH
           C          AMPLITUDES
           C
0002             COMMON Z11,Z21,Z22,HI,GI
0003             COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
               1        XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
               2        TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
               3        CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
               4        YY(201),DYY(50,201),
               5        F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
               6        CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
               7       ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004             COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
0005             IF(IZ.GT.0)GO TO 3
0006             E1(1)=E1(1)*.001
0007             E2(1)=E2(1)*.001
0008           3 CONTINUE
0009             DO 1 I=1,IX
0010             JH=JX(I)
0011             DO 1 J=1,JH
0012           2 ES(I,J)=ES(I,J)*.001
0013             IF(LX(I,J).EQ.0)GO TO 1
0014             M1=MR(I,J)
0015             M2=MR(I,J)+4*LX(I,J)-4
0016             DO 1 M=M1,M2,4
0017             X(M)=X(M)*.001
0018             X(M+1)=SIGN(SQRT(.001*ABS(X(M+1))),X(M+1))
0019             X(M+2)=SIGN(SQRT(.001*ABS(X(M+2))),X(M+2))
0020             X(M+3)=X(M+3)*.001
0021           1 CONTINUE
0022             RETURN
0023             END
```

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                 C                                                                          004220
 0001                  SUBROUTINE NGK                                                       004230
                 C                                                                          004240
                 C         NGK CALCULATES THE COEFFICIENTS OF THE NORMAL EQUATIONS        FA004250
                 C                                                                          004260
 0002                  COMMON Z11,Z21,Z22,HI,GI                                             004270
 0003                  COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),   004280
                      1       XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),                  004290
                      2       TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MO,E,FT,ST,SC,SG,        004300
                      3       CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,   004310
                      4       YY(201),DYY(50,201),                                          004320
                      5       F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),       004330
                      6       CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH   004340
                      7       ,QTL,IZ,ZIT,EPS,E1(5),E2(5)                                   004350
 0004                  DIMENSION ZZ(2048)                                                   004360
 0005                  COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI                             004370
                 C         INITIALIZATION                                                 FA004380
 0006                  DO 1 M=1,MA                                                          004390
 0007                  C(M)=0.                                                              004400
 0008                  DO 1 MM=1,MA                                                         004410
 0009                1 A(M,MM)=0.                                                           004420
 0010                  KN=1                                                                 004430
 0011                  DO 2 N=1,NX                                                          004440
 0012                  IF(N.GT.1)KN=KX(N-1)+1                                               004450
 0013                  KH=KX(N)                                                             004460
 0014                  V1=(TB(N)/1.667)**2                                                  004470
 0015                  V2=(DLFP(N)/FP(N))**2/6.                                             004480
 0016                  CN=(72.296*FP(N))**2                                                 004490
                 C         CALCULATE INTERNAL MESH WIDTH FOR RESOLUTION BROADENING        FA004500
 0017                  FT=TMX(N)-FLOAT(KH-KN)*TC(N)                                         004510
 0018                  RW=SQRT(V1+V2*FT**2)                                                 004520
 0019                  WN=AMIN1(QTL*FP(N),1.667*RW)                                         004530
 0020                  KC=3.*TC(N)/WN+1.                                                    004540
 0021                3 DL=TC(N)/FLOAT(KC)                                                   004550
 0022                  KR=2.*RW/DL+.5                                                       004560
 0023                  IF(KR.LE.100)GO TO 4                                                 004570
 0024                  WRITE(6,100)IZ,KR                                                    004580
 0025              100 FORMAT(1H //' WARNING: INTERNAL GRID WAS TOO FINE IN ITERATION',    004590
                      1I3,', KR REDUCED FROM',I6,' TO 100'//)                               004600
 0026                  KC=50.*TC(N)/RW                                                      004610
 0027                  GO TO 3                                                              004620
                 C         PREPARATION OF MAIN LOOP:                                      FA004630
                 C         KT LABELS CALCULATED VALUES,                                   FA004640
                 C         KT=1 CORRESPONDS TO LOWEST ENERGY FOR A GIVEN RUN (N).         FA004650
                 C         KK LABELS MEASURED VALUES,                                     FA004660
                 C         KK=KN CORRESPONDS TO LOWEST ENERGY FOR A GIVEN N.              FA004670
                 C         THE CALCULATION STARTS FROM THE LOWEST FLIGHT TIME             FA004680
                 C         (HIGHEST ENERGY) OF A GIVEN RUN.                               FA004690
 0028                4 KK=KH                                                                004700
 0029                  KT=KH-KN+1                                                           004710
 0030                  K1=101-KR                                                            004720
 0031                  K2=101+KR                                                            004730
 0032                  CALL AF(RW,DL,K2,RF)                                                 004740
 0033                  DO 5 K=K1,K2                                                         004750
 0034                  TK=FT+FLOAT(K-101)*DL                                                004760
 0035                  E=CN/TK**2                                                           004770
 0036                  CALL YT                                                              004780
 0037                5 F(K)=YY(K)*RF(K)                                                     004790
```

```
              CALL SIMP(F,K1,K2,Z(KK))
              Z(KK)=Z(KK)*DL
C                 Z(KK): CALCULATED TRANSMISSION
              ZZ(KT)=(Y(KK)-Z(KK))/DLY(KK)
              CHISQ=CHISQ+ZZ(KT)**2
              DO 6 M=1,MA
              DO 7 K=K1,K2
            7 F(K)=DYY(M,K)*RF(K)
              CALL SIMP(F,K1,K2,DZ(M))
              DZ(M)=DL*(DZ(M)/DLY(KK))
C                 COEFFICIENTS:
              C(M)=C(M)+DZ(M)*ZZ(KT)
              DO 6 MM=1,M
            6 A(M,MM)=A(M,MM)+DZ(M)*DZ(MM)
C                 MAIN LOOP:
              KH=KH-1
              DO 8 KKK=KN,KH
              FT=FT+TC(N)
              KK=KK-1
              KT=KT-1
              RW=SQRT(V1+V2*FT**2)
C                 RELABEL PREVIOUSLY CALCULATED INTEGRAND VALUES
              KR=2.*RW/DL+.5
              IF(KR.GT.100)KR=100
              KA=K1-KC
              KB=K2-KC
              K1=101-KR
              K2=101+KR
              KM=MAX0(KA,K1)
              DO 9 K=KM,KB
              KO=K+KC
              YY(K)=YY(KO)
              DO 9 M=1,MX
            9 DYY(M,K)=DYY(M,KO)
C                 NEWLY NEEDED INTEGRAND VALUES
              IF(KA.LT.K1) GO TO 10
              KAA=KA-1
              DO 11 K=K1,KAA
              TK=FT+FLOAT(K-101)*DL
              E=CN/TK**2
              CALL YT
           11 CONTINUE
           10 KBB=KB+1
              DO 12 K=KBB,K2
              TK=FT+FLOAT(K-101)*DL
              E=CN/TK**2
              CALL YT
           12 CONTINUE
              CALL AF(RW,DL,K2,RF)
              DO 13 K=K1,K2
           13 F(K)=YY(K)*RF(K)
              CALL SIMP(F,K1,K2,Z(KK))
              Z(KK)=Z(KK)*DL
              ZZ(KT)=(Y(KK)-Z(KK))/DLY(KK)
              CHISQ=CHISQ+ZZ(KT)**2
              DO 14 M=1,MA
              DO 15 K=K1,K2
           15 F(K)=DYY(M,K)*RF(K)
```

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 0091                CALL SIMP(F,K1,K2,DZ(M))                                                 005380
 0092                DZ(M)=DL*(DZ(M)/DLY(KK))                                                 005390
           C              COEFFICIENTS:                                                     FA005400
 0093                C(M)=C(M)+DZ(M)*ZZ(KT)                                                   005410
 0094                DO 14 MM=1,M                                                             005420
 0095             14 A(M,MM)=A(M,MM)+DZ(M)*DZ(MM)                                             005430
 0096              8 CONTINUE                                                                 005440
 0097              2 CONTINUE                                                                 005450
           C              END OF MAIN LOOP                                                  FA005460
 0098                DO 16 M=1,MA                                                             005470
 0099                MMX=M-1                                                                  005480
 0100                DO 16 MM=1,MMX                                                           005490
 0101             16 A(MM,M)=A(M,MM)                                                          005500
 0102                RETURN                                                                   005510
 0103                END                                                                      005520
```

```
               C
 0001                SUBROUTINE YT
               C
               C          YT YIELDS TRANSMISSION VALUES AND DERIVATIVES.
               C
 0002                COMMON Z11,Z21,Z22,HI,GI
 0003                COMMON TITLE(15),H(6),AG(6),SPIN(6),PP(6),X(200),DLX(200),ES(6,2),
                    1      XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                    2      TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
                    3      CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                    4      YY(201),DYY(50,201),
                    5      F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
                    6      CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
                    7      ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
 0004                COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
 0005                CALL GCS
 0006                YY(K)=EXP(-XN(N)*ST)
 0007                DO 1 M=1,MA
 0008                DYY(M,K)=-XN(N)*DST(M)*YY(K)
 0009              1 CONTINUE
 0010                RETURN
 0011                END
```

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FORTRAN IV G1  RELEASE 2.0           MAIN            DATE = 75336          20/33/10              PAGE 0001

                C                                                                                 005750
0001                    SUBROUTINE GQS                                                            005760
                C                                                                                 005770
                C            GQS YIELDS TOTAL CROSS SECTIONS AND DERIVATIVES.                   FA005780
                C                                                                                 005790
0002                    COMMON Z11,Z21,Z22,HI,GI                                                  005800
0003                    COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),        005810
                      1         XN(5),XR(5),FP(5),DLFP(5),TC(5),TE(5),TJ(5),                      005820
                      2         TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,            005830
                      3         CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,       005840
                      4         YY(201),DYY(50,201),                                              005850
                      5         F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),           005860
                      6         CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH       005870
                      7         ,QTL,IZ,ZIT,EPS,E1(5),E2(5)                                       005880
0004                    COMMON/GQSR/DR11(50),DR21(50),DR22(50)                                    005890
0005                    COMPLEX DR11,DR21,DR22                                                    005900
0006                    COMPLEX HI,GI,FE,F1,F2,EX1,EX2,U11,U21,DU11(50),DU21(50),                 005910
                      1          DET,Z11,Z21,Z22,R11,R21,R22                                      005920
0007                    M=0                                                                       005930
0008                    ST=0.                                                                     005940
0009                    PLQ2=1.3019/E                                                             005950
0010                    DO 1 I=1,IX                                                               005960
0011                    AL(I)=1.+1./AG(I)                                                         005970
                C            P-WAVE POTENTIAL SCATTERING:                                       FA005980
0012                    XK1=.21969*SQRT(E)/AL(I)                                                  005990
0013                    XO=XK1*RP(I)                                                              006000
0014                    X1=XO-ATAN(XO)                                                            006010
0015                    SP=H(I)*PLQ2*AL(I)**2*6.*SIN(X1)**2                                       006020
0016                    ST=ST+SP                                                                  006030
0017                    JH=JX(I)                                                                  006040
0018                    DO 2 J=1,JH                                                               006050
0019                    M1=MP(I,J)+2                                                              006060
0020                    M2=MP(I,J)-2+4*LX(I,J)                                                    006070
0021                    IF(X(M1-1).EQ.0..AND.DLX(M1-2).EQ.0..AND.DLX(M1-1).EQ.0.)GO TO 3          006080
                C            S WAVE:                                                              006090
                C            POTENTIAL-SCATTERING PHASE FACTOR                                  FA006100
0022                    AR1=(2.*E-E2(1)-E1(1))/(E2(1)-E1(1))                                      006110
0023                    AR1=AR1*.95                                                               006120
0024                    ATGH=.5*ALOG((1.+AR1)/(1.-AR1))                                           006130
0025                    AR2=SQRT(1.E6*E)*ATGH                                                     006140
0026                    AR3=X(M1-2)*AR2                                                           006150
0027                    XI1=-XK1*X(M1-1)+ATAN(AR3)                                                006160
0028                    EX1=CEXP(2.*GI*XI1)                                                       006170
                C            COLLISION MATRIX ELEMENT                                           FA006180
0029                    CALL RMAT                                                                 006190
0030                    U11=EX1*(2.*Z11-1.)                                                       006200
                C            TOTAL CROSS SECTION                                                FA006210
0031                    ST=ST+PLQ2*H(I)*G(I,J)*(1.-REAL(U11))*AL(I)**2                            006220
                C            DERIVATIVES WITH RESPECT TO POTENTIAL-SCATTERING PARAMETERS:       FA006230
0032                    MO=M                                                                      006240
0033                    IF(DLX(M1-2).EQ.0.)GO TO 8                                                006250
0034                    M=M+1                                                                     006260
0035                    ABL= AR2/(1.+AR3**2)                                                      006270
0036                    DU11(M)=2.*GI*ABL*U11                                                     006280
0037                  8 IF(DLX(M1-1).EQ.0.)GO TO 9                                                006290
0038                    M=M+1                                                                     006300
0039                    ABL=-XK1                                                                  006310
0040                    DU11(M)=2.*GI*ABL*U11                                                     006320
```

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0041              9 IF(LX(I,J).EQ.0.)GO TO 10
            C           DERIVATIVES WITH RESPECT TO RESONANCE PARAMETERS
0042                DO 11 MM=M1,M2,4
0043                DO 11 ML=1,4
0044                MK=MM+ML-1
0045                IF(DLX(MK).EQ.0.)GO TO 11
0046                M=M+1
0047                DU11(M)=GT*EX1*(Z11**2*DR11(M)+2.*Z11*Z21*DR21(M)+Z21**2*DR22(M))
0048             11 CONTINUE
0049             10 ML=MC+1
0050                IF(M.LT.ML)GO TO 2
0051                DO 12 MM=ML,M
0052             12 DST(MM)=-PLQ2*H(I)*G(I,J)*REAL(DU11(MM))*AL(I)**2
0053                GO TO 2
            C           P WAVE:
0054              3 DO 7 MM=M1,M2,4
0055                GT=X(MM+1)**2+X(MM+2)**2+X(MM+3)
0056                DD=1.012E-7*X(MM)/AG(I)
0057                WW=DD+GT**2/2.772
0058                W=SQRT(WW)
0059                XMM=(E-X(MM))/W
0060                XX=XMM*XMM
0061                STMM=0.
0062                IF(XX.LE.9.)
                   1STMM=PLQ2*H(I)*G(I,J)*X(MM+1)**2*EXP(-XX)*1.7725/W
0063                ST=ST+STMM
0064                IF(DLX(MM).EQ.0.)GO TO 4
0065                M=M+1
0066                DST(M)= STMM*2.*XMM/W
0067              4 IF(DLX(MM+1).EQ.0.)GO TO 5
0068                M=M+1
0069                DST(M)= STMM*(2./X(MM+1)-GT*X(MM+1)/1.386*(1.-2.*XX)/WW)
0070              5 IF(DLX(MM+2).EQ.0.)GO TO 6
0071                M=M+1
0072                DST(M)= STMM*(           -GT*X(MM+2)/1.386*(1.-2.*XX)/WW)
0073              6 IF(DLX(MM+3).EQ.0.)GO TO 7
0074                M=M+1
0075                DST(M)=-STMM*GT/2.772*(1.-2.*XX)/WW
0076              7 CONTINUE
0077              2 CONTINUE
0078              1 CONTINUE
0079                RETURN
0080                END
```

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                     C                                                                                006760
0001                        SUBROUTINE RMAT                                                           006770
                     C                                                                                006780
                     C          RMAT CALCULATES THE R MATRIX, ITS DERIVATIVES AND THE INVERSE FA006790
                     C          OF 1-I*R/2                                                          FA006800
                     C                                                                                006810
0002                        COMMON Z11,Z21,Z22,HI,GI                                                  006820
0003                        COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),       006830
                          1       XN(5),XR(5),FP(5),DLFP(5),TC(5),TE(5),TJ(5),                       006840
                          2       TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,             006850
                          3       CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,        006860
                          4       YY(201),DYY(50,201),                                                006870
                          5       F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),            006880
                          6       CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH       006890
                          7       ,QTL,IZ,ZIT,EPS,E1(5),E2(5)                                         006900
0004                        COMMON/GQSR/DR11(50),DR21(50),DR22(50)                                    006910
0005                        COMPLEX DR11,DR21,DR22                                                    006920
0006                        COMPLEX HI,GI,FE,F1,F2,EX1,EX2,U11,U21,DU11(50),DU21(50),                006930
                          1        DET,Z11,Z21,Z22,R11,R21,R22                                        006940
0007                        R11=(0.,0.)                                                                006950
0008                        R21=(0.,0.)                                                                006960
0009                        R22=(0.,0.)                                                                006970
0010                        IF(LX(I,J).EQ.0)GO TO 2                                                   006980
                     C          (GO TO 2 IF NO RESONANCES ARE GIVEN)                                FA006990
0011                        MO=M                                                                      007000
0012                        IF(DLX(M1-2).NE.0.)M=M+1                                                  007010
0013                        IF(DLX(M1-1).NE.0.)M=M+1                                                  007020
0014                        DO 3 MM=M1,M2,4                                                           007030
0015                        SQ1=(E/X(MM))**.25                                                        007040
0016                        ARG2=(E-ES(I,J))/(X(MM)-ES(I,J))                                          007050
0017                        IF(E.LT.ES(I,J))SQ2=0.                                                    007060
0018                        IF(E.GE.ES(I,J).AND.ARG2.GE.0.)SQ2=ARG2**.25                              007070
0019                        CE=(E-X(MM))**2+.25*X(MM+3)**2                                            007080
0020                        IF(CE.LT.1.E-60.AND.X(MM+3).EQ.0.)FE=(1.E30,0.    )                       007090
0021                        IF(CE.LT.1.E-60.AND.X(MM+3).GT.0.)FE=(1.E30,1.E30)                        007100
0022                        IF(CE.GE.1.E-60)FE=(X(MM)-E+HI*X(MM+3))/CE                                007110
0023                        W1=SQ1*X(MM+1)                                                            007120
0024                        W2=SQ2*X(MM+2)                                                            007130
0025                        F1=W1*FE                                                                  007140
0026                        F2=W2*FE                                                                  007150
0027                        R11=R11+F1*W1                                                             007160
0028                        R21=R21+F2*W1                                                             007170
0029                        R22=R22+F2*W2                                                             007180
0030                        IF(DLX(MM).EQ.0.)GO TO 4                                                  007190
0031                        M=M+1                                                                     007200
0032                        DR11(M)=-F1*F1                                                            007210
0033                        DR21(M)=-F2*F1                                                            007220
0034                        DR22(M)=-F2*F2                                                            007230
0035                      4 IF(DLX(MM+1).EQ.0.)GO TO 5                                                007240
0036                        M=M+1                                                                     007250
0037                        DR11(M)=F1*SQ1*2.                                                         007260
0038                        DR21(M)=F2*SQ1                                                            007270
0039                        DR22(M)=0.                                                                007280
0040                      5 IF(DLX(MM+2).EQ.0.)GO TO 6                                                007290
0041                        M=M+1                                                                     007300
0042                        DR11(M)=0.                                                                007310
0043                        DR21(M)=SQ2*F1                                                            007320
0044                        DR22(M)=SQ2*F2*2.                                                         007330
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0045          6 IF(DLX(MM+3).EQ.0.)GO TO 3                                          007340
0046            M=M+1                                                               007350
0047            DR11(M)=HI*F1*F1                                                    007360
0048            DR21(M)=HI*F2*F1                                                    007370
0049            DR22(M)=HI*F2*F2                                                    007380
0050          3 CONTINUE                                                            007390
0051            M=M0                                                                007400
        C             CALCULATE INVERSE OF 1-I*R/2                                FA007410
0052          2 DET=(1.-HI*R11)*(1.-HI*R22)+.25*R21**2                              007420
0053            Z11=(1.-HI*R22)/DET                                                 007430
0054            Z21=(   HI*R21)/DET                                                 007440
0055            Z22=(1.-HI*R11)/DET                                                 007450
0056            RETURN                                                              007460
0057            END                                                                 007470
```

```
              C
0001                SUBROUTINE YTAB
              C
              C          YTAB YIELDS TABLES OF MEASURED AND CALCULATED VALUES
              C          (DESCENDING FLIGHT TIME, ASCENDING ENERGY) AND PLOTS.
              C
0002                COMMON Z11,Z21,Z22,HI,GI
0003                COMMON TITLE(15),H(6),AG(6),SPIN(6),RP(6),X(200),DLX(200),ES(6,2),
                   1      XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                   2      TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MC,E,FT,ST,SC,SG,
                   3      CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                   4      YY(201),DYY(50,201),
                   5      F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),DZ(50),
                   6      CHISQ,CHISQO,MP(6,2),MR(6,2),DST(50),AL(6),RF(201),CC,KN,KH
                   7      ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004                DIMENSION TT(2),EE(2)
0005                COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
              C           ENERGY RANGE OF PLOT
0006                CC=(72.296*FP(1))**2
0007                TMIN=TMX(1)-FLOAT(KX(1)-1)*TC(1)
0008                EMAX=CC/TMIN**2
0009                EMIN=CC/TMX(1)**2
0010                IF(NX.EQ.1) GO TO 4
0011                DO 5 N=2,NX
0012                CC=(72.296*FP(N))**2
0013                TMIN=TMX(N)-FLOAT(KX(N)-KX(N-1)-1)*TC(N)
0014                EMX=CC/TMIN**2
0015                EMN=CC/TMX(N)**2
0016                IF(EMX.GT.EMAX) EMAX=EMX
0017                IF(EMN.LT.EMIN) EMIN=EMN
0018              5 CONTINUE
              C           ENERGY SCALE OF PLOT:
0019              4 EMAX=EMAX*1000.
0020                EMIN=EMIN*1000.
0021                EBER=1.04*(EMAX-EMIN)
0022                ILG=ALOG10(EBER)
0023                IF(EBER.LT.1.)ILG=ILG-1
0024                DEK=10.**ILG
0025                EBER=EBER/DEK
0026                BER=10.
0027                IF(EBER.LE.6.25)BER=6.25
0028                IF(EBER.LE.5.   )BER=5.
0029                IF(EBER.LE.4.   )BER=4.
0030                IF(EBER.LE.2.5 )BER=2.5
0031                IF(EBER.LE.1.25)BER=1.25
0032                BER=BER*DEK
0033                EMIN=FLOAT(INT(50.*EMIN/BER))*BER/50.
0034                EMAX=EMIN+BER
0035                SE=.00025*BER
              C           WRITE TABLES
0036                DO 1 N=1,NX
0037                WRITE(6,100)IZ,N,XN(N),FP(N)
0038            100 FORMAT(1H1//
                   1' COMPLETED ITERATIONS  :',I3                          /
                   2' TIME-OF-FLIGHT RUN NO.:',I3                          /
                   3' SAMPLE THICKNESS      :',1PE10.3,' ATOMS/B'/
                   4' FLIGHT PATH           :',1PE10.3,' M'          /)
0039                WRITE(6,101)
```

```
0040      101 FORMAT(1H0///
            1' FLIGHT        NEUTRON       MEASURED          CALCULATED   TOTAL'/
            2' TIME          ENERGY                 TRANSMISSION          X-SECTION'/
            3' (NS)          (KEV)                                        (B)'/)
0041          CC=(72.296*FP(N))**2
0042          FT=TMX(N)+TC(N)
0043          IF(N.EQ.1)KN=1
0044          IF(N.GT.1)KN=KX(N-1)+1
0045          KH=KX(N)
0046          DO 3 KK=KN,KH
0047          KT=KK-KN+1
0048          FT=FT-TC(N)
0049          E=CC/FT**2
0050          EZ(KT)=E*1000.
0051          CALL GQS
0052          WRITE(6,102)FT,EZ(KT),Y(KK),DLY(KK),Z(KK),ST
0053      102 FORMAT(F9.3,F11.3,F11.4,2H+-,F6.4,F9.4,F12.3)
0054        3 CONTINUE
      C         NP: NUMBER OF POINTS
0055          NP=KH-KN+1
      C         PLOT CALCULATED CURVE
0056          IF(N.EQ.1)
             1CALL PLOT(EZ,Z(KN),NP,2,0,1,3,0,4,EMAX,EMIN,SE,1.1,-.15,.00125,
             2TITLE,IZ)
0057          IF(N.GT.1)
             1CALL PLOT(EZ,Z(KN),NP,2,0,1,3,0,0,EMAX,EMIN,SE,1.1,-.15,.00125,
             20,0)
      C         PLOT MEASURED DATA
0058          IF(N.LE.3) NS=N-1
0059          IF(N.GE.4) NS=N+3
0060          CALL PLOT(EZ,Y(KN),NP,1,NS,1,0,0,0,EMAX,EMIN,SE,1.1,-.15,.00125,
             10,0)
      C         PLOT ERROR BARS
0061          DO 2 KK=KN,KH
0062          KT=KK-KN+1
0063          EE(1)=EZ(KT)
0064          EE(2)=EZ(KT)
0065          TT(1)=Y(KK)+DLY(KK)
0066          IF(TT(1).GT.1.1)TT(1)=1.1
0067          TT(2)=Y(KK)-DLY(KK)
0068          IF(TT(2).LT.-.15)TT(2)=-.15
0069          CALL PLOT(EE,TT,2,2,0,1,1,0,0,EMAX,EMIN,SE,1.1,-.15,.00125,0,0)
0070        2 CONTINUE
0071        1 CONTINUE
0072          CF=SQRT(CHISQ/FLOAT(KX(NX)-MA))
0073          WRITE(6,103)CHISQ,CF
0074      103 FORMAT(1H //28H CHI**2:                    ,1PE9.3/
            1           28H ERROR ADJUSTMENT FACTOR:    ,1PE9.3/1H1)
0075          RETURN
0076          END
```

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                C                                                                              008560
 0001                 SUBROUTINE ORTH(MX,A,B)                                                  008570
                C                                                                              008580
                C           ORTH YIELDS THE COVARIANCE MATRIX BY GRAM-SCHMIDT                FA008590
                C           ORTHOGONALIZATION OF THE COEFFICIENT MATRIX.                     FA008600
                C                                                                              008610
 0002                 DIMENSION A(50,50),B(50,50),UE(50,50),OM(50,50)                          008620
 0003                 DO 1 M=1,MX                                                              008630
 0004                 DO 2 N=1,MX                                                              008640
 0005               2 OM(M,N)=0.                                                               008650
 0006               1 OM(M,M)=1.                                                               008660
 0007                 CN=1./SQRT(A(1,1))                                                       008670
 0008                 DO 3 M=1,MX                                                              008680
 0009               3 OM(M,1)=OM(M,1)*CN                                                       008690
 0010                 DO 4 M=2,MX                                                              008700
 0011               4 UE(M,1)=A(M,1)*CN                                                        008710
 0012                 DO 5 N=2,MX                                                              008720
 0013                 SUM=0.                                                                   008730
 0014                 KX=N-1                                                                   008740
 0015                 DO 6 K=1,KX                                                              008750
 0016               6 SUM=SUM+UE(N,K)*UE(N,K)                                                  008760
 0017                 CN=1./SQRT(A(N,N)-SUM)                                                   008770
 0018                 DO 7 M=1,MX                                                              008780
 0019                 SUM=0.                                                                   008790
 0020                 DO 8 K=1,KX                                                              008800
 0021               8 SUM=SUM+UE(N,K)*OM(M,K)                                                  008810
 0022               7 OM(M,N)=(OM(M,N)-SUM)*CN                                                 008820
 0023                 MN=N+1                                                                   008830
 0024                 IF(MN.GT.MX)GO TO 5                                                      008840
 0025                 DO 9 M=MN,MX                                                             008850
 0026                 SUM=0.                                                                   008860
 0027                 DO 10 K=1,KX                                                             008870
 0028              10 SUM=SUM+UE(M,K)*UE(N,K)                                                  008880
 0029               9 UE(M,N)=(A(M,N)-SUM)*CN                                                  008890
 0030               5 CONTINUE                                                                 008900
                C           FORM COVARIANCE MATRIX AS PRODUCT OM*OM'                         FA008910
 0031                 DO 11 M=1,MX                                                             008920
 0032                 DO 12 N=M,MX                                                             008930
 0033                 B(M,N)=0.                                                                008940
 0034                 DO 13 K=1,MX                                                             008950
 0035              13 B(M,N)=B(M,N)+OM(M,K)*OM(N,K)                                            008960
 0036              12 CONTINUE                                                                 008970
 0037              11 CONTINUE                                                                 008980
 0038                 DO 14 M=2,MX                                                             008990
 0039                 NX=M-1                                                                   009000
 0040                 DO 15 N=1,NX                                                             009010
 0041              15 B(M,N)=B(N,M)                                                            009020
 0042              14 CONTINUE                                                                 009030
 0043                 RETURN                                                                   009040
 0044                 END                                                                      009050
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                C
 0001                 SUBROUTINE ADJ(MX,MA,X,DLX,B,C)
                C
                C         ADJ CALCULATES THE NEWLY ADJUSTED PARAMETERS
                C
 0002                 DIMENSION X(200),DLX(200),B(50,50),C(50)
 0003                 M=0
 0004                 DO 1 MM=1,MX
 0005                 IF(DLX(MM).EQ.0.)GO TO 1
 0006                 M=M+1
 0007                 XM=0.
 0008                 DO 2 MN=1,MA
 0009               2 XM=XM+B(M,MN)*C(MN)
 0010                 X(MM)=X(MM)+XM
 0011                 DLX(MM)=SQRT(B(M,M))
 0012               1 CONTINUE
 0013                 RETURN
 0014                 END
```

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               C
0001                 SUBROUTINE KEV
               C
               C          KEV CALCULATES RESONANCE PARAMETERS IN KEV AND WIDTH
               C          AMPLITUDES
               C
0002                 COMMON Z11,Z21,Z22,HI,GI
0003                 COMMON TITLE(15),H(6),AG(6),SFIN(6),RP(6),X(200),DLX(200),ES(6,2),
                   1        XN(5),XR(5),FP(5),DLFP(5),TC(5),TB(5),TJ(5),
                   2        TMX(5),ZH(5),Y(5120),DLY(5120),M1,M2,MO,E,FT,ST,SC,SG,
                   3        CS(6,2),G(6,2),I,IX,J,JX(6),K,KX(5),L,LX(6,2),M,MX,N,NX,MA,
                   4        YY(201),DYY(50,201),
                   5        F(201),A(50,50),B(50,50),C(50),EZ(2048),Z(5120),CZ(50),
                   6        CHISQ,CHISQO,MP(6,2),MR(6,2),CST(50),AL(6),RF(201),CC,KN,KH
                   7       ,QTL,IZ,ZIT,EPS,E1(5),E2(5)
0004                 COMPLEX Z11,Z21,Z22,DZ11,DZ21,DZ22,HI,GI
0005                 DO 1 I=1,IX
0006                 JH=JX(I)
0007                 DO 1 J=1,JH
0008               2 ES(I,J)=ES(I,J)*1000.
0009                 IF(LX(I,J).EQ.0)GO TO 1
0010                 M1=MR(I,J)
0011                 M2=MR(I,J)+4*LX(I,J)-4
0012                 DO 1 M=M1,M2,4
0013                 X(M)=X(M)*1000.
0014                 X(M+1)=X(M+1)*ABS(X(M+1))*1000.
0015                 X(M+2)=X(M+2)*ABS(X(M+2))*1000.
0016                 X(M+3)=X(M+3)*1000.
0017                 DLX(M)=DLX(M)*1000.
0018                 DLX(M+1)=DLX(M+1)*SQRT(ABS(X(M+1))*.001)*2000.
0019                 DLX(M+2)=DLX(M+2)*SQRT(ABS(X(M+2))*.001)*2000.
0020                 DLX(M+3)=DLX(M+3)*1000.
0021               1 CONTINUE
0022                 RETURN
0023                 END
```

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                C
 0001                 SUBROUTINE SIMP(Y,M,N,Z)
                C        THIS SUBROUTINE PERFORMS INTEGRATION BY SIMPSON'S RULE
 0002                 DIMENSION Y(201)
 0003                 IF(N-M-2)5,3,5
 0004               5 Z=0.
 0005                 K=M
 0006                 L=N
 0007               1 K=K+1
 0008                 L=L-1
 0009                 DO 2 I=K,L,2
 0010               2 Z=Z+Y(I)
 0011                 Z=2.*Z
 0012                 IF(M+1-K)4,1,4
 0013               3 Z=4.*Y(M+1)
 0014               4 Z=(Y(M)+Z+Y(N))/3.
 0015                 RETURN
 0016                 END
```

```
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                C
 0001                 SUBROUTINE AF(RW,DL,KX,RF)
                C
                C        AF YIELDS THE RESOLUTION FUNCTION
                C
 0002                 DIMENSION RF(201)
 0003                 RF(101)=.566870/RW
 0004                 F1=EXP(-(DL/RW)**2)
 0005                 F2=F1*F1
 0006                 DO 21 K=102,KX
 0007                 RF(K)=RF(K-1)*F1
 0008                 KK=202-K
 0009                 RF(KK)=RF(K)
 0010              21 F1=F1*F2
 0011                 RETURN
 0012                 END
```

Note added in print

The most recent version of FANAL (January 1976) has the statements 007040 and 007050 in subroutine RMAT replaced by

```
SQ1=(E/ABS(X(MM)))**.25
ARG2=(E-ES(I,J))/(ABS(X(MM)-ES(I,J))).
```

This permits inclusion of s-wave resonances with subthreshold resonance energies ($E_\lambda<0$ for the elastic channel, $E_\lambda<E_t$ for the inelastic channel). Their elastic and inelastic neutron widths must be taken as follows:

$$\Gamma_{\lambda n} = \Gamma^0_{\lambda n} \sqrt{|E_\lambda|/1eV},$$

$$\Gamma_{\lambda n'} = \Gamma^0_{\lambda n'} \sqrt{|E_\lambda - E_t|/1eV}.$$

(For the elastic channel this corresponds to e.g. the ENDF convention.)